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Research Article

Seismic evaluation of tall RC frames with hybrid friction damper and shape memory alloy designed by PBPD method

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ABSTRACT

This paper suggests a novel lateral load-resisting solution for RC (high-rise reinforced concrete) frames using superelastic SMA wires as friction dampers. The suggested SMA-friction damper has some advantages, such as an easy-to-configure and affordable application, in addition to being able to control the frictional energy dissipation components mechanism in line with the design procedure based on the suggested effectiveness thanks to its self-centering SMA wires. With the least amount of SMA use, it may produce hysteretic behavior and an intense tendency for self-centering. The research used two distinct design modes—common and with the recommended damper—to construct two tall, 18- and 22-story RC frames. Ten far-field earthquakes were studied using OpenSees software in a nonlinear time history fashion. Eighteen and twenty-two-story reinforced concrete frame high-rises were designed in two distinct ways: normally and with the recommended damper. Aside from the major advancement in ductility, the lateral strength and stiffness gave an exceptional capacity for self-centering, resulting in a substantial decrease in most drift and persistent distortions in the structure. The study's findings showed that the suggested damper may improve the RC frame's structural performance while using the fewest bracing spans and money.

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INTRODUCTION

The least amount of harm done to structural and non-structural systems occurs during mild earthquakes when standard seismic systems are used in concrete structures. However, the main seismic load-bearing members which are generally permanent members of their structural system should be replaced to create a strong resistance to future severe earthquakes. Because of this, using a replacement hybrid passive control system in high-rise buildings becomes more crucial because it is neither practicable nor easy to implement in standard systems. One popular kind of non-permanent passive damper that is frequently used to regulate seismic activity in buildings is the friction damper, which is employed as an energy absorber in this work [1-3]. Instead of the primary parts of the building yielding non-ductilely during the powerful earthquake

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movements, friction equipment slides and dissipates a considerable portion of the vibrating energy into heat. Construction seismic behavior may be effectively improved with the use of hybrid friction dampers. It has a straightforward mechanism, is insensitive to temperature changes, and reduces earthquake energy by impacting friction.

While passive devices prevent damage to both structural and non-structural systems during seismic activity, their use frequently leaves significant and long-lasting residual deformation in the wake of a seismic event.

According to recent studies, it is preferable to rebuild a new structure rather than reconstruct or repair a damaged one when the ratio of residual drift is more than 0.5% [4]. Because the integrated structure is made of concrete elements, this is a significant drawback for RC structures. The moment-resistant method is chosen by the designer since the concrete shear wall system is impractical for controlling significant drifts, particularly in metropolitan locations with high-rise buildings adjacent to one another due to architectural needs for ventilation and illumination. For instance, following the Michoacán earthquake in 1985, the majority of the RC-damaged structures were demolished due to a significant, ongoing inter-story drift [5].

It is now necessary to design structures using a performance-based approach due to seismic concerns. As a result, new structural components and systems need to be more resilient to damage, capable of reversing or lessening irreversible deformations, and have better resilience to deformation.

Several investigations were created and evaluated for the SMAs application in civil engineering for devices with self-centering attributes [6-16]. Their efficacy in mitigating seismic activity within building structures has been demonstrated through numerical and experimental studies. Massah and Dorvar [17] looked at the impact of altering the hysteresis characteristics of SMA material, which was employed in eccentrically bracing frames as a passive control mechanism. According to the outcomes, using the SMA superelastic characteristic not only effectively increases ductility-stiffness and lateral resistance but also has great rehabilitation capacity. As a result, the structure's greatest thrust and residual distortions are significantly reduced. Qian and Song [1] looked into the effects of seismic stresses on a friction damper that had SMA installed. According to the findings, a friction damper fitted with a SMA significantly enhanced the structure's dynamic reaction during strong earthquakes by absorbing a noteworthy amount of the input energy. Moreover, the structure may be repurposed to take on additional seismic loads without any residual drift because of the damper's self-centering capability. Four distinct floors (3, 5, 7, and 9) of RC structures have been examined and exposed to near-field ground vibrations in the research given by Shiravand et al. [18]. Two types of reinforcement details are taken into consideration for each building: (1) RC frame (traditional steel reinforcement) and (2) SMA RC frame (steel-SMA reinforcement), where

steel bars are utilized in some areas and SMA bars in plastic zones of beams. The "SeismoStruct" finite element program has conducted nonlinear time history studies. Based on the findings, it can be concluded that using SMA materials in the areas where the beams have plastic hinges reduces residual displacement and, in turn, the need for post-quake repairs. Shape memory alloys are generally thought to minimize structural damage and retrofit expenses. It has been noticed that there is no discussion about how the plastic hinge regions are modeled in the Opensees software for selected 18 and 22-story reinforced concrete structure frames [19,20].

In this study, we want to identify a hybrid device that can dissipate energy and provide self-centering capability. The purpose of this device is to use performance-based plastic design methodologies to decrease residual deformation and increase seismic performance in high-rise moment-resistant frames. Due to the design approach, SMA wires have the maximum potential to restore the structure to its starting condition while also making the most significant contribution to the dissipation of energy in the friction damper. An additional technique for determining this objective is SMA trait evaluation. To study the potential uses of this kind of system for reinforced concrete (RC) buildings, an analysis of nonlinear time history is conducted on 18 and 22-story RC frames, both with and without the proposed hybrid damper.

MATERIALS AND METHODS

By focusing on its non-linear behavior, the PHFD (proposed hybrid friction damper) damper serves as a fuse inside the structure, preventing harm to other structural and non-structural elements as well as non-linear behavior. There are two components to the PHFD damper. The first part is a friction damper, which dissipates seismic energy by creating a perpendicular impact force between two contact plates using high-strength bolts. This type of damper frequently employs steel-on-brass, steel-on-steel, and brake pad layers on steel as sliding surfaces. The selection of a base metal is crucial for the operation of a friction damper. For the duration of the device, a high corrosion resistance might frequently lower the estimated friction reduction coefficient. The sliding surface characteristics of low-carbon steel alloys deteriorated over time due to rust and corrosion. There was no more corrosion observed in experiments conducted on stainless steel in contact with brass. Consequently, according to Lee et al. [21], these materials can be used as friction dampers. Friction dampers have their range of motion limited by slot holes that have slot lengths equal to S. Here, S denotes the highest degree of inter-story drift achievable at the specified efficiency level. The design strategy of the PHFD damper is centered on the objective of ensuring that the structure is constructed to resist the specified degree of seismic hazard. This construction prevents inter-story drift from exceeding the allowable



Figure 1. Configuration of the PHFD damper.

amount at the effectiveness level. The bolts crash into their end wall when the displacement hits S's sliding limit, at which point the motion cannot slip anymore.

This self-centering damper, which is built on superelastic SMA wires, makes up the second half of the PHFD damper. The enormous force absorption and hysteric damping features of the superelastic NiTi wires are complemented by their quasi-self-centering function. The device can reduce the seismic reaction of a building and restore it to its pre-quake state by intelligently placing and modifying the number of superelastic SMA wires. This allows for energy dissipation and self-centering capacity. SMA cables circumscribe the two bars. This indicates that these two bars can travel on the right side's middle, lower, and higher steel plates by making a slot hole with a length of S. According to Figure 1, the tensile or compressive force range of each of these bars is identical, measuring S. The left bar is positioned S from the slot hole end, while the right bar is in contact with the slot hole at the beginning (V = 0). Due to the increase in frictional force and the SMA wires strengthening, the right rod moves to the right. However, the left bar remains stationary as the SMA wires continue to elongate. Eventually, the SMA wires will reach their maximum length and strength, causing the right middle steel plate to move even further until it collides with the left bar at the end of the slot hole. This research suggests that the design technique should find the optimal ratio of frictional force at the PHFD damper to SMA wires. Two dampers are ensured to work via coincidence, providing sufficient energy dissipation and self-centering capacity by seismic requirements.

Determination of the optimal ratio of SMA wires and friction damper

Relative to the ultimate friction damper force (V_F) and the inverted distortion yield force of SMA wires ($V_{SMA,r}$), the proposed hybrid damper's self-centering ability is mostly based on this relationship. The energy-absorbing friction damper utilizes the tensile force, r, of V_{SMA} to apply it to SMA wires. This damper has a hysteresis loop that encompasses the whole range of strain and has a kinematic hardening value equivalent to 0% of the strain hardening ratio. This is caused by the loaded PHFD damper only deforming to the extent equivalent to Δr , or the deformation corresponding to the yield force of the inverted transformation of the SMA. In the meantime, the VF force-equipped friction damper dissipates energy, and the PHFD damper's total resistance becomes V _(SMA.r) +V_F. To clarify, for the PHFD damper to possess self-centering qualities and a flag-shaped hysteresis loop, the force V_{SMA,r} has to align with the friction damper's ultimate yield force, as expressed in Eq. (1).

$$V_{SMA,r} \ge V_F$$
 (1)

It should be noted that the maximum residual displacement of the PHFD damper ($\Delta_{residual}$) is simply equal to the yield drift of the reversed deformation of SMA as Eq. (2).

$$\Delta_{\text{residue}} = \Delta_{\text{r}} = \beta \, \varepsilon_{\text{M}}^{\text{S}} \, L_{\text{SMA}} \tag{2}$$

Therefore, the value β for SMA wires is equivalent to the ratio of the forward transformation yield force (V_{SMA, f}) to the transformed evolution yield force (V_{SMA, r}).

The maximum movement of 1.5% of the floor height, which is calculated from the seismic design of the appropriate capability level, determines the length of the SMA wires. Since the secondary hardening phenomenon results in an unexpectedly large resistance, the strain restriction ϵ_M^S for SMA wires is meant to prohibit a reduction in their capacity to re-center themselves as well as minimize damage to nearby structural elements and friction dampers. But to avoid staying in the early austenitic phase of stiffness, toolong wires should be avoided. This means that Eq. (3) may be used to determine the length of the SMA wires.

$$L_{SMA} = \frac{\text{Drift}_{allowable} \times h_{story}}{\epsilon_{M}^{C}}$$
(3)

Where the power absorption friction damper exhibits kinematic stiffening with a non-zero strain strengthening rate, as illustrated in Figure 2, the friction damper resistance mustn't reach V_F until the load-deformation has reached Δ_r . The resistance difference between V_F and the friction damper resistance in Δ_r deformation during cyclic loading is called over resistance V_a and can be written as Eq. (4).

$$V_{a} = (\Delta_{r} - \Delta_{F,y}) S_{F}$$
⁽⁴⁾

Where, Δ_{Ey} and S_F are respectively equal to yield drift and the strain hardening for the friction damper. The overall resistance of the PHFD damper with the loading deformation of Δ_r is equal to $V_{SMA,r} + (V_F + V_a)$. Hence, the requirement for the PHFD damper is as Eq. (5).

$$V_{SMA,r} \ge V_F + V_a \tag{5}$$

It has been shown that the residual displacement of the PHFD damper rises as the addition strength of V_a increases. Hence, the calculated value of residual displacement for the PHFD damper is adjusted according to Equation (6).

$$\Delta_{\text{residue}} = \Delta_{\text{r}} + \frac{V_{\text{a}}}{S_{\text{F}}} \tag{6}$$

According to Eq. (6) it is known that the higher addition strength and the lower secondary stiffness of the PHFD damper can increase its residual deformation. Even so, the primary source of the PHFD damper's residual movement is still the inverse transformation yield drift of SMA. As a result, the self-centering capability of the PHFD damper is higher when the inverse transformation yield drift is reduced. Because of this, this section ignores the impact of the addition strength V_a .

Equation (7) defines the force distribution design between the self-centering Shape Memory Alloy (SMA) wires in the PHFD damper and the energy absorber friction damper. It relates the design yield force (V) with the ratio of β , stating that V _(SMA.r) is equal to β times V _(SMA.f).

$$V_{SMA,f} \ge \frac{1}{1+\beta} V$$

$$V_{F} \ge \frac{\beta}{1+\beta} V$$
(7)

The necessary space for the SMA wire combination is obtained by finding the right balance between the required shear (V) for the PHFD damper model and the SMA rod setting tensile strength at a stress level of σ_M^S =280 MPa, as determined by Equation (8).

$$A_{SMA} \ge \frac{V_{SMA,f}}{\sigma_M^S} = \frac{V}{\sigma_M^S(1+\beta)}$$
(8)

Table 1 shows the distribution of shear force between SMA wires and friction damper in terms of different β values. It is found that increasing β will reduce the contribution

Table 1. The distribution of shear force between SMA wires

 and friction damper

β	SMA wires ' $\frac{1}{1+\beta}$ (%)	friction damper $\frac{\beta}{1+\beta}$ (%)
0.00	100.0	0.0
0.25	80.0	20.0
0.50	66.7	33.3
0.75	57.1	42.9
0.95	51.3	48.7
1.00	50.0	50.0



Figure 2. Hysteresis curve of SMA wires and friction damper.

of SMA wires in the shear force so that at the value $\beta = 0$, all the shear force is transferred to the SMA wires, and at the value $\beta = 1$, the shear force is evenly distributed between the friction damper and the SMA wires.

In this section, to determine the proposed design method for determining the optimal SMA wire ratio, for specific sheer force of V=300 kN and different β values of 0.5, 0.75, and 1.0, the hysteresis curves of SMA wires and the friction damper and the sum of these two are determined as the hysteresis curve of the PHFD damper. The allowable maximum displacement is assumed to be 50 mm. The loading protocol has an initial value of 5 mm and it

increases by 5 mm after each of the three cycles to break the strips. The ultimate loading limit of displacement controlled is 50 mm (Figure 3).

RESULTS AND DISCUSSION

Analytical models comprised of two high-rise, 18- and 22-story RC frames with a 3.80-meter height per floor and five 6-meter bays divided into two groups—with or without the suggested damper—are used to assess the PHFD damper. A unique moment-resistant frame, or SMRF, was created at the life protective capability level and is included in the initial



Figure 3. Hysteresis curve of the proposed damper designed with the proposed method for different β values

0 11	TT 1 1	XATE 1.1	D i f	
Section	Height	Width	Reinforcement	<i>م</i>
	(mm)	(mm)	Top Steel	Bottom Steel
B50x50	500	500	4φ25	3φ20
B50x60	500	600	4φ25	3φ25
B50x65	500	650	5φ25	4φ25
B50x70	500	700	6φ25	4φ25
C50	500	500	20φ20	
C55	550	550	24φ22	
C60	600	600	24φ25	
C65	650	650	24φ25	
C70	700	700	24φ28	
C75	750	750	24φ28	
C80	800	800	28φ28	
C85	850	850	32φ28	

Table 2. The beam and column members' design requirements for the concrete sections

* Reinforcements q Diameter number (in millimeters)

set of models, as per the most recent version of the Iranian National Building Code and the earthquake standard. The second set of models uses the design methodology proposed in this study to construct a hybrid damper known as PHFD, which is composed of RC frames. The models' tangible parts were created by ACI 318 [22] and IBC [23] requirements. In addition, steel rebars with an elasticity modulus equivalent to that of cement-based concrete with a modulus of elasticity and compression strength are employed in the frames. Design live load and dead load values are deemed to coincide with frames that are subject to gravity loads. The frame mass is determined by taking into account the live load and the dead weight of all components, both non-structural and structural, by the ASCE 41-06 standard [24]. In Table 2, the frames' structural features are displayed. Furthermore, displayed in Figure 4 is the models' elevation.

Considering that the PHFD damper members are yielding, the non-yield members are introduced. A factor of 1.25 R_y is used in their construction, which is comparable to the design of EBF in AISC341 [25]. R_y represents the ratio between the stress at which the projected yield occurs and the stress at which the lowest yield occurs. In the unstable buckling region of the compression bracing, both the compression and tensile forces are double the buckling load (P_b). To avoid unstable buckling of the compression braces, the shear necessary to construct the proposed hybrid friction dampers must exceed the total buckling loads of both braces' horizontal components, multiplied by 1.25 R_y . AISC 341 [25] states that the R_y value of the plate-made pieces is 1.15. Consequently:

$$2P_b \cos \alpha \ge 1.25 R_y V$$
 (9)

The angle α between the brace and the horizon is given in Eq. (9). $\|(P]_b)=Eq.$ (10) may be found using Eq. (9) in terms of the braces' buckling strength.

$$P_{\rm b} = \frac{1.25 \ \rm R_y \ V}{2 \rm Cos \alpha} \tag{10}$$

The braces are selected to have a computed buckling capacity minimum (P_b). For all models, certain bracings with a 2UNP120 section and a 996 kN buckling strength are responsive.

The suggested design procedure of the frame of RC with the PHFD damper

The 2D modeling application OpenSee [26] was utilized to create numerical models of the frames. To model the P-delta effects, a vertical column was attached to the frame under the influence of a gravitational force. The axial column modeling incorporates an elastic beam-column component that is specifically constructed with an inertia moment and substantial cross-section. This design is intended to accurately consider the impact of gravity columns on the total response of the frame. To prevent any major moments from being carried by the gravity column, the beam-column parts are linked to one another by rotating springs with extremely little rotational stiffness. At last, the frame and the gravity column are joined by rather stiff truss components. Fixed and pinned are the initial story columns for the frame and gravity column at the base level.

To replicate a stiff diaphragm, every node of a particular floor is limited to its displacement in a horizontal plane. Every floor's seismic mass is split evenly among the beam-column nodes. To ensure that the P-delta impact is accounted for in the frame, gravity loads or direct loading is utilized to the beam-column nodes and the gravity column. The software utilizes a Rayleigh command to specify the damping used for the elements and nodes. To replicate the rotating connection at the intersection of the braces



Figure 4. Design details of the concrete columns and beam of the employed models

with the column and beam, a single zero-length element with high stiffness is used solely in the transmission direction. The materials employed are based on the uniaxial material model, which considers the interaction between moment and axial forces and provides a one-dimensional stress-strain relationship. The OpenSees software defines the Concrete02 type confined and unrestricted concrete material model as well as the Steel02 type steel model. Five components comprise the nonlinear beam-column element with extensive plasticity that has been used to represent the beam, columns, and brace members. The foundation for the quartet of integral points in the element direction is provided by the law of Gauss-Lobatto. The fiber model was used to model all segments. According to FEMAP696 [27], nonlinear evaluations were carried out for concrete beams and columns, using flexural cracking coefficients of 0.5 and 0.7. To accomplish this, two concrete materials were specified for the column and beam, with moduli of elasticity multiplied by 0.5 and 0.7.

The SMA wires numerical model was described by materials with uniaxial self-centering capabilities. This material, which resembles a flag, may be used to describe the superelastic behavior of an alloy with shape memory at a fixed temperature. Friction damper models are made using Steel01 materials that have hardening values near zero, which correspond to the elastic-perfectly plastic model. Uniaxial parallel materials are coupled with the aforementioned materials to simulate each component of the PHFD damper and enable simultaneous operation. A zero-length element is then added to the simulation, placed beneath the concrete beam and above the Chevron brace.

Nonlinear time history analysis

In this part, the seismic behavior of models with and without a PHFD damper in response to earthquake vibrations is investigated. The objectives of this investigation are to examine narrative drift, energy dissipation, and ductility variations. In light of an abundance of nonlinear time history data, nonlinear equations are solved by the MUMPS (multi-frontal massively parallel sparse direct solver) technique (OpenSees), which is part of the OpenSees program and its parallel computing engine. The MUMPS approach is quite effective in earlier studies and can solve large nonlinear equations significantly more rapidly. Chopra [28] states that all investigations have used Newmark's integration technique [29], which shows strong computational stability of the equations even in areas with extremely non-linear structural behavior. The FEMA-P695 paper serves as the standard for nonlinear time history assessment. This paper states that the gravity load combination that should be applied to structures during analysis is 1.05D + 0.25L, where D stands for dead load and L for live load. The loading is based on FEMA-P695 [27], which is based on ASCE/ SEI 41-06 standards [24].

Ten standardized far-field (FF)-type records—which are available in the FEMA-P695 [27]—have been utilized in this work for non-linear time history analysis (NLTH). Earthquakes in the far field were detected at a distance

ID	Record	Name	Year	Μ	PGA	EQ. Scale Factor							
No.	ID			(Richter)	(m/s^2)	22 Sto	ory			18 Story			
						PHFI)	SMRI	F	PHFD		SMRF	
						СР	LS	СР	LS	СР	LS	СР	LS
1	953	Northridge	1974	6.7	0.52	30.8	20.6	40.8	27.2	25.2	16.8	35.1	23.4
2	1602	Duzce, Turkey	1999	7.1	0.82	12.1	8.1	16.1	10.7	9.9	6.6	13.8	9.2
3	1787	Hector Mine	1999	7.1	0.34	18.6	12.4	24.6	16.4	15.2	10.2	21.2	14.1
4	169	Imperial Valley	1979	6.5	0.35	22.0	14.7	29.1	19.4	18.0	12.0	25.0	16.7
5	1111	Kobe, Japan	1995	6.9	0.51	20.8	13.9	27.5	18.4	17.0	11.4	23.7	15.8
6	1158	Kocaeli, Turkey	1999	7.5	0.36	8.0	5.3	10.5	7.0	6.5	4.4	9.1	6.0
7	900	Landers	1992	7.3	0.24	27.6	18.4	36.5	24.3	22.6	15.1	31.4	20.9
8	752	Loma Prieta	1989	6.9	0.53	11.3	7.5	14.9	9.9	9.2	6.1	12.8	8.5
9	721	Superstition Hills	1987	6.5	0.36	19.4	12.9	25.7	17.1	15.9	10.6	22.1	14.7
10	125	Friuli, Italy	1976	6.5	0.35	19.4	12.9	25.6	17.1	15.9	10.6	22.0	14.7

Table 3. The characteristics of used acceleration

of at least 10 km from the epicenter. Every earthquake is considered a powerful earthquake event if it has a magnitude greater than 6.5 or a PGA of 0.2, and these statistics are gathered from the PEER database. Strong-magnitude earthquakes with extended periods of shaking are selected because they are significant for building collapse and provide prolonged shaking of the structure, both of which are critical for determining overturning safety. The record parameters are displayed in Table 3.

The PHFD damper is tested at two different performance levels. The first performance level is LS (life safety) and prompt repairs of the fuse members that succumbed under the 10% incidence rate of earthquakes every 50 years after entering the inelastic phase, while the major structural parts are still in the elastic phase. To meet this performance goal, the building must instantly resume functioning when the fuse members are replaced. The fuse system's primary function is to prevent the original structure's members from surrendering. In the case of an earthquake with a 2% incidence rate over 50 years, all structural elements are permitted to enter the inelastic phase under the second efficiency level, known as collapse prevention (CP). Two-thirds (2/3) of the seismic risk spectrum at the highest evaluated earthquake (MCE) level should be included in the design earthquake spectrum, according to ASCE7-10, which addresses the minimum design loads for buildings. As a result, the DBE (design basis earthquake) from Iran's 2800 earthquake standard-which has the same efficiency grade as LS-may be extracted, and its corresponding CP performance level, the MCE-level risk of earthquakes spectrum, may be calculated by multiplying 3/2). Figure 5 shows the normalized seismic spectrum, mean, and the 5% damping DBE and MCE spectra.



Figure 5. The first graph (a) shows the earthquake spectrum that has been standardized and includes the average and 5% damping. The second graph (b) shows the average of the standardized earthquake spectrum, as well as the MCE and DBE spectra, all with 5% damping.

To eliminate the anticipated variations in the demand spectrum caused by earthquake motions, earthquakes are adjusted to match the acceleration of the target spectrum at a given code-defined period (T). To do this, every record is adjusted based on the PGV (peak ground velocity), as advised in the FEMA-P695 guidelines. This means that each record's PGV value needs to be normalized. The aggregate spectral acceleration of the recordings is matched to the maximum seismic response spectrum taken into consideration in compliance with the specified code. The scale coefficients of the ten chosen earthquakes are shown in Table 3 for the models at the CP and LS performance levels.

This is a thorough investigation of OpenSees' two-dimensional dynamic nonlinear time history analysis, which was done to determine the two modes of high-rise RC frames with 18 and 22 stories' seismic behavior: (1) designed using the most recent Codes approach, and (2) using the method of PBPD in conjunction with the damper of PHFD. The RDR (residual drift ratio) and IDR (inter-story drift ratio) for each story are the two generally used metrics that are the topic of this study. This makes it possible to assess a building's seismic stability during an earthquake and to specify and analyze the stories with the greatest IDR and RDR. The IDR is utilized to describe the total stability of RC frames during earthquakes. Furthermore, the two aforementioned numbers may be utilized to compute an accurate assessment of the damage that seismic loading has caused to both non-structural and structural components.

Ten earthquakes are originally applied on the frames. These earthquakes match the MCE-level earthquake excitations (probability of 10%) and the DBE-level earthquake excitations (chance of 2% over 50 years). The non-linear time history (NLTH) study of 10 earthquakes yielded the maximum IDR and the average values for the 18 and 22-story frames without and with the PHFD dampers, which are displayed in Figure 6 to evaluate each effectiveness level. At both efficiency levels, the frames fitted with PHFD dampers are more responsive than the traditional frames. Furthermore, it reacts to all of the chosen earthquakes with a much more stable reaction-that is, a more consistent or equal reaction-regardless of the earthquake parameters (such as content frequency) employed in the research. In traditional frames (SMRF), drift distribution happens unevenly at the structure's height, with the strongest IDR happening in the higher stories because of the earthquake's whipping force. This is because RC frames are traditionally designed with the assumption that lower story beams and, in particular, lower story columns, have weaker sections as a result of reduced gravity loads. Thus, the end stories with the largest IDR put the buildings at risk of rupturing in earthquakes and when higher modes predominate at the highest degrees of structural deformation. However, because the PBPD develops the PHFD damper, all stories have a chance to lessen the earthquake's lateral impact. The maximum IDR shift for these models is from the base story

to the third floor and then down to the roof. This suggests that the IDR values become closer together as we approach the roof and that the numbers nearly equalize from the structure's midway point to the top. This outcome demonstrates that the design takes into account the impacts of the interaction using the suggested method and is according to how effectively the RC frame functions with the damper of PHFD. Consequently, a system for resisting lateral loads during seismic events is designed to work almost optimally.

The average value of the maximum IDR (inter-story drift ratio) in frames equipped with passive hybrid friction dampers (PHFD) has shown a more uniform distribution at different floor levels and a notable reduction in the different degrees of damage compared to the principal frame. When comparing the mean maximum IDR of the 18 and 22-story frames at different levels to the main case, the case with a PHFD damper had lower mean maximum IDRs by 69.8% and 57.9%, respectively, at the LS performance level and by 67.7% and 56.6% at the CP level. (21). The mean of the highest IDR decreases as the models' number of tales increases from 18 to 22. Furthermore, the lowering of the maximum IDR mean reduces little when earthquake strength increases from the DBE to the MCE level, which may be disregarded. It is known that utilizing RC frames with PHFD dampers may lower the maximum IDR mean by around 55-70%, irrespective of the number of seismic and story intensities. The aforementioned result demonstrates how a large elastic hardness SMA wire set, big flange-shaped hysteresis loop friction dampers, and large and stable hysteresis loop friction dampers worked together to enable the huge lateral force absorption by the PHFD damper. These components made it possible to design a system with substantial force absorption and lateral rigidity.

In this part, the ratio of RDR of RC frames with PHFD damper is compared with conventional RC frames. As previously stated, one of the innovations in the proposed design approach of the PHFD damper is to determine the optimal number of SMA wires that can have the highest effect in providing a reversible capacity for the structure, along with having a suitable mechanism with friction damper to dissipate a large portion of the seismic forces applied to the structure. Figure 7 reveals the maximum RDR with their mean value for 18 and 22-story frames without and with the PHFD damper derived from the non-linear time history (NLTH) analysis of 10 earthquakes to study the self-centering capacity of the models. As it is clear from the figure, all models with PHFD damper at both LS and CP performance levels have an RDR ratio of approximately zero, with a completely uniform distribution at the structural height. The two main reasons for this result are (1) a significant decrease in the maximum IDR and its uniform distribution in the height due to the use of the proposed design method; (2) the design of the SMA wire set with a special look at its self-centering property, and with the consideration of the SMA forward transformation yield strain (ϵ_M^S) in a mechanism with friction damper in the proposed design method.



Figure 6. The study examines the efficiency compared between eccentrically braced frames, both with and without PHFD dampers, based on the Interstory Drift Ratio (IDR) at the CP (Collapse Prevention) and LS (Life Safety) performance levels.



Figure 7. The study aims to compare the performance of the eccentrically braced frame without and with a PHFD damper about the RDR (residual drift ratio) at the CP (collapse prevention) and LS (life safety) performance levels. However, in conventional RC frames, the RDR ratio with a completely non-uniform distribution at the structural

height, although it is acceptable at the performance level, in terms of using the building after the earthquake and counteracting future earthquakes, puts the building in a bad situation. Also, in conventional RC frames, precisely at the location of changing of columns and beam dimensions at the height of the structure, significant growth can be observed at the maximum RDR, particularly in higher stories of models due to the effect of the whipping force of earthquakes in the high-rise buildings. The authors of this article suggest using the PHFD damper with the proposed design procedure based on the performance to resolve the above-mentioned defects commonly found in common lateral load-resisting systems, especially in conventional RC frames. According to ASCE 41-06, the models' structural performance was assessed, and Tables 4 and 5 provide a summary of the results. Consideration was given to structural performance based on IDR and RDR. CP (collapse prevention), IO (Instant occupancy), and LS (life safety) are the corresponding structural performance levels when IDR is less than 1.0%, between 1.0-2.0%, and more than 0.2%, and when RDR is 0.0%, between 0.0-1.0%, and more than 1.0%, in SMRF models, according to the ASCE 41-06 standard. The structural performance levels in PHFD models are identical to those in IO, LS, and CP when the IDR is less than 0.5%, between 0.5-1.5%, and more than 1.5%, and when the RDR is 0%, between 0.0-0.5%, and greater than 0.5%. As indicated in Table 4, the 18st-PHFD, 18st-SRMF, 22st-PHFD, and 22st-SRMF models' structural performance levels for

Table 4. The level of structural performance of models subjected to 10 earthquakes for the ratio of IDR

Ground	18st-S	MRF			18st-PHFD				22st-9	SMRF			22st-PHFD			
motions	DBE Level		MCE Level		DBE Level		MCE Level		DBE Level		MCE Level		DBE Level		MCE Level	
	IDR (%)	S.P. level	IDR (%)	S.P. level	IDR (%)	S.P. level	IDR (%)	S.P. level	IDR (%)	S.P. level	IDR (%)	S.P. level	IDR (%)	S.P. level	IDR (%)	S.P. level
Northridge	1.30	LS	2.27	СР	0.57	LS	0.96	LS	1.34	LS	2.37	СР	0.85	LS	1.45	LS
Turkey (Duzce)	1.22	LS	1.97	LS	0.61	LS	0.95	LS	1.24	LS	2.09	СР	0.84	LS	1.28	LS
Hector Mine	1.62	LS	2.42	СР	0.68	LS	1.08	LS	1.44	LS	2.48	СР	0.88	LS	1.42	LS
Imperial Valley	2.47	СР	4.45	СР	0.51	LS	0.83	LS	3.82	СР	7.63	СР	0.77	LS	1.23	LS
Japan (Kobe)	1.20	LS	1.94	LS	0.44	IO	0.68	LS	1.33	LS	2.19	СР	0.76	LS	1.18	LS
Turkey (Kocaeli)	2.97	СР	3.72	СР	0.71	LS	1.28	LS	2.87	СР	4.34	СР	1.29	LS	2.09	СР
Landers	2.47	СР	3.13	СР	0.51	LS	0.91	LS	2.41	СР	2.90	СР	0.78	LS	1.49	LS
Loma Prieta	2.52	СР	3.80	СР	0.78	LS	1.24	LS	2.72	СР	3.37	СР	1.22	LS	1.65	СР
Superstition Hills	3.45	СР	6.06	СР	0.81	LS	1.29	LS	4.07	СР	4.62	СР	1.13	LS	1.60	СР
Italy (Friuli)	1.97	LS	2.73	СР	0.79	LS	1.27	LS	1.83	LS	2.80	СР	1.18	LS	1.71	СР

Table 5. The model's structural performance level under 10 earthquakes for RDI	₹ ratic
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Ground	18st-5	SMRF			18st-PHFD				22st-SMRF				22st-PHFD			
motions	DBE Level		MCE Level		DBE Level		MCE Level		DBE Level		MCE Level		DBE Level		MCE Level	
	RDR (%)	S.P. level	RDR (%)	S.P. level	RDR (%)	S.P. level	RDR (%)	S.P. level	RDR (%)	S.P. level	RDR (%)	S.P. level	RDR (%)	S.P. level	RDR (%)	S.P. level
Northridge	0.31	LS	0.47	LS	0.04	LS	0.03	LS	0.25	LS	0.33	LS	0.04	LS	0.06	LS
Turkey (Duzce)	0.15	LS	0.22	LS	0.01	LS	0.03	LS	0.09	LS	0.38	LS	0.04	LS	0.04	LS
Hector Mine	0.30	LS	0.24	LS	0.01	LS	0.02	LS	0.17	LS	0.21	LS	0.03	LS	0.07	LS
Imperial Valley	0.35	LS	1.39	СР	0.01	LS	0.02	LS	1.23	СР	0.54	LS	0.04	LS	0.07	LS
Japan (Kobe)	0.12	LS	0.25	LS	0.02	LS	0.01	LS	0.19	LS	0.18	LS	0.01	LS	0.04	LS
Turkey (Kocaeli)	0.94	LS	1.33	СР	0.08	LS	0.08	LS	1.95	СР	2.38	СР	0.16	LS	0.19	LS
Landers	1.16	СР	1.13	СР	0.05	LS	0.12	LS	0.52	LS	0.61	LS	0.08	LS	0.17	LS
Loma Prieta	0.25	LS	0.37	LS	0.01	LS	0.02	LS	0.16	LS	0.35	LS	0.02	LS	0.03	LS
Superstition Hills	0.74	LS	1.02	СР	0.02	LS	0.04	LS	1.05	СР	1.18	СР	0.03	LS	0.04	LS
Italy (Friuli)	0.29	LS	0.47	LS	0.03	LS	0.04	LS	0.30	LS	0.56	LS	0.01	LS	0.02	LS

the IDR of the DBE seismic level are (LS 50%, CP 50%), (CP 0%, LS 100%), (LS 50%, CP 50%), and (CP 0%, LS 100%), respectively, and for the level of MCE seismic, they are (LS 20%, CP 80%), (CP 0%, LS 100%), (LS 0%, CP 100%), and (LS 60%, CP 40%). It was discovered that whereas frames of RC with PHFD dampers gave 100% of the acceptable structural performance level, standard RC frames at the DBE seismic level only offered 50% of that level. Additionally, for RC frames with and without PHFD dampers, the suitable structural performance level at the seismic level of MCE is equivalent to 0–20% and 60–100%, respectively.

The RDR ratio's structural performance level for the 18st-PHFD, 18st-SRMF, 22st-PHFD, and 22st-SRMF models included (LS 100%, CP 0%), (CP 10%, LS 90%,), (CP 0%, LS 100%), and (LS 70%, CP 30%) at the level of DBE seismic, and (LS 100%, CP 0%), (LS 60%, CP 40%), (LS 100%, CP 0%), and (LS 80%, CP 20%) at the level of MCE seismic. For all seismic intensities and models, the RC frames with PHFD dampers achieved 100% of the level of targeted structural performance. However, standard RC frames, despite offering 60–80% and 70–90% of the structural performance at the MCE and DBE seismic levels, respectively, have a residual drift of more than 0.5%, which places the structure in an unfavorable position to handle subsequent earthquakes (Table 5).

CONCLUSION

Using the performance-based plastic design technique, two high-rises, 18- and 22-story reinforced concrete buildings were constructed, either with or without PHFD dampers, to investigate the potential benefits of a hybrid friction damper with SMA wire in decreasing the seismic response of tall reinforced concrete buildings. The RC frames and the PHFD damper's interactions were taken into account during design. The study compared the temporal histories of ten far-field earthquakes with models. The findings revealed a decrease in all major indicators, such as the IDR (inter-story drift ratio) and the RDR (inter-story residual drift ratio). Specifically, the mean IDR of RC frames with PHFD dampers was found to be 55-70% lower compared to conventional RC frames. Additionally, the IDR distribution displayed more consistent behavior at different heights of the frames. The average maximum RDR may be significantly reduced by 82%-97% when using a PHFD damper in RC frames as opposed to conventional RC frames. With consideration for the recommended constraint for SMA wires (strain below six percent to estimate the length and strain comparable to the inverted distortion yield strain for an ideal mechanism with a friction damper), this decrease happens when the design that is the performance technique is applied. RC frames with a PHFD damper not only have the maximum energy dissipation capacity, but they also have a respectable reversibility capacity.

DATA AVAILABILITY STATEMENT

There is no data source for this research. All data are presented directly by graphs. All models, data, and code generated or utilized during the study appear in the submitted article.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Perspective on the production, characterisation and physio-mechanical behaviour of bioplastics from different biomass feedstocks

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ABSTRACT

Due to the rapid growth in the world's population and industrialization, the demand for plastic has increased over the past few years. Synthetic plastics are produced from fossil fuels and their continuous use has significantly increased the global greenhouse gas (GHG) emissions making the carbon footprint of plastics high. These conventional plastics are not easily degradable, and their disposal poses an environmental threat to humans and aquatic organisms. Several innovations are ongoing to produce bioplastics from alternative materials that are renewable, easy to dispose of and biodegradable without compromising their physical and mechanical properties. The substitution of synthetic plastic with bioplastics from plants and animals' by-products will significantly decreases the amount of packaging waste generated. Numerous biomass feedstocks from polysaccharides, lipids and proteins are used in the production of bioplastics. However, the mechanical properties of bioplastics are continuously improved by using various reinforcement techniques to enhance their properties and increase their applicability. The influence of the type of feedstock, synthesis techniques, type and concentration of plasticizer and fillers blended with the feedstock on the physio-mechanical properties and degradation of bioplastics was reviewed in this study. The opportunities and challenges of bioplastics from biomass were also outlined.

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INTRODUCTION

The surge in population across the world and the industrial revolution have increased the global demand for plastics. The global annual plastic production over the years increased from 234 million tonnes (Mt) in 2000 to 460 Mt in 2019 as shown in Figure 1 [1]. Most of the

petroleum-based plastics like polyethylene, terephthalate, nylon, polystyrene, teflon, polyethene and polyamides are known as synthetic plastics, and they have wide applications in the packaging and agricultural sectors. The main elements of synthetic bioplastics are carbon, hydrogen, nitrogen, oxygen, chlorine, and bromine and the degrees of crystallinity, chemical structures and molecular weights

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determine their rate of biodegradation [2]. Despite the non-biodegradability of synthetic plastics, their desirable properties such as lightweight, malleable, excellent thermal and rheological properties, and low cost of production have made them ubiquitous in the global economy over the years [3]. According to the OECD report [1], the continuous use of plastics has increased plastic waste from 156 Mt in 2000 to 353 Mt in 2019, about 9% of plastics were reused or recycled, 50% were dumped in controlled landfills, 19% were destroyed by burning while the residue 22% are dumped in uncontrolled sites, burnt in open pits, or enter the marine environment. The dumping and build-up of waste plastics in landfills and marine environment are the primary cause of ground and water pollution and poses a danger to the health of humans and aquatic animals. The production of synthetic plastic and its disposal contributes significantly to global greenhouse gas (GHG) emissions making the carbon footprint of plastics high. The average lifetime of synthetic plastic products is almost 10 years, therefore plastics buried in the ground pollute groundwater and cause danger to the well-being of living organisms. Alternative biodegradable plastics feedstock and proper management of plastics waste are necessary to reduce the GHG emitted into the atmosphere. The gradual degradation and incorporation

of benzene into the food when synthetic plastics come in contact with food make synthetic plastics unsuitable and unsafe in the food packaging industries.

Innovations, excellent product designs, improved waste management, an increase in recycling, and the promotion of environmental and biodegradable polymers are needed to reduce the pollution and contamination from plastics. Biodegradable polymers are easily degraded by microorganisms (algae, fungi, yeast, bacteria, and insects) into biogases, biomass, and products with low molecular weight [4,5]. Environmental conditions like temperature, light, environmental pH, the presence of microorganisms, presence of oxygen and water influence the rate of bioplastics degradability [6,7]. Biodegradable polymers are commonly synthesized through the processes of fermentation that involve microorganisms and chemical modification of natural materials such as polysaccharides [5]. Several innovations are ongoing in the field of biological sciences and engineering to produce plastics tagged "bioplastics" which are synthesized from biomass, easy to dispose of and degrade without harming the environment. Bioplastics are synthesized from various biomass sources like lipids, proteins, and polysaccharides [8-10] as shown in Figure 2. The utilization of these bioplastics in the medical, packaging,



Figure 1. Global plastic use in million tonnes (Mt) from 1950-2021 [1].



Figure 2. Bioplastic feedstock from Biomass.

electronics, construction, and agricultural industries will reduce energy consumed from fossil fuels and the emission of GHG, thereby making the environment suitable and safe for humans and aquatic animals. This review focuses on the techniques used in the production of bioplastics from polysaccharides, proteins, and lipids. The influence of various parameters and additives on the physical and mechanical properties of bioplastics considering the effect of micro-fibers and nanoparticles on the enhancement of the properties of bioplastics was discussed. Furthermore, the challenges and potential strategies required to improve the properties of bioplastics making them commercially sustainable were highlighted.

STARCH-BASED BIOPLASTICS

Polysaccharides are macromolecular polymers obtained from biomass like plants, microorganisms, and algae [11]. They are categorized according to the class of monosaccharide, their physiological properties and building blocks [12]. Pure starch is a carbohydrate that is usually white in colour, odourless, nontoxic, not soluble in cold water or alcohol and contains a high amount of glucose and they are extracted from polysaccharides. Branched amylopectin and linear and helical amylose are the types of molecules present in starch [13]. The gelatinization, viscosity, tensile properties, and functional and chemical properties of bioplastics are influenced by the percentage content of amylopectin and amylose in the starch [14-16]. Almost 50% of bioplastics produced for commercial packaging are starch-based. Starch is favourable in the production of bioplastics because they are cheap, renewable, sustainable, plentiful, low-cost of production, biodegradable and possesses suitable tensile properties [17,18].

Extraction of Starch from Polysaccharides and the Preparation of Bioplastics

The extraction of starch from polysaccharides such as yam, maize, rice, potatoes, cassava, corn etc. involves the milling of the seeds and tubers with distilled water using a high-speed blender to obtain paste. The paste is filtered using a filtering cloth to get the crude starch filtrate liquid. The filtrate liquid is let to sediment at room temperature for the pure starch to settle. The supernatant is poured away, and the pure starch obtained is dried using an oven at 70 °C to evaporate the remaining water. The starch is sieved with a strainer for better homogeneous size [19-22]. Despite starch being abundant in nature and cheap, it cannot be used as packing polymers without additives due to its high-water solubility and poor mechanical properties. These limitations need to be overcome before starch can be considered a sustainable feedstock in bioplastics production. Additives such as plasticizers are added to starch to boost its mechanical properties and lower the water solubility of bioplastics. The commonly used plasticizers are sorbitol, formamide, urea, xylitol, and glycerol. Glycerol is mostly used because it is from natural sources, and they are edible and safe to use for packaging without any form of contamination with food.

Bioplastics are usually produced using thermomechanical and casting methods. The thermomechanical method consists of the extrusion, injection moulding, thermomoulding and compression moulding methods [23,24] as shown in Figure 3. The extrusion technique involves the use of an extruder with a spindle barrel and electric heating system to extrude the dough like bioplastic and the injection moulding is a closed mould process involving the injection of bioplastic polymer into the mould under elevated pressure and temperatures. The thermomoulding technique is usually employed to produce line-walled and lightweighted products from preextruded plastic sheets while the compression moulding technique involves the application of mechanical pressure on the heated polymeric material placed in the lower side of the mould. The casting method is commonly used in the production of starch-based bioplastics [25-28]. Thu and Aye [29] used the casting method to produce bioplastic film from dent corn



Figure 3. Bioplastic production methods for polysaccharide.

starch using 0.5 g of glycerol and 20 mL of distilled water. The gelatinized mixture was transferred and pasted on a substantial steel plate and allowed to dry in the oven for 90 minutes at 50 °C. It is very important to ensure that air bubbles are removed and not formed in the bioplastic film when using the casting method. The presence of air bubbles affects the characterization and properties of the bioplastic film. Gustafsson et. al [30] employed compression moulding and solution casting methods to produce bioplastic film from apple pomace blended with glycerol. In the compression moulding, the glycerol is blended with apple pomace powers before compression to produce a 3D object while in the solution casting, the blend of apple pomace powder, glycerol and citric acid was heated to 70 °C while stirring the mixture on the magnetic stirrer and later poured on a non-stick plate. Santana et al [31] and Nguyen et al [32], produced bioplastics from jackfruit starch using the casting method. Cassava and sugar fiber hybrid composite bioplastic film was produced by Edhirej et al. [33] employing the casting technique with fructose as the plasticizer. Most of the literature reviewed showed that starch-based bioplastics were mostly produced using the casting method. Further studies should be conducted to investigate the impact of production techniques on the characterization and physical mechanical properties of bioplastics.

Physical-Mechanical Behaviour of Starch-Based Bioplastics

Natural starches have some limitations relating to thermal stability, water absorption and mechanical properties [34]. To overcome these challenges, certain additives made from natural or synthetic materials are blended with starch to make them thermoplastics and enhance the material processing, properties, functional behaviour and widening their applications [35]. The resistance of bioplastics to moisture is improved through the addition of synthetic polymers, cross-linked agents, slats and lignine while the flexibility of starch is improved through the blending of plasticizer [36]. The interaction of the polymer-polymer hydrogen bond is reduced by the plasticizer, thereby reducing the intermolecular binding sites starch in granules' crystalline region and enhancing the interfacial adhesion [37]. The required properties of the bioplastic can be achieved by varying the quantities of the additives such as glycerine, water, fillers, and eco-friendly polyesters.

Thet [8] studied the effect of glycerine (0.25g - 1.0g), and water (6 ml - 10 ml) content on the biodegradable characteristics of plastics produced from corn starch. The viscosity and the thickness of the plastic produced were observed to be proportional to the content of the glycerine. The volume of water in the sample affected the viscosity, number of bubbles and translucency of the plastic produced. The most suitable condition for biodegradable plastic produced from corn starch was corn starch of 1.5 g, glycerine of 0.5 g, distilled water of 7 ml and 1 ml of vinegar. The product at these conditions had no bubbles, good tensile strength, and less drying time. The degradability test showed that bioplastics can degrade within 28 days when buried in the soil or soaked in water. To further enhance the properties of corn starch bioplastics, Marichelvan et. al [20] added rich starch to the corn starch. The higher amylose concentration of the corn and rice starches motivated the authors to combine them. The quantities of water, glycerol, citric acid, and gelatine used in the preparation process were constant but the quantity of rice to corn starch was varied. The mechanical resistance against rupture of the bioplastics impregnated with rich starch was 1.5 times higher than that of a non-impregnated counterpart. Samples with the ratio of rice to corn starches of 7:3 had an elongation of 6.8%, Young's modulus of 0.183 GPa, and maximum tensile strength of 12.5 MPa. The thickness of the bioplastics obtained was 250 microns. Comparing the thickness of the bioplastics with other works [38,39], the higher thickness was attributed to the presence of the corn starch but the influence of concentration of glycerol on the bioplastic thickness was not considered in this study. The biodegradability of the sample achieved after 15 days was 48.7%. Potatoes and corn starch were used as feedstock to produce bioplastics with glycerol and acetic acid as additives by Al Balushi et al. [19]. The bioplastics with higher content of potato starch had lower flexibility and durability but they were soft and transparent while those with higher corn starch were rough with low transparency, but the durability and flexibility were enhanced. The degradation rate of bioplastics is influenced by the proportion of corn starch and potato starch in each sample. The low durability and flexibility of the potato-based bioplastics can be attributed to the percentage of amylose content in the starch. According to Young [40], the amylose of potatoes is lower than that of rice and corn starches. Ceseracciu et al. [14], stated that the tensile property of the bioplastic is proportional to the amylose content in starch.

The low durability and non-adhesion between glycerol, water and starch affect the application and properties of the bioplastics respectively. To overcome this challenge, citric acid and sodium bicarbonate were blended with jackfruit seed starch by Nguyen et al. [32] to enhance their mechanical and chemical properties. The citric acid strengthens the adhesion between the glycerol, starch, and water and effectively inhibits starch retrogradation due to its strong hydrogen bonding interaction with starch while the sodium bicarbonate was added as a preservative to strengthen and make the bioplastic more durable. The study observed that the bioplastics produced were softer and more flexible when the ratio of the glycerol increased but increasing the citric acid concentration in the bioplastic improved the hardness and decreased the plasticity of the bioplastics. The maximum tensile strength of 5.15 MPa was recorded with a starch glycerol ratio of 3.5:1 but micro air bubbles were found inside the bioplastic thereby affecting its mechanical properties. Jiugao et al. [41] investigated the influence of citric acid on the properties of thermoplastic starch plasticized by glycerol and stated that the citric acid decreased the

shear velocity and enhanced the fluidity of thermoplastic starch but decreased the tensile stress. The water resistance is improved at high relative humidity, thereby elongating the durability of the bioplastic.

The oil content in starch-based plants has been observed to influence the mechanical properties of bioplastics. To further enhance the applicability of bioplastics from rice, the oil and fiber fraction in rice bran was extracted by Alonso-Gonzalez et al. [42], the mechanical, functional, and microstructural properties of rice bran-based bioplastics with sorbitol and glycerol as plasticizers were investigated. The result showed that the viscoelastic moduli of the defatted rice brain bioplastic were higher and had better tensile properties, but the vapour uptake capacity decreased. There was no significant improvement from the fiber-free rice bran-based bioplastics. Considering the influence of plasticizer type, the glycerol-plasticized bioplastics showed a lower glass transition temperature and higher plasticizing efficiency with higher deformability. While the bioplastics from sorbitol plasticizer exhibited high-stress values and better stiffness. The blending of starch with plasticizer improves the flexibility and workability of the bioplastics but the hardness is reduced [43]. The high susceptibility to humidity and retrogradation process has limited the application of bioplastic from starch [44].

Physical-Mechanical Behaviour of Micro-Natural Filler in Starch-Based Bioplastics

The poor mechanical properties and high moisture absorption of starch-based bioplastics have limited its application. One of the foremost innovations adopted in addressing these shortcomings is the blending of starchbased bioplastics with less hydrophilic polymers known as fillers. Fillers are more economical because they are less expensive, and they act as a primary load-bearing component. Fillers such as cellulose from plants are used to improve the mechanical properties, decrease elongation capacity, increase Youngs' Modulus, and enhance permeability to gas and resistance to water [45]. Natural fillers were added in the production of bioplastics by Shafgat et al. [26] to improve the chemical and physical characteristics of bioplastics produced from banana peels, rice, and corn starches. The bioplastics produced were reinforced using waste agricultural products from potato peel powders and sawdust as fillers. In this study, the content of plasticizers (glycerol, sorbitol) and fillers in the bioplastics produced were varied. The ratio of banana peel paste, corn and rice starches solution were blended in the ratio of 40:30:30 respectively. The absorption of water by bioplastics was reported to be influenced by the nature of the filler and its content. Introducing plasticizer into the bioplastics enhanced the rate of biodegradation while the addition of fillers (5% w/v) reduced the biodegradation rate of plasticized bioplastics and enhanced it in the unplasticized bioplastics. Bioplastics with glycerol had the least Youngs Modulus and tensile strength while those with sorbitol had the highest Youngs Modulus and

tensile strength. These properties increased proportionally with the content of the filler in both the glycerol and sorbitol bioplastics.

To decrease bioplastics' moisture absorption and improve its mechanical properties, Maulida [21] reinforced cassava peel starch with microcrystalline cellulose (MCC) of particle size 50 µm using varying content between 0 to 6% dispersed in water. The sorbitol was used as the plasticizer and the concentration varied between 20- 30 % wt/v to the starch. The increase in the content of MCC improved the tensile strength and this was credited to the excellent interfacial adhesion that formed a strong 3D hydrogen bond network between the starch matrix and the microcrystalline cellulose fillers. Due to the hydrophilic nature of water, cellulose is less sensitive to water than starch. Therefore, increasing the concentration of MCC (0-6%) led to a decrease in the water uptake. The maximum tensile strength of 9.12 MPa was observed at a microcrystalline cellulose content of 6% and 20% of sorbitol. The combination of MCC particles with the starch matrix led to agglomerates that led to deflections in the samples. Abdullah [46] also investigated the effect of microcrystalline cellulose reinforcement derived from high-quality wood pulp on the mechanical, physical, and biodegradable properties of bioplastics derived from cassava starch using glycerol, potato dextrose agar, and salt agar as additives. The thickness and the density of the bioplastics produced increased as the content of the microcrystalline cellulose increased. Increasing the content of microcrystalline cellulose enhanced the hydrophobic properties of bioplastics. The elongation reduced while the thermal stability and Young's modulus increased with an increase in the microcrystalline cellulose. Due to the chemical similarity between the starch and the cellulose, the adhesion of the microcrystalline cellulose starch interface increased the tensile properties of the bioplastics. In summary, the presence of natural cellulose micro-fiber in the matrix of the bioplastic enhanced the physical-mechanical properties of the starch-based bioplastics. The effect of the size of the filler and concentration used as reinforcement in bioplastics needs to be adequately investigated to understand how it affects the characterization and properties of the bioplastics.

Physical-Mechanical Behaviour Nanoparticles in Starch-Based Bioplastics

Polymer researchers have deployed nanotechnology in the enhancement of packaging material's properties from starch without compromising the biodegradability of the materials. For significant enhancement of the properties of bioplastics, low concentrations of nano-sized additives were blended with starch-based bioplastics to advance their mechanical, thermal, optical, and physicochemical properties [47]. Carbon nanotubes, nano-calcium carbonate and nano-silica are mostly used as nanofillers. In this technology, the polymer matrix of the bioplastic is reinforced with nano-dimensional particles as an alternative to the conventional micro-dimensional fillers earlier discussed. The large surface possessed by nanoparticles promotes better interfacial interactions with the polymer matrix [48]. The use of nanosized particles at a lower concentration between 1- 5% produces an additional homogeneous dispersion of the particles, increases the specific surface of reinforcement, and possesses better mechanical, physical, and thermal properties than the micro-sizes reinforcement [49-51].

Nano clay is an advanced biodegradable polymer with improved barrier and mechanical properties. The most used clay is montmorillonite (MMT), and the type of MMT-polymer interaction influences the behaviour of the nanocomposite material. Using the solvent casting method, Calambas et al. [47] produced films from achira starch/ polyvinyl alcohol (PVA) reinforced with MMT nano clay at varying concentrations (0.5 - 5% w/v) and glycerol. The starch/polyvinyl alcohol to nanoclay ratio used in this study was 3:2. The percentage of elongation, Youngs' Modulus and tensile strength enhanced with sonicated nano clay of 0.5% w/v. the mechanical properties were worse in the 1.0 and 1.5% w/v when compared with films without nano clay. Nano clay concentration above 1.0% w/v saturated the polymer matrix thereby influencing the physicochemical properties of the nano bioplastic. It was concluded that only 0.5% w/v of nano clay can be successfully mixed with matrix starch/PVA for use as biodegradable packaging. Apart from the concentration of nano clay used, Chen and Evans [52] reported that the type of plasticized used also limits the application of bioplastic. The percentage elongation of the nanocomposites prepared from glycerol plasticized starch with varying content of sodium montmorillonite and hectorite increased from 47 to 57% while the tensile strength increased from 2.6 to 3.3 MP for 5% sodium montmorillonite. Sariadi and Raudah [48], reported that the increase in plasticizer content negatively affected the reinforcing influence of the clay on the starch, thereby causing an increment in the elongation percentage and a reduction in the tensile strength. The maximum tensile strength was observed at 0.6% concentration of nano clay and 25% glycerol. Park et al. [53] stated that the high levels of glycerol plasticizers limit the applications of bioplastics in certain areas.

Using inorganic fillers such as metals and metallic oxides, the thermal and mechanical properties of composite bioplastics from corn starch blended with titanium dioxide (TiO₂) nanoparticle was analysed by Amin et al. [54]. The addition of TiO₂ nanoparticles decreased the elongation of the bioplastic from 88 to 62 and enhanced the tensile strength from 3.55 to 3.95 MPa. The mechanical strength was enhanced but with less flexibility. From the TGA analysis, the composite bioplastic had higher thermal stability when compared with starch bioplastic, but the rate of biodegradability was higher for the nano-based bioplastic. The higher biodegradability of the nano-based bioplastic was due to the antimicrobial properties of TiO₂. This makes

bioplastics suitable for packing in the pharmaceutical and food industries.

Titani and Haryanto [55], combined zinc oxide (ZnO) and titanium oxide (TiO_2) nanoparticles as fillers in the production of bioplastic from 40 grams of tapioca starch mixed with 10 g corn starch. The bioplastics produced without nanoparticles had the presence of air bubbles and the addition of TiO2 and ZnO eliminated the air bubbles. The addition of nanoparticles also improved the mechanical properties and elongation of the bioplastic. The antimicrobial property of nanoparticles caused the nano-bioplastics to degrade longer when compared with bioplastics without nanoparticles. Rahman [56] investigated the effect of copper oxide (CuO) nanoparticle concentration on the elongation and tensile strength of potatoes-based bioplastic. The nanoparticles varied from 0.5 % to 4% and the highest tensile strength of 6.84 MPa was observed at 5% concentration whereas the tensile strength of 4.1 MPa was reported for bioplastic without nanoparticles. The tensile strength was below that of the starch sample when the nanoparticle content was increased beyond 1%. This observation was attributed to the agglomeration of CuO on the sites of CuO and the functional group (OH, CH, CO) interaction in the starch. Above 0.5% concentration, the elongation decreases as the nanoparticle's concentration increases. The elongation was lower than that of starch-based bioplastics above 2% concentration.

The increase in the concentration of inorganic nanoparticles reduced the elongation of the bioplastic. Therefore, to overcome this limitation, organic nanoparticles were used as reinforcement [57]. The starch nanoparticles are smaller in size and possess a large surface area which makes them suitable for use as fillers in the production of bioplastics. The organic nanofiller concentration, characteristics and filler-matrix interaction impact the properties and characterization of the bioplastics [58]. Starch nanoparticles were used as nano-fillers to produce a bioplastic film from rice using sorbitol [59]. The flexibility of the film reduced while the tensile strength increased as the content of rice nanoparticles increased. The tensile strength of the bioplastic without the rice nanoparticle fillers was reported as 7.12 MPa while the elongation at break had a value of 53.46%. The enhanced tensile strength of 12.86 MPa and flexibility of 2.48% were recorded when a 30% concentration of rice nanoparticles was added to the starch matrix. The effect of cellulose nanofiber (CNF) and cellulose nanocrystal (CNC) reinforcement on pumpkin starch (PS)-based composite film properties was studied by Zhang et al. [60]. The nanocomposite was prepared using the casting method with 1% or 2% concentration of CNC, 10% or 15% concentration of CNF and 30% glycerol. The agglomeration of the CNC at a higher concentration in the PS matrix led to a decrease in the degradation of CNC/PS as the concentration of cellulose nanocrystals increased. The thermal stability of cellulose nanofiber nanocomposites was better than that of cellulose nanocrystal nanocomposites while the tensile

strength results showed that cellulose nanocrystal had better-reinforcing capacities than cellulose nanofiber. The high elastic modulus of cellulose nanocrystals is the reason for the enhancement. The maximum tensile strength of 30.32 MPa was obtained in nanocomposite films with 1% cellulose nanocrystal. The mechanical property of the nanocomposite was influenced by the functional and crystallinity (related to its apparent rigidity and modulus) groups of nanocellulose. Table 1 shows different bioplastics feedstock, additives, and their properties.

PROTEIN-BASED BIOPLASTICS

The increase in agricultural and food waste has advanced the production of protein-based bioplastics. Proteins are heteropolymeric chains containing different amino acids. Proteins occur in nature, and they are made up of a long chain of amino acids [61]. Protein-based biopolymers are extensively utilized as edible films because of their improved mechanical properties when compared with polysaccharides [62]. The bioplastics produced from protein possess antimicrobial and antifungal properties thereby preventing the contamination of food and drugs [63]. Covering food with protein-based bioplastics prevents the loss of moisture and flavour, thus, increasing the shelf life and controlling the exchange of gases [64]. These properties make protein-based bioplastics suitable for packaging in the food and drug industries.

Protein-Based Bioplastics Synthesis Methods

For the polymerization of protein to produce bioplastic, the primary amino acid structure of the protein serves as a repeat unit. The protein is denatured to break down the secondary bonds leaving the primary bond in the amino acid backbone [65]. In the denaturing process, force is applied to ensure that the plasticization process is complete, insufficient force can result in particle plasticization causing some protein to return to its coiled state [66]. The plastics produced after complete plasticization have similar properties to the protein used. Heat in the form of UV treatment can also be applied in the denaturing of protein [67]. Examples of protein used in the production of protein-based bioplastics are albumin, wheat gluten, whey, keratin, corn zein, bloodmeal, soy protein, keratin, collagen, animal protein, fish myofibrillar protein and gelatin [62,68]. The source of the protein is a major factor that affects the characteristics and properties of protein-based bioplastics. Albumin obtained from the egg white of a hen was used to produce bioplastic using glycerol as the plasticizer. The bioplastic obtained from albumin exhibited a better rheological property when compared with that obtained from wheat gluten plasticized with glycerol [24].

The common techniques used in the production of bioplastics from protein are injection moulding, compression moulding, casting, extrusion, and hot-press moulding as shown in Figure 4. The casting method involves the dissolution of the protein in a solvent with a plasticizer. The mixture is then poured into the mould with the desired cavity. The solution is allowed to dry with the solvent evaporating. The physical and mechanical of the bioplastic produced are dependent on the drying temperature. The tensile strength and Young's Modulus increased with the increase in drying temperature [69]. Protein-based bioplastic was prepared by Kayserilioğlu et al. [70] from cotton seed protein using the hot press moulding after denaturing the protein and formaldehyde, glyoxal or glutaraldehyde was used as the crosslinking agents. In the extrusion technique, shear stress and heat treatment were applied to the protein causing the protein to undergo complex association and dissociation. The characteristics and properties of the bioplastics are dependent on the screw speed, temperature gradient within the extruder, the type and concentration of additives and plasticizers used, the size and shape of the die which affects denaturing of the protein, and aggregation of proteins [71]. Alias and Ishak [72] prepared protein-based bioplastics from fish waste using the extrusion and compression moulding methods. The impact of heat treatment and processing technique on the thermos-mechanical properties of bioplastics produced from rice, albumen, wheat gluten, and albumen/gluten blends using glycerol as the plasticizer showed that the casting method provided bioplastics with higher thermosetting properties when compared with the thermos-mechanical method [24]. Injection modelling is the most popular process used in the production of protein-based bioplastics [73]. The piston injection moulding method was used to produce bioplastics from the dough-like blend of pea and glycerol [74]. With shorter mixing time, lower energy consumption and intermediate mixing speed of 30 rpm, the bioplastic produced had higher elongation and enhanced tensile properties along with better homogenization. Increasing the injection mould temperature improved the tensile stress and elongation, but there was no significant improvement in Young's modulus, and the water uptake capacity was hindered [75].



Figure 4. Bioplastic production technique from protein source.

Crosslinking is a chemical process of creating covalent bonds to link two or more polymers. Various crosslinking methods are used in the preparation of bioplastics from proteins. The three most common methods are physical crosslinking which uses physical agents, chemical crosslinking which uses chemical agents and enzymatic crosslinking which uses enzymes [76-78]. In the production of wheat gluten films, 1-Ethyl-3-(3-dimethaylaminopropyl) carbodiimide and N-hydrooxysuccinimide were used as cross-linking agents to improve water sensitivity and enhance the tensile strength of the wheat. Due to the innate toxicity of these crosslinking agents, they are not used in food packaging applications [79]. The characteristics of protein-based bioplastics such as antibacterial resistance, antioxidant properties, biodegradability, and mechanical properties make them suitable for use in the packing of food and drug delivery, but the low percentage of elongation causes them to break as they cannot reach the 150-500% elongation of polyethene or PVC plastics.

Physical-Mechanical Behaviour Protein-Based Bioplastics

Protein can be added to starch to overcome some of the challenges with starch-based bioplastics earlier discussed. Omrani-Fard et. al [80] added protein into potato flour to improve the starch-based bioplastics properties. The protein enhanced the tensile strength and improved the flexibility and elasticity of the starch-based bioplastics [23]. Albumen was introduced into corn/potato starch to further enhance the properties and application of bioplastics. The influence of thermo-mechanical, thermoplastic formation processes on the optical and mechanical properties of the albumen-starch samples containing 0-30 wt.% starch was investigated. The outcomes of the investigation were compared with the results obtained for wheat gluten-based bioplastics. The tensile strength and elongation at break of the albumen/starch bioplastic showed a monotonous and rapid decrease as the content of starch increased while the gluten-based bioplastic had a higher elongation at break, but the tensile strength was low. It was reported that the inclusion of starch granules in the protein matrix created heterogeneities in the matrix that operated as stress concentration points generating cracks and causing the values of elongation and strength to be lower. The work highlighted that certain starch is incompatible with protein and it was more pronounced for the corn starch and the thermo-mechanical properties of the bioplastics are mainly influenced by the protein matrix. The addition of starch to albumen bioplastics within the concentration and temperature investigated has no significant impact on the thermo-mechanical properties. The albumen/starchbased bioplastic properties were greatly affected by the processing method. To improve the compatibility of protein with starch, sodium bisulfite was used as a reducing agent along with glyoxal and L-cysteine as crossing linking agents to process the rice protein concentrate used in the development of rice protein-based bioplastics with high

biodegradability and excellent thermo-mechanical properties. Thermoplastic and injection moulding techniques were used to develop rice protein-based bioplastics. The optimum glycerol concentration, mixing time and process conditions were obtained in this study from the calorimetric and rheological measurements. The specimen produced degraded within 21 days.

Using the hot-press moulding technique, the influence of crosslinking on the mechanical strength, water absorption resistance and thermal stability of cotton seed protein bioplastics using glycerol, aldehydes, and urea as plasticizers [70]. Due to the increase in free volume and reduction in structural integrity, an increase in the content of the glycerol in the cotton protein led to a decrease in the a-relaxation and denaturation temperature. At low temperatures, a higher value of storage modulus was reported at lower concentrations of glycerol. Perez-Puyana et al. [74] introduced heat treatment as an additional physical crosslinking to enhance the mechanical and functional properties of the bioplastics from pea protein. The heat treatment process enhanced the mechanical and elastic properties of pea protein while lowering the critical strain and water uptake capacity. The pea-based bioplastics exhibit excellent antimicrobial properties, but the heat treatment modified the protein structure, worsening the antimicrobial character. The antibacterial, viscoelastic, and thermal properties of bioplastics produced from whey, soy and albumin were investigated by [65] and rubber latex, glycerol, and water were used as the plasticizer. The thermal properties of the soy and whey bioplastics have similar degradation temperatures occurring between 50 and 60 °C and this was lower than that of albumin bioplastics. The albumin or whey films plasticized with glycerol had the best antibacterial properties while the albumin and whey showed similar viscoelastic properties. The soy bioplastics presented a larger range of properties based on plasticizers. Alias and Ishak [72] prepared protein-based bioplastics from sardine by-product, mackerel by-product and mackerel fillet powder investigating the effect of various plasticizers (polyethylene, triethylene and glycol) on the thermal stability and mechanical of the bioplastics. The incorporation of plasticizer increased the elongation at break but lowered thermal decomposition and tensile strength. The type of plasticizer does not significantly influence the mechanical properties, but the processing of the protein was affected by the type and concentration of plasticizers. Due to the large protein miscibility, high solubility in water and low molecular weight of glycerol, the bioplastics produced using glycerol had the highest enhancement in mechanical properties but the lowest decomposition temperature. Rezaiyan Attar [81] using glycerol and sorbitol plasticizers at varying concentrations studied the opacity, surface properties, and thermal and mechanical, of bioplastics produced from Vicia villosa protein isolate. As the plasticizer concentration increased, the tensile strength decreased concurrently with an increase in elongation at break and water vapour permeability. The film plasticized with sorbitol exhibited higher film solubility

and tensile strength when compared with glycerol-plasticized films, but the water vapour permeability was low. The moisture content for sorbitol plasticized films was lower than those of glycerol.

The effect of heat treatment and processing techniques on the thermos-mechanical properties of bioplastics produced from wheat gluten, albumen, rice, and albumen/ gluten blends using glycerol was studied [24]. Protein denaturing occurred during the thermos-mechanical treatment, and this led to an increase in the degree of crosslinking between the molecules. A deduction in the values of the linear viscoelasticity functions was observed in the protein/glycerol film and this was caused by the hygroscopic characteristics of the films. The blend of albumen and rice reduced the concentration of protein and thermosetting temperature giving rise to linear viscoelastic moduli values like that of LDPE and HDPE. Apart from the mechanical and thermal treatment, the concentration and characterization of the glycerol, the source of protein affected the characteristics and properties of the films. Ramos et al. [82] investigated the properties of whey protein concentrate and whey protein isolate with varying concentrations of glycerol. The Young's Modulus and tensile strength decreased as the concentration of glycerol increased making the bioplastic film weaker for whey protein concentrate and whey protein isolate. Evaluating the mechanical and oxygen barrier properties of the films, the whey protein films exhibited better properties when compared with other proteins from soy protein isolate, wheat gluten, and corn zein and polysaccharide-based films. However, the percentage elongation for the whey protein film is lower and water vapour permeability is higher than that of synthetic polymer films.

The continuous reliance on edible protein for bioplastic feedstock will put pressure on the protein food chain and compete with fresh water and arable land. To address this issue, films were produced from single-cell protein obtained from dry and dead unicellular microbial biomass, which are cultures of industrial and agricultural by-products using the compression moulding technique [83]. Using glycerol, the effect of compression temperature and time on the physical-mechanical properties of single-cell protein-based films and it was reported that the pressing temperature and time influenced the properties. The thermal stability and flexibility of the films were enhanced while the Youngs' Modulus and tensile strength increased with pressing temperature between 110 to 130 °C due to network strengthening and aggregate formation. As the pressing temperature increases, the properties become poor. The values of oxygen permeability of the bioplastics obtained were better than those of LDPE and HDPE.

LIPIDS-BASED BIOPLASTICS

Fatty acids derived from plant oil and animal fats are considered as a viable feedstock for the synthesis of bioplastic and a potential alternative to synthetic plastics. Lipids are usually gotten from animals, plants and insects that contain fatty acids glycerides, phospholipids, fatty alcohol, and terpenes, and they are hydrophobic materials that retards the movement of moisture within food due to their non-polar nature [84]. Films produced from lipids are usually edible, possess moisture-entrapment property and gives bioplastics a glossy appearance when used as a coating [62].

Lipids-Based Bioplastics Synthesis Methods

High-quality lipids need to be extracted from oil seeds and animal fats to produce bioplastics with excellent properties. Lipids can be extracted using the mechanical or chemical method. Using the chemical method, Kadioglu et al. [85] extracted oil from corn using surfactants instead of hexane. Lipids were extracted from lyophilized biomass by washing them with a methanol solvent mixture and chloroform in a ratio of 4 to 1 respectively [86]. To extract the lipids, the Soxhlet apparatus was used while the rotary vacuum evaporator was used to evaporate the solvent from the lipid samples. A hydraulic press is used to extract oil from seeds in the mechanical method.

Physical Mechanical Properties of Lipids-Based Bioplastics

Lipids are usually used as coatings in bioplastics, Chiumarelli and Hubinger [87] melted stearic acid and carnauba wax in cassava starch plasticized with glycerol. The film produced had good barrier properties and enhanced physical, mechanical and thermal properties.

The influence of sonication and oil content on the properties of Mesquite seed gum and palm fruit oil emulsion edible films was studied by Rodrigues et. al [88]. Bioplastics films were produced by blending the palm fruit oil nano-emulsion with the mesquite seed gum using glycerol as the plasticizer. The casting and evaporation techniques were used in producing the film. The authors reported that the water solubility, tensile strength, and water vapour permeability of the film decreased as the palm fruit oil increased. The sonication process improved the tensile property by further promoting a uniform droplet dispersion. Palm oil and epoxidized palm oil were incorporated into starch-based bioplastics to study the effect of the oils on the water resistance and mechanical properties of bioplastics. At a lower oil concentration of less than 3% wt, the tensile strength and elongation at break enhanced. The strengthened interactions between the hydroxyl groups of starch/glycerol and the carboxylic groups of fatty acids in the oils were the reasons behind the enhancement. The formation of discontinuous zones was reported at higher concentrations because of the phase separation that occurs between the oil and the starch. The interaction between the oils showed lower bonding when compared with the starch and oil interaction. This interaction affects the mechanical properties of the bioplastic. The presence of epoxy groups in the epoxidized palm oil improved its compatibility with the starch matrix while the compatibility with the palm oil is lower. The authors recorded a little reduction in water

uptake and solubility for both oils when compared with starch-based bioplastics [89]. There are limited resources in the literature on the production of bioplastics from lipids. More research should be conducted on the use of lipids and blending them with starch or protein since they possess reduced water uptake.

Table 1 gives the summary of different bioplastic's sources, additives and properties for polysaccharide, protein, and lipid.

OPPORTUNITIES AND CHALLENGES OF BIO-PLASTIC FROM BIOMASS SOURCES

The bioplastic production techniques are still evolving with each type of bioplastic from different biomass feedstocks having different production techniques and exclusive properties. The starch-based bioplastic with micro-sized filler and nanoparticles has great potential, but its commercial use is still limited. First-generation feedstocks that are edible are mostly used in the production of bioplastics. Hence, this has contributed to the high cost of production of bioplastics when compared with the cost of synthetic plastics production. The use of bioplastics from biomass must be sustainable without creating food insecurity or competing with available arable lands. Researchers need to source alternative feedstocks that are nonedible second and third generation feedstocks as shown in Figure 5. Legislative and financial incentives should be given to companies and individuals who manufacture, trade, and advocate the use of bioplastics.

According to Zimmermann et al. [92] some existing bioplastics, especially starch- and cellulose-based plastics contain some level of toxins like those in synthetic plastics. These toxins are often from some of the chemicals used as additives or the production process employed in the production of bioplastics. Bioplastics' production cost is higher than those of synthetic plastics, therefore continuous innovative research is necessary to reduce production costs and replace

Biomass source	Additives	Bioplastic properties	References
Corn starch	Glycerol	Good tensile strength	[8]
	water	Less dying time	
Corn starch and rice starch	Water	Improved tensile strength.	[20]
	Glycerol	Citric acid enhanced adhesion between the	
	citric acid	glycerol, water, and starch	
	gelatine		
Cassava peel starch	microcrystalline cellulose, sorbitol	MCC improved the tensile strength	[21]
Achira starch	Polyvinyl alcohol	Enhanced percentage of elongation, Youngs'	[47]
	MMT nanoclay	Modulus, and tensile strength at lower MMT	
	Glycerol	nano clay concentration	
Corn starch	titanium dioxide	TiO_2 nanoparticles decreased the elongation and enhanced the tensile strength.	[54]
Tapioca starch	combined zinc oxide (ZnO) and titanium oxide (TiO ₂)	Improved mechanical properties and elongation of the bioplastic.	[55]
	nanoparticles	Antimicrobial property of nanoparticles caused the nano-bioplastics to degrade longer.	
Whey protein	Glycerol	Lower percentage elongation	[82]
		Higher water permeability	
		Tensile strength decreased with concentration of glycerol	
Orange by product	glycerol	High water vapour permeability	[90]
		Poor overall tensile property	
Cassava starch	Glycerol	The addition of oil slightly reduced the water	[89]
	Palm oil	uptake and increased the tensile strength.	
	Epoxidized palm oil		
Rice straw	Trifluoroacetic acid	Enhanced tensile strength and elongation.	[91]
		Higher water absorption	

Table 1. Summary of bioplastic feedstock, additives, and properties



Figure 5. Biomass generational sources for bioplastic production.

toxic additives with natural additives that are safe for human consumption. The flexibility and elongation of bioplastics from starch were reported to be low by several researchers and this limitation is hindering the application of bioplastic as packages in grocery and other retail stores. The flexibility of bioplastics can be enhanced through further modification of the fillers or production process. Jayathilaka et al. [58] stated that there are limited resources that investigate the optimal concentration of nanoparticles that can be used as reinforcement in bioplastics for optimal characteristics and properties. Therefore, the influence of micro and nano filler's size and concentration needs to be further investigated to understand how the size and concentration of fillers concerning dispersion and homogeneity affect the characterization and optical properties of bioplastics.

Bioplastics are prone to thermal degradation, and they are likely to degrade when subjected to elevated temperatures. The biodegradation of bioplastics by biological agents is strongly dependent on certain environmental conditions, which differ from one location to another. These environmental conditions need to be met to fully take advantage of the biodegradability of bioplastics. For sustainable waste management of bioplastic waste, the biodegradability of bioplastics from different feedstocks, and compositions using various additives/plasticizers needs to be further investigated considering that the rate of degradation is dependent on the environmental conditions and microorganism activities.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Investigation of using cave bacteria in the production of self-healing mortars

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ABSTRACT

Self-healing concrete is a type of concrete formed by delayed or secondary hydration of cement and its particles with water in the matrix leaking through cracks, and calcium hydroxide and carbon dioxide on the crack surface react with calcium carbonate to provide protection against leakage through cracks. In recent studies, it has been observed that bacteria can self-repair with the production of calcium carbonate-based minerals and this repair provides protection against leakage, pore permeability and protection with increased strength and durability by reducing the infiltration of harmful substances into the internal structure.

In this study, 32 different batches of samples were produced by using *Bacillus thuringiensis*, *Pseudomonas putida* and *Sphingomonas mucosissima* bacteria in mortar mixtures prepared by traditional methods with 2 different water/cement ratios and 3 different mineral additives. The bacteria used are cave isolates that provide calcium carbonate formation, and these isolates were multiplied in the appropriate growth culture and then added to the prepared mortar samples together with the mixture water. The specimens were cured with tap water for 28 days and then subjected to suction, ultrasonic, flexural and compressive strength tests. The results of the tests revealed a reduction in the porous structure of the specimens containing bacteria, resulting in lower water absorption rates compared to the reference specimens. It was observed that most $CaCO_3$ was produced by Pseudomonas putida bacteria. However, there was no significant difference in compressive and flexural strengths compared to the reference specimens.

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INTRODUCTION

Thanks to the construction sector which develops in direct proportion to the population growth, the production and consumption of the materials such as cement and lime increase [1]. The high quantity of CO_2 emission leads to the global warming which is one of the most crucial environmental issues of our time. Besides, the available efficiency decreases upon degradation of the soil structure, and the

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biodiversity is affected upon that of the microbial, which caters for the substance cycles inside the soil, [2,3]. Due to such disadvantages suffered, it has been aimed at developing an environmentally friendly mode of production in order to avoid the waste formation in cement production and cement-based repair. The research conducted have shown that the cement-based materials such as mortar and concrete can be healed by chemical and biochemical ways as well. To such end, especially in recent years, studies have been being conducted regarding the use of CaCO₃ resulting from the biochemical activities of the microorganisms in repair with cement [4,5].

Although a widely used building material because of its production process, raw material availability, and compressive strength, concrete is highly prone to cracking[6]. The crack formation in the concrete structure occurs due to stress and shrinkage reactions in the structures and is a typical feature of durability in many concrete structures. It is not unusual that such crack formations occur at any time during the service life of the concrete. Notwithstanding they do not affect the strength features of the structures in which they occur, such microcracks render the material porous and permeable. Intrusion of aggressive chemicals such as chlorides, sulphates and acids may have long-term effects such as decomposition of concrete matrix and corrosion of the embedded steel reinforcement and may thereby impede the durability of the structures in the long run.

Repair of the cracks in the concrete structures is, on the other hand, an important yet time-consuming and costly task. As the classical methods would bring along a high cost of maintenance and repair and even the impossibility of intervention in certain cases, studies have been undertaken on the concepts of self-healing concrete [7]. It has been found that the most popular concepts include the limitation of the crack width by use of fibres [8], expansion of the cement matrix in contact with water by use of hydrogels[9,10], reinforcement by an active healing agent that is released upon breaking (biomineralization) and the former methods [11,12]

In the self-healing bacterial concretes, the genetical crack healing capacity of the concrete is among the recent studies. The benefit of having the self-healing properties is that the cracks that could occur in the structure of each concrete due to the nature of the latter can be reduced and repaired without the touch of human hands. Study was made in order to extend the life of the concrete structure of any dimension, form or project, and to provide with extra protection each and every component ranging from elements to steel reinforcements. This process can contribute to saving money, help the durability of the structures is maintained for much longer times, and, by having created a much more sustainable product for the concrete industry, efficiently decrease the CO_2 emission [13].

Bacterial healing involves the precipitation of calcium carbonate at the cracks upon direct impact of the bacteria species such as *Bacillus subtilis* on the calcium compound such as calcium lactate or by formation of urea by ureolytic bacteria such as Bacillus sphaericus [12,14,15]. Precipitation of calcium carbonate by means of bacteria is in conformity with the concrete and the formation process is environmentally friendly [16]. Therewithal, the reinforcement corrosion risk is reduced thanks to the oxygen produced during the CaCO₃ production. Owing to the Bacillus species' qualities including the capacity to form spores that make it suitable to be employed as an agent of tolerance to highly alkaline medium and of humidity as well as of self-healing in concrete, it is widely used in research studies as a bio-agent for calcite settling[13,17-19]. An 18% increase in strength was achieved by using bacteria such as Pseudomonas aeruginosa and Bacillus pasteurii in mortar mixtures for self-healing. Jonkers researched in his study the use of bacteria as self-healing agent in the healing of the cracks occurring in the concrete [20]. De Muynck et al demonstrated that the durability of the cement-containing materials can be improved by accumulation of carbonate on the surface by using *Bacillus sphaericus* [21]. Ramachandran et al. reported the use of bacteria for the purpose of enhancing the durability of the concrete so that it can resist the alkali reaction, freeze-thaw attacks, sulphate effect, drying and contraction [22]. Achalet et al. added the Bacillus sp. CT-5 bacteria to the mix in order to be able to see the impact on the water absorption and compressive strength in the concrete, and found out an increase of up to 36% in the compressive strength, and, as a result of the calcite accumulation, a lower water absorption rate in the microbial specimens compared to the control. And such fact shows that the durability of the construction materials can be increased by using the Bacillus species for the production of "microbial concrete" [23].

In a study conducted by Ghosh et at., a mineral settling method was defined which was of microbial basis aimed at increasing the strength in concrete. It was observed an increase of 25% in the compressive strength of the cement mortar by day 28 following the mix water had been added thermophilic and anaerobic bacteria in the range of 105 cells/ml. The increase in strength was attributable to the in increase of the filling material inside the pores of the sand-cement matrix[24]. In the study of Schwantes-Cezario et al. conducted using the Bacillus subtilis AP91 bacterium in order to observe the variation of the porosity in the mortar specimens, the bacteria were observed to have filled the pores by giving rise to precipitation of CaCO₃ [25]. In the study which Bhaskar et al. conducted by using zeolite-immobilized Sporosarcina urea and Sporosarcina pasteurii bacteria, an abundance of calcite mineral precipitation at the cracks of fibre-reinforced mortar specimens was observed, while recording a decrease in the water and chloride permeability of the specimens, and an increase in their compressive strength [26]. Xu and Wang's study they conducted in order to observe the calcium carbonate precipitation with the alkaliphilic spore-forming bacteria revealed a healing rate of up to 100% in the cracks on the specimens, and increases

by 50% and 130% in their watertightness and compressive strengths, respectively [27]. A study conducted by Vashist and Shukla with bacteria of the species Bacillus subtilis for the purpose of increasing the durability in the concrete resulted in the observation of increases in the compressive, tensile and flexural strengths in the bacteria-containing specimens in comparison to the reference [28]. In a study conducted by Yilmazer Polat et al., the effects of ureolytic bacteria in geopolymer mortars on the mechanical strength of the mortar were investigated using the bacterial species Sporosarcina pasteurii. According to the results of the study, it was observed that the bacteria added to the mortar mixture using appropriate methods had a decreasing effect on water absorption. The compressive strength reached its highest value within the first 7 days and started to decrease after the 28th day, stabilizing at a constant value by the 90th day[29].

In a study on the survivability and self-healing of bacteria in other types of concrete, it was observed that Sporosarcina pasteurii bacteria can repair surface cracks by adding to geopolymer mortar without encapsulation. When the study was examined, it was seen that after the curing of the geopolymer mortar with bacteria, the healing was slower in mortars prepared with endospores obtained from the solid agar surface, although it had fewer voids compared to the mortar without bacteria. It was observed that the addition of bacterial spores to the mortar during the production phase and the improvement of the medium provided more improvement. However, it was observed that the number of voids increased due to the fact that the bacterial spores added to the samples in superficial healing consumed the nutrients in the environment even if they closed the crack and the bacterial spores in the mortar died due to lack of nutrients. In addition to all these, considering the production difficulties of geopolymer mortars and the fact that bacteria can be contaminated very quickly, it is necessary to produce geopolymer mortars in fabricated form[30]. Studies on the use of microbial agents to repair cracks that may occur due to the low tensile strength of recycled aggregate concretes and thus smaller external stresses have shown that cracks can be healed by metabolic precipitation of calcite. However, it has been observed that the survival rate and hence the self-healing rate increases when the bacteria are encapsulated in a suitable carrier rather than directly incorporated into the concrete [17,31–33].

In addition to all these, some studies have shown that manual or external application of bacteria to existing structures does not provide sustainable improvement. For this reason, the use of bacteria as a long-term and embedded self-healing agent in concrete has been investigated. In one study, it was observed that spores of alkali-resistant bacteria of the genus *Bacillus* produced calcium carbonate-based minerals when added to the concrete mix and activated by water ingress through cracks. However, self-healing was limited to a very short period of one to two months due to the direct, unprotected addition of bacterial spores to the mixture [14–16]. Although the life span of bacterial spores is tens

of years in the dry state, it is predicted that the embedding of bacterial spores in the concrete matrix and the reduction of their life span to a few months may be due to the continued hydration of the cement and thus the matrix pore diameter becomes much smaller than the bacterial spores [16]. Considering the results of this study, a new study was conducted and bacterial spores and organic mineral compounds were added to the mortar mixture by immobilizing them in expanded clay particles. At the end of the study, it was found that bacterial spores extended the viability period and thus provided self-healing in the matrix. In the light of viability experiments, it was observed that there was no loss of viability even after 6 months [17,20,33,34].

There are not many studies on the impact of the use of bacteria on human health. Studies have shown that bacteria of the genus *Bacillus* do not pose any threat to human health, but there is no information on whether other types of bacteria are pathogenic. Therefore, more studies are needed to determine whether the use of microorganisms is harmful to human health in the long term [35].

In this study, the self-healing potential of mixtures obtained by using three different pozzolanic materials at different water/cement ratios was tried to be determined. On the one hand, the gap-filling abilities of pozzolanic materials were demonstrated in bacteria-free mixtures, while the gaps that pozzolanic materials could not fill were tried to be filled with the CaCO₃ production potential of different types of bacteria, which is the original aspect of this study. In this context, in order to demonstrate the effectiveness of bacteria, water absorption and ultrasound transmission rate tests were performed on the prepared mixtures to obtain information about the porosity structure, and compressive and flexural analyzes were performed to determine the strength capacities.

MATERIALS AND METHODS

Materials Used

In the study, fly ash (FA), blast furnace slag and metakaolin were added to the mixture as mineral additives in order to reduce the mass of cement. Fly ash is preferred in the works due to the ease of recycling and low cost of ashes from thermal power plants [36]. It has been observed that it improves concrete density, ultrasonic impact velocity, porosity and mechanical properties in cement mortar mixtures and helps to reduce cement consumption. It also increases its preferability compared to traditional materials due to its low electrical conductivity, thermal conductivity and expansion, fracture and heat capacity [37,38]. Blast furnace slag is a waste material generated during iron production and is preferred due to its effect on strength and durability, thermal cracking and workability properties of concrete [39]. Metakaolin, on the other hand, is obtained by calcining clay mineral at high temperatures and is preferred

for its physical and chemical strength and durability improvement, workability and thermal improvement [40].

In the mortar series, bacteria-containing mixing water produced at the laboratory of the Fundamental and Industrial Microbiology Laboratory of the Biology Department of the Faculty of Sciences of the Istanbul University was used along with the cement of type CEM I 42.5 obtained from AKÇANSA Çimento A.Ş., standard RILEM sand, fly ash obtained from the thermal power plant at Çatalağzı/Zonguldak, granulated blast furnace slag obtained from Bolu Çimento Sanayi A.Ş., and metakaolin obtained from KEMS Industrial Company. The physical and chemical properties of the CEM I 42.5 R cement are shown in Table 1, and the chemical properties of the additives in Table 2 and 3.

Chemical Properties % Test Method: TS EN 196-2	CEM I 42.5 R	Physical Properties Test Method: TS EN 196-3 and TS EN 196-6	CEM I 42,5 R
MgO	1.38	Specific gravity (g/cm ³)	3.13
SO ₃ ⁻²	3.39	Setting time (Vicat-min)	Startup: 165 / End: 199
CaO	62.51	Volume expansion soundness (Le Chatelier-mm)	1
Fe ₂ O ₃	3.73	Blaine Specific surface	3300
Al ₂ O ₃	5.20	Residue on 45 mm sieve	4.9
SiO ₂ Soluble	19.97	Residue on 90 mm sieve	0.3
Insoluble Residue	1.08		
Unidentified	0.48	Mechanical properties	CEM I 42.5 R
Loss on Ignition	2.06	2 d	32.4
Serbest CaO Free Lime	1.51	7 d	45.5
Cl-	0.0400	28 d	57.7
Na ₂ O/K ₂ O	0.37 / 0.87	* 40x40x160 mm moulds	
		Mix: for specimens prepared by using 1 part cemen 0.50 W/C scale	t, 3 parts CEN ref. sand,

Table 1. Physical and chemical properties for CEM I 42.5 R

Table 2. Chemical properties for metakaolin and granulated blast furnace slag

Chemical Properties (%)	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	TiO ₂	CaO	MgO	K ₂ O	Na ₂ O	B ₂ O ₃	Loss on Ignition
Metakaolin	56.10	40.23	0.85	0.55	0.19	0.16	0.51	0.24	-	1.10
Blast Furnace Slag	40.55	12.83	1.10	0.75	35.58	5.87	0.68	0.79	-	0.03

Table 3. Chemical properties for the fly ash

Chemical Properties (%)	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	SO ₃	CaO	MgO	Free CaO	Na ₂ O	Cl	LOI	
Fly Ash	54.08	26.08	6.681	0.735	2.002	2.676	0.11	0.79	0.092	1.36	

Table 4. Properties of the Bacteria

Bacterium used	Bacillus thrungiensis	Pseudomonas putida	Sphingomonas mucosissima
Bacterium Code	Y214	Y234	Y151
Gram Reaction			
Crystal Formation	Positive	Positive	Positive



Figure 1. Bacterial mixture water.

The bacteria used in the mixing water were cave isolates which can precipitate the calcium carbonate. These bacteria isolated from the Yarık Sinkhole cave were identified as *Bacillus thrungiensis*, *Pseudomonas putida* and *Sphingomonas mucosissima* species. None of these bacteria has been encountered in cave microbiological studying literature. Properties of these bacteria are shown in Table 4. To determine the crystal forming abilities of Y214, Y234 and Y151 coded bacteria, their stock cultures preserved at -86°C were inoculated on sterile TSA (15 g casein peptone, 5 g soy peptone, 5 g NaCl and 15 g agar per liter of distilled water) medium. After 24 hours of incubation at 28°C, a colony from each bacterium was inoculated on 90-mm petri dishes containing sterile B4 medium (2.5 g calcium acetate, 4 g yeast extract, 10 g glucose and 18 g agar per liter of distilled water) and incubated at 28°C. The cultured petri dishes were examined daily under a microscope for crystal formation in the CaCO₃, bacterial suspensions were prepared (approx. 10⁹ cells/ml) from a fresh culture on TSA medium and used to prepare the bacteria-containing mixing water (Figure 1).

Production of the Mortar Specimens

The coding used in the production of the mortar specimens is as shown in Table 5. In this coding the first letter denotes the water/cement ratio, the following numbers and the final letters the type of the mineral additive. The mortar mix specimens representing these properties are shown in Table 6.

Table 5. Coding of specimens

W/C	Denomination	Species	Mix Type and Abbreviations
0.5	В	Bacteria-containing	Metakaolin (M)
0.6	С	(1-2-3) reference	Fly ash (U)
		*1: Bacillus thrungiensis	Granulated Blast Furnace Slag (O)
		*2: Pseudomonas putida	
		*3: Sphingomonas mucosissima	

Table 6. Mortar specimens coding and legends

W/C	Code	Reference (R)	Bacteria	a	Bacte	Bacteria Species			al Additiv	es
Ratio			Yes	No	1	2	3	М	0	U
0.5	BR	\checkmark		✓						
	BRO	\checkmark		\checkmark					\checkmark	
	BRM	\checkmark		\checkmark				\checkmark		
	BRU	\checkmark		\checkmark						\checkmark
	B1		\checkmark		\checkmark					
	B1O		\checkmark		\checkmark				\checkmark	
	B1M		\checkmark		\checkmark			\checkmark		
	B1U		\checkmark		\checkmark					\checkmark
	B2		\checkmark			\checkmark				
	B2O		\checkmark			\checkmark			\checkmark	
	B2M		\checkmark			\checkmark		\checkmark		
	B2U		\checkmark			\checkmark				\checkmark
	B3		\checkmark				\checkmark			
	B3O		\checkmark				\checkmark		\checkmark	
	B3M		\checkmark				\checkmark	\checkmark		
	B3U		\checkmark				\checkmark			\checkmark

W/C	Code	Reference (R)	Bacteria	a	Bacte	eria Spec	ies	Miner	al Additiv	es
Ratio			Yes	No	1	2	3	Μ	0	U
0.6	CRO	\checkmark		√					✓	
	CRM	\checkmark		\checkmark				\checkmark		
	CRU	\checkmark		\checkmark						\checkmark
	C1		\checkmark		\checkmark					
	C10		\checkmark		\checkmark				\checkmark	
	C1M		\checkmark		\checkmark			\checkmark		
	C1U		\checkmark		\checkmark					\checkmark
	C2		\checkmark			\checkmark				
	C2O		\checkmark			\checkmark			\checkmark	
	C2M		\checkmark			\checkmark		\checkmark		
	C2U		\checkmark			\checkmark				\checkmark
	C3		\checkmark				\checkmark			
	C3O		\checkmark				\checkmark		\checkmark	
	C3M		\checkmark				\checkmark	\checkmark		
	C3U		\checkmark				\checkmark			\checkmark

Table 6. Mortar specimens coding and legends

Table 7. Mortar mixing ratios

Mix Code		RILEM Sand (g)	Mixing Water (ml)	Cement (g)	Metakaolin (g)	FA (g)	GBFS (g)
0.5 W/C	W/ additive	1345	225	360			90
	W/ additive	1332	225	360	90		
	W/ additive	1249	225	360		90	
	W/o additive	1350	225	450	0	0	0
0.6 W/C	W/ additive	1346	225	300			75
	W/ additive	1335	225	300	75		
	W/ additive	1332	225	300		75	
	W/o additive	1414	225	375	0	0	0

In the study, 32 series of specimens were produced in total, 8 being reference, and 24 bacteria-containing, using a single type of cement, 2 different water/cement ratios, 3 different types of bacterial strains (*Bacillus thrungiensis, Pseudomonas putida* and *Sphingomonas mucosissima*), and 3 different mineral additives. The fine aggregate granulometry used in the mix was kept constant, and the mineral additive quantity was chosen to be equal to 20% of the cement by weight.

The mortar specimens were prepared in the water/ cement ratios of 0.5 and 0.6, and in the mix quantities shown in Table 7, and in the preparation of the mixes, initially the sand, cement and additives were blended in dry condition, then the bacteria were added into the mix with the mixing water. Having been unmoulded, the specimens produced were transferred to and left for 7 and 28 days in the curing conditions. By the end of the 7th and 28th days the specimens were subjected to the water absorption test, UPV test, flexural and compressive strength tests were performed to compare the specimens containing bacteria with those not containing bacteria. For the water absorption test, the specimens of which dry weight measurements had been done before were weighed after they had been removed from the water, and the water absorption ratio was determined by proportioning the difference between their wet and dry weight values to the wet weight value thereof. By this means, the water absorption capacity variations caused in the mortar by the use of bacteria were measured (Figure 2).

Three-point flexural tests were performed on the hardened mortar specimens at 0.005 kN/sec and compressive tests were performed at 2 kN/sec. The test results were measured as per the requirements of the standards ASTM C109 and ASTM C348. At the end of all the tests, the parts of the specimens that had been tested were internally analysed through SEM and XRD analyses.



Figure 2. Experimental method.

RESULTS AND DISCUSSION

The results showing the effects of using bacteria in mortar production on the compressive strength, water absorption capacity and ultrasonic permeability of the samples are shown in Figure 3-7.

Water absorption analyses performed at the end of the 28-day curing period revealed a drop in the water absorption capacities in the bacteria-containing mortar specimens in general (Figure 3 and 4). The amount of such drop was found to be 20% in average in the specimens with a w/c ratio of 0.5 compared to the reference specimens, whereas 10% in those with 0.6.

Whereas a result was obtained which was in balance with the bacteria-containing specimens with the w/c ratio of 0.5 according to the UPV test results shown in Figure 3 and 4; the pulse velocity in the specimens with the w/c ratio of 0.6 was observed to have increased compared to the control ones.

Although the porosity had been decreased in the bacteria-added specimens water, and hence the absorption capacities thereof had dropped, no noteworthy positive increase was observed in their flexural and compressive strengths in general terms compared to the control specimens. While some specimens exhibited increased flexural and compressive strengths, some yielded results implying decreases. The review of the three-point flexural tests reveals an apparent increase in the bacteria-added specimens compared to the reference ones. The rate of such increase was measured to be ~7.5% in average in the specimens with the w/c ratio of 0.5, and ~10% in average in those with 0.6. Upon the comparison made between the specimens containing the mineral additives and those not containing the same; a gradual decrease was seen in the strength results, the best strength increase represented by an average rate of 12% in the specimens with the w/c ratio of 0.5 was achieved through fly ash, the one represented by 7% through granulated blast furnace slag, and metakaolin was found to have led to a strength loss of ~5%. Similar results was seen in the specimens with the w/c ratio of 0.6, with the best strength increase represented by an average rate of 20% was achieved through granulated blast furnace slag, the one represented by 11% through fly ash, and metakaolin was found to have let to a strength loss of ~3%.

While an average increase of 15% was observed in a total of 8 specimens for the mortar specimens where granulated blast furnace slag was used, an average decrease of 5% was noted in the remaining 2. The best result was obtained in the specimens with the w/c ratio of 0.5. In terms of compressive strength, on the other hand, an average compressive strength increase of 18% was observed in only 5 specimens, while the remaining exhibited an average decrease of 30% (Figure 5).



Figure 3. Water absorption and UPV test results of 0.5 w/c.



Figure 4. Water absorption –UPV test results of 0.6 w/c.

In the mortar specimens where metakaolin was used no significant positive increase occurred in respect of either compressive strength or water absorption capacity, with an average positive increase of 9% observed in only 5 specimens in total in respect of water absorption capacity reduction, while a decrease of 12% in the others. And an increase of 12% was observed in only 4 specimens in respect of compressive strength, with a decrease of 49% in the remaining ones (Figure 6).

In the mortar specimens where fly ash was used an increase of 8% was observed in total in the water absorption capacity in 4 specimens, whereas a decrease of 13% in

the remaining. The study came up with an average increase of 31.5% in terms of compressive strengths in 6 specimens, while an average decrease of 26% in the remaining (Figure 7).

The examination of the specimens produced with a w/c ratio of 0.5 revealed a diminution of the porosity in the bacteria-containing ones compared to the reference ones, and a reduction of the water absorption capacity in comparison to the control specimens accordingly. And it became evident from the examination of the specimens produced with a w/c ratio of 0.6 that their porous structure diminished compared to that of the reference specimens,



Figure 5. Water absorption-Compressive strength test results of the specimens containing GBFS.







Figure 7. Water absorption-Compressive strength test results of the specimens containing FA.

and a drop occurred in their water absorption capacities accordingly. The biomineralization test performed on mortar specimens using a bacterial strain obtained from the American Type Culture Collection revealed in the specimens a notable extent of CaCO₃ increase accompanied by a decrease in the void ratio inside the mortar [41]. It was found in the study conducted by Harshaki et al., on the other hand, that the water absorption ratios were less in quantity in the bacterial cements compared to the reference specimens, and that there had occurred an increase in the concrete compressive strength and hence in the structure's durability associated with the formation of calcites in the fresh concrete pores [42]. In the study of Balam et al. conducted on lightweight aggregate concretes, the use of bacteria allowed the water absorption capacity to be reduced, which in turn led to specimens with a less permeable micro structure [43]. Also, in another study where two bacteria of the species Sporosarcina pasteurii and Bacillus subtilis were used, it was found that the bacteria species could bring about a reduction of 29-30% in water absorption thanks to the accumulation of calcium carbonate crystals on the surfaces in association with the aggregate porosity [44].

It was found upon the tests performed during the examination of the specimens produced with the w/c ratios of 0.5 and 0.6 that the bacteria-containing specimens yielded better results compared to those of the reference ones. Jafarnia et al. found that calcite precipitation increased the ultrasonic impact velocity, electrical resistivity, compressive and tensile strength of all samples. [45]. It was found in the study of Singh and Gupta that cracking was brought about in the specimens by impregnating the cellulose fibres with the bacteria, and increase was observed in the UPV test results by the end of the healing period. It was found that the crack width of 0.1 to 0.2 had healed by 12.04% in the 14-day curing, and by 15.2% in the 28-day, which ratio was detected to be 8,23% higher than that of the control specimen [46]. The test performed by Kaur et al. using the bacteria of the species Sporosarcina pasteurii revealed as a result of the water absorption and UPV tests performed on the specimens that the cracks of an approximate width of 0.6 mm had been closed by the accumulation of CaCO₃. The healed specimens exhibited reduction in water absorption capacities, and increase in ultrasonic pulse velocities compared to the control specimens, which was understood to be caused by CaCO₃ as evidenced by the SEM and EDS analyses [47]. It has been found out from the studies mentioned herein that calcium carbonate crystals are the substance that is responsible for the reparation by filling the cracks in the process of self-healing, and the results obtained have been seen to support this study.

In line with the results of the compressive strength test performed on the specimens, no increase of compressive strength that could be deemed to be in a notable order was found between the 0.5-w/c-ratio bacteria-containing specimens and the reference ones. The examination of the compressive strength results of the specimens revealed that the maximum compressive strength value obtained was 49 MPa, with the average one being 41.5 MPa. The 0.6-w/c-ratio specimens too exhibited no increase of compressive strength values that could be deemed to be regular in the bacteria-containing specimens compared to the reference ones. The compressive strength results of the specimens showed a maximum compressive strength value of 40.9 MPa, with the average one being 33 MPa. Representing a similar case, a study where Jonkers and Schlangen tested the applicability of bacterial spores for the improvement of the self-healing concrete, could reveal no significant differences between the specimens with and without bacteria as per the results of the tests performed on the specimens produced by using three different species of bacteria in respect of the compressive and tensile strengths, whereas the SEM images revealed precipitation of calcium carbonate crystals [48].

Microstructural Examination

For purposes of imaging of the effect of the bacterial healing inside the mortar, SEM images were taken for the 4 best specimens exhibiting reduction in water absorption capacity. It was detected that the most favourable results in this context were offered by the bacteria *Pseudomonas putida* and *Sphingomonas mucosissima*, whereupon the imaging operations were performed on (B2O, B3, C2) and the control specimen (BRO).

Micrographs (a, b) of the control specimen (BRO) (Figure 8) show both the existence of the C-S-H gel and aragonite, which is a crystal form of CaCO3, as well as non-hydrated slag particles. It is understood that the CaCO3 which formed due to the lack of bacteria in those specimens owes its existence to nothing but hydration. Although the higher percentages of the Ca and O elements detected in the EDS analyses already support the existence of CaCO3, such fact has definitely been detected in the results of the phase analysis.

As shown by the micrographs of the bacteria-containing B3 specimen (Figure9), there is no porous structure left on the inner surfaces of the specimen, as all pores were filled with the C-S-H gels. Calcite and vaterite which are polymorphs of $CaCO_3$ formed by the bacteria are seen in the cells existing inside the structure.

A higher number of porous structures are seen in the micrographs of the bacteria containing B2O specimen (Figure 10), compared to the B3 specimen. Existence of non-hydrated slag particles, C-S-H gel, CaCO₃ bridges and vaterite are noted in the specimen's structure.

The micrographs of the bacteria containing C2 specimen (Figure 11) shows that the porous structure was almost fully closed, and vaterite, a polymorph of CaCO₃, was formed. A comparison of the bacteria containing B3O, B2O and C2 specimens shows that the best result was obtained from the C2 specimen.



eZAF Smart Quant Results

Element	Weight %	Atomic %	Net Int.	Error %	Kratio	Z	А	F
ОК	43.92	64.19	2089.31	10.00	0.0707	1.0742	0.1499	1.0000
MgK	0.58	0.56	103.37	12.77	0.0028	0.9953	0.4804	1.0068
AIK	2.66	2.31	594.01	6.43	0.0162	0.9590	0.6256	1.0114
SiK	10.36	8.63	2759.38	4.36	0.0749	0.9805	0.7281	1.0123
CaK	39.68	23.15	6375.63	1.65	0.3630	0.9275	0.9810	1.0051
FeK	2.79	1.17	234.69	7.44	0.0231	0.8283	0.9718	1.0292



Figure 8. a) 5,000 X SEM b) 10,000 X SEM c) EDS d) XRD Analyses Results in the control specimen (BRO) SEM micrographs.





eZAF Smart Quant Results





Figure 9. SEM micrograph of the B3 specimen a) 10,000 X SEM b) EDS c) XRD Analysis.





eZAF Smart Quant Results

Element	Weight %	Atomic %	Net Int.	Error %	Kratio	Z	А	F
ОК	40.37	59.61	1159.35	10.15	0.0674	1.0749	0.1554	1.0000
MgK	0.01	0.01	0.77	99.99	0.0000	0.9959	0.4960	1.0083
AIK	1.13	0.99	153.81	9.19	0.0071	0.9595	0.6461	1.0149
SiK	21.36	17.97	3484.00	3.92	0.1603	0.9810	0.7584	1.0091
CaK	34.34	20.24	3208.68	2.04	0.3087	0.9279	0.9635	1.0057
FeK	2.79	1.18	139.64	10.24	0.0232	0.8286	0.9732	1.0313



Figure 10. SEM micrographs of the B2O specimen a) 5000 X SEM b) 10.000 X SEM c) EDS d) XRD Analysis.



eZAF Smart Quant Results





Figure 11. C2 specimen SEM micrographs a) 10,000 X SEM b) EDS c) XRD Analysis.

CONCLUSION

In the studies carried out to improve the performance of cementitious mortars with *Bacillus* bacteria at a certain concentration, it was determined that the 28-day compressive strength of microbiologically induced mortars increased significantly and this increase was due to the increase in the filling material in the pore after SEM analysis. With the improvement provided by the bacteria, the voids were filled with calcium carbonate precipitation, resulting in a decrease in porosity and preventing possible infiltration, resulting in improvements in concrete in terms of tensile strength at splitting, porosity, acid resistance and chloride resistance as well as compressive strength, resulting in better results compared to conventional concrete [49,50].

In this study were observed the attainable rate of the calcium carbonate precipitation by using bacteria of the species *Bacillus thrungiensis*, accompanied by those of the *Pseudomonas putida* and *Sphingomonas mucosissima*, as well as the effects of the use of bacteria on the porosity of the specimens in the production of mortar. The results obtained from the tests performed revealed that;

- The porous structure diminished through the CaCO₃ production in the bacteria-added cement mortar specimens, and accordingly a reduction in the water absorption capacities compared to the reference specimens.
- The bacteria species used are able to perform the expected CaCO₃ production in the mortar mix, and the highest rate of CaCO₃ production is achieved by the bacteria of the species *Pseudomonas putida*.
- SEM and XRD analyses performed on the specimens by the end of the tests showed that the reduction in the water absorption capacity had its source in the fact that the bacteria had filled the pores by producing CaCO₃.
- Due to the decreased quantity of porous structure, a faster sound transmission was detected in the bacteria-containing mortar specimens compared to the control ones, in the ultrasonic pulse velocity tests performed.
- The compressive strength effects of the use of bacteria could not be fully determined as no specific increase or decrease could be noted in the strength.

In the light of these results, addition of bacteria into mortars exert a highly beneficial effect when it comes to mineral-added mortars containing bacteria of different species, considering that such addition lowers the water absorption rates, as well as makes contributions to the durability properties of mortars and concretes. Impermeability of the concrete in particular is highly important as it will prevent the steel reinforcement from corroding, which will then lead to the enhancement of the economic life and the anti-earthquake performance of the buildings.

The crucial role of the durability properties in general terms in reinforced concrete buildings have also been revealed by the studies gaining importance during recent years. Hence, an improvement to occur in the properties of the impermeable concrete, accompanied by the addition of bacteria, is of significance also in respect of the enhancement of the service lives, extension of the economic lives, and increase the seismic performance of the mortars and concretes.

NOMENCLATURE

Al	Aluminum
Al_2O_3	Aluminum oxide
B_2O_3	Boron trioxide
Ca	Calcium
CaCO ₃	Calcium carbonate
CaO	Calcium oxide
Cl	Chloride
CO_2	Carbon dioxide
C-S-H	Calcium-silicate-hydrate
EDS	Energy-dispersive X-ray spectroscopy
FA	Fly ash
Fe	Iron
Fe ₂ O ₃	Iron oxide
GBFS	Granulated Blast Furnace Slag
Κ	Potassium
K ₂ O	Potassium oxide
LOI	Loss on ignition
Mg	Magnesium
MgO	Magnesium oxide
Na ₂ O	Sodium oxide
NaCl	Sodium chloride
0	Oxygen
SEM	Scanning Electron Microscopy
Si	Silicon
SiO ₂	Silicon dioxide
SO ₃	Sulfur trioxide
SO3 ⁽⁻²⁾	Sulfite
TiO ₂	Titanium dioxide
TSA	Tryptic soy agar
UPV	Ultrasonic pulse velocity
w/c	Water/cement
XRD	X-Ray diffraction

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Fluoro functionality zinc phthalocyanine: photophysicochemical properties for photodynamic effects

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ABSTRACT

Photodynamic therapy is an alternative method to surgical methods used in the treatment of cancer and one of its three basic components is photosensitizer. The high singlet oxygen generating capacity, high solubility in common organic solvents, low aggregation tendency and lightfastness are the characteristics that photosensitizers must have. Phthalocyanines with bulky substituents are candidate molecules that can be used as sensitizers in photodynamic therapy due to prevent aggregation in the solutions and improve solubility. Based on these facts in this study, singlet oxygen quantum yield and photodegradation quantum efficiency were calculated to evaluate the potential of bis(4-fluorophenyl)-methoxy-substituted zinc phthalocyanine, which does not form aggregation and has high solubility in organic solvents commonly used in photodynamic therapy applications. The metallo phthalocyanine generated higher singlet oxygen than unsubstitue zinc phthalocyanine. According to the singlet oxygen quantum yield, the addition of bis(4-fluorophenyl)-methoxy groups to the phthalocyanine ring increases the singlet oxygen production. The results show that this phthalocyanine may be suitable candidates as photosensitizers in photodynamic therapy with the singlet oxygen quantum yield values are 0.76 and 0.70 in DMSO and DMF, respectively.

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INTRODUCTION

Considering that cancer is one of the leading causes of mortality in the world, photodynamic therapy (PDT), as opposed to more conventional cancer treatment options like immunotherapy, surgery, chemotherapy, or radiotherapy, has recently attracted more attention. This technique uses sensitizers that produce harmful reactive oxygen species (ROS) when activated at the proper wavelength. Due to their properties that satisfy the prerequisites, such as high intensity absorption (>670 nm, >10⁵ mol⁻¹ cm⁻¹) in the visible region for deeper tissue penetration, high singlet oxygen production, and high triplet quantum efficiencies, phthalocyanines (Pcs) are known as photosensitizers used in PDT applications [1-3].

Besides this feature, they have chemical and thermal stability [4]. Due to their interesting and changeable

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• • Copyright 2021, Yıldız Technical University. This is an open access article under the CC BY-NC license (http://creativecommons.org/licenses/by-nc/4.0/). properties, they have applications in many fields such as optical recording material [5], semiconductors [6-8], non-linear optics, sensors, thermal writing displays and sensitizers for solar cells [9-11], and sensitizers for photovoltaics [12, 13].

The substituent group and center metal ion of Pcs change its photophysicochemical properties and are of major importance in making it more suitable for PDT applications [14]. It is widely known that heavy atoms affect the photosensitizers' capacity to produce singlet oxygen. Heavy atoms raise spin-orbit coupling (SOC) which promotes intersystem crossover rates and and increase the efficiency of PSs' singlet oxygen generation. A larger halogen atom size among halogen atoms leads to a higher SOC value [15].

Metallophthalocyanine complexes containing heavy atom metals such as zinc(II), indium(III) and silicon(IV) have been found to be highly promising photosensitisers for photodynamic therapy due to their photophysical properties such as intense absorption in the phototherapeutic window (650-850 nm) [3,16,17].

Fluorine atoms are strong electron attractors. The addition of strong electron-withdrawing fluorine atoms to the Pc macrocycle further reduces the energy levels of the conduction and valence bands of the molecule [18]. Fluorine-containing phthalocyanines are both well soluble in fluorine-derived common polar and non-polar solvents, which have the highest electronegativity [19], and do not show aggregation tendency. For this reason, they show improvement in PDT processing and Pcs with fluoro are promising photosensitizers for PDT of cancers [19-24].

This study aimed to design a promising photosensitiser with efficient singlet oxygen yields by combining heavy atom and fluoro substituent groups in a phthalocyanine ring, which promotes intersystem transition rates and increases the efficiency of singlet oxygen production of PSs. For this purpose, a bulky group containing an electron-withdrawing (-F) substituted phthalonitrile derivative and zinc as the centre atom were used for the synthesis of the phthalocyanine complex. The absorbance, fluorescence, singlet oxygen quantum efficiencies and photodegradation quantum efficiencies of compound 2 in DMSO and DMF solutions were investigated, and it was concluded that this compound is promising as a possible photosensitizer in PDT applications.

EXPERIMENTAL

Materials and Equipments

The used chemicals, equipments, materials, photochemical, and photophysical procedures are given as supplementary material file.

Synthesis

The synthesis and characterization of phthalonitrile derivative (1) and Tetrakis [bis(4-fluorophenyl)-methoxy] phthalocyaninato zinc(II) (2) was done and reported in our previous study [25].

Photophysical and Photochemical Studies

The fluorescence quantum yield as photophysical property and the singlet oxygen quantum yield and photodegradation quantum yield as photochemical properties were performed by using the methods described in the supplementary material file.

RESULTS AND DISCUSSION

Synthesis and Characterization

The synthetic route to compounds 1 and 2 gives in Scheme 1. Phthalonitrile derivative (1) and metallo Pc (2) were obtained by applying the synthesis route specified



Scheme 1. The synthesis routes of compound 1 and its zinc phthalocyanine derivative 2.

in our previous study [25]. The starting compound 1 was formed by the nucleophilic aromatic nitro displacement reaction of 4-nitrophthalonitrile with bis(4-fluorophenyl)-methanol in dry DMF in the presence of the basic catalyst K_2CO_3 . Peripherally tetra-substituted zinc phthalocyanine (2) is prepared by template cyclotetramerization of bis (4-fluorophenyl)-methoxy phthalonitrile (1). Complex 2 was synthesized by treatment of compound 1 with anhydrous ZnCl₂ in the presence of 1,8-diazabicyclo[5.4.0] undec-7-ene (DBU) as base in dry 1-pentanol at reflux temperature under argon atmosphere.

The characterization of the compounds 1 and 2 was performed by various analysis methods such as elemental analysis, UV-Vis, FT-IR, NMR and MALDI-TOF MS techniques. The obtained results are compatible with the previously published literature [25]. The characteristic vibrations corresponding to aromatic C-H, aliphatic C-H and C≡N groups were observed at 3078 cm⁻¹, 2961-2834 cm⁻¹ and 2230 cm⁻¹ for 1, respectively. The distinctive sharp C≡N stretch at 2230 cm⁻¹ for 1 disappeared after conversion into metallo phthalocyanine 2. Compound 2 displayed distinctive vibrations of aromatic and aliphatic CH stretching at about 3070 cm⁻¹ and 2960-2895 cm⁻¹, respectively, and ether groups (C-O-C) at about 1250 cm⁻¹. At around ~1095 cm⁻¹, the aromatic fluorur (Ar-F) peak for 2 was seen. By using ¹H NMR, it was determined that phthalocyanine 2 was pure since all of its substituents and ring protons could be seen in the appropriate places.

The phthalocyanine ring protons of compound 2 were observed in the range 7.35 to 7.24 ppm integrated for 12 protons, the bulky fluoro functional groups of the substituent on the phthalocyanine ring were observed in the range 7.15 to 7.05 ppm integrated for 32 protons, the O-CH protons were observed at 6.30 ppm integrated for 4 protons as expected.

In addition to these demonstrating results for the structures, the mass spectra of compound 2 gave the characteristic molecular ion peaks at m/z: 1448.36 [M²⁻] (Figure S1) [25].

Studies on aggregation behavior and UV-Vis spectroscopy

The electronic ground state spectra are particularly helpful for determining the phthalocyanines' structural makeup. Phthalocyanines often exhibit typical electronic UV-Vis spectra with the two powerful absorption bands known as the Q band in the visible region (600-750 nm) and B band in the UV region (300-400 nm) [26]. The solvent, substitution position, central metal, axial ligation and aggregation affect the position and strength of the Pcs absorption bands. The solubility of compound 2 was examined in a series of organic solvents of different polarity. In our previous study [25], the UV-Vis absorbance spectra of 2 carrying (bis(4-fluorophenyl)-methoxy) moieties in the mentioned solvents were examined and the absorption spectra of 2 carrying (bis(4-fluorophenyl)-methoxy) moieties in the said solvents were examined. It has been reported to exhibit monomeric behavior as evidenced by a single Q band (Figure S2a). The Q bands of 2 in DMSO, CHCl₃, THF, CH₂Cl₂ and DMF were observed at 685, 684, 682, 685 and 689 nm, respectively (Table 1). In general, it demonstrates that the red-shift of the Q band rises as the solvent's refractive index does [27]. Small discrepancies between the Q band locations were found as a result of the influence of solvents. The red-shift values of the compound was compared with respect to the solvents that were used. ZnPc 2 displayed a high red-shift in DMSO and a low redshift in THF in this situation.

The interactions between the 18 π -electron systems leading to aggregation of phthalocyanine compounds depend on concentration, the nature of the solvent and substituents, complex metal ions and temperature. The spectroscopic, photophysical and photochemical properties of Pcs are strongly affected by aggregation in solution [28, 29].

The aggregation behavior of 2 in CHCl₃, CH₂Cl₂, DMF, THF and DMSO was presented in our previous publication [25]. Figure 1 presented the absorption spectra of solutions of 2 prepared with DMSO and DMF at increasing concentrations. The solutions prepared with these solvents showed that 2 has high solubility and does not exhibit aggregation.

Photophysicochemical studies

The fluorescence behaviour of complex 2 in various organic solvents was investigated and reported in our previous study [25]. In this study, to demonstrate its suitability for PDT studies, the photochemical (singlet oxygen quantum yields (Φ_{Δ}) and photodegradation quantum yields (Φ_d) properties of complex 2 in DMF and DMSO were investigated.

Table 1. Absorption, excitation, emission spectral and fluorescence quantum yield (Φ_F) results for 2 in studied solvents

Solvent	Q band λmax, (nm)	log ε	Excitation λ_{Ex} , (nm)	Emission λ _{Em} ,(nm)	Stokes Shift Δ_{Stokes} , (nm)	$\Phi_{ m F}$
CHCl ₃	685	5.13	686	700	15	0.0830
CH_2Cl_2	684	5.08	685	696	12	0.0847
THF	682	5.15	684	694	12	0.0949
DMF	685	5.09	686	698	13	0.0775
DMSO	689	5.12	690	702	13	0.0780



Figure 1. UV–Vis absorption spectra of 2 for aggregation studies in (a) DMSO and (b) DMF at different concentrations. (Inset: Plot of absorbances versus concentrations).

Fluorescence spectra studies and Fluorescence quantum yields

In our previous study, the fluorescence behaviour of complex 2 was investigated in various solvents including $CHCl_3$, CH_2Cl_2 , DMF, THF and DMSO. The standart and the studied Pc 2 were excited at the same appropriate wavelength. Table 1 and Figure S2(b) give The resulting fluorescence data and quantum yields, respectively. Fluorescence properties of 2 were observed to be the lowest in DMF. Considering the fluorescence property of compound 2, it has been determined that it has the potential to be used as a photosensitizer in PDT.

Singlet oxygen quantum yields (Φ_{Λ})

PDT is based on the selective destruction of target tissue by " ${}^{1}O_{2}$ " produced as a result of the dynamic interaction between a Ps, light of a wavelength suitable for the excitation of Ps, and molecular oxygen. Singlet oxygen quantum yield (Φ_{Δ}) is a measure of the singlet oxygen generation capacity of a molecule and is one of the most important parameters in studying molecule potential to be used as a Ps for PDT applications [29,30].

For this reason, the search for suitable photosensitizers is a continuing investigation issue among researchers. In present study, the photochemical properties of fluoro-functional Zn(II) phthalocyanine 2 were investigated in DMSO and DMF due to lack of standart in CHCl₃, CH₂Cl₂. 1,3-diphenylisobenzofuran (DPBF) was used as the chemical extinguisher of singlet oxygen. In this study, singlet oxygen generation potentials of fluoro-functional Zn(II) phthalocyanine, which was synthesized to shift the absorption to the Vis region and whose photophemical properties were investigated in DMSO and DMF due to lack of standart in CHCl₃, CH₂Cl₂. Singlet oxygen quantum yields were calculated. Information about the singlet oxygen measurements conditions were given in the supplementary file. DPBF degradation at 417 nm (in DMSO) and 415 nm (in DMF) [3] was recorded by UV-Vis spectrophotometer (Figure 2). The absence of any changes in Q band intensities during singlet oxygen generation indicated that the complex was not degraded during Φ_{Δ} determinations.

The Φ_{Δ} values of the peripherally tetra [bis(4-fluorophenyl)-methoxy]-substituted Pc was calculated and this values are presented in Table 2. The Φ_{Δ} values are 0.76 and 0.70 in DMSO and DMF, respectively. The heavy atom effect of halogen atoms is weak because they are not very close to the Pc ring [31]. When the effect of halogen atom was examined, the Pc ring carrying F showed higher singlet oxygen



Figure 2. Absorption changes during the determination of singlet oxygen quantum yield in (a) DMSO and (b) DMF using DPBF as a singlet oxygen quencher.

Complex	Solvent	$\Phi_{\rm F}$	$\Phi_{\rm d}$	Φ_{Δ}	Reference
Compound 2	DMSO	0.0780	4.01x10 ⁻⁴	0.76	This study
	DMF	0.0775	6.03x10 ⁻³	0.70	
Std-ZnPc	DMSO	0.20	0.26x10 ⁻⁴	0.67	[3]
	DMF	0.17	0.23x10 ⁻⁴	0.56	
Compound 3c	DMSO	0.167	2.4x10 ⁻⁴	0.71	[22]
	DMF	0.19	-	0.04	[33]
Compound 2	THF	0.20	-	0.72	[34]
Compound 6	Toluene	0.035	1.39x10 ⁻⁶	0.60	[35]

Table 2. Comparison of Photophysical and photochemical parameters of different fluorinated phthalocyanines

activity in DMSO (Φ_{Δ} = 0.76) and DMF (Φ_{Δ} = 0.70) compared to unsubstituted zinc phthalocyanine ($\Phi_{\Delta DMSO} = 0.67$ and $\Phi_{\text{ADMF}} = 0.56$ [3]). Another factor affecting the photochemical properties is the polarity and coordination strength of the solvents [27]. This may be due to the attempt of the amine group in DMF to quench singlet oxygen. In general, the singlet oxygen quantum yield values of phthalocyanines are higher in DMSO than in DMF [3, 27], and results in complex 2 are in line with this trend. The data obtained determined that 2 has the potential to provide favorable singlet oxygen production in PDT, in agreement with the literature [16, 20-22]. Singlet oxgyen quantum yields were calculate only in DMSO and DMF due to luck of standart in in CHCl₃, CH₂Cl₂. Normally, water solubility is important properties of phthalocyanine compounds for PDT applications. But many Pcs are soluble in organic solvents such as DMSO, DMF etc. Our samples are not soluble in water but they have good singlet oxygen quantum yield in DMSO. DMSO is not toxic solvent for biological cell studies required concentration for PDT application. For many phthalocyanine complexes which is insoluble in water, biocompitable solvent DMSO is used as medium in in vivo or in vitro studies. Fluorinated phthalocyanines have been also reported to show improved

photosensitizer activity for PDT compared to nonfluorinated derivatives [32-35] as given in Table 2.

Photodegradation quantum yields (Φ_d)

In PDT applications, PSs that provide the formation of "1O2" molecule must be stable under the applied light. Because this stability is necessary to maintain its effectiveness and to keep the drug concentration unchanged. The Φ_d value is an indication that the molecule can be used in PDT as a photosensitizer. In this study, the photodegradation tendency of 2 in DMSO and DMF solutions was followed by exposure to visible light for certain periods of time, followed by changes in the maximum Q-band in the absorption spectra of this compound (Figure 3). Table 2 presents the Φ_d values of 2 in studied solvent. The Φ_d value of 2 was higher than the Φ_d value of standard zinc phthalocyanine in DMSO, but lower than that in DMF. The stable zinc Pcs compounds have Φ_d values as low as 10^{-6} however unstable derivatives have Φ_d values of the order 10⁻³[3]. For this reason, it was determined that the Fluoro-substituent attached to the phthalocyanine ring increases the resistance of the molecule to visible wavelength light in DMSO while destabilizing it in DMF.



Figure 3. UV–Vis absorption changes for a) 2 in DMSO and b) 2 in DMF during the determination of photodegradation quantum yield.

CONCLUSION

In summary, the effect of solvent on the singlet oxygen generating capacity and light stability of 2, whose synthesis, characterization and photophysical properties were examined in detail in our previous publication, was investigated and its photosensitizer candidacy for PDT was investigated. This complex exhibited good solubility and non-aggregated species in the previously mentioned solvents. The $\Phi_{\rm FP}$ singlet oxygen production ability and photostability of 2 was also examined in DMSO and DMF. The effects of bulky floro functional of the substituent on the Pc ring and the type of solvent on this properties were also evaluated. The complex 2 exhibited lower Φ_F compared to unsubstituted ZnPc. The Φ_A value of compound 2 was found higher than unsubstituted ZnPc in DMSO and DMF. The studied Pc showed a high stability in DMSO and this stability is suitable for PDT applications. Although these Pcs have high Φ_d in DMF, this has reasonable singlet oxygen production as photosensitizers for PDT. The results showed that the substitution [bis(4-fluorophenyl)-methoxy] group on the Pc ring effected on photophysicochemical properties of the studied Pcs. This study indicates that the photophysicochemical properties of the studied Pcs are satisfactory to be used as photosensitizer in PDT.

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AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Interacting with chat GPT: Impact on students and teaching-learning

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ABSTRACT

This paper presents a discussion of ChatGPT, an AI-powered chatbot developed by OpenAI, and the technology behind it. This work provides a brief history of the Generative Pre-trained Transformer (GPT) model, which is the backbone of ChatGPT, and its ability to perform various language-based tasks. It further explores how ChatGPT leverages GPT's capabilities to offer a sophisticated chatbot experience to users and its role in students' teaching-learning process. It includes an interview with ChatGPT, which highlights the potential benefits and threats of using this technology by students and for the purpose of teaching-learning and in academia. Finally, the article discusses on the outcomes of a survey conducted on undergraduate college students of Delhi and analyzes the responses to conclude on students' perception on the use of ChatGPT and its impact on teaching-learning processes, and subsequently presents some recommendations on the same.

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INTRODUCTION

In the last few years, there have been substantial progressions in the realm of education, driven by the advancements in artificial intelligence (AI) and machine learning. One of the noteworthy innovations is ChatGPT, a language model crafted to produce text responses that closely resemble human-generated content when provided with input prompts. ChatGPT has garnered significant attention for its capacity to generate coherent and contextually relevant responses in various domains, including the field of education. Figure 1 illustrates the trend in Google searches for AI, chatbots, ChatGPT, and Bard-related queries over the past six months in India (November 2022-April 2023). Introduced in February 2023, Google Bard utilizes the GPT-3 language model, just like ChatGPT, to offer comparable functionalities. Both ChatGPT and Google Bard are AI chatbots specializing in natural language processing, thus performing similar tasks.

Nonetheless, these two services exhibit certain distinctions and cater to slightly different usage scenarios. This paper presents an examination of the cutting-edge technology that empowers ChatGPT, an advanced chatbot that has recently gained considerable attention, and assesses its impact on contemporary student learning.

The article is organized as follows: In Section II, we provide an in-depth exploration of the Generative Pre-Trained Transformer (GPT), the foundational technology behind ChatGPT. This section delivers the essential background

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India. 01/11/2022 - 11/05/2023. Web Search.

Figure 1. Trend in Google searches for AI, Chatbot, ChatGPT, Bard related queries in India in the last 6 months (November 2022-April 2023). Retrieved from Google Trends[#]

information on the fundamental concepts associated with ChatGPT, encompassing natural language processing and artificial intelligence, while elucidating their respective roles within the technology. Moving on to Section III, we delve into the advantages and the wide array of language-based tasks that GPT can execute, ranging from text generation and question answering to interactive games. The fourth section provides a review of related literature on the technology in the domain of students and learning. Section V of the paper demonstrates the potential of ChatGPT by presenting the output of a series of questions put up with the chatbot regarding its impact on teaching-learning and today's students. In the sixth section, we have analyzed the responses to a survey conducted on college undergraduate students of Delhi, presented as objective wise discussions in section VII. This is followed by results in section VII and subsequent recommendations in section VIII and finally we have concluded the impact of ChatGPT on students and teaching-learning.

Objectives

The primary objective of this work is to explore the impact of ChatGPT on students' and on teaching-learning. Specifically, we aim to investigate how ChatGPT can enhance students' engagement, knowledge acquisition, and critical thinking skills when used as a learning tool. By analyzing the responses to a questionnaire circulated amongst undergraduate college students of Delhi, we have discussed the students' perception of using this tool and their level of engagement with ChatGPT in regards to teaching-learning. Further, through interactions with ChatGPT on questions relating to its impact on students, we aim to shed light on the potential benefits and challenges associated with incorporating AI language models into educational settings. The objectives behind framing the questions in the questionnaire for survey purpose can be summarized as:

- To explore the impact of ChatGPT on students and teaching-learning.
- 2) To investigate how ChatGPT enhances student engagement and knowledge acquiring.
- To discuss the perception of students on their use of ChatGPT tool

MATERIALS AND METHODS

The work was carried out in four phases:

- Firstly, related literature works on ChatGPT were reviewed and the capabilities, benefits and limitations offered by the model were explored.
- Next, questions relating to impact of ChatGPT in teaching-learning processes were put up to ChatGPT and the responses from the interaction were recorded and analyzed.
- Thirdly, a questionnaire was circulated among students of different age groups, studying in different undergraduate courses across institutes/universities of Delhi. The preliminary questionnaire with 13 close-ended questions was prepared for the students with the help of literature survey and discussions carried out with student representatives of different courses at Maharaja Surajmal Institute, Delhi. 408 students shared their perspective on the use of ChatGPT in learning through filling out the questionnaire.

Count	Age	Institute/university name	
(Total: 359) 5	17		
81	18		
103	19	Maharaja Surajmal Institute, Maharaj	
90	20	Surajmal Institute of Technology	
61	21		
19	22		
(Total: 21) 9	18		
10	19	Various colleges of GGSIPU (besides	
2	20	MSI/MSIT)	
(Total: 10) 1	18		
5	19		
3	20	Various colleges of DU	
1	21		
(Total: 18) 1	17		
4	18		
3	19		
6	20	Others like NIT, IGNOU, NSUT	
2	21		
2	22		

A handful of the original study participants were given the link to the survey Google form, and the snowball sampling/chain-referral method was used to spread the information to others via email and WhatsApp. The forms were closed once 400+ responses were received from the students. The distribution of the students who participated in the study is shown in Table 1. The questionnaire comprised 13 questions, and at least 3-4 questions were directed towards providing responses for each of the specified objectives.

• Finally, a statistical analysis of the received survey responses was carried out and based on all the collected data, we have suggested some recommendations for the integration of ChatGPT in teaching-learning processes and for use by students in academia.

SIGNIFICANCE

Understanding the impact of ChatGPT on students' learning outcomes is of paramount importance for educators, researchers, and policymakers. This research has the potential to inform the design and implementation of AI-driven educational technologies, leading to more effective and engaging learning environments. Furthermore, by identifying the advantages and limitations of ChatGPT, we can address concerns related to bias, ethical considerations, and the potential replacement of human instructors.

Background Information

Artificial intelligence

Artificial intelligence (AI) aims to develop machines capable of executing tasks that demand human-like intelligence. These tasks encompass activities such as image recognition, speech recognition, language comprehension, decision-making, and data-driven learning. AI is becoming more popular day by day because industries aim to develop machines that can perform tasks that were previously done by humans. Machine learning, deep learning, and neural language are used to approach AI [1].

Today AI is being used in various industries and fields including healthcare, finance, transportation, and consultation. For example:

- Tesla's self-driving cars use deep learning which can detect obstacles on the road and maintain the speed and controls the steering wheel.
- Snapchat filters use machine learning (ML) algorithms to separate human faces from backgrounds, track facial expressions, and modify the image on the screen depending on what the user is doing.

NLP

Natural language processing (NLP) represents the field of artificial intelligence (AI) dedicated to enabling computers to comprehend text and speech in a manner similar to human understanding. NLP leverages a combination of statistical, machine learning, and deep learning models, along with rule-based language modeling from computational linguistics. These technologies empower computers to grasp the meaning of text or audio data, discern the intention and sentiment of the speaker or writer. An example of this application can be seen in speech recognition, where the primary task involves accurately converting spoken language into written text, often referred to as "speech-totext." This technology ensures the reliable transformation of voice data into textual information [2].

Chatbot

Natural In the earlier stages of it, text-based chatbots were limited to answering the developers' questions. They worked like an interactive FAQs (frequently asked questions), but they failed when given with difficult or unanticipated inquiries.

Chatbots now may handle client interactions 24/7 and improve their responses by learning from user questions. Chatbots eliminate repetitive chores and streamline procedures. Since chatbots are available to any number of users at once, they can reduce phone-based customer service wait times. This way they offer a good user experience and satisfied customers tend to stay more loyal [3].

Unlike previous chatbots that used rule-based approaches, ChatGPT uses a neural network model that can learn from vast amounts of data to generate responses. It is pre-trained on a large corpus of text, making it capable of responding to a variety of questions in a conversational



Figure 2. Stages in GPT model.

manner. As such, ChatGPT is considered one of the most advanced chatbots in existence today [4].

A flowchart of a GPT model generally consists of the following main stages, as shown in Figure 2:

- 1. Data Preparation: In this stage, the raw input data is pre-processed and transformed into a format that can be used by the GPT model. This may involve tasks such as tokenization, encoding, and batching.
- 2. Model Architecture: This stage involves defining the architecture of the GPT model. This typically involves selecting the number of layers, hidden units, and attention mechanisms, as well as any other hyperparameters that may affect the performance of the model.
- 3. Fine-tuning: Once the GPT model has been pre-trained, it can be fine-tuned on a specific downstream task. This involves adjusting the model parameters and training it on a smaller dataset that is specific to the task. The goal of fine-tuning is to adapt the pre-trained model to the specific task and improve its performance on that task.
- 4. Inference: Finally, the trained GPT model can be used for inference, which involves generating text based on an input prompt or question. During inference, the input prompt is fed into the GPT model, and the model generates a text output based on the learned patterns and structures from the pre-training and fine-tuning stages.

Therefore, the flowchart of a GPT model involves several stages of data preparation, model architecture design, pre-training, fine-tuning, and inference, all of which are essential for developing a robust and effective natural language generation system.

ChatGPT

ChatGPT, a state-of-the-art language model developed by OpenAI, represents a significant breakthrough in artificial intelligence, specifically in natural language processing, and has the potential to revolutionize the way students engage with educational content [3]. Table 2 below showcases some of the guidelines on how to prompt your queries to ChatGPT for refined results.

ChatGPT Capabilities

- Text generation: ChatGPT can generate text on any topic given by the user. It can generate text in a particular word limit as user asked. Text can be generated in various forms like one can use ChatGPT for generate code of programs and it is most interesting too. It has ability to write the code from the scratch or you can modify pre-written code in every language you request.
- Question-Answering: ChatGPT can answer the almost all question with nearly accurate answer which can be used in different purposes. It can understand and respond to natural language questions with relevant information. This is useful in wide change field and can be used for educational purposes [5].
- Translation: it is not a new feature this was introduced much before ChatGPT. The feature of translating texts into another language quickly and accurately without changing the expression in the sentence is very appreciable.
- Interactive game: ChatGPT can be used for a fun and engaging way to kill some time. You can play various games simply by chatting with a bot using this OpenAI platform like simply asking ChatGPT to guess the movie name by using yes-no format [6].

Characteristics	Details
Tone	Indicate the preferred style, whether it be formal, informal, or any other.
Structure	Provide a description of the layout or arrangement, for instance, whether it should follow an essay format or use bullet points.
Role	Specify a role or point of view to take on (for example, expert or critic).
Purpose	Express the aim or intent of the response (for instance, to inform or persuade).
Situation	Supply relevant background details, data, or context.
Extent	Clarify the extent or breadth of the subject matter.
Keywords	Enumerate significant terms or phrases for inclusion.
Limitations	Specify restrictions, such as word or character limits.
Examples	Furnish instances of the preferred style, format, or content.
Comparisons	Request the AI to employ analogies or illustrations to elucidate concepts.

Table 2. ChatGPT prompting guide (Source: neatprompts.com)

ChatGPT benefits in advancing teaching-learning

- 24/7 availability: Nowadays, routine and sleep cycle of the student is changed because of various factors like

 Social media, extracurricular activities, traveling or maybe any side hustle. So they require study material according to their preference of time. That's why the availability of content is necessary to students at any time, regardless of their location or time zone.
- Personalized Learning: ChatGPT can be used to design individualized learning experiences for students by looking at their conduct, abilities, learning style, and capacity for understanding. It can provide customized learning plans, reports, and guidance based on individual needs and learning styles. It can assist student to clear doubt and to score more and more marks in exams/test [7].
- Unlimited material source: Benefit of using ChatGPT in advancing teaching-learning is providing unlimited source of study material to student as well as to teacher. ChatGPT act like one stop destination where student/ teacher can search relevant and optimized content for any subject in any language. This is very useful for those students who can't access the library or any traditional source of information [6].
- Teaching strategy: ChatGPT can help teachers to make lesson plan: ChatGPT can help teachers to make lesson plans by giving unique and creative ideas to make interesting resources like Notes, assessments and fun activity for learning purposes. It can be used to create

interactive learning experiences for students, such as quizzes, and games [1].

Possible drawbacks of using ChatGPT in teachinglearning

- Personal Interaction: ChatGPT or any AI model can provide you better learning experiences but can't provide human interaction experience. Surely, ChatGPT can provide better learning experiences but can't teach any student basic social manners like, "How to talk", "How to behave", "How to cooperate with coworkers" etc. As humans are social animals these factors are also important to teach the students, where ChatGPT totally fails.
- Total dependency on technology: More use of ChatGPT to provide answer to questions or get learning materials can reduce the proper functioning of human brain or we can say human will loss the skill of creative thinking and problem solving. Students more likely use ChatGPT instead of thinking for themselves and developing their own ideas [8].
- ChatGPT generate answers and texts based on existing data, which can limit the creativity and originality. This can become a reason in future that students cannot think of any innovative idea, which leads to student wouldn't get any innovative ideas and can have very limited perspectives or vision for future [2].

LITERATURE REVIEW

The related works in literature have been analyzed and compared in Table 3.

Table 3. Comparative analysis of related works

Similarity	Difference	Significance
Alshater [2] and Lund & Wang [3] acknowledge OpenAI's development of ChatGPT and its contributions to artificial intelligence. They discuss how ChatGPT may affect academia and libraries. They discuss ChatGPT's ethical issues, such as text biases and privacy concerns. Both works stress on ethical use of ChatGPT.	Alshater [2] covers ChatGPT's general features, while Lund & Wang [3] examine its implications for academia and libraries. Alshater covers ChatGPT technology and its applications across industries, while Lund & Wang examines its effects on research, scholarship, and library services. Lund & Wang feature ChatGPT- generated questions and answers for a more conversational approach.	Both Alshater [2] and Lund & Wang [3] discussed ChatGPT's advanced chatbot technology. They showed ChatGPT's skills and highlighted the ethics behind using chatbots.
Kalla & Smith [5] and Rospigliosi [4] examine how artificial intelligence affects learning outcomes and engagement. Technology-assisted learning: Both papers examine how AI-based tools can improve classroom learning or create new interactive learning experiences. Student engagement: Both papers discuss how AI tools can increase student engagement in learning. Interactive learning: Both papers emphasize the value of interactive learning environments and AI's role in facilitating dialogue, questions, and responses to encourage student participation.	Kalla & Smith [5] examine how AI affects classroom learning, while Rospigliosi [4] examines chatbot-assisted learning. Methodology: Kalla & Smith may use qualitative and quantitative data analysis, while Rospigliosi may use experimental or quasi-experimental designs to assess chatbot-assisted learning interventions. In [5], they examine adaptive learning systems or intelligent tutoring systems, while in [4], they focus on chatbot technology. Learning outcomes: Kalla & Smith (2023) examine how AI implementation affects knowledge acquisition, critical thinking, and problem- solving, while Rospigliosi (2023) measures student engagement.	Both papers [4] and [5] examine the pros and cons of AI in education, filling research gaps. Current educational theories and research emphasize student engagement as essential to effective learning. Theoretical frameworks would illuminate paper quality. Assessing the theories' application and empirical support is crucial. Valid and reliable measures, proper sampling, and control groups (if applicable) improve study quality and validity.

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Tab	le 3	. Con	parative	analysis	of related	l works ((continued))
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Similarity	Difference	Significance
Both papers [6] and [7] raise concerns about students' overreliance on AI tools like ChatGPT for homework and assignments. They worry about students becoming lazy thinkers and losing critical thinking, researching, and writing skills. Both papers discuss AI-enabled academic dishonesty and the potential damage it can cause to the educational system. They highlight instances where educational institutions have banned ChatGPT or similar AI tools due to concerns about student learning, content accuracy, and potential negative effects.	Baidoo-Anu & Owusu [6] addressed student fears and concerns about AI tool dependency and its potential negative effects on learning. It emphasizes caution and traditional learning approaches when using ChatGPT for assignments and essays. On the other hand, Huzaif [7] suggested using ChatGPT as a pedagogical tool to help students organize their thoughts and improve writing skills. It advocates for AI integration in the classroom and teaches students how to effectively use ChatGPT for writing.	Baidoo-Anu & Owusu [6] raise concerns about student reliance on AI tools and the potential loss of vital skills. It emphasizes academic integrity and highlights valid concerns about AI and its impact on learning. The paper effectively emphasizes the potential negative consequences and underscores the responsibility of educators in addressing them. On the other hand, Huzaif [7] proposes using ChatGPT as a teaching tool rather than banning it. It suggests that AI can provide structure and feedback for student writing, potentially improving writing skills when implemented well.
Malinka et al. [9] and Sullivan et al. [10] aim to increase sentiment categorization accuracy and effectiveness using machine learning and deep learning. They propose new methods to improve sentiment analysis. Both papers perform sentiment analysis using machine learning and deep learning techniques. They compare their proposed methods to existing sentiment analysis approaches using benchmark datasets.	Malinka et al. [9] used feature engineering and a typical machine learning method for sentiment analysis. They employ constructed characteristics to represent input data. On the other hand, Sullivan et al. [10] used deep learning techniques, such as CNN and RNN architectures, to improve sentiment analysis. They utilized word embeddings to automatically capture semantic information. Malinka et al. utilized a typical machine learning technique like Support Vector Machines (SVM), while [10] utilized deep learning models like CNN and RNN to capture complex sentiment analysis patterns and dependencies. The performance metrics of the approaches differ, with [9] achieving a sentiment analysis accuracy of 87% and [10] achieving a higher accuracy of 92%.	Both publications [9] and [10] demonstrate strong theories and concepts, proposing new methods to advance sentiment analysis. They show a good understanding of machine learning and deep learning approaches, which are considered cutting-edge techniques. The papers validate and verify their outcomes using benchmark datasets. Sullivan et al.'s use of deep learning and higher accuracy suggests a more advanced and effective strategy compared to Malinka et al.'s machine learning-based approach. Both papers contribute to the field of sentiment analysis research, with [10] offering more innovative concepts and achieving better performance.
Both papers [1] and [8] discuss the use of AI technologies, particularly ChatGPT, in education and learning. They acknowledge the potential benefits of AI technologies in facilitating learning and providing assistance to students. Additionally, both papers recognize the limitations of AI technologies, including their inability to replace human interaction and the challenges they pose in developing certain skills.	Adiguzel et al. [1] provide a broader overview of the use of AI technologies in education, offering insights beyond ChatGPT. It covers the pros and cons of AI technology, emphasizes the roles of teachers, and addresses the ethical use of technology. On the other hand, Shidiq [8] focuses specifically on the impact of ChatGPT on creative writing assignments. It narrows its scope to discuss the challenges and strategies related to using ChatGPT for creative writing. The methodology of [1] involves descriptive qualitative analysis, while the methodology of [8] is not specified.	Both papers contribute valuable insights into the use of AI in education. Adiguzel et al. [1] provides a comprehensive understanding of AI technologies in education, covering various aspects and considering the roles of teachers. It highlights the pros and cons of AI and its impact on students' creative writing skills. Shidiq [8] specifically examines the harmful effects of using ChatGPT for creative writing assignments and suggests alternative approaches to mitigate these downsides. It emphasizes the importance of maintaining teacher-student contact in creative writing. Both papers demonstrate a strong understanding of the subject matter and contribute to the existing body of knowledge in the field of AI in education.

Since the introduction of ChatGPT, there has been a notable increase in research and proposals for various methodologies, emphasizing its potential for integration into educational environments spanning diverse fields. This integration has sparked lively discussions among educators at various levels. Different studies and surveys have been carried out to experiment with the use of ChatGPT-

In a study conducted by Vázquez-Cano et al. in 2023, they investigated whether there are notable distinctions in the assessment of a summary generated by ChatGPT, which was intermingled with summaries produced by a standard group of 15-year-old students. These summaries were then evaluated by 30 Spanish language teachers with varying genders, ages, and levels of professional experience. The findings indicated that ChatGPT received a significantly higher score for its summary performance compared to the highest-scoring students [11].

In another study by Shoufan [12], 56 senior students enrolled in a computer engineering program served as participants for a two-stage study wherein they firstly evaluated ChatGPT in their own words after using it for completing a learning activity. This qualitative data was subsequently subjected to a rigorous analysis using Taguette tool for encoding and identifying patterns or themes within textual data. This thematic analysis of students' responses unveiled a multifaceted landscape of perceptions of ChatGPT and building on this analysis, a comprehensive 27-item questionnaire was developed to quantitatively assess students' levels of agreement with various positive and negative themes' statements related to ChatGPT [12].

Ali et al. [13] investigated through their study how ChatGPT impacts learning English by collecting data through an online questionnaire from 80 teachers and students who had used ChatGPT earlier. The quantitative analysis conducted with SPSS yielded results that are crucial for the development of research on recently introduced technological advancements in L2 teaching and recommend incorporating ChatGPT into English language programmes to support learners [13].

With an emphasis on the situation in Latinoamerican institutions of higher learning, study by Huallpa [14] examines the ethical conundrums that result from integrating ChatGPT into higher education. To understand more about their experiences with and reasons for utilising conversational agents powered by AI, he used an online survey to collect information from 220 participants. Results suggested that integration of AI in Latin American higher education is complicated as it is influenced by cultural and ethical factors and participants considered the incorporation of ChatGPT to be moderately accessible and held somewhat favorable social attitudes towards it. They recognized the importance and accountability of ChatGPT in facilitating personalized educational opportunities and emphasized the need for clear institutional regulations concerning privacy and data protection [14].

Interaction with ChatGPT

The following questions are put up by authors and each response is written entirely by ChatGPT [3]:

Question: How does ChatGPT impact college students' teaching-learning?

ChatGPT

ChatGPT, as an AI language model, can potentially impact college students' teaching and learning in several ways. Here are a few potential impacts:

1. Information and resource access: College students can use ChatGPT to quickly access information and

resources related to their coursework. They can ask questions about specific topics, receive explanations, and obtain references for further study. This can be particularly helpful when they need immediate assistance outside of regular class hours or when they have difficulty finding relevant information.

- 2. Concept clarification and explanations: ChatGPT can provide explanations and clarify complex concepts for students. It can break down difficult topics into simpler terms, provide examples, and help students grasp challenging ideas. This can be valuable when students need additional support or alternative explanations beyond what is available in their textbooks or lectures.
- 3. Study and research assistance: College students often engage in research projects or assignments that require extensive reading and analysis. ChatGPT can assist by suggesting relevant research articles, helping refine research questions, or offering insights into specific areas of study. It can also help with structuring essays, providing writing tips, or assisting in proofreading and editing.
- 4. Personalized learning experiences: ChatGPT can adapt to individual students' needs and provide personalized learning experiences. It can track a student's progress, understand their learning preferences, and offer tailored suggestions for further study or practice. By analyzing patterns in a student's questions and interactions, ChatGPT can provide targeted recommendations, adaptive feedback, and support their unique learning journey.
- 5. Language practice and feedback: Language proficiency is crucial for college students, especially for those studying in non-native languages. ChatGPT can serve as a language practice tool, allowing students to engage in conversations and receive feedback on their writing or speaking skills. It can help students improve their grammar, vocabulary, and overall language fluency.

However, it's important to note that while ChatGPT can be a valuable tool, it should not replace human instructors or personalized interactions. It should be seen as a supplement to traditional teaching methods and a means to augment learning experiences. The role of human instructors in providing guidance, mentorship, and individualized feedback remains crucial for comprehensive education.

Question: What is the effect of ChatGPT on students' critical thinking?

ChatGPT

The effect of ChatGPT on students' critical thinking can be both positive and negative, and it depends on how the tool is utilized and the context in which it is used. Here are some potential effects:

Positive Effects:

1. Exposure to diverse perspectives: ChatGPT can expose students to a wide range of perspectives and ideas that they might not have encountered otherwise. This

exposure can stimulate critical thinking by challenging students' existing beliefs and encouraging them to consider alternative viewpoints.

- 2. Promoting inquiry and exploration: ChatGPT can encourage students to ask questions, explore various topics, and delve deeper into their areas of interest. By providing quick access to information, it can facilitate independent research and investigation, allowing students to develop their critical thinking skills through active exploration.
- 3. Encouraging analysis and evaluation: ChatGPT can assist students in analyzing and evaluating information. It can help them assess the credibility of sources, identify biases, and critically examine arguments or claims. By engaging with ChatGPT, students can practice assessing the reliability and validity of information, which enhances their critical thinking abilities.
- 4. Problem-solving support: ChatGPT can aid students in problem-solving by offering suggestions, guiding them through logical reasoning, and providing alternative perspectives. By engaging with the model in problem-solving scenarios, students can refine their analytical skills and think critically about the steps needed to arrive at a solution. Negative Effects:
- Overreliance on information without verification: If students solely rely on ChatGPT for information, there is a risk of accepting answers without independently verifying their accuracy. This can hinder critical thinking by
- discouraging students from questioning or fact-checking the information they receive.2. Lack of real-time feedback: While ChatGPT can pro-
- vide responses and explanations, it may not always offer real-time feedback on students' thought processes or challenge their reasoning. This can limit opportunities for students to receive constructive feedback on their critical thinking skills and may hinder their growth in this area.
- 3. Absence of human interaction and collaboration: Critical thinking is often enhanced through discussions, debates, and collaboration with peers and instructors. If students excessively rely on ChatGPT as their primary source of information and interaction, it may reduce opportunities for engaging in critical dialogue and cooperative learning experiences.

To maximize the positive impact of ChatGPT on critical thinking, it is important for educators to emphasize the importance of independent thinking, verification of information, and critical evaluation. They should encourage students to use ChatGPT as a tool for exploration, analysis, and idea generation, rather than a definitive source of knowledge. Additionally, instructors should supplement the use of ChatGPT with activities that foster face-to-face discussions, critical analysis, and collaborative problem-solving to provide a balanced approach to developing critical thinking skills. **Question:** What is the effect of ChatGPT on research work writing?

ChatGPT

The effect of ChatGPT on research work writing can be both beneficial and potentially challenging. Here are some potential effects:

Benefits:

- 1. Access to information and resources: ChatGPT can assist with gathering information and accessing relevant resources for research work. It can provide suggestions for research topics, recommend scholarly articles or books, and offer insights into specific areas of study. This can save time and streamline the research process for students.
- 2. Idea generation and organization: ChatGPT can help students generate ideas, brainstorm research questions, and organize their thoughts. By engaging in conversations with ChatGPT, students can receive prompts, suggestions, and alternative perspectives, which can contribute to the development of their research work and aid in structuring their arguments.
- 3. Writing assistance and feedback: ChatGPT can support students in the writing process by providing suggestions for sentence construction, vocabulary choices, and overall writing style. It can also assist with grammar and syntax, proofreading, and identifying potential areas of improvement. This can enhance the clarity, coherence, and overall quality of students' research writing. Challenges:
- 1. Dependence on AI-generated content: One potential challenge is the risk of overreliance on ChatGPT for generating content. While it can offer valuable suggestions and ideas, students should exercise critical judgment and ensure that the generated content aligns with academic integrity standards. Relying too heavily on ChatGPT's responses without independent thought and originality can undermine the authenticity and credibility of the research work.
- 2. Limited context and subject expertise: ChatGPT has knowledge up until September 2021, and its responses are based on patterns and examples it has encountered during training. Therefore, it may not always possess the most up-to-date information or have domain-specific expertise in certain specialized fields. Students need to be aware of this limitation and complement ChatGPT's responses with additional research and consultation with subject matter experts.
- 3. Lack of individualized feedback: While ChatGPT can offer general suggestions and writing assistance, it may not provide personalized feedback tailored to each student's specific needs and writing style. It's essential for students to seek input from their instructors, peers, or writing centers to receive comprehensive feedback and guidance on their research work.

To make the most of ChatGPT's impact on research work writing, students should view it as a tool that

complements their own efforts and critical thinking skills rather than a substitute for independent research and original thought. It's crucial to maintain academic integrity, verify information from reliable sources, and engage in discussions with instructors and peers for thorough feedback and guidance throughout the research process.

Question: Is ChatGPT sufficient and will replace libraries and teachers in educational institutes?

ChatGPT

ChatGPT is a powerful tool that can provide information, explanations, and assistance in various educational contexts. However, it is not sufficient to replace libraries and teachers in educational institutes. Here's why:

- 1. Depth and breadth of knowledge: While ChatGPT has access to a vast amount of information, it does not possess the depth and breadth of knowledge that libraries offer. Libraries contain extensive collections of books, journals, and other resources covering diverse subjects, allowing students to explore topics comprehensively. Libraries also provide access to specialized databases and archives that may not be readily available through ChatGPT.
- 2. Human interaction and expertise: Teachers play a crucial role in education by providing guidance, mentorship, and personalized instruction. They bring their expertise, experience, and pedagogical skills to create engaging learning experiences. Teachers can adapt their teaching methods based on students' needs, offer realtime feedback, facilitate discussions, and foster critical thinking. Human interaction and the personalized support that teachers provide cannot be replicated by ChatGPT alone.
- 3. Critical thinking and creativity: Education is not solely about accessing information but also about developing critical thinking skills, creativity, and problem-solving abilities. Libraries offer resources that encourage independent thinking, research, and analysis. Teachers guide students in developing these skills through discussions, projects, and assignments that require higher-order thinking. ChatGPT, while helpful in certain aspects, cannot fully replace the multifaceted approach to learning facilitated by libraries and teachers.
- 4. Contextual understanding and adaptation: ChatGPT operates based on patterns and examples in its training data, which might not always capture the nuances and context of specific educational environments. Libraries provide resources that are carefully curated and evaluated for relevance and accuracy. Teachers, through their experience and understanding of the curriculum, can adapt and tailor the learning experience to suit the needs of their students, taking into account the specific context and learning goals.

While ChatGPT can supplement learning and provide valuable support, it should be seen as a tool that complements the role of libraries and teachers rather than a complete replacement. The combination of libraries, human instructors, and ChatGPT can create a comprehensive educational experience that incorporates access to knowledge, critical thinking, personalized guidance, and interaction necessary for effective learning.

Question: How can ChatGPT be integrated with classroom teaching-learning?

ChatGPT

ChatGPT can be integrated with classroom teaching-learning in various ways to enhance the educational experience. Here are some suggestions for integration:

- Research and information gathering: Students can use ChatGPT to assist in their research projects or assignments. They can ask questions to gather initial information, receive suggestions for relevant sources, or seek clarification on specific topics. This integration can help students efficiently access information and resources to support their learning.
- 2. Concept exploration and explanation: In the classroom, teachers can leverage ChatGPT to reinforce or expand on concepts discussed during lectures. They can use ChatGPT to provide alternative explanations, offer additional examples, or delve deeper into specific aspects of a subject. This integration can help students gain a deeper understanding of the topics covered.
- 3. Personalized learning support: ChatGPT can be used as a personalized learning tool to cater to individual student needs. Students can engage with ChatGPT to receive targeted practice exercises, obtain personalized feedback on their work, or access supplementary materials aligned with their learning goals. This integration can promote differentiated instruction and address the diverse learning needs of students.
- 4. Collaborative learning and discussions: ChatGPT can facilitate collaborative learning experiences within the classroom. Students can engage in group discussions or debates with ChatGPT as a virtual participant, encouraging critical thinking and providing different perspectives. Teachers can design activities that involve students interacting with ChatGPT to collectively solve problems or analyze complex scenarios.
- 5. Language learning and practice: ChatGPT can assist in language learning by providing opportunities for students to practice their language skills. Students can engage in conversations with ChatGPT to improve their writing, speaking, and grammar. Teachers can design language learning activities that involve students interacting with ChatGPT to enhance their language proficiency.
- 6. Formative assessment and feedback: ChatGPT can be utilized for formative assessment purposes. Students can submit their written work or responses to ChatGPT, which can provide automated feedback on grammar,

sentence structure, and overall coherence. This integration can help students improve their writing skills and receive immediate feedback on their work.

It's important to note that while integrating ChatGPT into the classroom, the role of human instructors remains vital. Teachers should guide students on the appropriate use of ChatGPT, help them critically evaluate the information received, and encourage independent thinking. They should also balance the use of ChatGPT with other teaching strategies to provide a comprehensive and interactive learning experience.

RESULTS AND DISCUSSION

On the basis of interview conducted with ChatGPT, it is analyzed that it has both positive and negative impacts on students' learning. It is a tool for exploration, analysis, and idea generation, rather than a definitive source of knowledge. Rather than looking at ChatGPT as a replacement, the combination of libraries and ChatGPT can create a comprehensive educational experience for students that incorporate access to knowledge, critical thinking, personalized guidance, and interaction necessary for effective learning. Teachers should integrate and balance the use of ChatGPT with other teaching strategies and guide students on the appropriate use of ChatGPT.

The survey results have been statistically analyzed and interpreted according to the defined objectives, as presented in Table 4.

The foundation of this research lies in acknowledging digital literacy education as an essential component of modern learning. In today's digital age, students and teachers must be equipped with the skills to navigate and harness technology effectively. Following results can be concluded for each of the objectives according to the discussions:

 To explore the impact of ChatGPT on students and teaching-learning: Around 47% of students rely on Internet-based searches and content for learning, with 38.5% using AI tools like ChatGPT. Classroom teaching and traditional books/e-books are less popular for learning. Students find ChatGPT helpful for assessments and assignments, with mostly positive impacts, although some negatives. Over 75% believe that ChatGPT has

Table 4. Analysis of survey responses



Discussion: Around 47% students nowadays rely on Internet based searches and contents for learning, followed by ChatGPT like AI tools (38.5%). Reliability of students on classroom teaching and use of books/e-books for learning is significantly low.

Most students also agree that using ChatGPT for assessment and assignment purposes has both positive as well as negative impacts on them, but mostly positive, as it proves to be helpful, resourceful and time saving.

Also, more than 75% students believe that the students' use of institute libraries and its resources has been affected in varying extents by the increasing use of ChatGPT nowadays. However, it can still not completely replace the libraries and the classroom teaching, as agreed by 85% of the respondents.

Table 4. Analysis of survey responses (continued)

Objective: To investigate how ChatGPT enhances student engagement and knowledge acquiring Results

• Method(s) required for building skills such as academic writing/creative writing/business writing etc.



Discussion: Only around 12% students believe that ChatGPT alone is sufficient for building skills such as academic writing/creative writing/business writing. Over 62% students feel that a combination of all-ChatGPT, classroom teaching and self-learning is required for developing such skills.

Majority of respondent students (almost 55%) are also of the opinion that through engaging activities like personalized tutoring, interactive games etc., ChatGPT has a positive impact on them, while 31% were not sure about the impacts of the same. However, 44.6% of students do feel that ChatGPT and alike tools are making students lazy thinkers, i.e. have a negative impact on their critical thinking abilities.

Objective: To discuss the perception of students on their use of ChatGPT tool

Crash studies

Yes, always

Gives idea only

No

Results

• Purpose for which students generally use ChatGPT



54.7%

As shortcut for problem solving
 As an aid in academic writing
 Fun interactions and games

• Answers provided by ChatGPT are suitable and satisfactory



• Threat posed by ChatGPT to replacing software developers/programmers



• Banning ChatGPT like models in educational institutes

44.6%



• Use of ChatGPT involves risk of getting inaccurate information and learning wrong



• Possibility of ChatGPT like AI models to replacing traditional search engines in the long run



Table 4. Analysis of survey responses (continued)

Discussion: A major section of students (60%) use ChatGPT as a shortcut to problem solving, followed by as an aid in academic writing and a very low percent use it for crash studies or fun interactive games. According to over 58% of the respondents, ChatGPT like models should be integrated with classroom teaching processes rather than putting a ban on their use in educational institutes. In their use of the tool, 50.5% students believe that they get suitable and satisfactory answers from ChatGPT. However, the risk of getting inaccurate information and learning wrong sometimes also exists, as agreed by over 63% students.

A good section of students (almost 43%) do not think that ChatGPT is posing a threat to replacing software developers/programmers. Also, there is a much divided opinion on the possibility of ChatGPT like AI models replacing traditional search engines in the long run, where 21% students believe that this will happen, but almost 30% students think that both will coexist and, around 22% say that traditional search models will have to incorporate AI.

affected institute libraries, but 85% agree it can't fully replace libraries and classroom teaching.

- 2. To investigate how ChatGPT enhances student engagement and knowledge acquiring: Only 12% of students believe ChatGPT is sufficient for building writing skills, with 62% advocating a combination of ChatGPT, classroom teaching, and self-learning. Approximately 55% of students find ChatGPT's engaging activities beneficial, while 44.6% think these tools may hinder critical thinking, though 31% are uncertain about their impact.
- 3. To discuss the perception of students on their use of ChatGPT tool: About 60% of students use ChatGPT for problem-solving, with fewer using it for academic writing or fun games. Over 58% believe ChatGPT-like models should be integrated with classroom teaching, not banned. While 50.5% get satisfactory answers, over 63% acknowledge the risk of inaccuracies. Most students (43%) don't see ChatGPT as a threat to replace software developers/programmers. Opinions are divided on ChatGPT replacing traditional search engines; 21% think it will, while almost 30% believe both will coexist, and 22% see traditional search models incorporating AI.

RECOMMENDATIONS

Few recommendations for teachers and students around teaching-learning processes and the use of ChatGPT like AI tools are:

- Students should gain a comprehensive understanding of the benefits of AI tools, such as augmenting creativity, streamlining processes, and solving complex problems efficiently. Acknowledging these advantages can inspire innovation.
- Also, rather than putting a ban on their use, integrating the use of ChatGPT, Grammarly or other AI tools in institute libraries and/or as part of teaching-learning processes through appropriate ways can serve to be beneficial. These tools have the potential to help spark the creative process when wielded thoughtfully
- Equally important is the awareness of AI's limitations. Students need to grasp that AI tools are not infallible and may not always provide perfect solutions.

Understanding these constraints encourages critical thinking and problem-solving skills.

- Academicians should redesign assessment tasks (such as examinations) in a way that they can't be completed as easily by AI tools and rather adopt more personalized reflective tasks which are contextualized to the subject content. Faculty should include concept-based/ innovative classroom assignments which invoke students' critical thinking rather than encouraging copy-pasting content from the Internet or books or from ChatGPT like tools.
- The use of authentic assessments, which are creative learning experiences that evaluate students' skills and knowledge in realistic situations, should be included by teachers. These assessments go beyond traditional tests to reflect real-world challenges' complexity, enhancing motivation and learning applicability for students.
- One approach advocates for a variety of assessment formats, including presentations, performances, and digital forms such as web pages, videos, and animations. This allows students to demonstrate their understanding and creativity through mediums they find comfortable and engaging.

CONCLUSION

ChatGPT, introduced by OpenAI in November 2022, is part of a lineage of AI language models that have evolved rapidly in the last decade. The proliferation of these large language models has ushered in a fundamental question for the field of education that whether these models are a blessing or a potential challenge to the existing teaching and learning paradigms. Understanding their viewpoints is imperative for comprehending the implications of AI-driven language models on the educational landscape. Through a four-phase methodology in this work, more than 400 students of different undergraduate courses in Delhi were surveyed on their perception and use of ChatGPT, and similar questions from the questionnaire were also put up for interacting with the tool. Several other authors have conducted studies and surveys on a range of participants to experiment with the use of ChatGPT with objectives varying from checking its capabilities to write summaries
in Spanish, or integrate into English language programs to promote learners to considering ethical impacts of integrating ChatGPT in higher education. The findings of our paper indicate a generally positive reception of ChatGPT among students. They appreciate its potential benefits for learning and professional life, such as motivation and valuable explanations. However, students also acknowledge the need for a solid subject knowledge foundation and express concerns about accuracy and potential drawbacks. Teachers therefore can and should integrate ChatGPT into teaching-learning processes. While the impact on academic integrity and job opportunities is a modest concern, the overall outlook remains optimistic. And as education keeps changing, it's going to be crucial to keep researching and figuring out how to make the most of AI like ChatGPT in the classroom.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Acoustic emission reduction in vehicles by using MPP structures in wheel ARCH liner structures

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ABSTRACT

Noise emission is an important problem of vehicles. An important part of the general noise of the vehicle, which is called pass-by noise, is composed of the wheels and the engine. In this study, it was aimed to design a wheel arch liner (WAL) that can absorb the sounds coming from the wheels of the vehicles by creating micro-perforated panel (MPP) structures. While examining the diameters, pattern, and frequency of the holes in the MPP structures within the scope of the research; The effect of the cavity, which can be left behind the wheel arch liner structure to be used in the vehicle, on the acoustic absorption values was also included in the scope of the research, and studies were carried out to reduce the acoustic emission. In order to observe the effect of this cavity, 2 different cavity sizes (18-28 mm) were used with a without cavity MPP structure. In the results of the research, the highest acoustic absorption value (*Sa*) was observed as 0.97 in the sample with 7% hole density and 3 mm hole diameter. In addition, when the cavity behind the MPP structure is examined, the best *Sa* value was found in the sample with an 18 mm cavity. This research, which sought to reduce pass-by noise, revealed the potential of integrating MPP structures into wheel arch liners to reduce wheel noise.

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INTRODUCTION

With the increasing population growth, the number of vehicles in our world is increasing day by day. The effect of this uncontrollable increase on the daily life of human beings is growing negatively. The most important of these negative effects are seen as emissions, and an important type of these emissions is noise emission. Noise generated by automobiles is one of the components of noise pollution in the environment. The outside noise of a moving vehicle is part of its character and can be an important aspect of its appeal; however, the public traffic noise from thousands of cars and trucks is considerable. In the design of a vehicle, external noise must be limited according to regulatory requirements and internal noise must be kept at

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a level acceptable to the customer [1]. Administrative regulations regarding noise from cars have become increasingly stringent in recent years [2]. While passing noise limits for all types of land vehicles are determined by government institutions to reduce the noise in our environment, these stand out as critical regulations that must be followed [3]. Pass-by noise measurement is mandatory for automotive manufacturers for the type approval and conformity of production. ISO 362 from April 2014 imposes 68 dB(A) as a maximum of noise in 2025 according to the 51-03 pass-by noise test procedure [4,5]. According to regulation, the pass-by noise should be decreased by 2 dBA every 2 years.

In a normal road vehicle, pass-by noise mainly consists of tires, powertrain, air intake systems, and exhaust. Tires make up most of the pass-by noise [6]. When the wheels of the vehicle rotate, acoustic waves are produced due to the contact between the tire and the road. In addition, acoustic waves are also generated by radiation from the tire itself when excited by contact. Acoustic waves are also produced by the impact of water droplets or gravel, which are reflected on the surface of the wheel arch by the rotation of the wheel when the vehicle is moving on a wet or gravel road. For certain wavelengths, a phenomenon of cavity resonance occurs for frequencies called modal frequencies. For these frequencies, there are standing waves, that is, waves whose pressure maxima are always at the same points. To avoid this phenomenon of cavity resonance, called Helmholtz resonance, it is necessary to absorb acoustic waves as they are reflected. Absorbing the noise generated by the tires will play an important role in adapting to the new noise regulations. For this reason, a significant majority of researchers have focused on reducing wheel noise. Bao et al. aimed to reduce tire acoustic cavity resonance (TACR) noise in a study. The researchers designed a tire-rim assembly using a Helmholtz resonator and worked to reduce the TACR value. In the tests performed, a decrease was observed at the peak of the noise and in the specified frequency range [7]. In another study, Wan et al. investigated the porous structure of the liner placed in the tire to reduce tire cavity resonance noise. The researchers explained that both resonance noise control and material configuration must be considered to decide the thickness and width of the porous material adhered to the inner surface of the tire. They also stated that thicker or larger porous material performed better in controlling cavity resonance noise [8]. The acoustic emission performances of porous and perforated geometric structures are higher than other structures. Cavity absorbs most of the noise. These structures have been popularly used and developed to reduce noise in developing technological areas [7,9,10]. Naderzadeh et al. studied the performance of noise barriers applied with different diffusers with or without perforated plates. The researchers, who stated that the diffuser performance increased with the addition of the perforated plate, also stated that

the acoustic performance of the structure formed by the addition of these perforated plates was improved by 3.59 dB [11]. In a study, Padavala et al. aimed to reduce the noise of the drivetrain of electric vehicles. To reduce powertrain noise and improve interior sound quality, the researchers applied a passive noise reduction method. The study also demonstrates the development of several types of mufflers, including a new innovative MPP muffler for reducing intake noise from the air compressor [12]. Allam and Abom explored the possibility of creating noise-absorbing mufflers for use in automotive exhaust or ventilation systems. In the research, MPP absorbers were placed in noise sources and acoustic tests were performed. The researchers have stated that micro-perforated muffler solutions for broadband damping of sound have the potential to be used in automobile noise sources [13]. The absorption properties of MPP structures are also investigated independently of the automotive field. The cavities between these structures also affect the noise absorption properties of the structure [14,15]. In a study, Yan et al. studied the sound absorption properties of a double-layer micro-perforated plate structure with a variable cross-section back gap. In the research, it was revealed that sound absorption properties improved by increasing the cavity distance and cross-sectional area of the MPP structure on the inner side. In the results of the tests performed on the impedance tube, it was stated that the sound absorption coefficient reached 0.8 with the increase in the cavities in the structure, while the noise reduction performance of the designed with cavity MPP structure rose [16]. In this current study, MPP structures on which many acoustic absorption studies were carried out were created to generate a Helmholtz resonator and tested in the acoustic cabin. Acoustic emission values were examined by focusing on the hole diameters, hole density, hole pattern, and the width of the cavity to be left behind the MPP structures in the created MPP structures, and the effects of these parameters on the acoustic absorption value were discussed. The aim and motivation of the research is to optimally configure these parameters in the designed MPP structures and to reveal the potential of these structures to be used as noise absorbing WAL in vehicles.

EXPERIMENTAL

Materials

Polypropylene, which is used for wheel arc liner in the study, is a preferred polymer in various industries such as aviation, construction, and automotive [17–19]. This raw material, which is a thermoplastic that can be easily shaped by applying heat and pressure; is frequently used in plastic automotive parts with its advantages such as lightness, durability, and cheapness [20–22]. This product, which can be shaped by plastic injection, is attractive to companies in serial production as it provides ease of

Features	Values
Thickness	1.7
Density (g/cm ³)	0.90-0.95
Melt flow rate (230°C; 2,16 kg) (g/10min)	9-14
Tensile stress (50 mm/min) (MPa)	≥16
Tensile strain at break (50 mm/min) (%)	≥40
Tensile modulus (1mm/min) (MPa)	≥750
Flexural modulus (2mm/min) (MPa)	≥700
Notched impact strength (Izod) (23°C) kJ/m ²	≥8
Hardness (D-shore)	56-60

Table 1. Used polypropylene's features for wheel arch liner

production. In addition, the recyclability of this material stands out as another feature that makes this material stand out [23,24]. Due to the superior properties of this material, the raw material of most wheel arch liners used in the automotive market has been polypropylene. The properties of the polypropylene used in the study are shown in Table 1.

Wheel arch liner in polypropylene doesn't bring any noise absorption. For this reason, absorbent material must be placed inside the hood. However, absorbent material has to be used and defined according to cost, package, and performance constraints. In the study, polyurethane foam which is used with acoustic absorber function in various sectors was used as an acoustic absorbent. Table 2 shows the properties of the absorbent product.

Table 2. Features of acoustic absorbent

eatures8hickness(mm)8fet density(g/m³)4ompression resistance (40%, 4th cycle) (kPa)2lammability (thickness 13 mm) (mm/min)2ompression set (50% compression, 70°C, 22 h)(%)3ensile strength (kPa)1longation at break (%)2ear resistance (N/cm)4dour (2h, 80°C) (rate)2opgging reflection (thickness 10 mm-3 h, 100°C)(%)8opgging gravimetric (thickness 10 mm-16 h, 100°C)(mg)2ormaldehyde content(ppm)2coustic on 10 mm (NRC value) (%)3		
Thickness(mm)	8	
Net density(g/m ³)	400	
Compression resistance (40%, 4th cycle) (kPa)	2.5 - 5	
Flammability (thickness 13 mm) (mm/min)	≤80	
Compression set (50% compression, 70°C, 22 h)(%)	3.1	
Tensile strength (kPa)	120	
Elongation at break (%)	200	
Tear resistance (N/cm)	4.5	
Odour (2h, 80°C) (rate)	2.5	
Fogging reflection (thickness 10 mm-3 h, 100°C)(%)	83	
Fogging gravimetric (thickness 10 mm-16 h, 100°C)(mg)	0.7	
Formaldehyde content(ppm)	2	
Acoustic on 10 mm (NRC value) (%)	30	
Acoustic on 20 mm (NRC value) (%)	46	

METHOD

Alpha Cabin

Acoustic absorption properties of structures are measured by several test methods such as impedance tubes and alpha cabins. In this study, Alpha Cabin was used as an acoustic emission test method. Alpha Cabins, named after the sound absorption coefficient "alpha", is a reverberating chamber prototype. The sound absorption coefficient of the sample tested in this system is determined from the basic formula based on Sabine's theory, consistent with the measurement made in a normal-sized reverberation chamber:

$$\alpha = \frac{0,163 \times V}{S} \left(\frac{1}{TR} - \frac{1}{TR_0} \right) \times C \tag{1}$$

- V is Cabin Volume
- *S* is Sample Area
- *TR* is Reverberation Time with the sample in the Cabin
- *TR*⁰ is Reference Reverberation Time without the sample in the Cabin
- *C* is the correction coefficient of the cabin

The sound absorption coefficient (α) is calculated using the difference between the reverberation time of the room with and without sample. The cabin correction coefficient (*C*) is found by comparing measurements of reference samples made in a reverberation chamber and an alpha cabin under the same conditions [25,26]. The alpha cabin volume of 6.98 m³ allows a cut-off frequency of almost 300 Hz. Above this, the acoustic field of the reverberation chamber has the potential to disperse and measurements are taken in the frequency range 400 Hz-10000 Hz [27-29]. The alpha cabin test setup schematic view is shown in Figure 1.

Sample Characteristic

In the wheel arch liners that are actively available in the market, there is the wheel arch liner itself, the absorbent placed on the wheel arch liner, and the cavity before



Figure 1. Alpha cabin test setup schematic view.



Figure 2. Sequence examples and placement of samples in the Alpha Cabin.

the engine part, according to the order of proximity to the wheel. The samples to be subjected to acoustic testing in Alpha Cabin are also listed in this order. As a result of the literature research, it was decided that the sample plates to be placed in the test cabinet should be a with surface 1x1.2 m^2 [30]. The absorbent product was used in the same thickness and properties in all samples produced within the scope of the study and tested in the Alpha Cabin. Sequence examples and placement of samples in the Alpha Cabin are shown in Figure 2.

Test Configurations

The first point was to list all the parameters that should impact acoustic performances on the roadside with absorbent that reach body side requirements from the original equipment manufacturer. Hole size and perforated area

Figure 3. The pattern of holes on MPP structure.

were taken into account. Preliminary studies have been made for the design of the MPP structure to be created. The optimum design was obtained by varying the hole diameters and the density of the holes. Holes with diameters of 2 mm, 3 mm, and 5 mm were used, while hole densities of 3% and 7% were used. According to the findings obtained from the pass-by-noise tests, the highest noise levels are seen in the range of 630-2000 Hertz. For this reason, acoustic emission values in this range are examined in this study. In the preliminary studies, the pattern of the holes in the plate was changed and positive results were obtained. In order to get a uniform hole pattern and to keep a high mechanical resistance, It was decided to use the model presented in Figure 3 as MPP structures.

In the continuation of the study, the effect of the cavity created in the MPP structure was examined. A total of 3 structures, 18 mm, and 28 mm, together with the structure without gaps, were examined in this content.

RESULTS AND DISCUSSION

Holes Diameter and Density

Hole diameter and density are important parameters to reduce acoustic emission in MPP structures. In the study, 3 different hole diameters, 2 mm, 3 mm, and 5 mm, together with the hole-free structure; Two different hole densities, 3%, and 7%, are combined. The test results performed in the Alpha cabin according to the relevant standards are as in Figure 4.

Acoustic absorption comparisons are made by examining $S\alpha$ values. When the test results are examined, it is seen that the acoustic absorption value of the sample with 3% hole density and 2 mm diameter is higher. However, the $S\alpha$ value of this sample is not in the frequency range where the



Figure 4. Effect of hole density and diameter on acoustic absorption value.

wheel and motor noise are intense and the pass-by noise is the highest (630-2000 Hertz). Comparisons of samples are made at 1000 Hertz. The optimum combination is observed in the sample with a hole density of 7% and a diameter of 3mm, with a value of 0.97 S α at a frequency of 1000 Hertz. Although the tendency of the other samples is different, the $S\alpha$ values at 1000 Hertz for two are 0.78. The 19.6% difference calculated according to the high $S\alpha$ value is of great importance when it is foreseen that these structures can be used in vehicles. Although combinations at different frequency values reach values as high as 0.99 (%3 hole density- 2 mm hole diameter), they are at low acoustic emission levels in the range where pass-by noise is most important. According to this result, it is obvious that while increasing the hole density increases the acoustic absorption performance, the hole diameter should be optimized. Because in the combination of holes with a diameter of 3 mm as an intermediate value, the higher $S\alpha$ value indicates that the increase or decrease in diameter does not have a linear correlation. As seen in the studies in the literature, it has been understood that hole diameters and patterns are of great importance in terms of acoustic emission [31]. In addition, in another study by Tayong, these results cannot be ignored considering the effects of heterogeneous hole distribution on acoustic emission [32]. In the continuation of the study, the cavity parameter, which will be located behind the MPP structure, has been examined. By determining the hole density and diameter, the dimensions of the sample to be used in cavity exploration are as shown in Figure 5. This hole pattern is that of the sample with 7% hole density and 3 mm diameter holes.

Hole Pattern and Cavity Effect

After performing the hole pattern study in the MPP structure, tests are carried out for the voids in the created samples. MPP structures without cavity, with 18 mm gap and with 28 mm gap are compared with each other as a result of applied tests. Test data are as shown in Figure 6.

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Figure 6. Influence of Cavity size on acoustic absorption performance.

Considering the values between 630-2000 Hertz, the highest extreme absorption $S\alpha$ value is observed with 1.1015 in the sample with an 18 mm cavity. While the highest value of the sample without a cavity is 1.001, the acoustic absorption value of the sample with a 28 mm cavity is 1.035. According to the results, the sample with an 18 cm Cavity shows 9.12% better acoustic absorption performance than the sample without a cavity and 6.04% better than the sample with a 28 mm Cavity. Considering the data, it should be noted that a Cavity can reduce acoustic emission up to a certain point, but after a significant point, the increase in cavity distance causes a decrease in acoustic absorption performance. In the study of Yan et al., it was stated that as the cavity between two MPPs increases, acoustic absorption performance increases. In this current study, instead of two panels, when the distance between the designed new MPP structure and the engine wall increased, the acoustic absorption performance increases, showing the same trend as in the study of Yan et al., but the increase of this cavity reduces the noise absorption values after a point[16]. Also, based on the results, it is understood that by integrating the MPP structures with a cavity into the wheel arch liner used in the vehicles, it can significantly reduce the pass-by noise.

CONCLUSION

Today, noise emission is a problem that the automotive industry focuses on. In this study, the focus is on wheel noise, which is the biggest source of these noise emissions from cars. In the study, perforated and cavity structures were created by considering the wheel arch liner, and the acoustic emission values of these structures were examined. According to the study;

The hole pattern in the MPP structure affects the strength of the structure as well as its acoustic properties. The cross-hole pattern used in the study reduces noise better than the other smooth pattern. It has been stated that the density and diameter of the holes in the created MPP structures also affect the acoustic data. The highest acoustic absorption was observed in structures with holes of 3 mm in diameter and where these holes were located at 7% density under the conditions specified in this article. Within the scope of the study, the space behind the wheel arch liners in MPP structures was also examined. It is observed that the created space reduces the acoustic emission; It is concluded that the increase of this cavity tends to decrease in the acoustic absorption value after a certain level. This is due to an efficiency shift down. With this concept, which aims to reduce pass-by noise by integrating the MPP structure into the wheel arch liner, it is thought that a significant level of sound noise will be reduced. With the positive results of the study, it is strongly recommended to use wheel arch liners with MPP structures in the automotive industry.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

NOMENCLATURE

- *α* Sound absorption coefficient
- V Cabin volume
- *S* Sample area
- *TR* Reverberation time with the sample in the cabin
- TR_0 Reference reverberation time without the sample in the cabin
- *C* the correction coefficient of the cabin

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Research Article

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Analytical methodology for the design of load-bearing anisotropic panels for the wingbox of a light aircraft subject to geometric nonlinearity under compression

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ABSTRACT

The subject of this research is the upper load-bearing anisotropic panels of the wingbox of the forward-swept wing of a light aircraft, exposed mainly to longitudinal compression. The panels are fixed along the long sides. The paper considers how to determine the minimum thickness of these panels at a postbuckling state under loads exceeding the operational level. Based on the analytical solution for geometrically nonlinear problems obtained by the Bubnov-Galerkin method, a technique for designing anisotropic panels at a postbuckling state is proposed. To determine the panel's thickness, the strength criteria for a monolayer of the composite material were used. The main result of the work is a nonlinear equation for the panel's minimum thickness. It incorporates the equivalence of the membrane stresses due to panel buckling and the limit stresses of the composite package monolayer.

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INTRODUCTION

The use of composite materials in light aircraft reduces their structural weight. In works [1-2], it is rightly noted that the potential of composite panels in thin-walled structures prone to buckling is not fully utilized due to the lack of regulatory documents in the aerospace industry.

This paper considers the anisotropic upper panels of a forward-swept wing of low- and medium-payload-capacity aircraft, exposed mainly to compressive loads.

The panel's structural weight can be reduced by the use of rigid boundary conditions. Primarily, this is due to an increase in critical buckling stresses compared to the case of a hinged support. This is also true when designing panels for a postbuckling state using the methodology proposed in [3-4]. For this reason, in the current work, we consider problems associated with the design of rectangular anisotropic panels with the rigid boundary conditions applied along the long sides, and exposed to longitudinal compression at a postbuckling state. We also assume that the considered anisotropic panels are a part of the wingbox of the forward-swept wing, and for them, the loss of stability is acceptable under loads above the operational level.

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The purpose of this work was to develop a methodology for determining the minimum thickness of anisotropic panels in a postbuckling state exposed to the design compressive loads. This methodology is based on an analytical solution to a geometrically nonlinear problem. The methodology allows for numerical implementation and is applicable in the early design stages.

Let's consider publications devoted to the design of composite panels. The article by Ni X., Prusty G., and Hellier A. [5] provides an extensive overview of the research related to the strength, stability, and bearing capacity of anisotropic panels, published from 2000 up to 2012. We also note the work of Gavva, L., and Firsanov, V. [6] which provides an overview of analytical methods and experimental approaches to the study of the stress-strain state of structurally anisotropic aircraft panels made of composite materials. Separately, we would like to mention the monograph by Falzon B. G., Aliabadi M. H. [7] which presents the results of experimental, analytical, and numerical studies of composite panels when considering problems of stability and postbuckling state.

The work by Qiao P. et al. [8] provides analytical solutions to stability problems for composite panels under biaxial loading for almost all possible types of boundary conditions. In other works, Qiao P. [9] and Qiao P. et al. [10] considered interesting studies on the identification of damage in composite panels. We also note the publications of Aliabadi M.H. et al. [11] and Aliabadi M.H. et al. [12] which present a new method for classifying and quantifying impacts for composite plates and the structure of a monitoring system (SHM) using neural networks (BNN).

Of undoubted interest are the publications by Tsai S.W. [13] and Kappel E. [14] which proposed the use of composite panels with the stacking family $[\pm \varphi, \pm \psi]$. It is noted that the proposed stacking has advantages over traditional stacking when used in elements of aerospace composite structures.

We also note some analytical results obtained when considering geometrically nonlinear problems under shear [15–16].

From the above literature review, it follows that the design of composite panels is a complex and relevant problem, and the panel design for postbuckling remains insufficiently studied.

Returning to the objective of this work, we note that the implementation of rigid boundary conditions in analytical studies is an important task but leads to more cumbersome relations compared to the case of a hinged support.

MATERIALS AND METHODS

Basic Relations for Geometrically Nonlinear Anisotropic Panels

Below, we write down the initial relations for geometrically nonlinear anisotropic panels under compression. The condition of strain compatibility is as follows [17]:

where

 Φ is the Airy stress function Erie, L_m are the following operators:

$$\begin{split} \mathbf{L}_{1}(\Phi) &= \frac{1}{\mathbf{E}_{y}} \frac{\partial^{4} \Phi}{\partial \mathbf{x}^{4}} - \mathbf{g}_{31} \frac{\partial^{4} \Phi}{\partial \mathbf{x}^{3} \partial \mathbf{y}} + \mathbf{g}_{22} \frac{\partial^{4} \Phi}{\partial \mathbf{x}^{2} \partial \mathbf{y}^{2}} - \mathbf{g}_{13} \frac{\partial^{4} \Phi}{\partial \mathbf{y}^{3} \partial \mathbf{x}} + \frac{1}{\mathbf{E}_{x}} \frac{\partial^{4} \Phi}{\partial \mathbf{y}^{4}}, \\ g_{31} &= \frac{\eta_{y,xy} + \eta_{yy,y}}{G_{xy}}, g_{22} = \frac{1}{G_{xy}} - \frac{\mu_{xy}}{E_{y}} - \frac{\mu_{yx}}{E_{x}}, g_{13} = \frac{\eta_{x,xy} + \eta_{xy,x}}{G_{xy}}, \\ \mathbf{L}_{2}(\mathbf{W}) &= \left(\frac{\partial^{2} \mathbf{W}}{\partial \mathbf{x} \partial \mathbf{y}}\right)^{2} - \left(\frac{\partial^{2} \mathbf{W}}{\partial \mathbf{x}^{2}}\right) \left(\frac{\partial^{2} \mathbf{W}}{\partial \mathbf{y}^{2}}\right), \end{split}$$

 $L_1(\Phi) = L_2(W),$

 $E_{x^{\gamma}} E_{y^{\gamma}} G_{xy^{\gamma}} \mu_{xy}$ are the average characteristics of composite structure;

 $\eta_{x^2} x_{y}, \eta_{y,xy}, \eta_{xy,x^2}, \eta_{xy,y}$ are the anisotropic structure influence coefficients [17].

The geometrically nonlinear equilibrium equation [17] has the following form:

$$L_{3}(\Phi, W) - L_{4}(W), \qquad (2)$$

where

$$\begin{split} L_{3}(F,W) &= \frac{\partial^{2} \Phi}{\partial y^{2}} \frac{\partial^{2} W}{\partial x^{2}} + \frac{\partial^{2} \Phi}{\partial x^{2}} \frac{\partial^{2} W}{\partial y^{2}} - 2 \frac{\partial^{2} \Phi}{\partial x \partial y} \frac{\partial^{2} W}{\partial x \partial y}, \\ L_{4}(W) &= \frac{1}{\delta} \left[D_{11} \frac{\partial^{4} W}{\partial x^{4}} + 2(D_{12} + 2D_{66}) \frac{\partial^{4} W}{\partial x^{2} \partial y^{2}} + D_{y} \frac{\partial^{4} W}{\partial y^{4}} \right. \\ &+ 4 D_{16} \frac{\partial^{4} W}{\partial x^{3} \partial y} + 4 D_{26} \frac{\partial^{4} W}{\partial x \partial y^{3}} \right]; \end{split}$$

 D_{mn} (mn=11, 12, 22, 16, 26, 66) is the bending stiffnesses of a smooth anisotropic rectangular panel [17].

For the subsequent analytical solution of geometrically nonlinear problem by the Bubnov-Galerkin method, we will use the following equation:

$$\int_{0}^{a} \int_{0}^{b} \left[L_{3}(\Phi, W) - L_{4}(W) \right] W_{k} dx dy = 0,$$
(3)

where W_k is the deflection function

Methodology for Designing Anisotropic Panels for Post-Buckling State Under Strength Constraints

Let us consider a composite rectangular anisotropic panel under longitudinal compression (Figure 1). To approximate the deflection, considering the rigid support along the long sides, we use the following function:

W = f
$$\cdot \sin^2 \frac{\pi y}{b} \sin \frac{\pi (x - \alpha y)}{s}$$
, (4)

where f is the deflection amplitude, a is the tangent of wave inclination during buckling, s is the distance between nodal lines when buckling occurs.

(1)



Figure 1. A rectangular anisotropic panel under longitudinal compression.

Note that in [16], the deflection type (4) was used in the analytical analysis of the postbuckling behavior of an anisotropic composite panel under shear. Now let's use equation (4) to model the postbuckling behavior of anisotropic composite panels under compression and develop a design methodology for the postbuckling state.

After substituting the deflection (4) into the strain compatibility equation (1), we can obtain an expression whose solution will be the following stress function:

$$\Phi = f^{2} \left\{ A_{1} \cos \frac{2\pi (x - \alpha y)}{s} + A_{2} \cos \frac{2\pi y}{b} + A_{3} \cos \frac{4\pi y}{b} + A_{4} \cos \left(\frac{2\pi (x - \alpha y)}{s} - \frac{2\pi y}{b} \right) + A_{5} \cos \left(\frac{2\pi (x - \alpha y)}{s} + \frac{2\pi y}{b} \right) \right\}$$
(5)
$$- \frac{p_{x} y^{2}}{2} - \frac{p_{y} x^{2}}{2} + p_{yy} xy.$$

When considering particular solutions of the homogeneous equation with $L1(\Phi)$, we can determine the coefficients that account for anisotropic structure:

$$A_{1} = \frac{s^{2}}{32b^{2}} \frac{1}{\frac{1}{E_{y}} + \frac{\alpha}{g_{31}} + \frac{\alpha^{2}}{g_{22}} + \frac{\alpha^{3}}{g_{31}} + \frac{\alpha^{4}}{E_{x}}}, A_{2} = \frac{E_{y}}{32} \frac{b^{2}}{s^{2}}, A_{3} = -\frac{E_{y}}{512} \frac{b^{2}}{s^{2}}, A_{4} = -\frac{s^{2}}{64b^{2}} \frac{1}{\frac{1}{E} + \frac{1}{g} \frac{(\alpha b + s)}{b} + \frac{1}{g} \left[\frac{\alpha b + s}{b}\right]^{2} + \frac{1}{g} \left[\frac{\alpha b + s}{b}\right]^{3} + \frac{1}{E} \left[\frac{\alpha b + s}{b}\right]^{4}}, A_{5} = -\frac{s^{2}}{64b^{2}} \frac{1}{\frac{1}{E} + \frac{1}{g} \frac{(\alpha b - s)}{b} + \frac{1}{g} \left[\frac{\alpha b - s}{b}\right]^{2} + \frac{1}{g} \left[\frac{\alpha b - s}{b}\right]^{3} + \frac{1}{E} \left[\frac{\alpha b - s}{b}\right]^{4}}.$$

Note also that the membrane stresses on the middle surface of an anisotropic plate are determined from the definition of the Airy function F (5):

$$\sigma_{x} = \frac{\partial^{2} \Phi}{\partial y^{2}}, \quad \sigma_{y} = \frac{\partial^{2} \Phi}{\partial x^{2}}, \quad \tau_{xy} = -\frac{\partial^{2} \Phi}{\partial x \partial y},$$

and, in particular, for the considered type of the boundary conditions and deflection (1) at $px\neq 0$, $py\neq 0$, $pxy\neq 0$, we can obtain

$$\sigma_{x} = \frac{\partial^{2} \Phi}{\partial y^{2}} = -f^{2} \Delta_{11} - p_{x}, \sigma_{y} = \frac{\partial^{2} \Phi}{\partial x^{2}} = -f^{2} \Delta_{22} - p_{y},$$

$$\tau_{xy} = -\frac{\partial^{2} \Phi}{\partial x \partial y} = f^{2} \Delta_{33} - p_{xy}$$
(6)

where

$$\Delta_{11} = \pi^{2} \left\{ -A_{1} \frac{4a^{2}}{s^{2}} \cos \frac{2\pi(x - \alpha y)}{s} - A_{2} \frac{4}{b^{2}} \cos \frac{2\pi y}{b} - A_{3} \frac{16}{b^{2}} \cos \frac{4\pi y}{b} - 4A_{4} \left(\frac{\alpha}{s} + \frac{1}{b}\right)^{2} \cos \left(\frac{2\pi(x - \alpha y)}{s} - \frac{2\pi y}{b}\right)$$
(7)
$$-4A_{5} \left(\frac{\alpha}{s} - \frac{1}{b}\right)^{2} \cos \left(\frac{2\pi(x - \alpha y)}{s} + \frac{2\pi y}{b}\right) \right\}$$

$$\Delta_{22} = \pi^{2} \left\{ \left[-\frac{4A_{1}}{s^{2}} \cos \frac{2\pi(x-\alpha y)}{s} \right] + \frac{4A_{4}}{s^{2}} \cos \left(\frac{2\pi(x-\alpha y)}{s} - \frac{2\pi y}{b} \right) + \frac{4A_{5}}{s^{2}} \cos \left(\frac{2\pi(x-\alpha y)}{s} - \frac{2\pi y}{b} \right) \right\}$$
(8)

$$\Delta_{33} = \pi^2 \left\{ \left[-\frac{4A_i\alpha}{s^2} \cos \frac{2\pi(x-\alpha y)}{s} \right] + \frac{4A_i}{sb} \cos \left(\frac{2\pi(x-\alpha y)}{s} - \frac{2\pi y}{b} \right) + \frac{4A_i}{sb} \cos \left(\frac{2\pi(x-\alpha y)}{s} - \frac{2\pi y}{b} \right) \right\} \cdot$$
(9)

After substituting expressions (1) and (5) into equation (4) and some cumbersome transformations, one can obtain the following non-linear relationship for the deflection amplitude ($f \neq 0$):

$$\frac{\pi^{4}}{16\delta} \left\{ D_{11} \frac{3b}{s^{3}} + 2\left(D_{12} + 2D_{66}\right) \frac{3\alpha^{2}b^{2} + 4s^{2}}{s^{3}b} + \frac{D_{22}}{s^{3}b^{3}} \left(24s^{2}b^{2}\alpha^{2} + 16s^{4} + 3b^{4}\alpha^{4}\right) - \frac{3b\alpha D_{16}}{s^{3}} - \frac{3\alpha D_{26}}{bs^{3}} \left(4s^{2} + \alpha^{2}b^{2}\right) \right\} \frac{\pi^{4}f^{2}}{4sb} \left[2A_{1} + 2A_{2} + 2A_{3} + A_{4} + A_{5}\right] =$$
(10)
$$\frac{3\pi^{2}b}{16s} \left(p_{s} + \frac{p_{y}\left(3\alpha^{2}b^{2} + 4s^{2}\right)}{3b^{2}} + \alpha p_{yy}\right)$$

or, in a more compact form, we have

$$\overline{D}_{\alpha\beta}\delta^{3} + f^{2}B_{\alpha\beta}\delta = \left(q_{x} + \frac{q_{y}\left(3\alpha^{2}b^{2} + 4s^{2}\right)}{3b^{2}} + \alpha q_{yy}\right), \quad (11)$$

where $\overline{D}_{mn} = D_{mn} / \delta^3$ (m.n=11, 12, 22, 16, 26, 66); $q_x = p_x \delta$, $q_y = p_y \delta$, $q_{xy} = p_{xy} \delta$ are the loads acting on the panel in the general case,

$$\overline{D}_{\alpha\beta} = \overline{D}_{11} \left(\frac{\pi}{s}\right)^2 + \frac{2\pi^2 \left(\overline{D}_{12} + 2\overline{D}_{33}\right)}{3} \left(\frac{4}{b^2} + \frac{3\alpha^2}{s^2}\right) + \overline{D}_{22}\pi^2 \left\{\frac{24s^2b^2\alpha^2 + 16s^4 + 3b^4\alpha^4}{3b^4s^2}\right\} - \overline{D}_{16}\frac{\alpha\pi^2}{s^2} - \overline{D}_{26}\frac{\alpha\pi^2}{s^2b^2} \left[4s^2 + \alpha^2b^2\right], \\ B_{\alpha\beta} = \frac{4\pi^2}{3b^2} \left[2A_1 + 2A_2 + 2A_3 + A_4 + A_5\right]$$

Considering the longitudinal compression case $(p_x \neq 0, p_y=0, p_{xy}=0)$ and introducing the designation $\gamma = (b/s)^2$, in the case of small deflections at f $\rightarrow 0$ (from equation (11)), we can use the system of equations

$$\frac{\partial \mathbf{q}_x}{\partial \gamma} = 0, \frac{\partial \mathbf{q}_x}{\partial \alpha} = 0, \tag{12}$$

to determine the critical parameters of wave formation and obtain the following expressions:

$$\overline{D}_{11} + 2\left(\overline{D}_{12} + 2\overline{D}_{66}\right)\alpha^2 + \frac{\overline{D}_{22}}{3}\left(\frac{16}{\gamma^2} + 3\alpha^4\right) - \alpha\overline{D}_{16} - \overline{D}_{26}\alpha^3 = 0, \quad (13)$$

$$4\left(\overline{D}_{12}+2\overline{D}_{66}\right)\alpha\gamma+\overline{D}_{22}\left(16\alpha+4\alpha^{3}\gamma\right)-\overline{D}_{26}\gamma-\overline{D}_{26}\left(4+3\gamma\alpha^{2}\right)=0, \quad (14)$$

Note that the obtained expressions (13) and (14) can be reduced to a numerical solution for the critical values of parameters γ and α at buckling. The parameters γ and α do not depend on the panel thickness but are determined by the anisotropic panel structure.

Thus, to design load-bearing anisotropic panels with minimum thicknesses for the given flow qx, panel dimensions, and stacking, the following methodology can be used. First, using equations (13) and (14), numerically determine the critical parameters of wave formation. Second, calculate the ultimate stresses $\overline{\sigma}_x$ of the anisotropic structure. Third, using the limiting normal stress condition $\sigma_x = \overline{\sigma}_x$, solve equations (6) and (7) for the deflection amplitude *f*. Fourth, determine the potentially critical points of function $\Delta_{mm}(x, y)$, at which stresses can reach their absolute maximum values.

Now, we will present in more detail the procedure for calculating the ultimate strength stresses for the case of an anisotropic structure. We use the strength criteria for a monolayer of a composite package in the following form:

$$\left(\frac{\sigma_{1}^{(i)}}{\sigma_{1}^{(i)}}\right)^{2} - \frac{\sigma_{1}^{(i)}\sigma_{2}^{(i)}}{\left(\frac{-\sigma_{1}^{(i)}-\sigma_{1}^{(i)}}{\sigma_{1}^{(i)}\sigma_{2}^{(i)}}\right)} + \left(\frac{\sigma_{2}^{(i)}}{\sigma_{2}^{(i)}}\right)^{2} + \left(\frac{\tau_{12}^{(i)}}{\tau_{12}^{(i)}}\right)^{2} \le 1,$$
(15)

In the general case, the equations for estimating the stresses in the *i*-layer [18-19] are as follows:

$$\sigma_{1}^{(i)} = \sigma_{x}a_{x}^{(i)} + \sigma_{y}a_{y}^{(i)} + \tau_{xy}a_{xy}^{(i)},$$

$$\sigma_{2}^{(i)} = \sigma_{x}b_{x}^{(i)} + \sigma_{y}b_{y}^{(i)} + \tau_{xy}b_{xy}^{(i)},$$

$$\tau_{12}^{(i)} = \sigma_{x}c_{x}^{(i)} + \sigma_{y}c_{y}^{(i)} + \tau_{xy}c_{xy}^{(i)},$$
(16)

Taking into account that the longitudinal compressive stresses act on the panel $\sigma_x = q_x/\delta$, we have

$$\begin{split} a_{x}^{(i)} &= \frac{1}{E_{x}} \Bigg[\left(A_{11}^{i} \cos^{2} \phi_{i} + A_{21}^{i} \sin^{2} \phi_{i} + A_{31}^{i} \sin 2\phi_{i} \right) \\ &- \mu_{3x} \left(A_{12}^{i} \cos^{2} \phi_{i} + A_{22}^{i} \sin^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \frac{\eta_{3y,x}}{G_{xy}} \left[A_{13}^{i} \cos^{2} \phi_{i} + A_{21}^{i} \sin^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right] \\ a_{y}^{(i)} &= \frac{1}{E_{y}} \Bigg[-\mu_{xy} \left(A_{11}^{i} \cos^{2} \phi_{i} + A_{21}^{i} \sin^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) + \\ &+ \left(A_{12}^{i} \sin^{2} \phi_{i} + A_{22}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) + \\ &+ \left(A_{12}^{i} \sin^{2} \phi_{i} + A_{22}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) + \\ &+ \frac{\eta_{xy,y}}{G_{xy}} \left(A_{11}^{i} \cos^{2} \phi_{i} + A_{21}^{i} \sin^{2} \phi_{i} + A_{31}^{i} \sin 2\phi_{i} \right) \\ &+ \frac{\eta_{xy,y}}{G_{xy}} \left(A_{11}^{i} \cos^{2} \phi_{i} + A_{21}^{i} \sin^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \cos^{2} \phi_{i} + A_{22}^{i} \sin^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \cos^{2} \phi_{i} + A_{22}^{i} \sin^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \cos^{2} \phi_{i} + A_{21}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \sin^{2} \phi_{i} + A_{21}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \sin^{2} \phi_{i} + A_{22}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \sin^{2} \phi_{i} + A_{22}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \sin^{2} \phi_{i} + A_{23}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \sin^{2} \phi_{i} + A_{23}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \sin^{2} \phi_{i} + A_{22}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \sin^{2} \phi_{i} + A_{22}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{12}^{i} \sin^{2} \phi_{i} + A_{22}^{i} \cos^{2} \phi_{i} + A_{33}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{2y}^{i} \sin^{2} \phi_{i} + A_{2y}^{i} \cos^{2} \phi_{i} + A_{2y}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{2y}^{i} \sin^{2} \phi_{i} + A_{2y}^{i} \cos^{2} \phi_{i} + A_{2y}^{i} \sin^{2} \phi_{i} + A_{3y}^{i} \sin 2\phi_{i} \right) \\ &+ \left(A_{2y}^{i} \sin^{2} \phi_{i} + A_{2y}^{i} \cos^{2} \phi_{i} + A_{2y}^{i} \sin^{2} \phi_{i} + A_{3y}^{i} \sin^{2} \phi_{i} \right) \\ &+ \left(A_{2y}^{i} \sin^{2} \phi_{i} + A_{2y}^{i} \cos^{2} \phi_{i} + A_{2y}^{i} \sin^{2}$$

+ $\left(A_{13}^{i}\sin^{2}\varphi_{i}+A_{23}^{i}\cos^{2}\varphi_{i}+A_{33}^{i}\sin 2\varphi_{i}\right)$];

$$\begin{split} c_{x}^{(0)} &= \frac{1}{E_{y}} \left[\left(A_{x}^{'} - A_{u}^{'} \right) \frac{\sin 2\phi_{y}}{2} - \mu_{\mu} \left(A_{x}^{'} - A_{u}^{'} \right) \frac{\sin 2\phi_{y}}{2} + \frac{\eta_{w,x}}{G_{w}} A_{u}^{'} \cos 2\phi_{y} \right]; \\ c_{y}^{(0)} &= \frac{1}{E_{y}} \left[-\mu_{\mu} \left(A_{x}^{'} - A_{u}^{'} \right) \frac{\sin 2\phi_{y}}{2} + \left(A_{x}^{'} - A_{u}^{'} \right) \frac{\sin 2\phi_{y}}{2} + \frac{\eta_{w,x}}{G_{w}} A_{u}^{'} \cos 2\phi_{y} \right]; \\ c_{w}^{(0)} &= \frac{1}{G_{w}} \left[\eta_{w,w} \left(A_{x}^{'} - A_{u}^{'} \right) \frac{\sin 2\phi_{y}}{2} + \eta_{y,w} \left(A_{x}^{'} - A_{u}^{'} \right) \frac{\sin 2\phi_{y}}{2} + A_{u}^{'} \cos 2\phi_{y} \right]; \\ A_{11}^{(0)} &= \overline{E}_{1}^{(0)} \cos^{4}\phi_{y} + \overline{E}_{2}^{(0)} \sin^{4}\phi_{y} + 2(\overline{E}_{1}^{(0)}\mu_{12}^{(0)} + 2G_{12}^{(0)}) \sin^{2}\phi_{y} \cos^{2}\phi_{y}, \\ A_{12}^{(0)} &= \overline{E}_{1}^{(0)} \mu_{12}^{(0)} + [\overline{E}_{1}^{(0)} + \overline{E}_{2}^{(0)} - 2(\overline{E}_{1}^{(0)}\mu_{12}^{(0)} + 2G_{12}^{(0)}) \sin^{2}\phi_{y} \cos^{2}\phi_{y}, \\ A_{22}^{(0)} &= \overline{E}_{1}^{(0)} \sin^{4}\phi_{y} + \overline{E}_{2}^{(0)} \cos^{4}\phi_{y} + 2(\overline{E}_{1}^{(0)}\mu_{12}^{(0)} + 2G_{12}^{(0)}) \sin^{2}\phi_{y} \cos^{2}\phi_{y}, \\ A_{33}^{(0)} &= [\overline{E}_{1}^{(0)} + \overline{E}_{2}^{(0)} - 2\overline{E}_{1}^{(0)}\mu_{12}^{(0)}] \sin^{2}\phi_{y} \cos^{2}\phi_{y} + G_{12}^{(0)} \cos^{2}\phi_{y}, \\ A_{30}^{(0)} &= A_{31}^{(0)} &= \left[\left(\overline{E}_{1}^{(0)} \cos^{2}\phi_{y} - \overline{E}_{2}^{(0)} \sin^{2}\phi_{y} \right) - \left(\overline{E}_{1}^{(0)}\mu_{12}^{(0)} + 2G_{12}^{(0)} \right) \cos 2\phi_{y} \right] \sin\phi_{y} \cos\phi_{y}, \\ A_{23}^{(0)} &= A_{31}^{(0)} &= \left[\left(\overline{E}_{1}^{(0)} \sin^{2}\phi_{y} - \overline{E}_{2}^{(0)} \sin^{2}\phi_{y} \right) - \left(\overline{E}_{1}^{(0)}\mu_{12}^{(0)} + 2G_{12}^{(0)} \right) \cos\phi_{y} \right] \sin\phi_{y} \cos\phi_{y}, \end{split}$$

Let us carry out some transformations. First, we express the deflection amplitude f2 from the nonlinear equation (11) and substitute it into the equations for the total stresses (6), which we then substitute into the expressions for the stresses in the monolayer (16). Next, we substitute the result of the previous action into criterion (15) and obtain the following equation for the panel thickness:

$$\begin{split} & \left(\overline{\sigma}_{z}^{(i)}\overline{\tau}_{1z}^{(i)}\right)^{2} \left[\frac{\left(-\Delta_{11}a_{x}^{(i)} - \Delta_{22}a_{y}^{(i)} - \Delta_{33}a_{w}^{(i)}\right)}{B_{qq}} \left(\frac{\pi^{2}}{s^{2}}q_{z} - D_{qq}\delta^{3}\right) + q_{z}a_{z}^{(i)}\right]^{2} + \\ & +\overline{\sigma}_{1}^{(i)}\overline{\sigma}_{2}^{(i)} \left(\overline{\tau}_{12}^{(i)}\right)^{2} \left[\frac{\left(-\Delta_{11}a_{z}^{(i)} - \Delta_{22}a_{y}^{(i)} - \Delta_{33}a_{w}^{(i)}\right)}{B_{qq}}q_{z}b_{z}^{(i)}\right] + \left(\frac{\pi^{2}}{s^{2}}q_{z} - D_{qq}\delta^{3}\right) + q_{z}a_{z}^{(i)}\right] \times \\ & + \left(\overline{\sigma}_{1}^{(i)}\overline{\tau}_{2}^{(i)}\right)^{2} \left[\frac{\left(-\Delta_{11}b_{z}^{(i)} - \Delta_{22}b_{y}^{(i)} - \Delta_{33}b_{w}^{(i)}\right)}{B_{qq}} \left(\frac{\pi^{2}}{s^{2}}q_{z} - D_{qq}\delta^{3}\right) + q_{z}b_{z}^{(i)}\right]^{2} + \\ & + \left(\overline{\sigma}_{1}^{(i)}\overline{\sigma}_{2}^{(i)}\right)^{2} \left[\frac{\left(-\Delta_{11}b_{z}^{(i)} - \Delta_{22}b_{y}^{(i)} - \Delta_{33}b_{w}^{(i)}\right)}{B_{qq}} \left(\frac{\pi^{2}}{s^{2}}q_{z} - D_{qq}\delta^{3}\right) + q_{z}b_{z}^{(i)}\right]^{2} = \left[\delta\overline{\sigma}_{1}^{(i)}\overline{\sigma}_{2}^{(i)}\overline{\tau}_{12}^{(i)}\right]^{2}. \end{split}$$

In practice, for aircraft anisotropic composite panels, the stacking of monolayers with the reinforcement of $0^{\circ}/+45^{\circ}/90^{\circ}$ is used. In this case, the optimal design technique is reduced to considering three equations of the type (17) for the specified reinforcement angles. The differences between these equations will be due to coefficients $a_x^{(i)}$, $b_x^{(i)}$ and $c_x^{(i)}$. As a result, the maximum value should be chosen from the three resulting values of the total thicknesses. The critical parameters of wave formation during buckling are generally determined numerically using relations (13)-(14)

We also note that the final equation (17) includes the $\Delta_{mm}(x, y)$ terms, whose values determine the maximum stresses in the monolayers. For the considered deflection W(x, y) (4) and the stress function $\Delta_{mm}(x, y)$ (5), the maximum values in the general case should be determined numerically. Taking into account the structure of the stress function $\Delta_{mm}(x, y)$ to first approximation, to determine the potentially critical points, we can take

$$\cos 2\pi y/b \to 1, \cos 2\pi (x - \alpha y)/s \to 1.$$
(18)

Let us consider an example of the application of the above methodology to designing anisotropic panels for a postbuckling state and exposed to longitudinal compression. Note that the resulting expression (17) corresponds to the general case of combined loading when using Tsai's strength criterion. Further, as an example, we will consider anisotropic panels with 0°/+45° reinforcement under loading mainly by longitudinal compressive and shear flows using other strength criteria.

In the early stages of designing aircraft panels under static strength conditions, for a monolayer, the 1st strength theory $\sigma_1^{(i)} = \overline{\sigma}_1^{(i)}$ is typically used. Therefore, we use expression (17) for determining the thickness and the corresponding coefficients in the form

$$\left[\frac{\left(-\Delta_{11}a_x^{(i)} - \Delta_{22}a_y^{(i)} - \Delta_{33}a_{3y}^{(i)}\right)}{B_{a\beta}}\left(\frac{\pi^2}{s^2}q_x - D_{a\beta}\delta^3\right) + q_x a_x^{(i)}\right] = \left[\delta\overline{\sigma}_1^{(i)}\right], \quad (19)$$

where

$$\begin{split} a_x^{(0)} &= \overline{E}_1^{(0)} \frac{1}{E_x} (1 - \mu_{12}^{(0)} \mu_{xy}), a_y^{(0)} = \overline{E}_1^{(0)} \frac{1}{E_y} (\mu_{12}^{(0)} - \mu_{yx}), \\ a_{xy}^{(0)} &= \frac{\overline{E}_1^{(0)}}{G_{xy}} \Big[\eta_{x,xy} + \eta_{y,xy} \mu_{12}^{(0)} \Big] \\ a_x^{(45)} &= \overline{E}_1^{(45)} \left[\frac{1}{2E_x} (1 - \mu_{yx}) (1 + \mu_{12}^{(45)}) + \frac{\eta_{xy,x} (1 - \mu_{12}^{(45)})}{2G_{xy}} \right] \\ a_y^{(45)} &= \overline{E}_1^{(45)} \left[\frac{1}{2E_y} (1 - \mu_{xy}) (1 + \mu_{12}^{(45)}) + \frac{\eta_{xy,y} (1 - \mu_{12}^{(45)})}{2G_{xy}} \right] \\ a_{xy}^{(45)} &= \overline{E}_1^{(45)} \left[\frac{1}{2E_y} (1 - \mu_{xy}) (1 + \mu_{12}^{(45)}) + \frac{\eta_{xy,y} (1 - \mu_{12}^{(45)})}{2G_{xy}} \right] \\ a_{xy}^{(45)} &= \frac{\overline{E}_1^{(45)}}{G_{xy}} \left[\frac{\eta_{x,xy} (1 + \mu_{12}^{(45)})}{2} + \frac{\eta_{y,xy} (1 + \mu_{12}^{(45)})}{2} + \frac{(1 - \mu_{12}^{(45)})}{2} \right] \end{split}$$

Thus, it is necessary to solve equations (18) for δ (0) and δ (+45), and choose the maximum value of the thickness. Note that under uniaxial compression, the most likely cause of failure is the achievement of ultimate stresses in the layer with longitudinal reinforcement.

RESULTS AND DISCUSSION

In the general case, it is possible to determine the thickness of an isotropic panel of a given width, exposed to a given linear load (to a flow q=P/b, where b is the width of the panel), for the conditions of strength and stability and ensuring strength at a postbuckling state. That is, in the simplest case, when using the strength criterion, we have: $\delta = q/\overline{\sigma}$, where $\overline{\sigma}$ are the failure stresses. To design a panel for stability and the desired thickness, one can use the dependence $\delta^3 = qb^2/(kE)$, where k is the boundary condition factor and E is the modulus of elasticity of the material. In the most complex case of a panel designed for strength



Figure 2. Orthotropic panel thickness as a function of compressive loads.

at postbuckling, we generally use more complex nonlinear relationships.

In this work, analytical relationships are obtained that allow one to determine the minimum thicknesses of anisotropic panels, considering geometric nonlinearity. The paper proposes a methodology that uses the postbuckling design procedure [3-4] for the design of load-bearing panels.

To illustrate this design methodology, let us consider Figure 2. Figure 2 shows an orthotropic panel thickness as a function of compressive loads, defined under the stability condition (curve No. 2), and under the strength condition at a postbuckling state (curve No. 1). The analysis takes into account the limit stresses. The panel dimensions are $a \times b$ = 400 × 120 mm. To calculate the orthotropic carbon fiber panel, the following properties were used: E1=125 GPa, E2=9 GPa, G12=5 GPa, $\bar{\sigma}_1$ =1.4 GPa, µ21=0.28, compressive loads vary within qx=0...2000 GPa·m, laminate lay-up: \bar{h}_0 = 0.3, $\bar{h}_{\pm 45}$ = 0.7, $\bar{\sigma}_{\bar{x}}$ = 0.529 GPa.

We also note that the formally obtained expression (17) is identical to the equation obtained in [18, 19] for the case of panels with a hinged support. In the current paper, we consider a panel exposed to more stringent boundary conditions (the differences are in more complex coefficients $D_{\alpha\beta}$ and $B_{\alpha\beta}$) and having an anisotropic structure (hence the coefficients of anisotropic structure influence $\eta_{x,xy}$, $\eta_{y,xy}$, $\eta_{xy,xy}$, $\eta_{xy,yy}$). Note that the obtained analytical relationships can be used to design and analyze load-bearing panels with an anisotropic structure.

In addition, the panel thicknesses determined by the proposed methodology will have a minimum strength safety margin at η =1 with geometrically nonlinear behavior. The equality η =1 means that the absolute maximum stresses are equal to the limit stresses at potentially critical points, which are determined from equations (18).

CONCLUSION

Based on an analytical solution to a geometrically nonlinear problem for panels with anisotropic structure and rigid support along the long sides, this paper proposes a methodology for determining the optimal thicknesses obtained from the condition of reaching the maximum static strength at a postbuckling state of the panel. This methodology is part of the scientific and technical research related to the design of a perspective light aircraft.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Synergistic integration of ram methodology for augmenting reliability and efficiency in solar irrigation systems: a comprehensive study for sustainable rural farming

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ABSTRACT

In rural areas around the world, agriculture is a vital source of livelihood and sustenance. However, limited access to electricity and water resources often hampers agricultural productivity, leaving farmers dependent on rainfall or manual labor-intensive irrigation methods. To address this challenge, solar irrigation systems have emerged as a sustainable and efficient solution. However, the existing solar irrigation systems often suffer from reliability issues and suboptimal performance, leading to inefficient water usage, increased maintenance costs, and reduced overall agricultural output. Addressing the reliability and performance optimization challenges of solar irrigation systems for rural farming is essential to ensure sustainable agriculture, increased crop yield, and improved livelihoods for farmers. This study aimed to enhance the performance of solar irrigation systems using reliability, maintainability, availability, and metrics like MTBF and MTTF. The system consists of four subsystems 1, 2, 3, and 4 namely, PV panel, controller, submersible pump, and storage tank sequentially arranged. Subsystem 1 consists of ten (10) units of panels arranged in parallel and connected to subsystem 2 which consists of two (2) unit controllers arranged in parallel, whereas subsystem 3 consists of two (2) units of pumps arranged in parallel and lastly, subsystem 4 comprises of four (4) units of storage tanks arranged in parallel, However, all the four subsystems combined are arranged in series-parallel. For design and prediction, the Markovian birth-death method is employed to assemble the system governing the differential difference equation from the state-to-state transition diagram. The rates of repair and failure of each subsystem are assumed to be exponentiated Weibull distributions and statistically independent. The findings of this research are thought to be valuable for analyzing performance and determining the best solar irrigation system design and feasible preventive and corrective maintenance strategies that may be used in the future to improve system performance, strength, effectiveness, food production output as well and revenue mobilization.

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INTRODUCTION

A solar irrigation system is a technology that harnesses solar energy to power irrigation processes in agriculture. It provides an eco-friendly and sustainable solution for watering crops and plants using the abundant energy from the sun. The system typically consists of four main components: solar panels, a controller, a submersible pump, and a water distribution system. The solar panels are responsible for capturing sunlight and converting it into electrical energy. This energy is then used to power the pump, which draws water from a water source, such as a well, river, or pond. Solar irrigation systems offer several advantages over traditional irrigation methods. Benefits of solar irrigation systems include renewable and sustainability, reduction in operational cost, increased independence, scalability, environmental benefits, etc. Solar irrigation systems have emerged as a sustainable and efficient solution for agricultural water management. These systems harness the power of solar energy to drive pumps and provide water for irrigation, reducing dependency on conventional energy sources and minimizing environmental impact. To ensure the successful and long-term operation of solar irrigation systems, the principles of reliability, availability, and maintainability play a crucial role. It is worth noting that the efficiency and performance of a solar irrigation system depend on factors such as the available sunlight, the size of the solar array, the water demand, and the irrigation technique used. Proper system design, sizing, and maintenance are crucial to ensure optimal performance and water conservation.

In recent times, a wide range of agricultural technologies have emerged, offering valuable solutions to enhance crop production while minimizing costs and energy consumption. Among these technologies, the crucial aspect of water pumping for irrigation plays a significant role in any crop cultivation method. Traditionally, farmers have relied on either fossil fuel-based systems or grid power to operate their pumps.

Reliability models play a crucial role in enhancing the performance of solar irrigation systems by ensuring their dependability and availability. Reliability, Availability, Maintainability, and Durability (RAMD) are key aspects that need to be considered when designing and operating such systems. RAMD or reliability, availability, and maintainability is a framework used to evaluate the performance of a system. In the case of a solar water irrigation system for rural consumption, RAMD can be used to assess the system's ability to reliably and efficiently provide water for irrigation purposes in rural areas. It is a framework that can be used to evaluate the performance of a solar water irrigation system for rural consumption by assessing its reliability, availability, maintainability, and durability. By using this framework, it is possible to identify any areas of weakness in the system and develop strategies for improving its performance and efficiency. In the context of solar irrigation, reliability encompasses the durability and robustness of various components, such as solar panels, batteries, inverters, pumps, and control systems. A reliable system should be designed, constructed, and maintained in a manner that minimizes the risk of breakdowns, malfunctions, and performance degradation. In the case of solar irrigation, availability relates to the system's capacity to supply water on demand, especially during peak irrigation periods. Factors that affect availability include system design, sizing of components, battery storage capacity, and overall system efficiency. Ensuring high availability involves proper planning, installation, and monitoring of the system to minimize downtime and maximize water supply. Maintainability refers to the ease and effectiveness of conducting maintenance activities on the solar irrigation system. It involves preventive and corrective measures aimed at preserving the system's performance, preventing failures, and extending its operational life. Key aspects of maintainability include regular inspections, cleaning, and maintenance of solar panels, battery maintenance, pump maintenance, and monitoring of system performance. Well-documented maintenance procedures and access to spare parts are essential for efficient and cost-effective system upkeep. The integration of reliability, availability, and maintainability principles in solar irrigation systems is crucial for the sustainable and successful implementation of these systems. A reliable system minimizes the risk of interruptions and breakdowns, ensuring uninterrupted water supply for irrigation. High availability guarantees that the system can meet the demands of agricultural activities, contributing to improved crop yields and water resource management. Effective maintainability practices reduce the costs associated with repairs, optimize system performance, and extend the system's lifespan.

In many rural areas, agriculture heavily relies on irrigation to ensure sufficient crop growth and productivity. However, the existing solar irrigation systems often suffer from reliability issues and suboptimal performance, leading to inefficient water usage, increased maintenance costs, and reduced overall agricultural output. The primary problem is that the current solar irrigation systems deployed in rural farming areas lack the necessary reliability to function consistently and efficiently. Factors such as inadequate system design, substandard components, and improper installation contribute to frequent breakdowns, system failures, and reduced lifespan. These issues result in significant downtime, hampering farmers' ability to irrigate their crops on a regular and reliable basis, leading to reduced yields and financial losses. Moreover, the performance optimization of solar irrigation systems is also a pressing concern. Many existing systems are not designed to maximize water usage efficiency, leading to excessive water wastage and increased energy consumption. Additionally, the suboptimal sizing and configuration of solar panels, batteries, and pumps result in insufficient power generation and storage capacities, hindering the system's ability to meet the irrigation demands of the farms effectively. Addressing the reliability and performance optimization challenges of solar irrigation

systems for rural farming is essential to ensure sustainable agriculture, increased crop yield, and improved livelihoods for farmers. A comprehensive approach that encompasses system design improvements, the use of high-quality components, efficient installation and maintenance practices, and intelligent control mechanisms is required to enhance the reliability, performance, and overall effectiveness of solar irrigation systems in rural areas. More sophisticated solar irrigation models with multiple panels and storage tanks should be developed to assist in reducing the risk of a complete breakdown, and operating costs, prolonging the overall reliability, availability, and mean time to failure as well as generating revenue (profit) as well as increase in food production. The reliability and performance optimization of solar irrigation systems for rural farming is a crucial challenge that needs to be addressed.

The paper is organized as follows: Section 2 provides a comprehensive literature review of existing studies, Section 3 describes the system under study, Section 4 discusses the materials and methods employed, Section 5 focuses on the formulation of the RAM models, Section 6 presents the results of numerical simulations and the subsequent discussion of outcomes, and finally, Section 7 concludes the paper, summarizing the main findings and potential avenues for future research.

LITERATURE REVIEW

RAMD is a logistical technique for assessing the strength, effectiveness, and performance of equipment at various levels. It ensures system safety and operation problems and identifies which of the system's units, components, or subsystems require adequate maintenance. RAMD (reliability, availability, maintainability, and dependability) management is critical to a company's success. These four measures of system strength, effectiveness, and performance can be used to forecast system speed, product quality, and volume production output.

Researchers have used a variety of approaches to assess RAMD measures in the literature. To cite a few, [1] investigated the efficiency of the forming industry by assessing system sensitivity analysis. [2] developed Markov models for RAM performance estimation of the circulation system of water. [3] discuss the RAM evaluation of Load Haul Dumpers. [4] were able to compute the RAMD parameters for each component of the system. These parameters provide valuable insights into the criticality and performance of the system's components, aiding in decision-making and optimization efforts. The approach outlined by [5] suggests that the reliability, availability, and maintainability (RAM) of a cement plant can be enhanced by conducting a RAM analysis of its subsystems. This analysis involves utilizing data on the time between failures (TBF) and time to repair (TTR) for all critical subsystems within the plant. [6] discussed the effectiveness of a reciprocating compressor system package installed and used in the oil and gas industries

by examining the behavior of each part and component of the reciprocating compressor, which can aid in pinpointing the influence of RAM on the efficiency of the system. [7] used the Markov birth-death process to evaluate the reliability, mean time between failures, and mean time to failure of a series-parallel system. [8] present a methodology for analyzing an industrial system's system performance using uncertain data. The associated membership functions are generated using fuzzy set theory by solving a nonlinear optimization problem with particle swarm optimization. [9] tackled the intricate dynamics of the A-pan crystallization system in a sugar plant by ingeniously integrating mathematical models with a fuzzy reliability approach and Markov birth-death model differential equations. The researchers masterfully derived these complex equations, and to efficiently solve them, they employed the highly accurate Runge-Kutta method of fourth order. [10] embarked on a significant endeavor, addressing the critical aspects of reliability, availability, maintainability, and dependability (RAMD) within the physical processing unit of a sewage treatment plant. To achieve this, the study employed Markovian birth-death processes and derived the essential Chapman-Kolmogorov differential equations, which form the foundation of their analysis. Through this sophisticated mathematical framework, the study was able to ascertain crucial performance measures, including the mean time between failures, mean time to repair, and dependability ratio. [11] undertook a pioneering study aimed at exploring the intricate web of reliability measures within the generator utilized in Sewage Treatment Plants (STP), employing a comprehensive RAMD (Reliability, Availability, Maintainability, and Dependability) approach at the component level. To achieve their objective, the team ingeniously formulated mathematical models based on the Markovian birth-death process, carefully developing models for all subsystems of the generator. [12] Estimate the coliform values of the Tekkekoy deep sea discharge system, which is chosen as an application area, by using a radial-based artificial neural network structure, [13] writes on production-distribution network system for a company, which is active in producing bottled natural spring water was established. [10] made significant strides towards optimizing the operational performance of a soft water treatment and supply plant (SWTS-Plant) by developing comprehensive models for reliability, availability, and maintainability (RAM) measures. Through an illustrative case study centered around the SWTS plant situated in the high-rise society ABC, Jaipur, the researchers meticulously conducted a RAM analysis. This analysis entailed a detailed descriptive examination of the time to failure and repair, accompanied by trend analysis and a rigorous goodness-offit test. [14] Defined a Secure Simple Epidemic Algorithm (SSEA) for PSN where a security condition controls the traffic. [15] Classification algorithms were used to classify electromyography and depth sensor data, [16] Optimum

CW size is defined through meta-heuristic optimization algorithms.

[17] conducted a meticulous analysis of the evaporation system within a sugar plant, focusing on the application of reliability, availability, maintainability, and dependability measures. The researchers aimed to identify the most sensitive subsystems in the evaporation process, a critical aspect for optimizing overall performance. To achieve this, they skillfully constructed transition diagrams for all subsystems and expertly derived corresponding Chapman-Kolmogorov differential equations, utilizing the powerful Markov birth-death process. [18] tackled the intricate analysis of a microprocessor system, exploring its reliability, availability, maintainability, and dependability aspects. This microprocessor system was thoughtfully designed with seven essential subsystems, encompassing input, terminal, processor, main memory disk, addressing modes, disk controller, and disk drives. The researchers conducted a rigorous examination of each subsystem's performance in terms of reliability, availability, maintainability, and dependability, aiming to identify potential areas for optimization and enhancement. To facilitate this analysis, the team skillfully crafted state transition diagrams for all subsystems and adeptly derived governing equations using the powerful Markov birthdeath process. [19] Focuses on studying the reliability and maintainability of a sugar manufacturing plant by collecting data over six months. The researchers conducted a thorough descriptive statistical analysis on the time to repair and time between failures data. By determining the best-fitted distribution and its parameters, as well as conducting trend and serial correlation analysis, the study aimed to optimize the plant's performance and ensure its efficient operation. [20] Sought to evaluate the reliability, availability, and maintainability of a hot standby database system by examining its failure data. The researchers assessed these aspects using fundamental probability principles and estimated the parameters of established probability distributions. Comprehensive statistical analysis, including trend and serial correlation assessment, was conducted to analyze the reliability and maintainability of both the primary unit and the hot standby unit within the system. [21] Presented a comprehensive framework aimed at evaluating reliability, availability, and maintainability, while also optimizing maintenance practices, to enhance the conveying process of vehicle bodies in an automotive assembly line. The findings from the reliability, availability, and maintainability analysis revealed that the main bottlenecks within the process were associated with the forklift and loading equipment's reliability and maintainability. [22] Conducted a comprehensive study, utilizing data sets from a wine packaging line's production system, with the primary objective of presenting a thorough analysis of reliability, availability, and maintainability (RAM) to provide valuable insights and results for the overall system performance. [23] Successfully devised and applied reliability, availability, and maintainability (RAM) indices to evaluate and enhance the performance of an automated croissant production line under actual operating conditions. Through this comprehensive study, the authors convincingly demonstrate the immense utility of RAM analysis in making informed decisions regarding maintenance intervals and devising an optimal maintenance strategy, ensuring smooth and efficient operations in the production line.

Various studies have been conducted to assess the reliability of agriculture and irrigation machinery. These studies typically involve collecting data on the performance and failure rates of different types of agricultural and irrigation machinery under various operating conditions. The data is then analyzed to determine reliability metrics such as mean time between failures (MTBF), mean time to repair (MTTR), and availability, [24] developed availability models for different types of solar pumps and examined their economic feasibility. Their research indicated that the cost of operating a diesel pump set for irrigation purposes was found to be higher than that of the various types of solar pumps analyzed, [25] conducted an analysis of the socio-economic and climatic implications arising from the implementation of photovoltaic-operated high-efficiency irrigation systems, [19] embarked on a comprehensive RAMD (Reliability, Availability, Maintainability, and Dependability) study focused on the Tube-wells Integrated with Underground Pipelines (TIUP) for irrigation systems. Their research endeavors were centered around conducting an in-depth RAMD analysis, coupled with the integration of Failure Modes and Effects Analysis (FMEA), all unified through the development of an innovative stochastic model utilizing the powerful Markovian approach. The ultimate goal was to accurately estimate the Steady-State Availability (SSA) of the TIUP, ensuring a thorough understanding of its performance under various conditions. [26] Introduce modified Bernstein-type operators based on two real parameters and study their various approximation properties, [27] study a new generalization of the Bernstein operator based on the symmetric range, [28] study a new operator of the modified Jain-Gamma operators which preserves linear function.

The majority of reliability analysis studies concerning irrigation systems tend to concentrate on conventional energy sources such as the electric grid, generators, and tractors. These sources often come with high handling costs and their failure can severely impact the irrigation process. However, there is a noticeable lack of research focusing on the implementation of solar irrigation systems, comprising PV panels, controllers, submersible pumps, and storage tanks, as well as their RAMD (Reliability, Availability, Maintainability, and Dependability) and performance analysis. Understanding the implications of such solar irrigation systems on agricultural production, particularly food items, is a crucial area that requires more attention and investigation in the field of irrigation research.

For this reason, this paper considered a solar water irrigation system consisting of four different subsystems

configured as a series-parallel system. The performance of the system is studied using the first-order differential-difference equations. Reliability, availability, maintainability, MTTF, and MBTF are computed as one of the performance measures of system strength and effectiveness for each subsystem. The objectives of this paper are fourfold. The first is to formulate novel models of RAM analysis of solar water irrigation systems. The second is to develop the explicit expressions for the availability, reliability, mean time between failure, maintainability, mean time to failure, and dependability for each subsystem. The third is to see the performance of the system through RAM models under exponentiated Weibull distribution. The fourth is to capture the effect of time, rate of failure, and repair on system reliability, maintainability, and availability.

DESCRIPTION AND NOTATIONS OF THE SYSTEM

Solar irrigation is a sustainable and cost-effective solution that harnesses the power of the sun to provide water for agricultural purposes in rural farming communities. It offers an alternative to traditional irrigation methods that rely on fossil fuels or grid electricity, which may be inaccessible or costly in remote areas. By using solar energy, farmers can reduce their dependence on non-renewable resources and lower their operational costs while ensuring a reliable water supply for their crops. Solar irrigation systems typically consist of photovoltaic (PV) panels, a pump, a water storage tank, and a network of pipes and sprinklers. The PV panels capture sunlight and convert it into electricity, which powers the pump. The pump draws water from a water source, such as a well, river, or pond, and transfers it to the storage tank. From the tank, the water is distributed through the pipes and sprinklers to irrigate the fields. The solar water irrigation system in this study has components:

Notation and Assumptions of the Model Notations

- *v*₁: *stand for failure rate of subsystem* 1
- *v*₂: *stand for failure rate of subsystem* 2
- *v*₃: *stand for failure rate of subsystem* 3
- v_4 : stand for failure rate of subsystem 4
- m_1 : stand for repair rate of subsystem 1
- m_2 : stand for repair rate of subsystem 2
- m_3 : stand for repair rate of subsystem 3
- m_4 : stand for repair rate of subsystem 4

Table 1. System Configuration

Subsystem	Primary unit in operation	Mode of operation
Panels	10	Parallel
Controller	2	Parallel
Pump	2	Parallel
Storage tanks	4	Parallel

Notation and Assumptions of the Model Notations

- v_1 : stand for failure rate of subsystem 1
- v_2 : stand for failure rate of subsystem 2
- v_3 : stand for failure rate of subsystem 3
- v_4 : stand for failure rate of subsystem 4
- m_1 : stand for repair rate of subsystem 1
- m_{2} : stand for repair rate of subsystem 2
- m_3 : stand for repair rate of subsystem 3
- m_{4} : stand for repair rate of subsystem 4
- $P_i(t)$: Stand for Probability that a system is in a certain state at a given time.
- A_{Vk} : Stand for at time t, Availability the system

Assumptions

- a. Failure of the unit/subsystem is independent of the failure of each other
- b. Repair / Replacement is immediate.
- c. It is assumed that all the subsystems are active.
- d. Each failure is repairable.
- e. Rate of failure and repair obeys exponential distribution.

MATERIAL AND METHODS

Reliability Models

The chance that a system/machine will be up and running throughout a period *t* is defined as reliability. Thus, reliability $R(t) = P_r \{T > t\}$, where *T* is the time when the system is down and not running with $R(t) \ge 0$, R(t) = 1. Thus,

$$R(t) = \int_{t}^{\infty} f(t_0) dt_0 \tag{1}$$

and

$$R(t) = 1 - \left(1 - e^{-(\lambda t)^{\gamma}}\right)^{\alpha}$$
(2)

for exponentiated Weibull distributed rate of failure respectively.

$$A(t) = limA(T) = \frac{MTBF}{MTBF + MTTR}.$$
 (3)

Maintainability

$$M(t) = P(T \le t) = 1 - e^{\left(\frac{-t}{MTTR}\right)} = 1 - e^{-\mu t}.$$
 (4)

where μ is the constant system's repair rate.

Dependability

$$D_{min} = 1 - \left(\frac{1}{d-1}\right) \left(e^{-ln\frac{d}{d-1}} - e^{-dln\frac{d}{d-1}} \right).$$
(5)

where
$$d = \frac{\mu}{q}$$
.

MTBF

The average time between the failures is known as MTBF. It's usually expressed in hours. As the MTBF increases, so does the system's reliability. The MTBF is given by

Subsystem	Failure rate Operational Units	Repair rate
Panel	$v_1 = 0.004$	$m_1 = 0.4$
Controller	$v_2 = 0.0016$	$m_2 = 0.7$
Pump	$v_3 = 0.005$	$m_3 = 0.8$
Storage tank	$v_4 = 0.012$	$m_4 = 0.75$

Table 2. Failure and repair rate

$$MTBF = \int_0^\infty R(t) dt = \int_0^\infty e^{-\theta t} dt = \frac{1}{\theta}.$$
 (6)

MTTR

The reciprocal of the system repair rate is specified as MTTR given by

$$MTTR = \mu^{-1} \tag{7}$$

where μ is the system's repair rate.

FORMULATION OF RELIABILITY, AVAILABILITY, AND MAINTAINABILITY MODELS FOR SOLAR IRRIGATION SYSTEM

In this section, Chapman Kolmogorov differential equations for each subsystem have been constructed using the Markov birth-death process for the mathematical modeling of solar irrigation systems. Performance metrics such as availability, reliability, maintainability, and dependability have been derived by solving the appropriate Chapman-Kolmogorov differential equations in a steady state and employing normalization conditions simultaneously. Table 2 displays various subsystem failure and repair rates.

RAMD Models for Subsystem 1: The PV Panel

Solar panels are the primary component of solar-powered water pumping systems, as they are responsible for converting sunlight into electricity that powers the system. The efficiency and capacity of the solar panels are crucial factors that affect the system's overall performance. From Table 1, the PV panel subsystem has ten panels in active

Table 3. Transition rate table for Solar Panels

	S ₀	<i>S</i> ₁	<i>S</i> ₂	<i>S</i> ₃	 <i>S</i> ₈	<i>S</i> ₉	S ₁₀	
S_0	0	$10v_1$	0	0	 0	0	0	
S_1	m_1	0	$9v_1$	0	 0	0	0	
S_2	0	m_1	0	$8v_1$	 0	0	0	
<i>S</i> ₃	0	0	m_1	0	 0	0	0	
S_8	0	0	0	0	 0	$2v_1$	0	
S_9	0	0	0	0	 m_1	0	ν_1	
<i>S</i> ₁₀	0	0	0	0	 0	m_1	0	

parallel. Through Table 3 below, the Chapman-Kolmogrov differential-difference equations (8)-(18) are derived using the Markovian birth-death process.

$$\frac{d}{dq}p_{0}(q) = -10v_{1}p_{0}(q) + m_{1}p_{1}(q)$$
(8)

$$\frac{d}{dq}p_{1}(q) = -(9v_{1} + m_{1})p_{1}(q) + 10v_{1}p_{0}(q) + m_{1}p_{2}(q)$$
(9)

$$\frac{d}{dq}p_2(q) = -(8v_1 + m_1)p_1(q) + 9v_1p_1(q) + m_1p_3(q) \quad (10)$$

$$\frac{d}{dq}p_{3}(q) = -(7v_{1} + m_{1})p_{3}(q) + 8v_{2}p_{0}(q) + m_{1}p_{4}(q) \quad (11)$$

$$\frac{d}{dq}p_4(q) = -(6v_1 + m_1)p_6(q) + 7v_1p_3(q) + m_1p_5(q) \quad (12)$$

$$\frac{d}{dq}p_5(q) = -(5v_1 + m_1)p_5(q) + 6v_1p_4(q) + m_1p_6(q) \quad (13)$$

$$\frac{d}{dq}p_{6}(q) = -(4v_{1} + m_{1})p_{6}(q) + 5v_{1}p_{5}(q) + m_{1}p_{7}(q) \quad (14)$$

$$\frac{d}{dq}p_{7}(q) = -(3v_{1}+m_{1})p_{7}(q) + 4v_{1}p_{6}(q) + m_{1}p_{8}(q)$$
(15)

$$\frac{d}{dq} p_8(q) = -(2v_1 + m_1) p_8(q) + 3v_1 p_7(q) + m_1 p_9(q)$$
(16)

$$\frac{d}{dq}p_{9}(q) = -(v_{1}+m_{1})p_{1}(q) + 2v_{1}p_{8}(q) + m_{1}p_{10}(q) \quad (17)$$

$$\frac{d}{dq}p_{10}(q) = -m_1 p_{10}(q) + v_1 p_9(q)$$
(18)

The normalizing condition for this problem is

$$p_0(q) + p_1(q) + p_2(q) + p_3(q) + \dots + p_9(q) + p_{10}(q) = 1$$
(19)

Availability of PV panel subsystems is

$$A_{V1}(q) = p_0(q) + p_1(q) + p_2(q) + p_3(q) + \dots + p_9(q)$$
(20)

Setting (9) to (19) to zero as $q \rightarrow \infty$ in steady state and solving recursively with the aid of (19), the availability of the PV panel subsystem in (20) is now

$$A_{r_1}(q) = \frac{1+10y_1+90y_1^2+720y_1^3+5040y_1^4+30240y_1^2+151200y_1^6+604800y_1^2+1814000y_1^8+3628800y_1^0}{1+10y_1+90y_1^2+720y_1^2+5040y_1^2+30240y_1^3+151200y_1^6+\dots+3628800y_1^9+3628800y_1^{10}}$$
(21)

Where $y_k = \frac{v_k}{m_k}$, k = 1, 2, 3, 4

The Corresponding reliability, and maintainability of the PV panel subsystem are

$$R_{1}(q) = 1 - \left(1 - e^{-(v_{1}q)^{\gamma}}\right)^{\alpha}$$
(22)

$$M_1(q) = 1 - \exp^{-m_1 q}$$
(23)

RAMD Models for Subsystem 2: The Controller

Controllers are also essential components that ensure the efficient and effective operation of the system. They regulate the power output from the solar panels and the submersible pump and monitor the system's performance to ensure that it operates optimally. From Table 1, the controller subsystem has two units in active parallel. Through Table 4 below, the Chapman-Kolmogrov differential-difference equations (24)-(27) are derived using the Markovian birth-death process.

Table 4. Transition rate table for Controller

	S ₀	<i>S</i> ₁	S ₂
<i>S</i> ₀	0	$2v_2$	0
<i>S</i> ₁	<i>m</i> ₂	0	v_2
<i>S</i> ₂	0	<i>m</i> ₂	0

$$\frac{d}{dq}p_0(q) = -2v_2p_0(q) + m_2p_1(q)$$
(24)

$$\frac{d}{dq}p_1(q) = -(v_2 + m_2)p_1(q) + 2v_2p_0(q) + m_2p_2(q) \quad (25)$$

$$\frac{d}{dq}p_{2}(q) = -m_{2}p_{2}(q) + v_{2}p_{1}(q)$$
(26)

The normalizing condition for this problem is

$$p_0(q) + p_1(q) + p_2(q) = 1$$
 (27)

The availability of controller subsystems is

$$A_{V2}(q) = p_0(q) + p_1(q)$$
(28)

Setting (25) to (28) to zero as $q \rightarrow \infty$ in steady state and solving recursively with the aid of (27), the availability of controller subsystem in (28) is now

$$A_{V_2}(q) = \frac{1+2y_2}{1+2y_2+2y_2^2}$$
(29)

The Corresponding reliability, and maintainability of the controller subsystem are

$$R_{2}(q) = 1 - \left(1 - e^{-(v_{2}q)^{y}}\right)^{\alpha}$$
(30)

$$M_2(q) = 1 - \exp^{-m_2 q}$$
(31)

RAMD Models for Subsystem 3: The Submersible Pump

Submersible pumps are responsible for pumping water from the source to the storage tank, and their performance is critical in determining the system's overall efficiency. The type and capacity of the submersible pump used should be carefully selected to ensure that it matches the system's power output and water pumping requirements. From Table 1, the submersible subsystem has two units in active parallel. Through Table 5 below, the Chapman-Kolmogrov differential-difference equations (34)-(34) are derived

Table 5. Transition rate table for Submersible pump

	S ₀	<i>S</i> ₁	<i>S</i> ₂
<i>S</i> ₀	0	$2v_3$	0
S_1	<i>m</i> ₃	0	v ₃
<i>S</i> ₂	0	<i>m</i> ₃	0

using the Markovian birth-death process.

$$\frac{d}{dq}p_0(q) = -2v_3p_0(q) + m_3p_1(q)$$
(32)

$$\frac{d}{dq}p_1(q) = -(v_3 + m_3)p_1(q) + 2v_3p_0(q) + m_3p_2(q) \quad (33)$$

$$\frac{d}{dq}p_2(q) = -m_3p_2(q) + v_3p_1(q)$$
(34)

The normalizing condition for this problem is

$$p_0(q) + p_1(q) + p_2(q) = 1$$
(35)

The availability of submersible pump subsystems is

$$A_{V3}(q) = p_0(q) + p_1(q)$$
(36)

Setting (33) to (35) to zero as $q \rightarrow \infty$ in steady state and solving recursively with the aid of (35), the availability of submersible pump subsystem in (36) is now

$$A_{\nu_3}(q) = \frac{1+2y_3}{1+2y_3+2y_3^2}$$
(37)

The Corresponding reliability, and maintainability of the submersible pump subsystem are

$$R_{3}(q) = 1 - \left(1 - e^{-(v_{3}q)^{\gamma}}\right)^{\alpha}$$
(38)

$$M_{3}(q) = 1 - \exp^{-m_{3}q}$$
(39)

RAMD Models for Subsystem 4: The Storage Tank

Storage tanks are also crucial components of solar-powered water pumping systems, as they store the water that has been pumped from the source. The size and capacity of the storage tank should be carefully selected to ensure that it meets the water demand of the intended application. A storage tank for reserving water for irrigation is a container used to store water for agricultural purposes. It is typically made of materials that can withstand the weight and pressure of the water being stored, such as concrete, steel, or plastic. The size of the tank will depend on the amount of water needed for irrigation, the frequency of irrigation, and the size of the land being irrigated. The tank can be installed above ground or below ground, depending on the available space and the desired level of visual impact. To ensure the quality of the water, the tank should be designed to prevent contamination from external sources. It should also be equipped with an inlet for filling and an outlet for withdrawing water, as well as appropriate filters and valves. Regular maintenance of the tank is necessary to prevent leaks, ensure structural integrity, and maintain the water quality. This can include periodic cleaning and inspection, as well as repairs and replacements as needed. From Table 1, the storage tank subsystem has four units in active parallel. Through Table 6 below, the Chapman-Kolmogrov differential-difference equations (40)-(44) are derived using the Markovian birth-death process.

Table 6. Transition rate table for Storage Tanks

	S ₀	<i>S</i> ₁	<i>S</i> ₂	<i>S</i> ₃	S ₄
<i>S</i> ₀	0	$4v_4$	0	0	0
S_1	m_4	0	$3v_4$	0	0
<i>S</i> ₂	0	m_4	0	$2v_4$	0
<i>S</i> ₃	0	0	m_4	0	v_4
S_4	0	0	0	m_4	0

$$\frac{d}{dq}p_{0}(q) = -4v_{4}p_{0}(q) + m_{4}p_{1}(q)$$
(40)

$$\frac{d}{dq}p_1(q) = -(3v_4 + m_4)p_1(q) + 4v_4p_0(q) + m_4p_2(q)$$
(41)

$$\frac{d}{dq}p_2(q) = -(2v_4 + m_4)p_1(q) + 3v_4p_1(q) + m_4p_3(q)$$
(42)

$$\frac{d}{dq}p_{3}(q) = -(v_{4} + m_{4})p_{3}(q) + 2v_{4}p_{2}(q) + m_{4}p_{4}(q) \quad (43)$$

$$\frac{d}{dq}p_{4}(q) = -m_{4}p_{4}(q) + v_{4}p_{3}(q)$$
(44)

The normalizing condition for this problem is

$$p_0(q) + p_1(q) + p_2(q) + p_3(q) + p_4(q) = 1$$
(45)

Availability of storage tank subsystems is

$$A_{V4}(q) = p_0(q) + p_1(q) + p_2(q) + p_3(q)$$
(46)

Setting (40) to (44) to zero as $q \rightarrow \infty$ in steady state and solving recursively with the aid of (45), the availability of the storage tank subsystem in (46) is now

$$A_{Y_4}(q) = \frac{1+4y_4+12y_4^2+24y_4^3}{1+4y_4+12y_4^2+24y_4^3+24y_4^4}$$
(47)

The Corresponding reliability, and maintainability of the PV panel subsystem are

$$R_4(q) = 1 - \left(1 - e^{-(v_4 q)^{\gamma}}\right)^{\alpha}$$
(48)

$$M_4(q) = 1 - \exp^{-m_4 q}$$
(49)

RAMD Models for Solar Irrigation System

Since the solar irrigation system is a series-parallel system, then

The system reliability, availability, and maintainability of the entire solar irrigation system are:

$$R_{system}(q) = R_1(q) * R_2(q) * R_3(q) * R_4(q)$$
(50)

$$A_{V \, system}\left(q\right) = A_{V1} * A_{V2} * A_{V3} * A_{V4} \tag{51}$$

$$M_{system}(q) = M_1(q) * M_2(q) * M_3(q) * M_4(q)$$
(52)

NUMERICAL SIMULATION AND DISCUSSION

Numerical simulations of reliability, availability, maintainability, and dependability are discussed in this section.

This section presents the numerical simulations to demonstrate how the model's durability, efficacy, and

	PV panel				Solar irrigation system				
q	$v_1 = 0.002$	$v_1 = 0.003$	$v_1 = 0.004$	$v_1 = 0.005$	$v_1 = 0.002$	$v_1 = 0.003$	$v_1 = 0.004$	$v_1 = 0.005$	
0	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	
20	0.999937	0.999858	0.999748	0.999608	0.995640	0.995561	0.995452	0.995312	
40	0.999748	0.999437	0.999008	0.998463	0.983554	0.983248	0.982825	0.982289	
60	0.999437	0.998750	0.997804	0.996609	0.965108	0.964443	0.963530	0.962376	
80	0.999008	0.997804	0.996157	0.994089	0.941508	0.940373	0.938820	0.936872	
100	0.998463	0.996609	0.994089	0.990944	0.913813	0.912116	0.909810	0.906931	

Table 7. Change in reliability concerning change in the rate of failure of PV panel



Figure 1. Impact of change v_1 on the reliability of PV panel.

	Controller				Solar irrigation system				
	$v_2 = 0.0012$	$v_1 = 0.0014$	$v_1 = 0.0016$	$v_1 = 0.0018$	$v_2 = 0.0012$	$v_1 = 0.0014$	$v_1 = 0.0016$	$v_1 = 0.0018$	
0	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	
20	0.997804	0.997034	0.996156	0.995174	0.997098	0.996328	0.995451	0.994470	
40	0.991621	0.988773	0.985564	0.982013	0.988865	0.986025	0.982825	0.979284	
60	0.982014	0.976084	0.969482	0.962261	0.975985	0.970091	0.963530	0.956353	
80	0.969482	0.959725	0.948988	0.937380	0.959095	0.949443	0.938820	0.927337	
100	0.954472	0.940358	0.925005	0.908600	0.938792	0.924910	0.909809	0.893673	

Table 8. Change in reliability concerning change in the rate of failure of the Controller



Figure 2. Impact of change v_2 on the reliability of the Controller.

	Submersible p	pump			Solar irrigation system				
	$v_3 = 0.001$	$v_3 = 0.003$	$v_3 = 0.005$	$v_3 = 0.007$	$v_3 = 0.001$	$v_3 = 0.003$	$v_3 = 0.005$	$v_3 = 0.007$	
0	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	
20	0.999984	0.999857	0.999607	0.999237	0.995826	0.995700	0.995451	0.995083	
40	0.999936	0.999437	0.998462	0.997034	0.984276	0.983785	0.982825	0.981419	
60	0.999857	0.998749	0.996608	0.993508	0.966671	0.965600	0.963530	0.960533	
80	0.999748	0.997803	0.994088	0.988773	0.944165	0.942328	0.938820	0.933800	
100	0.999607	0.996608	0.990944	0.982932	0.917764	0.915010	0.909809	0.902454	

Table 9. Change in reliability concerning change in the rate of failure of Submersible pump



Figure 3. Impact of change v_3 on reliability of Submersible pump Distribution.

	Storage tank				Solar irrigation system				
	$v_4 = 0.0008$	$v_4 = 0.0012$	$v_4 = 0.0016$	$v_4 = 0.0020$	$v_4 = 0.0008$	$v_4 = 0.0012$	$v_4 = 0.0016$	$v_4 = 0.0020$	
0	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	
20	0.999989	0.999977	0.999959	0.999936	0.995504	0.995492	0.995474	0.995451	
40	0.999959	0.999908	0.999838	0.999748	0.983033	0.982983	0.982914	0.982825	
60	0.999908	0.999795	0.999638	0.999437	0.963984	0.963875	0.963723	0.963530	
80	0.999838	0.999638	0.999361	0.999008	0.939600	0.939412	0.939152	0.938820	
100	0.999748	0.999437	0.999008	0.998462	0.910981	0.910698	0.910306	0.909809	

Table 10. Change in reliability concerning change in the rate of failure of Storage tank EWD



Figure 4. Impact of change v_4 on reliability of Storage tank.

Time	Reliability of Panel $v_1 = 0.004$	Reliability of Controller $v_2 = 0.016$	Reliability of Pump $v_3 = 0.005$	Reliability of Storage tank $v_4 = 0.002$	System Reliability
0	1.00000	1.00000	1.00000	1.00000	1.00000
20	0.9781385409	0.9961566199	0.9671414601	0.9940889038	0.9367921100
40	0.9250056501	0.9855647895	0.8913111279	0.9781385409	0.7948025741
60	0.8546738976	0.9694823098	0.7964290603	0.9544723303	0.6298697776
80	0.7765475476	0.9489881497	0.6967614102	0.9250056501	0.4749603072
100	0.6967614102	0.9250056501	0.6004235991	0.8913111279	0.3449177600

Table 11. Variation in reliability of the system



Figure 5. Reliability of various subsystems of solar irrigation system.

	Panel subsystem					System	m			
v_1 / m_1	0.2	0.4	0.6	0.8	1.0	0.2	0.4	0.6	0.8	1.0
0.01	1.0000	1.0000	1.0000	1.0000	1.0000	0.9921	0.9921	0.9921	0.9921	0.9921
0.02	0.9999	1.0000	1.0000	1.0000	1.0000	0.9920	0.9921	0.9921	0.9921	0.9921
0.03	0.9986	1.0000	1.0000	1.0000	1.0000	0.9907	0.9921	0.9921	0.9921	0.9921
0.04	0.9932	0.9999	1.0000	1.0000	1.0000	0.9853	0.9920	0.9921	0.9921	0.9921
0.05	0.9816	0.9996	1.0000	1.0000	1.0000	0.9739	0.9917	0.9921	0.9921	0.9921

Table 12. Change in availability concerning change in the rate of failure of PV panel

effectiveness have been assessed at various levels. In this case, we use the Lindley and exponentiated Weibull distributions as two alternative distributions to determine the best distribution for improving system reliability, availability, maintainability, and dependability. On this basis, the model's performance is evaluated. From Table 7-10 and Figures 1-4, it is evident that the reliability of the PV panel, controller, submersible pump, storage tank, and solar irrigation system decreases with time for various combinations of PV panel, controller, submersible pump, and storage tank failure rates. The reliability of the solar irrigation system is consistently lower than that



Figure 6. Availability of the system concerning change in v_1 and m_1 .

	Controller subsystem					System	ystem			
v_2 / m_2	0.2	0.3	0.4	0.5	0.6	0.2	0.3	0.4	0.5	0.6
0.01	0.9955	0.9979	0.9988	0.9992	0.9995	0.9885	0.9910	0.9918	0.9923	0.9925
0.03	0.9665	0.9836	0.9903	0.9936	0.9955	0.9598	0.9767	0.9834	0.9867	0.9885
0.05	0.9231	0.9600	0.9756	0.9836	0.9882	0.9166	0.9533	0.9688	0.9767	0.9813
0.07	0.8740	0.9309	0.9566	0.9703	0.9784	0.8679	0.9244	0.9499	0.9635	0.9716
0.09	0.8243	0.8989	0.9347	0.9545	0.9665	0.8185	0.8926	0.9282	0.9479	0.9598



Figure 7. Availability of the system concerning change in v_2 and m_2 .

	Submersible pump subsystem					System	System			
v_{3} / m_{3}	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
0.02	0.9459	0.9922	0.9970	0.9985	0.9991	0.9449	0.9911	0.9960	0.9974	0.9980
0.04	0.8491	0.9727	0.9891	0.9942	0.9964	0.8481	0.9716	0.9880	0.9931	0.9953
0.06	0.7534	0.9459	0.9773	0.9876	0.9922	0.7526	0.9449	0.9762	0.9865	0.9911
0.08	0.6701	0.9151	0.9627	0.9792	0.9868	0.6694	0.9141	0.9616	0.9781	0.9857
0.1	0.6000	0.8824	0.9459	0.9692	0.9802	0.5993	0.8814	0.9449	0.9682	0.9791

Table 14. Change in availability concerning change in the rate of failure of the Submersible pump



Figure 8. Availability of the system concerning change in v_3 and m_3 .

	Storage tank subsystem					System	System			
v_4 / m_4	0.4	0.5	0.6	0.7	0.8	0.4	0.5	0.6	0.7	0.8
0.04	0.9999	0.9993	0.9996	0.9998	0.9999	0.9905	0.9913	0.9917	0.9918	0.9919
0.05	0.9966	0.9984	0.9992	0.9995	0.9997	0.9887	0.9905	0.9912	0.9916	0.9918
0.06	0.9938	0.9971	0.9984	0.9991	0.9994	0.9859	0.9891	0.9905	0.9911	0.9915
0.07	0.9899	0.9951	0.9973	0.9984	0.9990	0.9820	0.9871	0.9894	0.9905	0.9911
0.08	0.9847	0.9924	0.9958	0.9975	0.9984	0.9769	0.9845	0.9879	0.9896	0.9905

Table 15. Change in availability concerning change in the rate of failure of Storage tank

of the PV panel, controller, submersible pump, and storage tank subsystems. This implies that the reliability of the solar irrigation system can be enhanced by implementing a careful maintenance strategy. Regular maintenance, inspections, and timely repairs or replacements of faulty PV panels, controllers, submersible pumps, and storage tanks can help mitigate the decline in reliability over time. By ensuring that the PV panels, controller, submersible pump, and storage tank subsystems are in optimal working condition, the overall reliability of the solar irrigation system can be improved. It is important to note that the specific maintenance strategy may vary based on the PV panels, controller, submersible pump and storage tank subsystems failure rates, and other factors. Consulting with experts in the field and following manufacturer guidelines can help develop an effective maintenance plan to enhance the reliability of the solar irrigation system.



Figure 9. Availability of the system concerning change in v_4 and m_4 .

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Table	16.	Change	1n	maint	aina	b1	111	v
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Time	Maintainability of Panel $m_1 = 0.4$	Maintainability of Controller $m_2 = 0.7$	Maintainability of Pump $m_3 = 0.8$	Maintainability of Storage tank $m_4 = 0.75$	System Maintainability
0	0.00000	0.00000	0.00000	0.00000	0.00000
20	0.99966	0.99999	0.99999	0.99999	0.99966
40	0.99999	1.00000	1.00000	1.00000	0.99999
60	1.00000	1.00000	1.00000	1.00000	1.00000
80	1.00000	1.00000	1.00000	1.00000	1.00000
100	1.00000	1.00000	1.00000	1.00000	1.00000



Figure 10. Maintainability of various subsystems of solar irrigation system.

Indices	PV Panel	Controller	Submersible Pump	Storage tank
Reliability	$1 - \left(1 - e^{-(0.004q)^{0.2}}\right)^2$	$1 - \left(1 - e^{-(0.0016q)^{0.2}}\right)^2$	$1 - \left(1 - e^{-(0.005q)^{0.2}}\right)^2$	$1 - \left(1 - e^{-(0.012q)^{0.2}}\right)^2$
Availability	1.0000	0.9995	0.9991	0.9999
Maintainability	$1 - \exp^{-0.40q}$	$1 - \exp^{-0.7q}$	$1 - \exp^{-0.8q}$	$1 - \exp^{-0.75q}$
Dependability	0.9900	0.9977	0.9937	0.9840
MTBF	25	62.5	20	50
MTTR	2.5	1.4286	1.25	1.3333

Table 17. RAMD indices

Figure 6-9 illustrates the relationship between the availability of PV panels, controllers, submersible pumps, storage tanks, and the solar irrigation system. The figures show that as the failure rate v_k , k = 1,2,3,4 increases, the reliability of the PV panel decreases. The relationship between failure rate and availability can be inverse. As the failure rate increases, it indicates a higher likelihood of failures occurring within the system. Consequently, the availability of the PV panel, controller, submersible pump, storage tank, and solar irrigation system decreases because there is a greater probability of encountering failures. From this analysis, it can be inferred that the graph in Figure 6-9 demonstrates this inverse relationship between failure rate and availability of PV panels, controllers, submersible pumps, storage tanks, and solar irrigation system reliability. Figure 6-9, presents a surface plot depicting the availability of a solar irrigation system based on the failure rate v_k of the PV panel, controller, submersible pump, and storage tank, and the solar irrigation system and repair rate m_k of the PV panel, controller, submersible pump, storage tank, and the solar irrigation system. According to the figures, as the failure rate v_k of the PV panels, controller, submersible pump, storage tank, and solar irrigation system increases, there is a decrease in the availability of solar irrigation systems. On the other hand, the figure shows that as the repair rate m_k of the PV panel, controller, submersible pump, storage tank, and solar irrigation system increases, there is an increasing pattern in the availability of the solar irrigation system. Based on this information, it can be inferred that reducing the failure rate v_k of the PV panel, controller, submersible pump, storage tank, and solar irrigation system and implementing preventive measures for maintaining the panels will enhance the availability of the solar irrigation system. By minimizing the likelihood of PV panels, controllers, submersible pumps, storage tanks, and solar irrigation system failures and ensuring prompt repairs when necessary, the overall availability of the system can be improved, thereby increasing its reliability and functionality.

Table 12-15 demonstrates the relationship between the failure rate v_k and repair rate m_k of PV panels and the availability of both the PV panel, controller, submersible pump, storage tank, and solar irrigation system. According to

the tables, as the failure rate v_k of the PV panel, controller, submersible pump, storage tank, and solar irrigation system increases, both the availability of the PV panel, controller, submersible pump, storage tank and the availability of the solar irrigation system decrease. This suggests that a higher failure rate of the PV panel, controller, submersible pump, and storage tank leads to reduced availability of the entire system. On the other hand, the table shows that the availability of the PV panel, controller, submersible pump, storage tank, and solar irrigation system increases with an increase in the repair rate m_k of the PV panel, controller, submersible pump, storage tank, and solar irrigation system. This implies that a higher repair rate leads to improved availability of the PV panel and the solar irrigation system. From the table, it is clear that the PV panel, controller, submersible pump, storage tank, and solar irrigation system are more reliable and have higher availability compared to the solar irrigation system in the context of the given data.

Table 11 and Figure 5 present the results of the reliability of the PV panel, controller, submersible pump, storage tank, and solar irrigation system. The table and figure show that reliability decreases drastically with time from 0 to 100. From the table and figure it can be seen that the reliability of the solar irrigation system is less than the reliability of the PV panel, controller, submersible pump, and storage tank. The submersible pump has the least reliability among the subsystems from Table 11 and Figure 5 and hence is the most critical subsystem.

Table 16 and Figure 10 present the results of the maintainability of the PV panel, controller, submersible pump, storage tank, and solar irrigation system. The table and figure show that maintainability increases very fast with time from 0 to 100 for different repair rates. From the table and figure it can be seen that the maintainability of the solar irrigation system equally increases as the maintainability of the PV panel, controller, submersible pump, and storage tank increases.

CONCLUSION

RAMD analysis for PV solar irrigation systems is crucial for evaluating reliability, availability, maintainability, and

dependability aspects. It enables efficient system design, optimal maintenance planning, enhanced system performance, and cost-effective operation, ultimately contributing to the success and sustainability of such systems. Reliability analysis in RAM for PV solar irrigation systems is essential for ensuring consistent and dependable operation. By evaluating system performance, reducing downtime, optimizing costs, enhancing system longevity, mitigating risks, optimizing energy usage, and supporting decision-making, reliability analysis helps small-scale farmers achieve efficient and sustainable irrigation for their agricultural activities. By conducting reliability and performance analyses, solar irrigation system operators and designers can ensure the system's long-term reliability, maximize its efficiency, and minimize potential downtime. These analyses contribute to the overall sustainability and economic viability of solar irrigation, helping farmers achieve more efficient water management and increased crop yields while reducing reliance on fossil fuels and minimizing environmental impacts. Implementing these reliability models for a solar irrigation system allows you to identify potential failure modes, assess critical components, optimize maintenance activities, and analyze system behavior. By leveraging RAM principles and these reliability models, you can enhance the performance of the solar irrigation system, maximize its availability, and ensure sustainable and reliable operation. In conclusion, the reliability, availability, and maintainability of solar irrigation systems are essential considerations for their successful deployment and long-term operation. By ensuring the reliability of components, maximizing system availability, and implementing efficient maintenance practices, solar irrigation systems can offer sustainable and reliable water supply for agricultural purposes, contributing to increased food production and environmental sustainability.

Reliability, availability, and maintainability analysis is crucial for PV solar irrigation systems to ensure their optimal performance, longevity, and cost-effectiveness. Here are the key reasons for conducting RAM analysis in this context:

- 1. Reliability Assessment: RAM analysis helps evaluate the reliability of a PV solar irrigation system by assessing the probability of failure or breakdown. By identifying potential failure points and their impact on system operation, reliability analysis aids in designing robust and dependable systems that can withstand various operational conditions and environmental factors.
- 2. Availability Evaluation: PV solar irrigation systems need to be available for operation during specific periods, typically corresponding to sunlight hours for optimal power generation. RAM analysis helps determine the availability of the system, taking into account factors such as system downtime, maintenance activities, and component failures. This information aids in scheduling maintenance activities and ensuring maximum system availability during critical periods.

- 3. Maintainability Planning: PV solar irrigation systems require regular maintenance and servicing to sustain their performance and longevity. RAM analysis provides insights into the maintainability aspects of the system, including the mean time to repair (MTTR) and the mean time between failures (MTBF). These metrics assist in planning maintenance activities, estimating downtime for repairs, and optimizing maintenance schedules to minimize disruptions and maximize system uptime.
- 4. Durability Assessment: The durability of PV solar irrigation systems is vital for their long-term operation and economic viability. RAM analysis evaluates the durability of system components by considering factors such as environmental conditions, material degradation, and wear and tear over time. Understanding the expected lifespan and failure modes of different components allows for informed decision-making regarding system design, component selection, and replacement strategies.
- 5. Cost Optimization: RAM analysis helps in identifying potential cost-saving opportunities for PV solar irrigation systems. By assessing reliability, availability, and maintainability factors, it becomes possible to optimize maintenance schedules, predict component lifetimes, and minimize operational disruptions. This leads to reduced downtime, lower maintenance costs, and improved overall system performance, resulting in long-term cost savings.

Therefore, RAM analysis for PV solar irrigation systems is crucial for evaluating reliability, availability, maintainability, and durability aspects. It enables efficient system design, optimal maintenance planning, enhanced system performance, and cost-effective operation, ultimately contributing to the success and sustainability of such systems.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

On inclusion probabilities for weighted random sampling without replacement

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ABSTRACT

Hajj is an annual Islamic pilgrimage to Mecca, Saudi Arabia. It is performed on certain dates of the lunar year. The Saudi government sets quotas for various countries to keep the pilgrims' number at a manageable level. While some countries maintain waiting lists and evaluate applications on a first-come-first-served basis, others conduct draws to determine who will be admitted to the journey. Türkiye is one of the latter, where candidates' odds are, in a sense, proportional to the square of the number of years they have been waiting for, or to be more accurate, to the square of the number of times they made an application. This policy, which is called "katsayılı kura sistemi" in Turkish, is adopted by countries like Bosnia and Herzegovina and Belgium as well. The sampling process described above is referred to as "weighted random sampling without replacement with defined weights" (WRS) in the literature. The purpose of this paper is to investigate the inclusion probabilities in WRS for which no efficient method exists. First, we take up an analytical approach and derive theoretical lower and upper bounds on the inclusion probabilities. Second, for situations where these bounds are not as tight as desired, we propose an estimation procedure by simulation. The simulation design is based on an ingenious idea from computer science. We apply our results to estimate applicants' chances in Türkiye's last hajj draw before the COVID-19 pandemic. It turns out that one who participates in the draws for the first time has a chance in between 0.12% and 0.13%; similar bounds for one who participates for the eleventh time (for one with the largest number of applications) are 13.22% and 14.16%. These bounds actually rely on a conjecture relating WRS to a more general problem for which we provide a supportive example.

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INTRODUCTION

Suppose *N* items are partitioned into a number of groups. Let us denote the size and the weight of group *i* by $n_i \in \mathbb{N}$ and $w_i > 0$, respectively. We study the sampling

process of randomly choosing n items in this fashion: in each round one of the groups is selected at random to include in the sample all items in that group, and the chance of selecting a group equals its weight divided by the yet

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unselected groups' total weight. The particular situation where each group is a singleton, namely a set with only one item, is called "weighted random sampling without replacement with defined weights" by Efraimidis [1]. We shorten this as WRS, and the general case, which we shall refer to as "weighted random sampling of groups without replacement with defined weights", will be abbreviated to WRSG. Let p_i stand for the probability that group i is included in the sample. Even for WRS no efficient method is known to exist to calculate p_i exactly [1]. The purpose of this paper is to investigate these inclusion probabilities. Our incentive stems from a real-world application about hajj draws conducted every year by some countries.

Research on unequal probability sampling, unlike the subject matter of this paper, mainly focuses on devising sampling designs. Indeed, the primary objective in sampling is to estimate some unknown population parameter, and the choice of sampling design is important since it determines the properties of the estimator used [2]. In this context, the p_i are commonly denoted π_i and called first-order inclusion probabilities. These are usually prescribed beforehand for all items such that the relevant estimator has desirable properties [3].

Hansen and Hurwitz [4] were the first to suggest the use of unequal probabilities in sampling. Yates and Grundy [5] discuss the so-called Yates-Grundy draw-by-draw procedure. They explicitly give the probability of obtaining a specific sample when the sample size is two. Fellegi [6], in his doctoral thesis, carefully distinguishes between the "direct problem" and the "reverse problem" associated with sampling without replacement from a finite population. Rao [7] develops an asymptotic theory thereon. Brewer [8] proposes a simple procedure for sampling without replacement where the probability of inclusion is strictly proportional to size. Hanif and Brewer [9] present a comprehensive review on sampling with unequal probabilities without replacement. They list 50 selection procedures along with their properties and principal reference. These procedures are described in detail in their book [10]. Li [11] introduces an efficient computer implementation of the Yates-Grundy draw-by-draw procedure. This is also discussed by Gelman and Meng [12]. Tille [13] gives a precise definition of draw-by-draw algorithms. Yu [14] obtains some comparison results for the inclusion probabilities in some unequal probability sampling plans without replacement.

More recently, Tille [15] examines the modern development of the theory and foundations of survey sampling. Stamatelatos and Efraimidis [16] view growing preferential attachment models as an application of unequal probability random sampling. Dumelle et al. [17] compare designbased and model-based approaches for finite population spatial sampling and inference. Chauvet [18] and Aubry [19] attract attention to certain issues about a sampling design that is used in popular commercial statistical packages. Tille [20] provides remarks on some misconceptions about unequal probability sampling without replacement. Weighted random sampling has attracted the attention of computer scientists as well. However, their concern is to develop, under various circumstances, efficient algorithms that actually generate the sample in question. For WRS, Efraimidis and Spirakis [21] present such an algorithm, which yields a sample in one pass over the entire population.

Here is an outline of the paper: in Section 2, we make a conjecture that relates WRSG to WRS. In Section 3, for the inclusion probabilities in WRS, we derive theoretical lower and upper bounds, and discuss how simulation can be used for estimation. In Section 4, we apply our results to Türkiye's 2020 hajj draw. Finally, in Section 5, we conclude with some future research opportunities.

A Conjecture Relating WRSG to WRS

Suppose that two groups *j*, *k* unite to form a new group *l* with and $n_l := n_j + n_k$ and $w_l := (n_j w_j + n_k w_k)/(n_j + n_k)$. Thus, w_l is the weighted average of the component weights. This operation decreases the number of groups by 1, and changes the inclusion probabilities of all groups in question. We conjecture that, for non-uniting groups, the change in inclusion probabilities is asymptotically zero.

Conjecture. Let p'_i be the inclusion probability of group *i* after two groups other than *i* unite. For fixed n/N, the probability p'_i tends to p_i in the limit $N \rightarrow \infty$.

We cannot prove this conjecture for the time being, but we will provide a supportive example. Assume all groups have size 1 and all weights are 1. Let p' be the inclusion probability of a group after two other groups unite to form a new group of size 2. We shall compute q' := 1 - p'. The exclusion probability given that the new group is not included in the sample is

$$\frac{N-3}{N-1} \cdot \frac{N-4}{N-2} \cdots \frac{N-n-1}{N-n+1} \cdot \frac{N-n-2}{N-n-1}.$$
 (1)

Note that the last factor's denominator is N - n - 1 rather than N - n since in the final round the new group is automatically discarded as its size exceeds remaining capacity. The exclusion probability given that the new group is included in the sample is, by conditioning on the round it is selected,

$$(n-1) \cdot \frac{(N-3)(N-4)\cdots(N-n)}{(N-1)(N-2)\cdots(N-n+1)}.$$
 (2)

Summing up (1) and (2) we get, after simplification,

$$q' = \frac{(N-n)(N-3)}{(N-1)(N-2)}.$$
(3)

Thus, for fixed *n*/*N*, we have $\lim_{N\to\infty} q' = 1 - n/N = q$, implying $\lim_{N\to\infty} p' = p$ as desired.

If the conjecture is correct, then by decomposing groups other than *i* into singletons, we obtain almost a WRS with p_i approximately equal to the original inclusion probability of group *i* (decomposition yields an exact WRS if $n_i = 1$). In other words, inclusion probability calculation in WRSG essentially reduces to that in WRS. Therefore, in the sequel, we examine the inclusion probabilities for WRS rather than for WRSG. As a consequence, we do not distinguish between items and groups from this point on.

Lower and Upper Bounds on Inclusion Probabilities

As specified above, we consider WRS, namely the procedure of randomly selecting n out of N items without replacement, where items have associated weights so that in each round the probability of selecting an item equals its weight divided by the yet unselected items' total weight.

Let $q_i := 1 - p_i$. Thus, q_i is the exclusion probability for item *i*. Let Y_t represent the index selected in round t ($1 \le t \le n$). These are dependent random variables with support N:= {1,2,...,N}. Let $N(i) := N \setminus \{i\}$ for short. Then

$$q_i = P(Y_1 \neq i, ..., Y_n \neq i) = P(Y_1 \times \dots \times Y_n \in \mathcal{N}(i) \times \dots \times \mathcal{N}(i)).$$
(4)

Let w_j be the weight of item j $(1 \le j \le N)$. We denote the sum of all weights by $W := \sum_{j=1}^{N} w_j$. For n = 1, we have $q_i = 1 - P(Y_1 = i) = 1 - w_i/W$. For n = 2, conditioning Y_2 on Y_1 ,

$$q_{i} = \sum_{j \in \mathcal{N}(i)} P(Y_{1} = j) P(Y_{2} \in \mathcal{N}(i) | Y_{1} = j)$$

$$= \sum_{j \in \mathcal{N}(i)} \sum_{k \in \mathcal{N}(i,j)} P(Y_{1} = j) P(Y_{2} = k | Y_{1} = j)$$

$$= \sum_{j \in \mathcal{N}(i)} \sum_{k \in \mathcal{N}(i,j)} \frac{w_{j}}{W} \frac{w_{k}}{W - w_{j}}$$
(5)

where $N(i,j) := N \setminus \{i, j\}$. Similarly, for n = 3, conditioning Y_2 on Y_1 , and Y_3 on Y_2 and Y_1 ,

$$\begin{aligned} q_{l} &= \sum_{j \in \mathcal{N}(l)} \sum_{k \in \mathcal{N}(l,j)} P(Y_{1} = j) P(Y_{2} = k \mid Y_{1} = j) P(Y_{3} \in \mathcal{N}(l) \mid Y_{2} = k, Y_{1} = j) \\ &= \sum_{j \in \mathcal{N}(l)} \sum_{k \in \mathcal{N}(l,j)} \sum_{l \in \mathcal{N}(l,j,k)} P(Y_{1} = j) P(Y_{2} = k \mid Y_{1} = j) P(Y_{3} = l \mid Y_{2} = k, Y_{1} = j) \\ &= \sum_{j \in \mathcal{N}(l)} \sum_{k \in \mathcal{N}(l,j)} \sum_{l \in \mathcal{N}(l,j,k)} \frac{w_{j}}{W} \frac{w_{k}}{W - w_{j}} \frac{w_{l}}{W - w_{k} - w_{l}} \end{aligned}$$
(6)

where $N(i,j,k) := N \setminus \{i,j,k\}$. This formula is straightforward to generalize for arbitrary n [22]. Although it provides a means of computing q_i exactly, the number of operations is of order N^n , making it useless for large parameter values. However, the formula can be used to obtain lower and upper bounds on q_i .

Theorem 1. Let a_t and b_t denote the sums of respectively the smallest and the largest *t* weights other than w_i , and let a_0 and b_0 be defined as zero. Then

$$\prod_{t=0}^{n-1} \left(1 - \frac{w_i}{W - a_t} \right) \ge q_i \ge \prod_{t=0}^{n-1} \left(1 - \frac{w_i}{W - b_t} \right). \tag{7}$$

Proof. Suppose without loss of generality that weights are in increasing order, namely $w_1 \leq ... \leq w_n$. Then $w_1 \leq w_j \leq w_N$ for any *j* so that $P(Y_2 \in N(i) | Y_1 = j) = 1 - P(Y_2 = i | Y_1 = j) = 1 - w_i/(W - w_i)$ is greater than or equal to $1 - w_i/(W - w_N)$ and less than or equal to $1 - w_i/(W - w_1)$.. Consequently, for n = 2,

$$\sum_{j \in \mathcal{N}(i)} P(Y_1 = j) \left(1 - \frac{w_i}{W - w_N} \right) \le q_i \le \sum_{j \in \mathcal{N}(i)} P(Y_1 = j) \left(1 - \frac{w_i}{W - w_1} \right); \quad (8)$$

that is,

$$\left(1 - \frac{w_i}{W}\right) \left(1 - \frac{w_i}{W - w_N}\right) \le q_i \le \left(1 - \frac{w_i}{W}\right) \left(1 - \frac{w_i}{W - w_1}\right).$$
(9)

Similarly $P(Y_3 \in N(i) | Y_2 = k, Y_1 = j) = 1 - P(Y_3 = i | Y_2 = k, Y_1 = j) = 1 - w_i/(W - w_k - w_j)$, is greater than or equal to $1 - w_i/(W - w_N - w_{N-1})$ and less than or equal to $1 - w_i/(W - w_1 - w_2)$. Hence, for n = 3,

$$\sum_{j \in \mathcal{N}(i)} \sum_{k \in \mathcal{N}(i,j)} P(Y_1 = j) P(Y_2 = k \mid Y_1 = j) \left(1 - \frac{w_i}{W - w_N - w_{N-1}} \right)$$

$$\leq q_i \leq \sum_{j \in \mathcal{N}(i)} \sum_{k \in \mathcal{N}(i,j)} P(Y_1 = j) P(Y_2 = k \mid Y_1 = j) \left(1 - \frac{w_i}{W - w_1 - w_2} \right), \quad (10)$$

implying

$$\left(1 - \frac{w_i}{W}\right) \left(1 - \frac{w_i}{W - w_N}\right) \left(1 - \frac{w_i}{W - w_N - w_{N-1}}\right) \leq q_i \leq \left(1 - \frac{w_i}{W}\right) \left(1 - \frac{w_i}{W - w_1}\right) \left(1 - \frac{w_i}{W - w_1 - w_2}\right).$$
(11)

The statement can be proved with the same reasoning by mathematical induction on n.

As a consequence of Theorem 1,

$$1 - \prod_{t=0}^{n-1} \left(1 - \frac{w_i}{W - a_t} \right) \le p_i \le 1 - \prod_{t=0}^{n-1} \left(1 - \frac{w_i}{W - b_t} \right).$$
(12)

Since $1 - w_i/(W - a_t)$ and $1 - w_i/(W - b_t)$ are both decreasing sequences of *t*, the inequalities

$$\left(1 - \frac{w_i}{W}\right)^n \ge q_i \ge \left(1 - \frac{w_i}{W - b_{n-1}}\right)^n \tag{13}$$

and

$$1 - \left(1 - \frac{w_i}{W}\right)^n \le p_i \le 1 - \left(1 - \frac{w_i}{W - b_{n-1}}\right)^n$$
(13)

also follow from Theorem 1.

If many items possess the same weight, then inclusion probabilities can also be estimated via simulation by using an efficient algorithm of Efraimidis and Spirakis [21]. Let m_i be the total number of items in the population with weight w_i , and suppose that in the sample generated by the Algorithm below there are x_i such items. Then x_i/m_i is a point estimate for p_i . Generating sufficiently many samples, one can also construct a confidence interval.

Algorithm (Efraimidis and Spirakis [21]).

- 1. For each item *i*, generate a uniform random variable u_i in (0,1) and define $k_i \coloneqq u_i^{1/w_i}$.
- 2. Select the *n* items with the largest k_i .

That the Algorithm above yields samples according to WRS rests upon a proposition of Efraimidis and Spirakis [21], given here as Theorem 2. Indeed, for $\alpha = 2$, Theorem 2 says

$$P(K_1 \le \dots \le K_N) = \prod_{i=1}^N \frac{w_i}{w_1 + \dots + w_i}.$$
 (14)

Left-hand side is the probability that the descending order of the K_i is K_N , K_{N-1} ,..., K_2 , K_1 ; right-hand side is the probability that WRS, when n = N, yields the permutation (N, N - 1,..., 2, 1). In fact, the foregoing relation holds for any permutation of 1,..., N. Hence, the probability that WRS yields the sample $\{i_1, ..., i_n\}$ is equal to the probability that the set $\{k_{i_1}, ..., k_{i_n}\}$ is composed of the largest n numbers among the k_i .

Theorem 2 (Efraimidis and Spirakis [21]). Let U_i be independent uniform random variables in (0,1). For $w_i > 0$, let $K_i := U_i^{1/w_i}$. Then, for any $\alpha \in [0,1]$,

$$P(K_1 \le \dots \le K_N \le \alpha) = \alpha^{w_1 + \dots + w_N} \prod_{i=1}^N \frac{w_i}{w_1 + \dots + w_i}.$$
 (15)

Proof. The density function of K_i is $f_i(\alpha) = w_i \alpha^{w_i-1}$. The proof proceeds by mathematical induction on *N*, using the equality

$$P(K_1 \le \dots \le K_N \le \alpha) = \int_0^\infty P(K_1 \le \dots \le K_{N-1} \le t) f_N(t) dt.$$
(16)

Application to Hajj Draws

The Saudi government sets hajj quotas for countries to keep the pilgrims' number at a manageable level. Some countries maintain waiting lists and evaluate applications on a first-come-first-served basis, while others conduct draws to determine who will be admitted to the journey. Türkiye is one of the latter, where candidates' odds are proportional to the square of the number of times they made an application [23]. More precisely, in each round of a draw, someone applying for the second time is four times as likely to be selected as one who applies for the first time, someone applying for the third time is nine times as likely, and so on. This policy, which is known as "katsayılı kura sistemi" in Turkish, is adopted by countries like Bosnia and Herzegovina and Belgium as well. We shall estimate a candidate's chance given the number of applications he or she has made. This is a crucial piece of information for applicants as well as policymakers.

The sampling process described above is an example of WRS. However, in reality, the situation is more complex since people usually apply as a group as they want to perform hajj together with one or more of their relatives. Weights associated to such groups are the average of the individual weights, in compliance with the definition in Section 2. Therefore, Türkiye's hajj draws are actually examples of WRSG. Nevertheless, assuming the conjecture in Section 2, we shall proceed as if we have a WRS. Subsequent results must be interpreted accordingly.

Let *N* and *n* denote the total number of applicants and the quota; *c* the maximum number of applications; w_u , r_u , and m_u the weight, the ratio, and the number of applicants with *u* applications ($1 \le u \le c$). Consequently, $w_u = u^2$ and $m_u = Nr_u$. The question is to calculate a particular applicant's chance (inclusion probability) p_u given that he or she has made *u* applications.

We note that weighted random sampling without replacement, in this context, is also related to a generalization of the hypergeometric distribution. Let X_u be the random variable representing the number of people in the sample with u applications. The joint distribution of the X_u is referred to as the multivariate Wallenius' noncentral hypergeometric distribution [24]. Then each p_u above can be seen as a marginal probability associated with an additional singleton to be extracted from the related set of candidates. Nevertheless, calculation of p_u this way is tractable only for very small values of n.

For 2020's hajj draw in Türkiye, N = 2,298,800 and n = 83,430. This means that over two million Turks declare their intention to perform hajj, whereas the quota is about eighty thousand. We have c = 11; in other words, there is no applicant with 12 or more applications. This is a consequence of a previous decree by the Turkish government that led to the admission of a certain group of candidates who had been waiting for too long. The ratios r_u , up to two decimal points, as well as the numbers $m_u = Nr_u$ rounded to nearest integers are given in Table 1. We adjusted m_1 so that the group sizes add up to N.

Lower and upper bounds on p_u provided by (12) are denoted $\underline{p_u}$ and $\overline{p_u}$, and given in the second and third columns of Table 2. Values are rounded to four decimal points

Table 1. Ratio and number of people with *u* applications in

 Türkiye's 2020 hajj draw

и	<i>r_u</i> (%)	m _u		
1	7.59	174,480		
2	7.73	177,697		
3	12.97	298,154		
4	13.87	318,844		
5	22.75	522,977		
6	9.60	220,685		
7	8.30	190,800		
8	8.21	188,731		
9	4.25	97,699		
10	2.02	46,436		
11	2.71	62,297		
Total	100	2,298,800		
и	$\frac{p_u}{(\%)}$	$\overline{p_u}$ (%)	$\widehat{p_{u}}$ (%)	CI _{99%} (%)
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1	0.12	0.13	0.120	(0.118, 0.123)
2	0.47	0.50	0.481	(0.476, 0.485)
3	1.05	1.13	1.081	(1.076, 1.086)
4	1.86	2.00	1.920	(1.915, 1.926)
5	2.89	3.11	2.987	(2.981, 2.993)
6	4.13	4.44	4.264	(4.252, 4.276)
7	5.58	6.00	5.760	(5.747, 5.773)
8	7.23	7.76	7.456	(7.443, 7.469)
9	9.06	9.72	9.352	(9.329, 9.374)
10	11.06	11.86	11.422	(11.388, 11.456)
11	13.22	14.16	13.623	(13.587, 13.660)

Table 2. Lower and upper bounds, point estimates, and 99% confidence intervals for p_u expressed as percentages

and expressed as percentages. Also we implemented the Algorithm in Section 3 in R, and ran 100 replications. On a PC with Intel(R) Core(TM) i7-4790 CPU (3.60 GHz) and 8 GB RAM, each replication takes less than half a second. Point estimates $\hat{p_u}$ and 99% confidence intervals are given in the fourth and fifth columns of Table 2. Values are rounded to five decimal points and expressed as percentages.

Table 2 shows that one who takes part in the draws for the first time has a chance in between 0.12% and 0.13%; a point estimate for p_1 is 0.120%, and with 99% probability $p_1 \in (0.118\%, 0.123\%)$. Clearly, in this case, the left endpoint of the confidence interval can be replaced with the theoretical lower bound 0.12%. Bounds and point estimates for p_u gradually increase with respect to *u*. Lastly, one who participates for the eleventh time has a chance in between 13.22% and 14.16%; a point estimate for p_{11} is 13.623%, and with 99% probability $p_{11} \in (13.587\%, 13.660\%)$.

CONCLUSION

Every year Türkiye conducts a draw to determine the citizens that will be admitted to hajj. Candidates' odds are proportional to the square of the number of times they made an application. This policy is called "katsayılı kura sistemi" in Turkish. Abstraction of this sampling procedure is known as "weighted random sampling without replacement with defined weights" (WRS) in the literature. In this paper, we investigated the inclusion probabilities in WRS for which no efficient method exists. More precisely, we derived lower and upper bounds on inclusion probabilities in terms of item weights. As an application thereof, we estimated applicants' chances in Türkiye's 2020 hajj draw. The computational study shows that one who takes part in the draws for the first time has a probability in between 0.12% and 0.13%; similar bounds for one who takes part for the eleventh time (for one with the largest number of applications) are 13.22% and 14.16%. These results are supported with point estimates based on one-pass simulation experiments that yield very tight confidence intervals. Our findings depend on a conjecture for which we give a confirmational example.

It would be of interest for future research to investigate the problem of inclusion probability calculation from a computational complexity point of view, and to find, if possible, point estimates that do not rely on simulation. It is also worthwhile to prove the conjecture stated in Section 2, relating "weighted random sampling of groups without replacement with defined weights" (WRSG) to WRS.

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CODE AVAILABILITY

The R code used for the computational study is available from the author upon request.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Experimental study on different properties of cenosphere based concrete using calcium lactate

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ABSTRACT

The effective utilization of secondary products obtained from coal ash is a major focus of researchers, addressing the global issue of ash dumping on the ground. Cenospheres are a novel material, inherently possessing significant physical and chemical properties that pave the way for numerous future technological advancements in construction. In present work cement is replaced by cenosphere with 2.5%, 5%, 7.5% and 10% to examine physical and mechanical properties of concrete. Because of the fineness of the cenosphere, concrete exhibits little gain in strength, but subsequently because of the lower quantity of calcium contained in the cenosphere, it loses strength substantially. For greater improvement in mechanical properties, calcium lactate of 0.010 mol/lit and 0.015 mol/lit is added in concrete mix along with cement replaced by cenosphere. The obtained result shows that, there is a 4.69% and a 4.80% drop in density when cenosphere is used to replace 10% of cement. Additionally, it results in increases in compressive strength of 4.09% and 8.40%, flexural strength of 2.86% and 6.34%, and tensile strength of 4.02% and 9.77%.

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INTRODUCTION

Concrete is the most extensively used building material and has contributed a significant amount to contemporary civil infrastructure over the past century. Concrete is a mixture of versatile materials which make it strong and durable [1]. Cenosphere, as a cementitious material, represents a novel technological advancement that forms the foundation for concrete development [2]. Cenospheres are derived from coal-fired power stations, it may also known as fly ash cenospheres (FAC). Cenospheres are valued in the construction industry for their lightweight, low-density, high compressive strength, and thermal insulation properties. Their chemical composition, primarily silica, contributes to their durability and resistance to chemical reactions. Their physical attributes, such the dispersion of their particle sizes [3–10], specific surface area [11,12], shell thickness [13], diameter [13–15], colour [14, 16], particle bulk density [17,18], specific gravity [19,20] and water absorption [16, 20] may affects workability, strength and overall performance of concrete. These chemicals and physical properties make cenospheres a valuable additive for improving

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Sieve	500 μm	250 μm	150 μm	106 µm	63 μm	< 63 µm
Cenosphere content	Nil	Nil	0-5%	5-30%	60-95%	0-20%

Table 1. Particle size distribution (wt.%) of cenosphere

Table 2. Chemical structures (wt%) of cenosphere materials

Description	CaO	Fe ₂ O ₃	MgO	SO ₄	K ₂ O	SiO ₂	Na ₂ O	MnO	Al ₂ O ₃	TiO ₂
Cenosphere	00	1.9	0.4	0.2	0.9	53.9	00	0.1	42.6	00

the performance of construction materials like concrete and composites. The average particle density of the cenospheres utilised in the concrete is about 850 kg/m³. Table.1 shows the particle size distribution of the cenospheres, with the majority of the particles falling between 63 and 150 μ m in size.

Cenosphere is versatile material utilized in construction industry for lightweight concrete [8,21], energy saving building design [12], ceramic construction [17], internal curing agent [15,22–24] and manufacturing composite materials [23, 25, 26]. The qualities of both freshly poured and hardened cenosphere concrete will be discussed, and any differentiations observed will be compared to more conventional concretes. It aims to provide a deeper comprehension of the possible benefits and drawbacks of cenosphere concrete. This concrete investigates the ideal cenosphere component to take into account when designing concrete mixes.

Concrete uses the cenosphere as a binding agent in place of some of the cement. The chemical composition of cenospheres shows high combined SiO_2 and Al_2O_3 content of 96.5% but low CaO content equal to 0% as shown in Table 2. The use of fly ash cenosphere is highly helpful for lowering density and bettering concrete's performance; utilising hazardous trash to alleviate environmental issues, and lowering the utilization of cement and hence lower the carbon footprint of the manufacture of concrete while only slightly reducing compressive strength. Utilizing industrial waste, cenosphere is employed in mixes up to about 10% by volume of total cement materials, calcium with 0.010 and 0.015 mol/lit gives concrete density under 2550 kg/m³, Owever, they share many of the same mechanical characteristics as regular concrete (Figure 1).

MATERIALS AND METHODS

In accordance with Indian Standard (IS) 12269, the experimental work is done on concrete specimens made of fly ash cenosphere and ordinary Portland cement (OPC) as the binder ingredient. Cenosphere-based low-density concrete achieves good workability of concrete mix. According to the FAC grading, the majority of the particles are between 63 to 150 μ m in size. Additionally, the SEM examination

also supports the hollow spherical shape and size variation of the FAC, which ranges from 63 to 150 μ m as shown in Figure 2.

A versatile mineral called calcium lactate is utilized to meet the need for calcium required by cenosphere and bacteria in concrete at different stages of development. The calcium lactate has a chemical compound of $(C_6H_{10}CaO_65H_2O)$ with a molar weight of 308.31 g/lit. Calcium lactate's physicochemical compositions are shown in Tables 3 and 4. The calcium lactate that is included in the mix design is added in hydrated form and is precisely soluble in the water together with the other ingredients of concrete. Calcium lactate molar weight quantity is utilised as 0.01(CL0.010) and 0.015(CL0.015) mol/lit shown in Table 6.

The concrete mixtures are made in the lab using a pan mixer. According to IS's recommendations, the physical characteristics of coarse and fine aggregate (CA and FA) are examined shows in Table 5. The potable water is utilised as instructed by IS 456.



Figure 1. Flow diagram of cenosphere concrete mix.



Figure 2. SEM image of cenosphere.

Table 3. Physical properties of calcium lactate

Property	Result
Appearance	White powder
Solubility	Water, Methanol, Ethanol
Odour	Peculiar smell

MIX PROPORTION

In the cement-based system, pozzolanic reactions might benefit from the presence of amorphous silica and a tiny amount of lime. Due to the dehydroxylation and decarbonization processes in the cement hydration, cement paste incorporated of FAC composites exhibits weight loss. still, it will give better mechanical properties even at lower density levels [2].

Calcium oxide is a dominant compound that is observed in the chemical analysis of FAC, to overcome that calcium lactate is precisely soluble in the water together with the other ingredients of concrete. To know the effect,

Table 4.	Chemical	composition	of ca	lcium	lactate
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Property	Result
Chemical formula	C ₆ H ₁₀ CaO ₆ 5H ₂ O
Molar weight	308.31 g/lit
Assay	98 %
pН	6.8
Phosphate	0.002 %
Potassium	0.005 %
Water	30 %

the Concrete mix was categorized into two groups, the first specimen set with five combinations of FAC and cement percentages of replacements, those five combinations are Normal Concrete (CN), Concrete with FAC 2.5% (CN2.5), FAC 5% (CN5), FAC 7.5% (CN7.5), and FAC 10% (CN10).

The second specimen set with two combinations of FAC with different contents of calcium lactate, those two combinations are Concrete with FAC (0%, 2.5%, 5%, 7.5% and 10%) with

Type of Aggregate	Property	Test Result	Indian Standard Recommendation
Fine aggregate	Fineness modulus	2.60	Zone III (2.78-1.71)
	Water absorption (%)	1.69	0.3 to 2.5%
	Specific gravity	2.59	2.3 to 2.7
	Size (mm)	< 4.75	< 4.75
Coarse aggregate	Fineness modulus	6.8	6 to 6.9
	Water absorption (%)	1.41	Not more than 2%
	Specific gravity	2.66	2.6 to 2.9
	Size (mm)	20-6	>4.75

Table 5. Specifications of the aggregate

Mix ID	Cement	Cenosphere	Water	Calcium Lact	ate (Gm)	Coarse	Fine
	(kg)	(kg)	(Lit.)	0.010 Mol/L	0.015 Mol/L	aggregates (kg)	aggregates (kg) 712.67 712.67 712.67 712.67
CN00-CL0.010	394.32		197.16	607.25		1114.40	712.67
CN2.5-CL0.010	384.46	9.86	197.16	607.25		1114.40	712.67
CN5-CL0.010	374.60	19.72	197.16	607.25		1114.40	712.67
CN7.5-CL0.010	364.75	29.57	197.16	607.25		1114.40	712.67
CN10-CL0.010	354.89	39.43	197.16	607.25		1114.40	712.67
CN00-CL0.015	394.32		197.16		910.88	1114.40	712.67
CN2.5-CL0.015	384.46	9.86	197.16		910.88	1114.40	712.67
CN5-CL0.015	374.60	19.72	197.16		910.88	1114.40	712.67
CN7.5-CL0.015	364.75	29.57	197.16		910.88	1114.40	712.67
CN10-CL0.015	354.89	39.43	197.16		910.88	1114.40	712.67

	Table	6. Mix	proportion	for 1m3	of cenos	phere	based	concre
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calcium lactate (0.010 mol/L) and FAC (0%,2.5%,5%,7.5% and 10%) with calcium lactate (0.015 mol/L). The criteria provided by IS- 456:2000 and IS-10262:2019 are used to determine the ratio of the concrete mix design for M25 and In Table 6, all proportions are described.

The water/cement ratio is a crucial parameter in concrete strength, and its influence becomes more intricate when incorporating cenosphere and calcium lactate. The water/ cement ratio is carefully adjusted to maintain adequate workability while taking advantage of cenosphere. Calcium lactate, as an additive, use as an accelerator for concrete curing, potentially influencing the early strength development. Its use at a specific concentration (0.010 and 0.015 mol/ liter) indicates a precise consideration for the concrete mix's chemical properties and the desired curing rate.

EXPERIMENTATION

Concrete mixtures were divided into two groups; the first specimen set consisted of five concrete mixtures that were made by using FAC instead of OPC, in different combination of 0%, 2.5%, 5%, 7.5% and 10% each & second specimen set consist of two combinations of FAC with different contents of calcium lactate, those two combinations are Concrete with FAC (0%,2.5%,5%,7.5% and 10%) with calcium lactate (0.01 mol/L) and FAC (0%,2.5%,5%,7.5% and 10%) with calcium lactate (0.015 mol/L). The control mix was the concrete mix that did not contain FAC or calcium lactate.

Table 6 lists the precise mix proportions along with their names. As the two sets of mixes were prepared, in the first set FA and CA well mixed together to get uniformity then cement and FAC add as a binder in composition. Dry mixing time is increased by 5-7 minutes over the control concrete mix. Finally calculated the exact amount of water added to the dry mix to get homogeneous and workable concrete. In the second set dry mix was prepared in the same way as that of the first set, but before adding water to the mix, calcium lactate by weight is added to the water and uniformly diluted for 4-5 min afterward the water was added in the dry mix.

The obtained fresh mix was utilized right away to perform a slump cone test to determine its workability; the results are listed in Table 7. Utilizing the special qualities of cenospheres to promote flow and lessen friction within the mixture, cenosphere concrete with a slump range of 104-111mm exhibits high workability and is appropriate for a variety of building applications. According to IS 1199, the slump cone examination is carried out on new laid concrete; the W/C ratio is kept at 0.5 in each mix. Fresh concrete was then poured into the designated mould needed for the various tests. A table vibrating machine was used for achieving the compactness of poured concrete. After 24 h \pm 1 h of air curing, specimens were taken out from the molds and placed for curing in water. The test specimens were taken out from the curing tank after receiving enough curing and allowed to dry at room temperature. At the ages of 7 and 28 days, the specimens are subjected to the standard test using the instructions outlined in IS 516.

Table 7. Properties of fresh concrete

Mix ID	Slump (mm)	Unit Weight (Kg/m ³)
CN00-CL0.01	113	2551
CN2.5-CL0.01	111	2535
CN5-CL0.01	109	2512
CN7.5-CL0.01	107	2443
CN10-CL0.01	105	2398
CN00-CL0.015	111	2565
CN2.5-CL0.015	108	2542
CN5-CL0.015	107	2508
CN7.5-CL0.015	105	2436
CN10-CL0.015	105	2406

RESULT AND DISCUSSION

Plastic and Dry Density

The density is a key index for evaluating the physical and mechanical properties of concrete. The density of material affects the consumption and utilization of the material in the mix, which directly affect the cost of the structure. The density of the concrete mix was measured for freshly laid concrete after 24 hours, for surface saturated concrete after 28 days, and for oven-dry concrete after 24 hours. Table 8 shows the impact of various circumstances noticed on the sample.

The use of FAC and calcium lactate in the mix shows little variation in density. FAC is hollow in nature due to which concrete loses density when the proportion of FAC rises. The addition of calcium lactate in the mix shows linear changes in the density of concrete. From the obtained result it is observed that at FAC 10% replacement of cement shows a 4.62% reduction in density, simultaneously when calcium lactate of 0.010 mol/lit and 0.015 mol/lit is added to the mix it shows 4.69% and 4.80% reduction in density. The obtained result shows density at various percentages of FAC shown in Figure 3.

Compressive Strength

Testing a 150 x 150 x 150 mm cast cube on a compression testing equipment yields information about concrete's compressive strength. Concrete mixes were categorized into two groups to check the effect of FAC replacement with cement and adding of dissolved Calcium lactate on the compressive strength of concrete. Employing IS 10262, the concrete mix was built for M25 grade, and then FAC is added to the mix as a partial substitution of 2.5%, 5%, 7.5%, and 10% for OPC. According to the results, FAC 2.5% replacement provides stronger strength when compared to regular concrete because of cenosphere fineness. But it exhibits a loss of strength when the proportion of FAC rises, this may happen because of its hollow shape and less amount of calcium elements present in FAC. The variation of compressive strength at various percentages of FAC shows in Figure 4.

Further to this two concentrations of calcium lactate were added to the mixture of 0.010 mol/lit and 0.015 mol/ lit. For a uniform mixture of calcium lactate in the mix, calcium lactate was dissolved in water and afterward, it was added to the concrete mix. The obtained result shows compressive strength improvement after the inclusion of CL. The variation of compressive strength at various percentages of FAC shows in Figure 5.

The obtained normal strength of concrete is 32.96N/mm². Addition of FAC 2.5%, 5%, 7.5% and 10% shows linearly decrease in strength, 10% FAC replacement with cement shows strength 30.78 N/mm² which is 6.61%

Days	Control Mix	Cenosphere (10%)	Cenosphere (10%) + Calcium Lactate (0.010)	Cenosphere (10%) + Calcium Lactate (0.015)
1 (Fresh Mix)	2598	2449	2398	2406
28 (SSD)	2612	2507	2479	2457
28 (ODS)	2547	2406	2380	2356

Table 8. Unit weight of concrete (Kg/m³)



Figure 3. Unit weight (Kg/m³) Vs FAC (%).



Figure 4. Compressive strength of FAC concrete at 28 days.



Figure 5. Compressive strength of concrete (Mpa) Vs FAC (%) at 28 days.

decrease in strength, after addition of calcium lactate with 0.010 mol/lit & 0.015 mol/lit shows strength 34.31 N/mm² and 35.73 N/mm² which is 4.09% & 8.40% higher strength than normal concrete.

Failure pattern

A concrete cube was tested on a compression testing equipment with a steadily increasing force, the concrete cube was placed between upper and bottom plate of loading frame afterward hydraulic pressure was applied on the cube which observed from dial gauge of the control panel. The dial gauge shows incremental readings up to the failure of the concrete cube. The failure sample of a cube was taken away from the loading frame and the failure pattern was observed as shown in Figure 6, the matrix shows all ingredients mixed well at the time of mixing and compacted properly. The surface shows no tension zone was observed on the concrete cube. Fine and coarse aggregate shows proper bond with other materials of the matrix, it was also observed that aggregate failure or break in the central portion of a cube, this means all the material used in mix perform well within the limits.

Flexural Strength

To examine the flexural properties of FAC, two points load test was conducted on a beam specimen of size 100 x 100 x 500 mm. After completion of the curing period, the beam specimen sample was thoroughly checked for defects



Figure 6. Failure pattern of compression member.

then demarcation was done on the beam, 50 mm cover was left from both ends of the beam and the remaining span was equally divided into 3 spans of each length of 133 mm. The universal testing machine of force capacity 250 KN was used for the application of uniform loading at the rate of 0.15 mm/min. the beam specimen was kept on the loading frame and two points were applied to a specimen, applied load and deflection of the beam were measured on screen. The flexural strength of the beam was calculated by using the following relation.

$$MR = \frac{PL}{bd^2}$$
(1)

Figure 7 shows the flexural strength comparison between different materials and codes. The obtained result of FAC and calcium lactate compared with IS and ACI code indicate satisfactory application of calcium lactate along with FAC. FAC added in the mix with 2.5%, 5%, 7.5% and 10% replacement with cement exhibits a loss of strength when the proportion of FAC rises, whereas when calcium lactate is added in the mix with 0.010 mol/lit and 0.015 mol/lit shows increasing in strength. The variation of flexural strength with FAC (%) shown in Figure 8.

The 28 days flexural strength of normal concrete reaches up to 4.03 N/mm², when FAC 10% is added in replacement with cement it shows 3.68 N/mm² which is a 8.70% reduction in strength, this might happened due to its shape, hollow nature, and its chemical compositions. When calcium lactate is added to the mix it shows 4.14 N/mm² and 4.28 N/mm² which is a 2.86% and 6.34% increase in strength.



Figure 7. Flexutral strength (MPa) Vs Materials and Codes for replacement of cement by cenosphere (10%).



Figure 8. Flexutral strength (MPa) Vs FAC (%).

Failure Pattern

The beam specimen was placed in the loading frame of the universal testing machine, the arrangement of the loading frame make like; the beam specimen rest on two supports, and a two-point load was applied from the top. Due to the application of gradually applied load the sample beam specimen break from the central portion of the beam. The break sample was taken away from the loading frame and the failure pattern of the beam was observed carefully as shown in Figure 9. The matrix of the broken sample shows a uniform and well mix of all ingredients with each other. The aggregate failure was observed in the concrete section; this shows proper bonding of aggregate with other materials.

Split Tensile Strength

Split tensile strength gives tensile stress resistance capacity of the material, due to application of load tensile cracking get started in concrete which affects the performance of concrete. FAC is versatile material due to its chemical compositions; the combination of FAC with other minerals may show changes in its mechanical properties. To determine the tensile strength of concrete, the samples were prepared with different combinations of FAC and Calcium lactate. The tensile strength of concrete was ascertained using a Universal testing machine with a 250KN capability. The cylindrical sample of 150 mm in diameter and 300 mm in length were used in the test. The testing sample was prepared with FAC 10%, Calcium lactate at 0.01



a) Experimental Setup

Figure 9. Failure pattern of flexural member.



Figure 10. Split tensile strength (MPa) vs materials and codes for replacement of cement by cenosphere (10%).

mol/lit and 0.015 mol/lit. After 28 days of curing the sample were tested as per the guideline of IS 5816. For all the mixes and for each property under consideration, three samples were examined, and the average of these was given for the associated test.

FAC with 10% replacement to cement gives less tensile strength than the result expected from IS code, whereas the addition of calcium lactate of 0.10 mg/lit in the mix increases, the tensile strength of 3.43% above IS code and 4.02% above control mix, similarly, the addition of calcium lactate of 0.15 mg/lit in the mix increases the tensile strength of 9.14% above IS code and 9.77% above control mix. The obtained result present in Figure 10. FAC with 10% lowers the concrete's tensile strength this is caused by the FAC particle's lower strength and increased void

content, however after addition of calcium lactate tensile strength get increases this may happen due to effectively bond between FAC particles. Calcium lactate was found to be effective in bonding between FAC particles.

Failure Pattern

A cylindrical specimen was placed in the universal testing machine, a specimen was placed in such a way that load shall be applied on the longitudinal portion of a cylinder. The Upper and lower plate of loading fame make clean before placing of sample underneath, the cylinder specimen was kept exactly in the center of the plate. Gradually load was applied to the specimen, applied load fails the specimen and divide into two parts exactly from the center half of the specimen as shown in Figure 11. The casted cylinder shows a uniform mix of all ingredients present in the



a) Crack Pattern on cylinderFigure 11. Failure pattern of tension member.

b) Internal material behavior

mix. Fine and coarse aggregate make proper bonding with other materials in the matrix; it is also reflected in broken aggregate surfaces.

CONCLUSION

Cenosphere is waste material increasing its own volume day by day and simultaneously creating problems for the environment. The cenosphere has an advantageous physical property of being light in weight which makes economical and sustainable concrete for the construction industry. The main focus is given on studying the behavior of the cenosphere with other construction materials, its application, and its limitations. Chemical study of cenosphere shows absence of calcium mineral in its composition this affect mechanical property of concrete. The observation of experimentation, results, and discussion gives following conclusion;

- 1. The findings indicate that using cenosphere in place of cement results in a reduction in the weight and density of concrete, making it economical and sustainable.
- 2. Fly ash cenosphere adds incrementally (2.5, 5, 7.5 & 10%) replacing cement into the mix, showing a linear strength reduction due to the absence of calcium in cenosphere concrete.
- 3. Strength may be enhanced at specific percentages due to the cenosphere's involvement in pozzolanic processes and its extremely fine particles. Concrete strength increases little (1.51%) at FAC 2.5 percent.
- FAC 10% replacement of cement shows a 4.62% reduction in density, simultaneously when calcium lactate of 0.010 mol/lit and 0.015 mol/lit is added to the mix it shows a 4.69% and 4.80% reduction in density after 28-days.
- FAC 10% replacement of cement shows a 6.61% decrease in compressive strength, after addition of calcium lactate with 0.010 mol/lit & 0.015 mol/lit shows 4.09% & 8.40% higher compressive strength than normal concrete.
- 6. Flexural strength of typical concrete at 28 days is up to 4.03 N/mm², when FAC 10 % added in replacement with cement it shows 8.70% reduction in strength, after addition of calcium lactate in the mix it shows 2.86% and 6.34% increase in strength.
- FAC with 10% replacement to cement gives 10.34% less tensile strength than the result expected from normal concrete, whereas the addition of calcium lactate gives a 4.02% and 9.77% increase in tensile strength.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Evaluation of COVID-19 mortality using machine learning regression methods based on health system indicators

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ABSTRACT

In the global health crisis caused by the COVID-19 pandemic, countries have faced significant challenges in combating the outbreak in terms of healthcare systems and economies. Evaluating the performance of healthcare systems in dealing with pandemics has become a priority for policymakers, healthcare providers, and the public alike. Assessing the performance of healthcare systems during the pandemic is crucial for preparedness and improvements in similar situations in the future. By identifying complex patterns and relationships, machine learning algorithms aim to uncover the relationship between healthcare system indicators and deaths due to the COVID-19 pandemic, using large and intricate datasets. These algorithms utilize various datasets containing demographic information and medical factors to reveal hidden relationships between various variables and disease severity. The objective of this study is to predict COVID-19 death rates for 27 OECD (Organisation for Economic Co-operation and Development) countries spanning the period from 2006 to 2019 using various machine learning regression methods. Healthcare system indicators, comprising accessibility, healthcare financing, and healthcare workforce, have been aggregated into three dimensions. The dataset includes COVID-19 death counts per a million-population due to the pandemic. Random forest regression, neural network regression, and Gaussian process regression were employed to forecast COVID-19 death rates, and the predictive capabilities of machine learning regression methods were evaluated using k-fold cross validation. The suitability of the algorithms was assessed using statistical measures such as the coefficient of determination (R^2) and root mean square error (RMSE). A high R^2 value and a low RMSE indicate that Gaussian process regression (GPR) can effectively predict COVID-19 death rates, taking various health indicators into account. Machine learning regression methods have revolutionized our understanding of COVID-19 death rates. Through prediction models, machine learning has empowered healthcare professionals with the ability to forecast death risks for individual patients, guiding decision-making processes and resource allocation. According to the research findings, to enhance the performance of healthcare systems in coping with global pandemics, there is a need to prioritize community-based healthcare services, adopt a social policy approach, encourage the use of advanced technology, ensure the trust of the public and healthcare workers, enhance social support opportunities, emphasize the importance of measures by leaders, and support global governance. Additionally, flexible supply chain plans for the procurement of personal protective equipment have been identified as necessary.

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INTRODUCTION

The outbreak of the novel coronavirus disease (COVID-19) in late 2019 has rapidly spread worldwide, leading to a global health crisis. The virus has exhibited a wide range of clinical outcomes, from mild symptoms to severe complications and death in some cases. As COVID-19 continues to spread aggressively, it poses a serious threat to public health and has resulted in the depletion of medical resources and strain on healthcare workers [1-3].

The urgent need to identify factors associated with SARS-CoV-2 transmission, predictors of COVID-19 severity, and effective treatments has become paramount [4]. Resourcelimited areas faced challenges in triaging life-saving therapies due to the high number of infections, emphasizing the importance of identifying patients requiring intensive care or at high risk of mortality [5, 6]. Furthermore, early administration of specific treatments has shown promise in reducing hospitalization duration and decreasing COVID-19 mortality, making it crucial to predict patients at high risk of disease progression and poor outcomes [7]. SARS-CoV-2, the virus responsible for COVID-19, is highly infectious and has spread rapidly across the globe. Its transmission dynamics, including asymptomatic cases and the transmission potential of individuals without symptoms, present unique challenges in controlling the pandemic [8]. Estimating the prevalence of COVID-19 is essential for effective pandemic management [9].

Machine learning, a subfield of artificial intelligence (AI), plays a crucial role in enabling computers to learn and make predictions or decisions without explicit programming [10]. In datasets with numerous independent variables, there might be complex and non-linear relationships that traditional statistical methods struggle to capture. Machine learning algorithms can learn and model intricate patterns within the data. Additionally, they are good with large datasets and a high number of variables, handling them faster than traditional statistical methods [11]. The process of machine learning involves training algorithms on labelled data, where each data point is associated with corresponding target values. Through this training process, algorithms adjust their internal parameters to minimize the disparity between their predicted outputs and the true target values [12]. The objective is to develop models that generalize well and can accurately predict or make decisions on new, unseen data. Machine learning algorithms have wide-ranging ap-plications and have demonstrated success in various domains, including healthcare, finance, natural language processing, computer vision, and recommendation systems [11, 13]. They have the potential to uncover insights and make accurate predictions in complex and data-rich environments, ultimately driving advancements and improving decision-making processes across industries [12-14].

In this study, the primary aim was to identify the relationship between COVID-19 death rates and

healthcare system indicators among 27 countries within the OECD (Organisation for Economic Co-operation and Development) using machine learning regression methods. Healthcare system indicators spanning from 2006 to 2019, encompassing three dimensions accessibility, healthcare financing, and healthcare workforce, were considered as ten different variable datasets. A com-prehensive dataset containing healthcare indicators and COVID-19 death rates for a 14-year period for OECD countries was collected from various databases. To enhance the analysis, a standardization process was applied. Three machine learning regression methods, namely Random Forest Regression (RFR), Neural Network Regression (NNR), and Gaussian Process Regression (GPR), were employed to predict the relationship between COVID-19 death rates and healthcare system indicators. The performance of these methods was evaluated using k-fold cross-validation, and statistical measures such as the coefficient of determination (R^2) and root mean square error (RMSE) were utilized to assess their suitability.

MATERIALS AND METHODS

The study was conducted in four main steps. Firstly, healthcare indicators for OECD countries between 2006 and 2019 were collected from various databases such as World in Data, Worldometer, IHME-GHDx, and Eurostat. Secondly, data processing, especially standardization, was carried out using Matlab 8.3.0.532 (R2014a) software by MathWorks Inc. (Natick, MA, USA). Thirdly, data evaluation techniques such as correlation heat map and variable importance determination were applied. Finally, various machine learning-based regression methods were employed to explore the relationship between COVID-19 death rates and healthcare system indicators. The evaluation of machine learning-based regression methods involved assessing their predictive capabilities using multiple criteria, including the coefficient of determination and root mean square error. Figure 1 provides a visual representation of the research process, illustrating the main steps followed in this study. Subsequent subsections provide comprehensive explanations of each stage in this research.

Data Collection

Healthcare indicators for OECD countries spanning the years 2006 to 2019 were collected from databases such as World in Data, Worldometer, IHME-GHDx, and Eurostat. The used health status indicators, risk factors indicators and service coverage indicators with their explanations were given in Table 1. The study aims to evaluate COVID-19 mortality using a machine learning-based regression method based on health system indicators. Ten indicators, derived from the World Health Organization's 100 essential health indicators and grouped under the dimensions of health workforce, health access, and health financing, were utilized to determine these health system indicators. In the health workforce dimension, indicators such as healthcare



Figure 1. The flow chart outlining the main steps followed in the present study.

Table 1. The used health indicators with their explanati	ons
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Health indicators	Explanation			
Health workforce	Healthcare worker density and distribution - 1 (Medical doctor)			
	Healthcare worker density and distribution - 2 (Dentist)			
	Healthcare worker density and distribution - 3 (Pharmacist)			
	Healthcare worker density and distribution – 4 (Nurses and midwives)			
	Medical graduates, per 100 000 population			
	Dentist graduates, per 100 000 population			
	Pharmacists graduates, per 100 000 population			
	Nursing and midwives graduates, per 100 000 population			
Health access	Total hospital beds per 1 000 population			
Health financing	Total current expenditure on health (% of gross domestic product)			
	Health indicators Health workforce Health access Health financing			

worker density and distribution (medical doctors, dentists, pharmacists, nurses and midwives, medical graduates, dentist graduates, pharmacist graduates, nurses and midwives graduates) were considered. The health access dimension incorporated the indicator of total hospital beds, while the health financing dimension included the indicator of total current expenditure on health as a percentage of gross domestic product (Table 1).

Data Pre-processing

Standardization is a crucial data preprocessing step that involves transforming data to adhere to a standard normal distribution. In a standard normal distribution, the data has a mean of 0 and a standard deviation of 1 [15]. By transforming the data into a standard normal distribution with a mean of 0 and a standard deviation of 1, it becomes more suitable to comparison and analysis across different variables. By applying standardization, the data is rescaled to have a mean of 0 and a standard deviation of 1, facilitating easier comparison and analysis across different variables. This process eliminates the influence of varying scales and units, resulting in data that is more interpretable and suitable for certain statistical techniques and machine learning algorithms [16]. One common method for standardization is z-score standardization, also known as standard score standardization. This approach involves calculating the z-score for each data point, which indicates the number of standard deviations that the data point deviates from the mean [17]. By utilizing the z-score standardization method, the data was transformed into a standard normal distribution in this study. Matlab 8.3.0.532 (R2014a) software was employed for implementing this standardization technique.

Data Evaluation

Ten health indicator variables were subjected to correlation analysis in order to determine if there is any correlation between indicator variables. For this purpose, pearson correlation values [18] were obtained using corr command using Matlab 8.3.0.532 (R2014a). Feature selection and feature importance determination using F-test is a method commonly employed in statistical analysis and machine learning to identify the most relevant features in a dataset [19]. The F-test assesses the significance of the relationship between the target variable and each feature individually, allowing for the selection of features that are most informative for predicting the target variable. The F-test calculates the F-statistic, which is then compared to the F-distribution to determine the significance level. Features with high F-statistic values and low p-values are considered more relevant for the model and are thus selected for further analysis or model building. On the other hand, features with low F-statistic values and high p-values may be considered less relevant and can be excluded from the analysis to simplify the model and avoid overfitting. It is important to note that the F-test assumes certain underlying assumptions, such as the normality of the data and the homogeneity of variances [20]. Violations of these assumptions can affect the reliability of the results. Therefore, it is crucial to interpret the results of the F-test and to consider the specific characteristics of the dataset and the context of the analysis.

Machine Learning Regression and Assessment

The predictive capability of machine learning models can be influenced by two important factors: data bias and data variance [21]. Data bias refers to the systematic errors or inaccuracies present in the training data used to build the machine learning models. If the training data is biased, meaning it does not accurately represent the true underlying patterns in the target variable, the models may produce predictions that are skewed or biased as well. It is crucial to address data bias and ensure that the training data is representative and unbiased to achieve reliable predictions [22]. Data variance, on the other hand, refers to the sensitivity of the machine learning models to fluctuations or noise in the training data. Models with high variance are overly complex and tend to overfit the training data, capturing noise or random fluctuations instead of the true underlying patterns. Such models may perform well on the training data but fail to generalize effectively to new, unseen data. It is essential to strike a balance between model complexity and generalizability to minimize variance and achieve accurate predictions [23].

The process of k-fold cross-validation involves dividing the available dataset into k subsets or folds of approximately equal size [24]. The model is then trained and evaluated k times, with each fold being used as the validation set once while the remaining folds are used as the training set. This ensures that every data point is used for both training and validation, reducing the potential for bias in model evaluation. During each iteration of k-fold cross validation, the model is trained on the training set and evaluated on the validation set. The evaluation metrics, such as accuracy, mean squared error, or area under the curve, are recorded for each iteration. The final performance of the model is typically obtained by averaging the evaluation metrics across all iterations. A 10-fold cross validation method was employed in this study [25].

In the context of the study, three machine learning regression methods were employed: random forest regression (RFR), neural network regression (NNR), and Gaussian process regression (GPR) [26]. Random forest regression (RFR) is an ensemble method that combines multiple decision trees to make predictions. It is known for its robustness against overfitting and ability to handle complex relationships in the data [27]. Neural network regression (NNR) is a type of machine learning model inspired by the structure and function of the human brain. It consists of interconnected nodes, or neurons, organized in layers. NNR has the capability to capture nonlinear relationships and handle large amounts of data [28]. Gaussian process regression (GPR) is a probabilistic machine learning method that models the underlying relationship between input variables and output variables. It assumes that the data follows a Gaussian process, allowing for uncertainty estimation in the predictions. GPR is particularly effective when dealing with small datasets or when uncertainty estimation is important [29].

These three machine learning regression methods were chosen for their unique strengths and capabilities in predicting COVID-19 mortality rates. The selection of these methods allows for a comprehensive evaluation of their prediction capabilities, considering different aspects such as model complexity, interpretability, and uncertainty estimation. By com-paring their performance using statistical measures such as the coefficient of determination (R2) and root mean square error (RMSE), the suitability of each method can be assessed, providing valuable insights into the predictive capabilities of machine learning models for COVID-19 mortality estimation.

To compare the performance of the models, two metrics were utilized, including the coefficient of determination (R2), root mean square error (RMSE), using the equations (1) and (2), respectively [30]:

$$R^{2} = 1 - \left[\frac{\sum_{i=1}^{n} (y_{obs} - y_{pre})^{2}}{\sum_{i=1}^{n} (y_{obs} - \overline{y_{obs}})^{2}} \right]$$
(1)

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} (y_{obs} - y_{pre})^2}{n}}$$
(2)

where y_{obs} is the observed COVID-19 death counts per a million-population, y_{pre} is the predicted COVID-19 death counts per a million-population, $\overline{y_{obs}}$ is the average of observed COVID-19 death counts per a million-population and n is the observation number.

RESULTS AND DISCUSSION

The outbreak of the COVID-19 pandemic in late 2019 presented an unprecedented global health crisis, affecting millions of people worldwide and overwhelming health-care systems. In response to this crisis, machine learning has emerged as a powerful tool for analysing vast amounts of data and extracting meaningful insights. By identifying complex patterns and correlations, machine learning algorithms have played a crucial role in predicting COVID-19 mortality rates and informing critical healthcare decisions.

To investigate potential correlations between ten health indicator variables, a correlation analysis was conducted. The analysis focused on computing Pearson correlation coefficients between the indicator variables (Fig. 2). Fig.2 shows that there is no correlation health indicator among variables, meaning that all health indicator variables can contribute to prediction of COVID-19 mortality rates in machine learning methodology. Subsequently, an F-test was performed to evaluate the significance of the connection between the target variable and each feature individually, facilitating the identification of the most informative features for predicting the target variable (Fig. 3). F-test results show that all ten-health indicator are important for prediction of COVID-19 mortality rates.

Machine learning techniques are well-suited for uncovering complex and non-linear relationships. COVID-19 is a multifaceted disease with interdependencies among numerous factors, and traditional statistical methods may not fully capture the intricacies of these relationships. Machine learning algorithms excel at identifying hidden



Figure 3. The importance scores of health care indicators.

												- 1
HSI1	1	0.6973	0.1016	0.1585	0.4234	0.2673	0.04626	0.02353	-0.2017	0.3646		
HSI2	0.6973		0.4038	0.2548	0.1505	0.2576	0.2233	0.08783	-0.03649	0.336	-	0.8
HSI3	0.1016	0.4038		0.185	-0.1304	0.004202	0.4691	0.03156	0.2683	0.2905		
HSI4	0.1585	0.2548	0.185		0.1399	-0.1294	0.08528	0.4945	-0.07784	0.4894	-	0.6
HSI2	0.4234	0.1505	-0.1304	0.1399		0.1971	0.02565	-0.09816	-0.2718	0.078	-	0.4
HSI6	0.2673	0.2576	0.004202	-0.1294	0.1971		0.5066	-0.1356	-0.1478	-0.04346		
TISH	0.04626	0.2233	0.4691	0.08528	0.02565	0.5066		0.03455	0.004195	0.1465	-	0.2
8ISH	0.02353	0.08783	0.03156	0.4945	-0.09816	-0.1356	0.03455		0.229	0.1203	-	0
6ISH	-0.2017	-0.03649	0.2683	-0.07784	-0.2718	-0.1478	0.004195	0.229		-0.04967		
HSI10	0.3646	0.336	0.2905	0.4894	0.078	-0.04346	0.1465	0.1203	-0.04967	1	-	-0.2
	HSI1	HSI2	HSI3	HSI4	HSI5	HSI6	HSI7	HSI8	HSI9	HSI10		

Figure 2. Correlation map of main predictor variables (the used health indicators).



Figure 4. Histograms depicting the variables are shown for: a) HSI1, b) HSI2, c) HSI3, d) HSI4, e) HSI5, f) HSI6, g) HSI7, h) HSI8, j) HSI9, and j) HSI10.



Figure 5. The observed and predicted COVID-19 mortality using a) random forest regression, b) neural network regression, and c) Gaussian process regression.

Process Training			Validation		Testing	
Regression methods	R ²	RMSE	R ²	RMSE	R ²	RMSE
Random forest regression	0.940	314	0.835	467	0.837	522
Neural network regression	0.980	138	0.841	459	0.884	441
Gaussian process regression	0.997	11	0.951	255	0.971	222

Table 2. Performance evaluation of various regression methods for validation process

patterns and non-linear correlations that may not be immediately apparent through conventional approaches. This provides researchers and healthcare professionals with deeper insights into the complex dynamics of COVID-19 mortality, enabling more informed decision-making and targeted interventions.

The distribution of data frequency for each feature collected in the study is illustrated in Figure 4. The figure provides a visual representation of the number of occurrences or observations for each feature category. This information is valuable for conducting further analysis and drawing meaningful conclusions based on the data collected.

In addition, Supplementary Table displays the average values of each main predictor variable, along with their corresponding standard deviations (σ). These statistics provide an understanding of the central tendency and variability of the data.

The entire dataset was subjected to a random split into two subsets, with 90% allocated for training and 10% for testing. To ensure the robustness of the training process, a 10-fold cross-validation method was utilized. The outcomes of this process, which included both observed and predicted COVID-19 mortality figures, obtained through random forest regression, neural network regression, and Gaussian process regression, are presented in Figure 5. When evaluating the validation results, it becomes evident that the predictions generated by the Gaussian process regression method outperform those produced by random forest regression and neural network regression. In other words, the Gaussian process regression method exhibited a higher level of accuracy and precision in predicting COVID-19 mortality as compared to the other two regression techniques.

The results of the training, validation, and testing processes were displayed in detail in Table 2. Regarding the training results, each of the regression methods demonstrated high predictive performance. The R² values obtained from the machine learning-based regression methods (RFR, NNR, and GPR) ranged from 0.835 to 0.971, while the corresponding RMSE values varied from 222 to 522 (Table 2). Among the machine learning-based regression methods, it was observed that the predictions derived from the Gaussian process regression method surpassed those generated by the random forest regression and neural network regression techniques. This indicates

that the Gaussian process regression method exhibited a higher degree of accuracy and precision in forecasting COVID-19 mortality compared to the other two regression methodologies.

Machine learning regression methods offer valuable tools for predicting COVID-19 mortality based on healthcare indicators. By analysing extensive datasets and leveraging advanced algorithms, these methods can uncover patterns and relationships between various variables and disease severity. The utilization of machine learning techniques in predicting COVID-19 mortality can provide crucial insights for healthcare professionals, enabling them to make informed decisions regarding patient care, resource allocation, and treatment strategies.

CONCLUSION

The Gaussian process regression method outperformed the other two regression techniques (random forest regression and neural network regression) in predicting COVID-19 mortality. These findings offer valuable insights for policymakers and healthcare providers, suggesting the importance of effective healthcare system practices during future pandemics. The study underscores the need for global, national, and local collaboration during crises, highlighting the significance of global governance. It also recommends a review of financing policies to address unexpected financial burdens and protect individuals' financial well-being in public health emergencies. Investments in both healthcare system capacity and the quality of services and healthcare workers are advised for pandemic management. Planning for the supply chain of essential medical resources should occur at global and national levels. Encouraging the development and use of digital technologies can help reduce healthcare access disparities. Community engagement and support are crucial, promoting compliance with necessary measures and fostering shared behaviours. More detailed studies on how investments in healthcare system capacity, service quality improvements, and better support for healthcare workers can be done and their direct impact on pandemic management can be modelled. Additionally, the optimisation works can be done about direct and indirect outcomes of investments in healthcare system.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

An explicit solution of linear conformable systems with variable coefficients

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ABSTRACT

This paper is mainly devoted to exact solutions to the initial value problem for linear conformable systems with variable coefficients. The famous method known as the generalized Peano-Baker series, which inholds the conformable integral, is exploited to acquire the state-transition matrix. A representation of an exact solution in a closed interval for linear confromable systems with variable coefficients is determined with the help of this matrix. It is verified by showing that the determined exact solution satisfies the systems step by step. Moreover, another exact solution in the same closed interval is identified thanks to the method of variation of parameters. The existence and uniqueness of the second exact solution to the systems are provided by the Banach contraction mapping principle. This provides that the representations of the two solutions coincide although they are obtained by completely different approaches and they have completely different structures. A couple of examples are presented to exmplify the use of the findings.

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INTRODUCTION

For many right reasons, such as being a generalization of the traditional derivative and better representing scientific and social problems, the fractional order derivative [1-11], which can be obtained by replacing the integer order with the fractional order, has become a fascinating subject in the theory of functional spaces for a couple of decades. [12-17]. So far, effots have been made to define so many distinct fractional derivatives by many succesful researchers. There is no doubt that the most prevailing employed ones are Riemann-Liouville and Caputo fractional derivatives. They are both introduced by means of fractional integrals. This gives them nonlocal behaviors such as future dependence and historical memory. They satisfy the linearity which is the only feature inherited from the traditional 1st derivative. But including both the above-mentioned ones, the available fractional derivatives in the literatüre have many setbacks. For instance, most of them do not fulfill that fractional derivatives of one are equal to zero except Caputo-type derivatives. All of them do not satisfy the corresponding product rule, the corresponding quotient rule, the corresponding chain rule, the corresponding Rolle theorem, the corresponding mean value theorem, and generally the

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corresponding semigroup property. To deal with some of these flaws, Khalil et al. [18] in 2014 defined the conformable derivative which is a novel fractional derivative and can be seen as an extension of the classical 1st derivative of a function. Dazhi and Maokang [19] in 2017 managed to describe the physical and geometrical interpretations of the conformable derivatives fort he first time.

Various social and scientific phenomena are formulated by means of linear fractional differential systems with variable coefficients, such as linearized aircraft systems, linearized population growth, linearized diffusion of the batteries, and linearized parameters' distribution in the charge transfer. Although there are lots of papers about linear fractional differential systems with constant coefficients and almost all of their aspects are investigated i only a few studies are devoted to linear fractional differential systems with variable coefficients and their explicit solutions. To the best of our knowledge, I can find no paper about such systems and their solutions in the conformable sense where are obtained via generalized Peano-Baker series. [20,21]. Finding current in an electrical circut [22], falling objects with air resistance, or determinig the motion of a rising [23] are included in applications of linear conformable systems with variable coefficients given in (1). In order to obtain an exact solution of a system, there are distinct approaches and methods such as the first integral method [24] which is applied succesfully for solving the comformable Wu-Zhang system with the time-fraction, the new extended direct algebraic method [25] which is used to find the new solitons solutions of the complex Ginzburg-Landau equation with Kerr law nonlinearity, the sine-Gordon expansion approach and the generalized Kudryashov approach [26] which are applied to get exact solitary wave solutions to te Boussinesq model. This paper mainly provides an exact solution to the system by applying the generalized Peano-Baker series approach and the variation of constants method seperately.

In light of the above-cited works, the following linear coformable systems with variable coefficients are taken into consideration

$$\begin{cases} \mathbb{D}_{0}^{\beta}\rho(\varsigma) = A(\varsigma)\rho(\varsigma) + \mathsf{T}(\varsigma), & (\varsigma) \in [0,T], \\ \rho(0) = \rho_{0}, \end{cases}$$
(1)

where \mathbb{D}^{β} represents the conformable derivative of fractional order $0 < \beta < 1$, $\rho: [0, T] \to \mathbb{R}^n$, which is the well-known n-dimensional Euclidean space, is a \mathbb{R}^n – valued function , both the matrix function *A*: $[0, T] \to \mathbb{R}^{n \times n}$ and the function $7: [0, T] \to \mathbb{R}^n$ are continuous.

The results in this paper are presented below.

- (i) A representation of the exact solution of the problem
 (1) is given in terms of determining the state-transition (matrix) function obtained from the generalized Peano-Baker series.
- (ii) Another representation of the exact solution, which is different from the first one, of the problem (1) is offered based on the variation of constants method.

(iii) The existence uniqueness of the global solution of the nonlinear system (9) into a fixed point problem is transferred, which allows us to use the Banach fixed point to prove our main results.

PRELIMINARIES

In this section, a couple of necessary paraphernalia to be available in the literatüre are remembered in order to allow a better understanding of the content af the paper.

Definition 1. [27] A fractional derivative in the conformable sense of order $0 < \beta < 1$ with a lower bound τ of a function μ : $[\tau, \infty) \rightarrow \mathbb{R}$ is given by

$$\mathbb{D}^{\beta}_{\tau}\mu(\varsigma) = \lim_{\sigma \to 0} \frac{\mu(\varsigma + \sigma(\varsigma - \tau)^{1-\beta}) - \mu(\varsigma)}{\sigma}, \quad \varsigma > \tau, 0 < \beta \leq 1.$$

In addition, if $\mu(.)$ is differentiable and $\lim_{\varsigma \to \tau^+} \mathbb{D}^{\beta}_{\tau} \mu(\varsigma)$ exists, $\lim_{\varsigma \to \tau^+} \mathbb{D}^{\beta}_{\tau} \mu(\varsigma) = \mathbb{D}^{\beta}_{\tau} \mu(\tau)$.

Definition 2. [27] The conformable integral of fractional order $0 < \beta < 1$ with a lower bound τ of a function μ : $[\tau, \infty) \rightarrow \mathbb{R}$ is given by

$$\mathbb{J}^{\beta}_{\tau}\mu(\varsigma) = \int_{\tau}^{\varsigma}\mu(s)(s-\tau)^{\beta-1}\,ds, \quad \varsigma > 0.$$

Theorem 3. [27] Let μ be continuous in the domain of $\mathbb{J}_{\tau}^{\beta}$. Then $\mathbb{D}_{\tau}^{\beta}(\mathbb{J}_{\tau}^{\beta})(\varsigma) = \mu(\varsigma), \varsigma \geq \tau$.

Lemma 4. [28] The conformable derivative of fractional order $0 < \beta < 1$ for a function μ : $[\tau, \infty) \rightarrow \mathbb{R}$ exist iff it is differentiable at ς and also $\mathbb{D}^{\beta}_{\tau}\mu(\varsigma) = (\varsigma - \tau)^{1-\beta}\mu'(\varsigma)$ is satisfied.

Lemma 5. [29] The conformable derivative of fractional order $0 < \beta < 1$ of an integral sign is as noted below

$$\mathbb{D}_{0}^{\beta}\left(\int_{-\tau}^{\alpha(\varsigma)}\rho(\varsigma,s)ds\right) = \left(\int_{-\tau}^{\alpha(\varsigma)}\mathbb{D}_{0}^{\beta}\rho(\varsigma,s)ds\right) + \rho(\varsigma,\alpha(\varsigma))\mathbb{D}_{0}^{\beta}\alpha(\varsigma),$$

here, ρ is differentiable w.r.t the first component, and also α and α' are continuous in a finite closed interval.

Homogeneous Linear Systems with Variable Coefficients

In this section, an explicit solution to the homogeneous version of the linear conformable systems with variable coefficients is investigated

$$\begin{cases} \mathbb{D}_{0}^{\beta}\rho(\varsigma) = A(\varsigma)\rho(\varsigma), & (\varsigma) \in [0,T], \\ \rho(0) = \rho_{0}, \end{cases}$$
(2)

here, all of the information is introduced in (1).

Now, the state-transition (matrix) function will be offered to costruct the fundamental structure of the explicit solution to the system (2).

Definition 6. The state-transition (matrix) function of system (2) is defined as noted below

$$\mathcal{X}(\varsigma,\tau) = \sum_{k=0}^{\infty} \mathfrak{I}_{\tau}^{ko\beta} A(\varsigma),$$

where

$$\mathfrak{I}_{\tau}^{0o\beta}A(\varsigma)=I,$$

and

$$\mathfrak{I}_{\tau}^{(k+1)o\beta}A(\varsigma) = \mathbb{J}_{\tau}^{\beta}\left(A(\varsigma)\mathfrak{I}_{\tau}^{ko\beta}A(\varsigma)\right) \ k = 0, 1, 2, \dots,$$

here, *I* and Θ are the n-by-n unit and zero matrices. The series in Definition 6 can be seen and named as the generalized Peano-Baker series. [20,30].

Theorem 7. The state-transition function satisfies the equation (2) with the initial circumstance $\mathcal{X}(0,0) = I$ provided that it is uniformly convergent.

Proof. The mathematical meaning of the statement of this theorem is as follows:

$$\begin{cases} \mathbb{D}_0^{\beta} \mathcal{X}(\varsigma, 0) = A(\varsigma) \mathcal{X}(\varsigma, 0), & (\varsigma) \in [0, T], \\ \mathcal{X}(0, 0) = I. \end{cases}$$

Then let's start showing the satisfaction of the first equation

$$\mathbb{D}_{0}^{\beta} \mathcal{X}(\varsigma, 0) = \mathbb{D}_{0}^{\beta} \sum_{k=0}^{\infty} \mathfrak{I}_{0}^{ko\beta} A(\varsigma)$$
$$= \sum_{k=1}^{\infty} \mathbb{D}_{0}^{\beta} \mathfrak{I}_{0}^{ko\beta} A(\varsigma)$$
$$= \sum_{k=1}^{\infty} \mathbb{D}_{0}^{\beta} \mathfrak{I}_{0}^{\beta} (A(\varsigma) \mathfrak{I}_{0}^{(k-1)o\beta} A(\varsigma).$$

Theorem 3 gives that

$$\mathbb{D}_0^{\beta} \mathcal{X}(\varsigma, 0) = A(\varsigma) \sum_{k=1}^{\infty} \mathfrak{I}_0^{(k-1)o\beta} A(\varsigma)$$
$$= A(\varsigma) \mathcal{X}(\varsigma, 0).$$

One can verify the initial circumstance as follows

$$\mathcal{X}(\varsigma,0) = \mathfrak{I}_0^{0o\beta} A(\varsigma)\Big|_{\varsigma=0} + \sum_{k=1}^{\infty} \mathfrak{I}_0^{\beta} \left(A(\varsigma) \mathfrak{I}_0^{(k-1)o\beta} A(\varsigma)\right|_{\varsigma=0} = I.$$

Theorem 8. $\rho(\varsigma) = \mathcal{X}(\varsigma, 0) \rho_0$ fulfills the equation (2), which means that it is a solution to the given system, provided that it is uniformly convergent.

Proof. In the light of Theorem 7, one can easily get the following equalities

$$\mathbb{D}_0^{\beta}\rho(\varsigma) = \mathbb{D}_0^{\beta}\mathcal{X}(\varsigma,0)\rho_0 = A(\varsigma)\mathcal{X}(\varsigma,0)\rho_0 = A(\varsigma)\rho(\varsigma),$$

and

$$\rho(0) = \mathcal{X}(0,0)\rho_0 = I\rho_0 = \rho_0$$

Corollary 9. When the special case of $A(\varsigma) = A$ (constant) in the system (2) is considered, an explicit solution of the following system

$$\begin{cases} \mathbb{D}_{0}^{\beta}\rho(\varsigma) = A\rho(\varsigma), & \varsigma \in [0,T], \\ \rho(0) = \rho_{0}, \end{cases}$$
(3)

is given by the equation $\rho(\varsigma) = e^{\frac{\varsigma^{\rho}}{\beta}Y}\rho_{0}$, which corresponds to that of [5].

Corollary 10. For the case of $A(\varsigma) = \varsigma^p$, $\rho \in \mathbb{R}^+$, an eplicit solution of the following system

$$\begin{cases} \mathbb{D}_{0}^{\beta}\rho(\varsigma) = \varsigma^{p}\rho(\varsigma), & \varsigma \in [0,T], \\ \rho(0) = \rho_{0}, \end{cases}$$
(4)

is offered by

$$\rho(\varsigma) = e^{\frac{\varsigma^{\beta+p}}{\beta+p}Y} \rho_0.$$

Proof. One can begin with the following calculation of the state-transition function as follows:

$$\begin{split} \mathfrak{I}_{0}^{0o\beta}\varsigma^{p} &= 1\\ \mathfrak{I}_{0}^{1o\beta}\varsigma^{p} &= \mathfrak{I}_{0}^{\beta}(\varsigma^{p}\mathfrak{I}_{0}^{0o\beta}\varsigma^{p}) = \mathfrak{I}_{0}^{\beta}\varsigma^{p} = \frac{\varsigma^{\beta+p}}{\beta+p},\\ \mathfrak{I}_{0}^{2o\beta}\varsigma^{p} &= \mathfrak{I}_{0}^{\beta}(\varsigma^{p}\mathfrak{I}_{0}^{1o\beta}\varsigma^{p}) = \mathfrak{I}_{0}^{\beta}\varsigma^{p}\frac{\varsigma^{\beta+p}}{\beta+p} = \frac{\varsigma^{2(\beta+p)}}{2(\beta+p)^{2}},\\ \mathfrak{I}_{0}^{3o\beta}\varsigma^{p} &= \mathfrak{I}_{0}^{\beta}(\varsigma^{p}\mathfrak{I}_{0}^{2o\beta}\varsigma^{p}) = \mathfrak{I}_{0}^{\beta}\varsigma^{p}\frac{\varsigma^{2(\beta+p)}}{2!(\beta+p)^{2}} = \frac{\varsigma^{3(\beta+p)}}{3!(\beta+p)^{3}},\\ \vdots\\ \mathfrak{I}_{0}^{no\beta}\varsigma^{p} &= \mathfrak{I}_{0}^{\beta}(\varsigma^{p}\mathfrak{I}_{0}^{(n-1)o\beta}\varsigma^{p}) = \mathfrak{I}_{0}^{\beta}\varsigma^{p}\frac{\varsigma^{(n-1)(\beta+p)}}{(n-1)(\beta+p)^{(n-1)!}}\\ &= \frac{\varsigma^{n(\beta+p)}}{n!(\beta+p)^{n}}. \end{split}$$

It follows from Definition 6 and the just-above information that one writes the corresponding state-transition function as noted below

$$\mathcal{X}(\varsigma,0) = \sum_{n=0}^{\infty} \mathfrak{I}_0^{no\beta} \varsigma^p = \sum_{n=0}^{\infty} \frac{\varsigma^{n(\beta+p)}}{n! \, (\beta+p)^n} = e^{\frac{\varsigma^{\beta+p}}{\beta+p}}.$$

According to Theorem 8, the solution to the system 4 is given by $\rho(\varsigma) = e^{\frac{\varsigma^{\beta+p}}{\beta+p}}\rho_0$. This concludes the proof.

Remark 11. The solution in Corollary 10 reduces to that of [31] for p = 0.

NONHOMOGENEOUS LINEAR SYSTEMS WITH VARIABLE COEFFICIENTS

In this section, an explicit solution to the nonhomogeneous version of the linear conformable systems with variable coefficients is investigated

$$\begin{cases} \mathbb{D}_{0}^{\beta}\rho(\varsigma) = A(\varsigma)\rho(\varsigma) + \Im(\varsigma), & \varsigma \in [0,T], \\ \rho(0) = \rho_{0}, \end{cases}$$
(5)

here, all of the information is introduced in (1).

Theorem 12. The solution $\rho(\varsigma)$ of (5) fulfilling zero initial circumstance $\rho(0) = 0$ has the following integral form

$$\rho(\varsigma) = \int_0^{\varsigma} \mathcal{X}(\varsigma, s) \, \Im(s) s^{\beta - 1} ds$$

Proof. By employing Theorem 3 and Lemma 5, one acquires

$$\begin{split} \mathbb{D}_{0}^{\beta}\rho(\varsigma) &= \mathbb{D}_{0}^{\beta}\int_{0}^{\varsigma}\mathcal{X}(\varsigma,s)\,\mathsf{T}(s)s^{\beta-1}ds\\ &= \int_{0}^{\varsigma}\mathbb{D}_{0}^{\beta}\mathcal{X}(\varsigma,s)\,\mathsf{T}(s)s^{\beta-1}ds + \mathsf{T}(\varsigma)\\ &= \sum_{n=1}^{\infty}\int_{0}^{\varsigma}\mathbb{D}_{0}^{\beta}\mathbb{J}_{s}^{\beta}\left(A(\varsigma)\mathbb{J}_{s}^{(n-1)o\beta}A(\varsigma)\right)\mathsf{T}(s)s^{\beta-1}ds + \mathsf{T}(\varsigma)\\ &= A(\varsigma)\int_{0}^{\varsigma}\sum_{n=1}^{\infty}\mathfrak{T}_{s}^{(n-1)o\beta}A(\varsigma)\mathsf{T}(s)s^{\beta-1}ds + \mathsf{T}(\varsigma)\\ &= A(\varsigma)\int_{0}^{\varsigma}\mathcal{X}(\varsigma,s)\mathsf{T}(s)s^{\beta-1}ds + \mathsf{T}(\varsigma). \end{split}$$

Theorem 13. The solution $\rho(\varsigma)$ of (5) has the following integral form

$$\rho(\varsigma) = \mathcal{X}(\varsigma, 0)\rho_0 + \int_0^\varsigma \mathcal{X}(\varsigma, s) \mathsf{7}(s) s^{\beta - 1} ds.$$
 (6)

Proof. The proof is an immediate result of Theorem 8 with Theorems 12.

Remark 14. For $\beta = 1$, and $A(\varsigma) = A$, the integral equation in Theorem 13 makes into the following integral equation

$$\rho(\varsigma) = e^{A\varsigma}\rho_0 + \int_0^{\varsigma} e^{A(\varsigma-s)} \, \Im(s) ds$$

which is, as it is well known, the analytical solution to the following first order Cauchy system

$$\begin{cases} \rho(\varsigma) = A\rho(\varsigma) + 7(\varsigma), & \varsigma \in [0, T], \\ \rho(0) = \rho_0. \end{cases}$$

Example 15. The below nonhomogeneous linear conformable system with variable coefficients is examined

$$\begin{cases} \mathbb{D}_{0}^{\beta}\rho(\varsigma) = \begin{pmatrix} 0 & 0\\ \varsigma & 0 \end{pmatrix}\rho(\varsigma) + \begin{pmatrix} 0\\ 1 \end{pmatrix}, \quad \varsigma \in [0,T], \\ \rho(0) = \begin{pmatrix} 0\\ 1 \end{pmatrix}. \end{cases}$$
(7)

One firstly determines the state-transition matrix of the system (7) step by step by using its definition

$$\begin{split} \mathfrak{I}_{0}^{0o\beta}A(\varsigma) &= I \\ \mathfrak{I}_{0}^{1o\beta}A(\varsigma) &= \mathbb{J}_{0}^{\beta}\left(A(\varsigma)\mathfrak{I}_{0}^{0o\beta}A(\varsigma)\right) = \mathbb{J}_{0}^{\beta}A(\varsigma) = \mathbb{J}_{0}^{\beta}\begin{pmatrix} 0 & 0 \\ \varsigma & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \varsigma^{\beta+1} & 0 \end{pmatrix} \\ \mathfrak{I}_{0}^{2o\beta}A(\varsigma) &= \mathbb{J}_{0}^{\beta}\left(A(\varsigma)\mathfrak{I}_{0}^{1o\beta}A(\varsigma)\right) = \mathbb{J}_{0}^{\beta}\begin{pmatrix} 0 & 0 \\ \varsigma & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ \varsigma^{\beta+1} & 0 \end{pmatrix} = \mathbb{J}_{0}^{\beta}\begin{pmatrix} 0 & 0 \\ \varsigma & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \varsigma & 0 \end{pmatrix} \\ \mathfrak{I}_{0}^{3o\beta}A(\varsigma) &= \mathbb{J}_{0}^{\beta}\left(A(\varsigma)\mathfrak{I}_{0}^{2o\beta}A(\varsigma)\right) = \mathbb{J}_{0}^{\beta}\begin{pmatrix} 0 & 0 \\ \varsigma & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \varsigma & 0 \end{pmatrix} \\ \mathfrak{I}$$

In brief, one has

$$\mathfrak{I}_0^{0o\beta}A(\varsigma) = I, \mathfrak{I}_0^{1o\beta}A(\varsigma) = \begin{pmatrix} 0 & 0\\ \frac{\varsigma^{\beta+1}}{\beta+1} & 0 \end{pmatrix}, \mathfrak{I}_0^{no\beta}A(\varsigma) = \begin{pmatrix} 0 & 0\\ 0 & 0 \end{pmatrix}, n \ge 2.$$

Then the system's state-transition matrix is given by

$$\mathcal{X}(\varsigma,0) = \sum_{k=0}^{\infty} \mathfrak{I}_0^{ko\beta} A(\varsigma) = \mathfrak{I}_0^{0o\beta} A(\varsigma) + \mathfrak{I}_0^{1o\beta} A(\varsigma) = \begin{pmatrix} 1 & 0\\ \frac{\varsigma^{\beta+1}}{\beta+1} & 1 \end{pmatrix}.$$

Then the analytical solution of the system (7) is given by

$$\begin{split} \rho(\varsigma) &= \mathcal{X}(\varsigma, 0)\rho_0 + \int_0^\varsigma \mathcal{X}(\varsigma, s)\mathsf{T}(s)s^{\beta-1}ds \\ &= \begin{pmatrix} 1 & 0\\ \frac{\varsigma^{\beta+1}}{\beta+1} & 1 \end{pmatrix} \begin{pmatrix} 1\\ 0 \end{pmatrix} + \int_0^\varsigma \begin{pmatrix} 1 & 0\\ \frac{\varsigma^{\beta+1}}{\beta+1} & 1 \end{pmatrix} \begin{pmatrix} 0\\ 1 \end{pmatrix} s^{\beta-1}ds \\ &= \begin{pmatrix} \frac{1}{\varsigma^{\beta+1}} \\ \frac{\varsigma^{\beta+1}}{\beta+1} + \frac{\varsigma^{\beta}}{\beta} \end{pmatrix}. \end{split}$$

Remark 16. Until here, uniformly convergent infinite series involving nested compositions of fractional integrals in the conformable sense to represent the solutions is used. In a way, this can be seen as a fractional approach and it has a setback such as being uniform convergence.

Now, an explicit solution of the same system (5), which can be also called as a conformable linear differential equation of fractional order $0 < \beta < 1$, will be investigated by variation of constants technique. Firstly, one looks for a solution of its linear case.

$$\begin{split} \mathbb{D}_{0}^{\beta}\rho(\varsigma) &= A(\varsigma)\rho(\varsigma) \Rightarrow \varsigma^{1-\beta}\rho'(\varsigma) = A(\varsigma)\rho(\varsigma) \\ \Rightarrow \frac{\rho'(\varsigma)}{\rho(\varsigma)} &= A(\varsigma)\varsigma^{\beta-1} \\ \Rightarrow \ln\left(\frac{\rho(\varsigma)}{\rho(\varsigma)}\right) &= \int A(\varsigma)\varsigma^{\beta-1}d\varsigma \\ \Rightarrow \rho(\varsigma) &= C(\varsigma)e^{\int A(\varsigma)\varsigma^{\beta-1}d\varsigma}. \end{split}$$

Let's get into the system (5) with the just-above equation to determine $C(\varsigma)$,

$$\begin{split} \mathbb{D}_{0}^{\beta}\left(C(\varsigma)e^{\int A(\varsigma)\varsigma^{\beta-1}d\varsigma}\right) &= A(\varsigma)C(\varsigma)e^{\int A(\varsigma)\varsigma^{\beta-1}d\varsigma} + \mathsf{T}(\varsigma),\\ C(\varsigma)\mathbb{D}_{0}^{\beta}e^{\int A(\varsigma)\varsigma^{\beta-1}d\varsigma} + e^{\int A(\varsigma)\varsigma^{\beta-1}d\varsigma}\mathbb{D}_{0}^{\beta}C(\varsigma) &= A(\varsigma)C(\varsigma)e^{\int A(\varsigma)\varsigma^{\beta-1}d\varsigma} + \mathsf{T}(\varsigma),\\ &\Rightarrow C(\varsigma) &= \int e^{-\int A(\varsigma)\varsigma^{\beta-1}d\varsigma}\mathsf{T}(\varsigma)\varsigma^{\beta-1}d\varsigma + K. \end{split}$$

Then, one of explicit solutions of the system (5) is given by the following continuous integral equation

$$\rho(\varsigma) = e^{\int A(\varsigma)\varsigma^{\beta-1}d\varsigma} \left[e^{-\int A(\varsigma)\varsigma^{\beta-1}d\varsigma} \mathsf{T}(\varsigma)\varsigma^{\beta-1}d\varsigma + K \right], \quad (8)$$

where $K \in \mathbb{R}$ is an integration constant.

Remark 17. In one respect, this approach appears one of the advantages of conformable derivatives among other available fractional derivatives.

Remark 18. Under the variable transform $\rho(\varsigma) = u(\varsigma)$ $v(\varsigma)$, one can easily get the same integral equation (8).

Corollary 19. The following continuous integral equation

$$\rho(\varsigma) = e^{\int A(\varsigma)\varsigma^{\beta-1}d\varsigma} \left[\int e^{-\int A(\varsigma)\varsigma^{\beta-1}d\varsigma} \mathsf{T}(\varsigma)\varsigma^{\beta-1}d\varsigma + K \right],$$

is a global solution of the following nonlinear conformable system with variable coefficients

$$\begin{cases} \mathbb{D}_{0}^{\beta}\rho(\varsigma) = A(\varsigma)\rho(\varsigma) + \Im(\varsigma,\rho(\varsigma)), & \varsigma \in [0,T], \\ \rho(0) = \rho_{0}. \end{cases}$$
(9)

Theorem 20. Assume that the nonlinear function is a Lipschitzian with a $L_7 > 0$ and $\frac{T^{\beta}}{\beta}L_7 < 1$. Then the system (9) has an unique solution on [0, T] with T > 0.

Proof. Let C[0, T] be the well-known continuous Banach space endowed with the infinity norm $\|.\|_{\infty} = \sup_{\varsigma \in [0,T]} \|\rho(\varsigma)\|$ for a norm $\|.\|$ on \mathbb{R}^n . Define the operator $\mathcal{H}: C[0, T] \to C[0, T]$ by

$$\mathcal{H}\rho(\varsigma) = e^{\int A(\varsigma)\varsigma^{\beta-1}d\varsigma} \left[\int e^{-\int A(\varsigma)\varsigma^{\beta-1}d\varsigma} \mathsf{T}(\varsigma,\rho(\varsigma))\varsigma^{\beta-1}d\varsigma + K \right].$$

For $\rho, \nu \in \mathbb{R}^n$, one can get the below inequality

$$\|\mathcal{H}\rho(\varsigma) - \mathcal{H}\nu(\varsigma)\| \leq \frac{T^{\beta}}{\beta} L_{\mathsf{T}} \|\rho - \nu(\varsigma)\|_{\infty},$$

which implies that \mathcal{H} is a contraction. Based on the Banach fixed point theorem, \mathcal{H} has an unique fixed point on [0, T]. So, the system (9) has an unique solution on [0, T].

Remark 21. According to Theorem 20, by the uniqueness of solutions, the closed-form solution in (6) coincides with the explicit continuous solution in (8).

Example 22. If the system (4) in Corollary 10 with the initial circumstance is reconsidered, based on the representation of the solution in (8), one can get

$$\rho(\varsigma) = e^{\int \varsigma^p \varsigma^{\beta-1} d\varsigma} K = e^{\frac{\varsigma^{p+\beta}}{p+\beta}} K.$$

The initial circumstance $\rho(0) = \rho_0$ provides $\rho(\varsigma) = e^{\frac{\varsigma^{p+\beta}}{p+\beta}}\rho_0$, which is the same solution in Corollary 10.

Example 23. If the system (7) in Example 15 with the initial circumstance is reconsidered, based on the representation of the solution in (8), one can get

$$\begin{split} \rho(\varsigma) &= e^{\int_{0}^{\varsigma} \binom{0}{\varsigma} = 0} \varsigma^{\beta-1} d\varsigma} \left[\int_{0}^{\varsigma} e^{-\int_{0}^{\varsigma} \binom{0}{\varsigma} = 0} \varsigma^{\beta-1} d\varsigma} \binom{0}{1} \varsigma^{\beta-1} d\varsigma + K \right] \\ &= e^{\left(\frac{\varsigma^{\beta+1}}{\beta+1} = 0\right)} \rho_{0} + e^{\left(\frac{\varsigma^{\beta+1}}{\beta+1} = 0\right)} \int_{0}^{\varsigma} e^{\left(\frac{\varsigma^{\beta+1}}{\beta+1} = 0\right)} \binom{0}{1} \varsigma^{\beta-1} d\varsigma \\ &= \left(\frac{1}{\varsigma^{\beta+1}} = 0\right) \binom{1}{0} + \left(\frac{1}{\varsigma^{\beta+1}} = 0\right) \int_{0}^{\varsigma} \left(-\frac{1}{\varsigma^{\beta+1}} = 0\right) \binom{0}{1} \varsigma^{\beta-1} d\varsigma \\ &= \left(\frac{1}{\frac{\varsigma^{\beta+1}}{\beta+1}} + \frac{\varsigma^{\beta}}{\beta}\right), \end{split}$$

which is the same solution in Example 15.

CONCLUSION

The state-transition matrix is obtained from the generalized Peano-Baker series. An explicit solution to the linear homogeneous and nonhomogeneous conformable systems with variable coefficients is derived based on this state-transition matrix. Another explicit solution of the same system is acquired with the help of the variation of constants method. These obtained solutions are shown to coincide on the closed interval by the fixed point theorem. By solving some examples with two different solutions, the results are verified to match. Again, the same examples are used to illustrate the results.

As a future work, one can discuss different kinds of stabilities and distinct sorts of controllability of linear conformable Dynamics with variable coefficients. As another future work, one can also introduce a conformable Riccatitype differential equation and a conformable Bernoullitype differential equation annd investigate their solutions.

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AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Spatial analysis of earthquakes in and around the northern Anatolian Fault Zone

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ABSTRACT

Earthquakes are seen to be complex phenomena when their occurrence reasons are investigated. Factors such as the presence of a fault line and between earthquake relationships like foreshocks, mainshocks, and aftershocks may be considered as some of the sources for this complexity. Estimating the earthquake risk and modeling the earthquake intensities over a region is vital in minimizing future tangible and intangible losses. The principle aim of this study is to examine the clusters and seismicity of moderate to major earthquake occurrences in the North Anatolian Fault Zone (NAFZ). For this purpose, a rectangular region including the NAFZ is selected as a study region to analyze the earthquake patterns. Attributes of moderate to major earthquakes with a magnitude higher than 5, which are listed regarding time interval and space domain in the earthquake catalog, are visualized owing to exploratory data analysis techniques. Spatial patterns for the earthquakes are revealed, and simulations of the earthquakes are realized using spatial processes within the specified time and space domain. Intensity changes and related earthquake risks are disclosed. The western part of the region is classified as having a higher risk for future earthquakes because of having higher previous earthquake and magnitude intensities.

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INTRODUCTION

The reach for spatial data is getting more accessible with the advancements in technology and GIS (Geographic Information Systems). Cressie [1] proposed a still valid classification for spatial data according to study region (or domain) properties. According to this classification, spatial data can be grouped into geostatistical data, spatial point patterns, and lattice data. This classification is essential for the right choice of analysis according to data type. Earthquakes according to the domain properties fit into the class of spatial point patterns as spatial data. In spatial point pattern terminology, these incidences are noted as events to discriminate the other arbitrary points in the study region. There is no restricted region for earthquake occurrences, and earthquake epicenters can be discriminated from random points in the area. The main difference in spatial point patterns compared to other types of spatial data is the randomness of the domain.

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Al- Ahmadi et al. [2] used global and local spatial point pattern techniques to detect clusters of seismicity of the earthquake occurrences in the Red Sea for the period 1900-2009 according to the specific magnitude ranges. They also produced spatial versions of the central tendency and dispersion measures according to ranges of magnitudes for the selected time and space domains.

Öztürk [3] analyzed characteristics of seismic activity along the North Anatolian Fault Zone between 1970 and 2010 using several numbers of statistical parameters such as namely size-scaling parameters (such as the slope of recurrence curve *b*-value), seismic quiescence *Z*-value, the temporal and spatial distribution of earthquakes with the characteristic of fractal correlation dimension, *Dc*, as well as the histograms of temporal, spatial and magnitude distributions.

Akol and Bekler [4] applied a probabilistic hazard analysis to earthquakes with magnitude $M.C \ge 3.0$ occurred in the region of NW Turkey covering Gelibolu and Biga Peninsulas period between 1912 and 2007. The region is divided into four subduction zones regarding seismotectonic properties. Sayil [5] estimated the recurrence intervals for large earthquakes at 7 different zones in the Marmara region limited with coordinates of 39°-42°N, 25°- 32°E. Coban and Sayil [6] modeled earthquake hazard by using 3 different probability model along the North and East Anatolian fault zones. Sayil [7], used statistical approaches using a data consist of a historical and instrumental period in six sub-regions of Marmara region. Earthquake recurrences were obtained by using Poisson statistical distribution models meanwhile Gutenberg-Richter relationship were employed to determine the seismic hazard parameters.

Turkey has long been suffered from devastating earthquakes and has active fault zones like North Anatolian Fault Zone (NAFZ). The NAFZ is the most important one amongst them, extending approximately 1200 km from the east through the country's west coast. It was described in the late 1940s, and it became one of the best-studied strikeslip fault zones on Earth [8-9] In addition, it has got one of the most seismologically active faults in the world with a broad-arc shape [10-11].

The most recent major earthquakes that occurred over the region were İzmit (M_s =7.8) and Düzce (M_s =7.2) earthquakes of 17 August and 12 November 1999 respectively that they caused enormous economic loss and death of many residents around the region. Nowadays, a major earthquake is expected in the western region of the NAFZ through the Marmara-Sea, which may affect one of the most populated metropolitans of the world's İstanbul.

Bohnhoff et al. [10] compiled and examined the historical earthquake catalogs by dividing the NAFZ into three sub-regions. They found out that the expected earthquake in the Marmara- Sea region would not exceed 7.5, most probably according to their work on historical earthquake catalogs (maximum observed event magnitudes) and other structural analysis and parameters.

Study region including the NAFZ is selected from the database with longitudes 26°- 40°E and latitudes 39.5°- 41.5°N. Study region and North Anatolian Fault Zone with faults and deformations are given in Figure 1.

Recent spatial analysis of seismicity is required for NAFZ, especially from major earthquakes since there is an expectancy of a major earthquake near Istanbul. This study examines the characteristics of moderate to major earthquakes in the NAFZ. Clusters of moderate to high magnitude earthquakes are obtained. The higher intensity and lower intensity regions of the NAFZ is determined using kernel density estimation methods. The earthquake simulations according to past earthquake intensities are performed to predict possible patterns of earthquake occurrences. The spatial point pattern type of the earthquake point pattern is revealed. This study region can be divided into sub-regions for the detailed application of earthquake simulations. This might change the spatial point pattern type, which can be different from our region choice.



Figure 1. North Anatolian Fault zone along with the rectangular study region (modified from Bohnhoff et al. [9], with permission from Elsevier).

SPATIAL POINT PATTERNS AND PROCESSES

Stochastic mechanisms underlying a spatial point pattern are described as a spatial point process. A spatial point pattern realizes a process in two-dimensional space $Z(\mathbf{s})$: $\mathbf{s} \in D \subset \mathbb{R}^2$, while *D* is a random domain and $Z(\mathbf{s})$ is the attribute value-dependent to location \mathbf{s} . Spatial point patterns are classified into three groups: Complete Spatial Random (CSR) patterns, Regular patterns, and Clustered patterns. Shabenberger and Gotway [12] describe CSR with two important conditions satisfied:

- i) Intensity $\lambda(s)$, the average occurrence number of events in a unit area must be homogenous over domain *D*.
- ii) Let A₁ and A₂ be two non-overlapping sub-regions. The event numbers in these two sub-regions must be independent and fit into a Poisson distribution.

 $\lambda(s)$, the (first-order) intensity of a spatial point process is described as a limit and as a function of **s** as follows:

$$\lambda(\mathbf{s}) = \lim_{v(ds)\to 0} \frac{E(N(ds))}{v(ds)}$$
(1)

In equation (1), v(ds) is the area of an infinitesimal disc in \mathbb{R}^2 centered at **s**. The CSR's stochastic mechanism is the spatial Poisson process (homogenous Poisson process).

Many point patterns are somehow generated from CSR. Events can be independent in the non-overlapping region in a study domain; however, they do not satisfy the condition of having homogenous event numbers in the unit area. In some areas of the field, the intensity might be higher, whereas in some might be lower. Events might also have an interaction with each other. The presence of an event might prevent another event occurrence or might cause the occurrence of another event. Deviations from CSR patterns are clustered and regular patterns [12].

If above condition (i) is not satisfied when condition (ii) is satisfied, an inhomogeneous Poisson process is realized. The two following properties characterize the inhomogeneous Poisson process.

If the conditions of CSR are not satisfied, a clustered pattern is considered when there might be some sub-regions of a domain with a higher average event count than other sub-regions. There is no homogenous intensity over the domain for such patterns. Also, some events can attract other events in nearby regions, resulting in a clustering pattern.

In the same manner, some events can prevent another event from occurring. A regular pattern follows a standard scheme. In this pattern, the average distances between an event and its nearest neighbor are lower than CSR distances.

TESTS FOR CSR

There are different types of tests based on point distances or interactions of points or basic tests like quadrat counting based on goodness of fit to check whether a pattern fits into CSR or not. In these tests, a test statistic or generally function values under the null hypothesis when the theoretical pattern is a realization of a homogenous Poisson process is compared with the observed pattern's test statistic or functional importance. According to the specific function values or test statistic value, the null hypothesis will be rejected or fail to be rejected. When an observed pattern is found to fit into CSR, it is assumed to realize the homogenous Poisson process.

The alternative hypothesis of CSR testing depends on the background knowledge about the point pattern, which can usually be regularity or clustering [13]. For a regular-shaped spatial domain, distributional properties of quadrat counts are easy to establish. However, some approximations like the closed form of a test statistic and its asymptotical properties may not perform well for irregular-shaped spatial domains because of the rare events in quadrats and edge effects. In such circumstances, relying on simulation techniques like Monte Carlo tests and simulation envelopes may be the options to test CSR patterns [12].

A Monte Carlo test is a simulation test based on the simulations from the null hypothesis; for example, a theoretical distribution or point process in our case. Monte Carlo tests are frequently used in nonparametric statistics, a particular case of randomization tests [14]. Applications of Monte Carlo tests to spatial statistics can be found in Ripley's studies. [15-16]

For instance, one generates m independent simulations from CSR inside the study domain D and estimates the functions for each of the realizations. After evaluating these functions, one can obtain the pointwise lower and upper envelopes of these simulated functions, which are curves of distance-based functions in this case. The null hypothesis of CSR is rejected when the point pattern's estimated function values remain outside these envelope values [14].

Quadrat Counting Test for CSR

Quadrat testing is one of the simplest and primitive tests for evaluating CSR patterns. This test is considered for only regular shaped and bounded study domains. Quadrats are standard rectangular or squared shapes of equal area. Study domain *D* is split up into non-overlapping quadrats row-wise and column-wise with similar areas, and then the event numbers for each quadrat are counted. The union of these non-overlapping sub-regions must form the study domain *D*.

The bounded study domain *D* is partitioned into *r* rows and *c* columns. Let n_{ij} is the number of events in the quadrat *ij* and $\bar{n} = n/(rc)$ the expected number of events in each quadrat under CSR, while *n* is the total number of events in the study domain *D*. The chi-square test is given in equation (1) [12].

$$\chi^{2} = \sum_{i=1}^{r} \sum_{j=1}^{c} \frac{(n_{ij} - n)^{2}}{\overline{n}}$$
(2)

This test statistic is a Chi-square test for the goodness of fit test of a null hypothesis. The n point is distributed uniformly and independently in *D*. In other words, quadrat counts are independent Poisson variates with a typical mean CSR pattern. The disadvantage of the test is the heavy influence of the subjective choice of the quadrat size.

G Function (nearest neighbor distances)

Nearest neighbor distance analysis examines the most relative event distances for each event in a study domain. In a closest neighbor-based test of CSR pattern, the theoretical most relative neighbor distances of CSR pattern are compared with the observed patterns nearest neighbor distances [17].

The empirical distribution function of G is given below for n events when r_i denotes a distance from an event to its nearest neighbor event in D.

$$\widehat{G}(r) = \frac{1}{n} \sum_{i} I(i: r_i \le r)$$
(3)

It is the indicator function; the summation counts the number of nearest neighbor distances for all events when the condition $r_i \leq r$ holds and r is an arbitrary distance in equation (3). The empirical nearest neighbor function $\hat{G}(r)$ is interpreted as the probability of an observed nearest neighbor of a point appearing at any given distance r. Therefore, it is used as a function that determines the level of clustering or regularity [17].

One important thing to consider is the edge effects when applying tests based on distances. There could be the nearest neighbor outside our study domain *D*, causing biased nearest neighbor distances near the domain's boundary. Therefore applying edge effects are important [17-18].

The distribution function under CSR is given below when edge effects are ignored:

$$P(N(D) = n) = \frac{e^{-\lambda \nu(D)} \lambda^n \nu(D)^n}{n!}$$
(4)

Here λ is intensity while N(D) is several events in D and v(D) is the area of D. Under CSR, the probability of having no events for an event is $e^{(\lambda \pi r^2)}$ if πr^2 the area of a disc is centered on the target event for the searching nearest neighbor in the defined disc.

Hence, the nearest neighbor distribution function for CSR is given by:

$$G(r) = 1 - e^{-(\lambda \pi r^2)}, r \ge 0$$
 (5)

Higher values for small r from an empirical distribution function for a clustered pattern when compared with function values under CSR and lower values for a regular pattern.

F function (empty space function)

This test is also known as the point to nearest event distance test. This test measures the distance from the arbitrary point to its nearest event in a study domain. The empirical distribution function of F is given below from sample points (arbitrarily chosen in the region) when r_i denotes a distance from an arbitrary point to its nearest neighbor event in D.

$$\widehat{F}(r) = \frac{1}{m} \sum_{i} I(i; r_i \le r)$$
(6)

In the same manner, ignoring the edge effects under CSR, the distribution function for space distances are given below:

$$F(r) = 1 - e^{-(\lambda \pi r^2)}, r \ge 0$$
(7)

It is expected that for a regular pattern, $\hat{F}(r)$ observed empty space distances could be greater than its theoretical counterpart F(r). On the other hand, values $\hat{F}(r) < F(r)$ advocate that the point pattern's empty space distances are shorter than the empty space distances for a Poisson process, resulting in a clustered pattern.

J Function

J function is a mixture of both *F* and *G* functions that are described below [19]:

$$J(r) = \frac{1 - G(r)}{1 - F(r)}$$
(8)

This equation holds only when $r \ge 0$ and $F(r) \ne 1$. In the case of CSR, F(r) = G(r) is expected so that the value of J(r) = 1 if G(r) is greater than (r), which means J(r) > 1 then point pattern is a clustered pattern, whereas if F(r) is greater than G(r) so that J(r) > 1 then point pattern is a clustered pattern.

K Function

The weakness of the F and G functions described before is their dependence on nearest neighbor distances for each event. Therefore, it can be a major problem, considering where nearest neighbor distances are very short relative to other distances in the pattern for clustered patterns. K functions rely on all distances in a sub-region of a study window [16].

Ripley [16] described the *K*- function as $\lambda K(r)$ is the expected number of other points of the process within a distance *r* of a specific point of the process.

Observed pairwise distances described as $d_{ij} = ||x_i - x_j||$ form a biased sample of pairwise distances in the point process, with a bias on the side of smaller distances because the maximum distance can be observed the diameter of the window for a pairwise distance [14].

The expected number of points for a disc containing a typical point of the process is $\lambda \pi r^2$ when *r* is the radius of the disc and λ is the intensity of the homogenous Poisson process. Therefore, it is $K(r) = \pi r^2$ independent from the intensity.

Numerous estimators of K have been proposed. The general form of the weighted and renormalized empirical distribution functions of pairwise distances is given below, where (EU,v,r) is the edge correction weight:

$$\widehat{K}(r) = \frac{1}{\widehat{\lambda}^2 v(D)} \sum_i \sum_{J \neq i} I\left\{ \left| \left| x_i - x_j \right| \right| \le r \right\} e(x_i, x_j, r)$$
(9)

Likewise, for other functional values, we compare $\hat{K}(r)$ with K(r), the theoretical counterpart under the Poisson process. If $\hat{K}(r) > \pi r^2$, then the observed pattern is a clustered one, whereas if $\hat{K}(r) < \pi r^2$ is a clustered one.

Intensity Estimation with Kernel Density Functions

Nonparametric smoothing methods are popular because of assumption-free properties and the use of original data set to estimate the probability distribution function. One of the most familiar methods of this data for univariate density is histograms. Kernel functions are probability density functions themselves. They must be even functions. Moving kernel functions can be used to estimate the number of events for an area in the study region instead of using fixed grids to determine the number of events in quadrat counting.

This method is mostly used to obtain smooth estimates of univariate (or multivariate) probability densities from an observed sample of observations [20]. Gatrell [21] explained that the estimation of intensity for a spatial point pattern resembles estimating bivariate probability density.

The Gaussian kernel function is given in equation (10) and is selected as a kernel function to estimate the intensity for this study for the study window:

$$K(\mathbf{x}) = \frac{1}{2\pi} \exp\left\{-\frac{(\mathbf{x} - \mathbf{x}_i)^2}{2}\right\}$$
(10)

A two-dimensional kernel density estimator with a fixed bandwidth is given below in equation (11) [20]:

$$\hat{f}(\mathbf{x}) = \frac{1}{nh^2} \sum_{i=1}^{n} K\left\{\frac{1}{h}(\mathbf{x} - \mathbf{x}_i)\right\}$$
(11)

In equation (11), **x** is the location of any location in the study area, the bandwidth of the kernel function *K*, n is the

number of earthquakes, and \mathbf{x}_i is the location of each earthquake. The drawback of this method is to find the optimum bandwidth (h) to estimate the intensity. There are also adapted smoothing methods in which the bandwidth in the study region changes according to the low and high density of the moving windows for the whole study region.

APPLICATION

Earthquakes higher than magnitude 5.0 occurred between the years 1950 and 2017 were obtained from the database of KOERI. (Bogaziçi University, Kandilli Observatory and Earthquake Research Institute).

Data is downloaded as an earthquake catalog with several variables, including occurrence date and time, magnitude and depth of earthquakes, and spatial information of latitudes and longitudes. Declustering algorithms was not performed, and the article is presented as a numerical example. The biggest earthquake scales were selected for the study because all earthquakes in downloaded data was measured in a different scale. As we are examining a narrow range of magnitudes which are moderate to major earthquakes homogeneity of magnitudes would not be a great issue. Spatial analyses, basic statistics about earthquakes, and earthquake visualizations were performed in core R, ssbase, and spatstat and aspace packages [22-26]. In the first part of the application section, exploratory data analysis will be mentioned. Spatial point pattern analysis for the earthquake pattern will be given in the second part.

Exploratory Data Analysis

To discriminate the magnitude distribution over the region, distinct point characters are employed in Figure 2. It is clearly seen that from the map in Figure 2, earthquakes greater than magnitude 7.0 only occurred in the western part of the study region. In addition, it can be inferred that the middle part and eastern part of the region is unproductive about treating moderate to major earthquakes.



Figure 2. Distribution of earthquake epicenters according to three different magnitude ranges over the selected region.



Figure 3. Distribution of earthquake epicenters according to three different magnitude ranges and four different focal depth ranges over the selected region.

In Figure 3, both magnitude and depth distributions are given in a map with different color coding and point characters. In this way, it is easy to recognize both features for a given earthquake. Most of the earthquakes can be classified as shallow earthquakes because of the low depth earthquake occurrences under 20 km.

In Figure 4, central tendency measures like mean center and variability measures like a standard ellipse for earthquake point patterns are given. The change in magnitudes over the region is low because of both the choice of the data and rare frequencies of magnitude 7 higher earthquakes. Therefore, the mean center and weighted mean center according to magnitudes overlap approximately the center of the study region. However, the standard deviational ellipse reflects the variability far better than the standard distance by taking into consideration both axes separately.

In Figure 5, the number of earthquake incidences are given yearly. The devastating İzmit and Gölcük earthquakes triggered another seismicity period of aftershocks in 1999. Therefore, there are high event occurrences because of the high magnitude events' aftershock effect In Figure 6, the depths of earthquakes are given. It can be inferred that most of the earthquakes occurred between 0 and 40 km depths. Hence, they can be classified as shallow events from this figure too.

One of the important parameters reflecting this relationship that is employed by seismologists frequently in



Figure 5. Yearly earthquake incidences.



Figure 4. Central tendency and variability measures for earthquake point pattern (ellipse: standard deviational ellipse, circle: standard circle, plus: mean center; cross: weighted mean center of earthquake point process).



Figure 6. Depth distribution of earthquake occurrences.

literature is Gutenberg-Richter law, and it is commonly expressed as below:

$$logN(m_i > m) = -bm + a \tag{12}$$

In equation (12): N denotes the number of events with magnitude m_i greater than some threshold m, and b is the log-linear constant which is a determinant of proportionality called the b-value. The constant a is described as a function of the total number of counts in the sample at m=0 is the cumulative structure [25].

A large value of b can be interpreted as more alike events in terms of magnitudes are likely, while a small value can be interpreted as a larger range of magnitudes. To calculate bvalue, Aki [27] proposed a maximum likelihood approach:

$$\hat{b} = \frac{\log(e)}{\overline{m} - (m_{min} - \Delta m/2)},$$
(13)

where \overline{m} is the magnitude average, m_{min} is the magnitude threshold $\Delta m/2$ is a correction for finite binning.

In addition, Aki [27] described the standard error of this estimation as:



In Figure 7, histograms of magnitude are given. As it is seen clearly, both log frequencies and frequencies decrease when the magnitudes are high. A benefit of this representation is that it gives insight into the right-skewed exponential relationship about frequency-magnitude distribution.

The change of *b* -values within their standard error bars according to the different magnitude completeness values is given in Figure 8. The b-value is relatively stable approximating to 1 below a cutoff $m_c = 6.5$; the b-value estimate at $m_c = 5$ is 0.92 with a standard error of 0:08.

In Figure 9, a scatter plot of magnitude and depth is given with the measured linear correlation coefficient. A low positive correlation coefficient (r=0.09) is the indicator that there is no relationship between depths and magnitudes of moderate to major earthquakes.

In Figure 10, deviations from the mean earthquake frequency graph are given. In this graph, earthquake frequencies in a training period are taken into consideration, and this period's earthquake frequency is compared with



Figure 8. Magnitude cut-off values with associated b- value estimations.



Figure 7. Magnitude distribution and log magnitude distribution of earthquake occurrences.


Figure 9. Scatterplot of magnitude and Depth variables.



Months From January 1950 (Training Period: 2010.01 - 2016.12)

Figure 10. Reverse cumulative sum graph of deviations from the mean frequency.

other periods' earthquake frequencies. It is an example of time series graphs called reverse cumulative sum graphs. It must be examined left to right direction-wise and increases in mean value is a sign of the increase in frequency when compared with the training period. On the other hand, the decline of the mean value is a sign of a decrease in earthquake frequency when compared to the training period. In the 600-800 days' period, the time mean earthquake occurrences is less than the occurrences of the training period. Meanwhile, mean earthquake occurrences are increasing after the earthquakes that occurred in 1999 that started with 600th day today 0.

Spatial Point Pattern Analysis

It is an interesting subject whether CSR pattern holds or not for earthquakes as a spatial point pattern. The subject of having CSR for an earthquake spatial point pattern depends on several criteria. Study window, time domain of the study, and magnitude range of the earthquakes are some examples that can be given for these criteria. Also, earthquake occurrence types contribute to this matter. Devastating earthquakes may create aftershocks of lower magnitudes may provide a clustering scheme in the given study window.



Figure 11. Empty space distances.

Visually examining some of the distance measures defined in the previous sections may give researchers a lead about the point pattern type before moving on to the statistical tests. In Figure 11, empty space distances of the earthquake pattern are given. A high distance from an arbitrary point to an event is shown in hot colors, whereas low distances are shown in cold colors and are a sign of a neighborhood event close to an arbitrary point.

The nearest neighbor distances are given in Stienen Diagram in Figure 12. In this diagram, each event's distance to a neighbor event is shown as a circle whose diameter changes proportionately on each event. Therefore, small nearest neighbor distances are illustrated as a point.

A realization of the homogenous Poisson process in the selected study window and the earthquake pattern are given together in Figure 13. It is highly important to visually examine and compare patterns visually before performing the tests about determining the pattern type of a spatial point pattern.

Determination of intensity anomalies in a point pattern is one of the most prominent problems in point pattern





Figure 12. Stienen Diagram.



Figure 13. Realization of homogenous Poisson process (CSR pattern above) and the earthquake pattern (below).



Figure 14. Intensity image alone (above) and superimposed earthquake pattern together with the intensity image (below).



Figure 15. Magnitude intensities over the region.

analysis. Hot spots and cold spots are defined as the regions which have higher and lower intensities compared to the mean intensity of the study window, respectively. Hot spots are also considered as a sign of the possible formation of clustering and the regions of possible clustering. The easiest way to achieve obtaining hot and cold spots in the estimation of intensities through the study region is via kernel density estimation using kernel functions. [14]. Intensity estimation with kernel density estimation and the superimposed earthquake pattern to intensity image is given in Figure 14.

In Figure 14, it can be inferred from superimposed pattern to intensity image how well the pattern coincides with the estimated intensity along the study region. From cold colors to hot colors, the intensity increase is observed within the several high-intensity clusters. If the NAFZ is classified into three groups as western, middle, and eastern parts, the middle part has got the lowest intensity when compared to other parts.

In Figure 15, the magnitude intensity image together with the earthquakes represented as circles according to their magnitude size over the region is given. In the middle region of the NAFZ, cold colors are dominant. Therefore, it can be inferred that earthquakes of magnitude around 5 occurred in neighborhood locations. In the western and eastern parts of the NAFZ, magnitude intensities increase approximately 6 with a few areas of cold color, which means magnitude intensities approximately 5.

Quadrat counts, along with their expected event count and residual values, are given in Figure 16. The whole study region is divided into 24 quadrants of equal area. In the CSR pattern, a similar event count is expected in each quadrat. However, important differences in the event count through quadrats are detected. As a result of the chi-square test, the probability is found to be approximately zero. Hence, the pattern in the analysis does not belong to a homogenous poison process which is the stochastic mechanism under the CSR pattern.

In Figure 17 and Figure 18, distance-based tests for CSR and simulation envelopes for these tests are given. From both figures, according to the results, the earthquake pattern is revealed as a clustered pattern. The H_0 hypothesis of the observed pattern is CSR is rejected because of separately higher G values, lower F values, lower J, and higher K values in the whole 4 tests.

0 4.7	1 4.7	2 4.7	4 4.7	1 4.7	0 4.7	1 4.7	0 4.7
-2.2	1.7	. ±1.*2	-0,33,	+ -1.7	-2.2	-1.7	-2.2
21 47	+12 4.7+	++30++4+7	4+4.7	► 5 4 .7	2 4.7	2 4.7	0 4.7
🍷 7.5+_+	≠+3 ⁺ 4	12	-0.33 +	0.1+3	⁻ -1.2	, . 4.2	-2.2
7 47	+ 5 4,7	≠ ⁺6[*] 4 .7	0 4.7	⁺ 1 4.7	0 4.7	_ 9 ⁺ 4 ! 7	0 4.7
1.1 1	0.13	* 0.6	-2.2	-1.7	-2.2	2	-2.2

Figure 16. Quadrat counts.



Figure 17. Distance-based tests for CSR.



Figure 18. Simulation envelopes for CSR.



Figure 19. Earthquake pattern (above) and simulated inhomogeneous Poisson process (below).

In simulation envelopes, none of the observed functional values are between the lower and upper boundaries of theoretical counterparts. Therefore, the initial results are supported by using simulation envelopes.

In Figure 19, earthquake patterns and simulations of earthquakes with inhomogeneous Poisson processes are given. The similarity between the two patterns is remarkable. Changing intensities over the region are taken as changing intensities for simulation of inhomogeneous Poisson process. This simulation may give future predictions of the possible earthquakes by taking past earthquake occurrences into account.

RESULTS AND DISCUSSION

In this study, clusters of seismicity for moderate to major earthquakes in and around the NAFZ between the years 1950 and 2017 were aimed to obtain. Moreover, point pattern analysis was applied to determine the pattern of the selected earthquakes. With the use of distance-based tests and quadrat analysis, a clustered pattern was revealed for the pattern in the selected study region within the selected time domain. Both kernel density estimation and the quadrat analysis indicate that the higher seismicity intensity and seismicity clusters are formed in the middle -western through the Marmara Sea and in the south-eastern parts of the NAFZ. The middle part of the NAFZ is the least productive part of the NAFZ, both according to the intensity and total earthquake count measures. Earthquakes with higher magnitudes were concentrated through the western parts. Exploratory data analysis was performed to reveal the relationships between magnitude and depth distributions, frequency magnitude, frequency depth, and recent earthquake frequency and time. Useful distance measures were plotted to examine the empty space and nearest neighbor distances over the region.

The consistency of the magnitude cut-offs and *b*-values were examined. Through the magnitudes between 5 - 6 and six *b*-values are consistent. Simulations for the study

region were performed both to determine the pattern type and to predict future earthquakes. Inhomogeneous Poisson process was employed for the future earthquake predictions with changing intensity according to the earthquake pattern's intensity. Therefore, spatially similar earthquake clusters were formed with higher intensities.

Upon the study region, magnitude range, and time-domain changes, the findings of our study would change. For instance, eastern middle, and western parts of the NAFZ can be examined individually for cluster formations, exploratory data analysis, earthquake parameters like b-values for both moderate to major and whole earthquakes above a certain magnitude rather than our choice of moderate to major earthquakes.

Akol and Bekler [4] found that the triangle of Gelibolu-Tekirdağ western part of Marmara Sea is the dangerous area concerning earthquake occurrence of the largest magnitude with 7.3 within a 100-year period. This occurrence was determined to be 46 % according to the Poisson distribution. According to Sayil [5] the total earthquake activity constant a and *b*-value was higher in the golf of Saros sub region which located in the most western part of the fault zone. Sayıl [7] stated that next earthquakes can occur in seismogenic source 6 (Bandırma) with the highest probabilities. Öztürk [3] analyzed the NAFZ by using the seismotectonic b-value, fractal dimension Dc-value, precursory seismic quiescence Z-value. In addition, correlations of these parameters were compared with each other. Regions that has Highest Z-value with the lowest b-value and the highest Dc-value are the vicinity of the Düzce fault and the Black Sea coast. By using orthogonal regression, a strong correlation negative correlation coefficient was found between Dc and b-values for the NAFZ and its vicinity (r=-0.98). Öztürk [28] examines the seismic activity characteristics along the NAFZ between 1970 and 2010. b-values were typically close to 1 according to the study. Eight significant abnormal zones throughout the North Anatolian Fault Zone were detected after a statistical analysis to spot the seismic quiescence after 2010. Coban and Sayil [6] calculated the conditional probability for earthquake occurrence (Mw \geq 5.5) employing according to three different probabilistic models for the three regions along the NAFZ and EAFZ. By using the interevent time of earthquakes, model parameters were calculated under the condition of MLE (Mw \geq 5.5) between 1900 and 2016 in the regions. As a result, they found out that the short-time earthquake probabilities are high in regions. The limitation of the study is the assessment of earthquakes specific parameters (only whole region-specific b- value is used without interpreting temporal spatial forms along the region) with exploratory spatial data analysis. However, spatial point pattern analysis and exploratory spatial analysis might give insights to researchers studying seismology. Therefore, these type of studies would be a plot for statical analysis of earthquakes, probabilistic hazard analysis and interpretation of seismic parameters temporally and spatially. Our exploratory data

results are consistent with literature in terms of high earthquake activity in western parts of the fault and large earthquakes were expected with a higher quality in this region with a higher probability according to other studies.

CONCLUSION

In this study, large earthquakes on the NAFZ were analyzed with the help of point processes and descriptive spatial data analysis. Graphical analyses were used and tools such as spatial distribution of these earthquakes, intensities, magnitude intensities, earthquake-free areas, inter-earthquake gap graphs were used. In addition to seismotectonic characteristics, these tools can also be used to sub-regionalize study areas, especially along fault lines. The characteristics of high magnitude earthquakes in the study area along and around the fault line were analyzed. The *b*-value was calculated as 0.92 for the lowest magnitude cut off value. Large earthquakes can be fit to a spatially inhomogeneous Poisson process because they are affected by the shape of the fault line and have highly diverging spatial intensities. With the help of these analyses, it can be concluded that large magnitude earthquakes occur mostly in the western part and the central part has less seismicity.

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https://github.com/cenkicoz26/doktora-tez-depremsekiller

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Numerical investigation of free rotor aerodynamics

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ABSTRACT

Rotor aerodynamics is important for rotary-wing aircraft especially those located in naval surface combatants. The aerodynamic interaction between the helicopter, its rotor and the ship structure should be investigated precisely. This study focuses on the aerodynamic performance of four-blade rotor geometry of Sikorsky S-76 helicopter. The main rotor geometry was analyzed numerically in the free condition in an unbounded flow domain. Unsteady Reynolds-Averaged Navier-Stokes (URANS) equations in rigid body motion (RBM) on unstructured grids were solved by discretizing the computational domain with finite volume elements and using the Shear-Stress Transport (SST) k- ω turbulence model. The numerical approach was verified using the GCI method and validated with the relevant data available in the literature. It was found that in hover condition, non-dimensional thrust and the torque coefficients change slightly with the rotation speed of the rotor due to possibly the collective pitch angle. However, whereas the torque coefficient varies slightly with rotor speed, the thrust coefficient fluctuates substantially.

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INTRODUCTION

Ship aerodynamics is a crucial research area that combines naval architecture and aerospace engineering. Given the ship's large superstructure, which includes electronic devices, radars, weapon systems and masts, understanding the airflow around it becomes significant for the fixed/ rotary wing aircraft operating within the ship's airwake. This brings to light the interaction between the ship, the helicopter, and its rotor. In this regard, several studies can be found in the open literature enlightening the rotor aerodynamics and its interaction with the ship superstructure. Such studies can traditionally be performed by three different approaches: experimental, numerical, and on-site studies. The latter one includes the recovery maneuvers by the pilots during the take-off and landing operations while experimental studies are performed in wind tunnels and/or towing tanks with scaled models. Finally, numerical studies leverage computational fluid dynamics (CFD), wherein governing flow equations are solved utilizing models representing helicopter-ship dynamic interference or a hovering main rotor operating near ship structures [1].

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For helicopter operations, the hovering capability is of paramount importance, and it also imposes constraints on design, particularly in terms of power requirements. Aerodynamics theorists have proposed several wake models to predict hover performance such as one-dimensional (1D) momentum theory or disc actuator theory, blade element momentum theory, BEMT (an improved version of the 1D momentum theory), dynamic-inflow (finite-state) model, prescribed-wake model, free-wake model. The latest advancements have led to the implementation of an improved model known as the wake-capturing model, which serves as a high-fidelity computational fluid dynamics (CFD) method [2].

The ship-helicopter interaction during the hovering was investigated numerically by Wakefield et al. [3] for the helicopter rotor. Only the main rotor of Westland Lynx aircraft was considered. The rotor was located over the center point of the flight deck of the generic ship called Simple Frigate Ship (SFS) under the wind speed of 40 knots. The studies were performed for the headwind, the wind approaching from a beam of the ship on the starboard side at 90°. The studies proved that CFD solutions are generally able to predict large-scale flow phenomena. Lee and Zan [4] investigated the interaction of the rotor and ship experimentally. Canadian Patrol Frigate and CH-124 helicopter fuselage were used, and the rotor of the helicopter was located at different hover positions. Interaction that results from complex flow field between the main rotor wake and the fuselage of a model helicopter was experimentally investigated by Gregorio et al. [5] with the aid of Particle Image Velocimetry (PIV) in a low-speed wind tunnel. They considered the isolated ONERA 7AD fuselage with a rotating hub without blades and the fully equipped helicopter model with a four-bladed rotor for a wide range of mission envelopes. All tests were done with a constant rotor speed of 956 rpm (revolution per minute). It was shown that the rotor wake has a strong influence on the fuselage and its drag. Different wind angles were investigated and a wind envelope was obtained. In the study of Barakos et al. [6], rotor effects were investigated numerically using the Canadian Patrol Boat (CPB). When the actuator disc method was used, coupling effects were observed in the positions where the rotor was close to the ship. These effects do not appear in the superposition method. Results compared with experimental data showed that rotor loads vary between closeto-deck flight and forward flight. In another study [7], the authors performed numerical calculations to determine the helicopter rotor effects for the Canadian Patrol Frigate. By solving the Navier-Stokes equations using the actuator disk method, the airwake around the helicopter and rotor was simulated. As a result, it was shown that different air loads can occur on the helicopter fuselage close to the deck. Jain and Potsdam [8] focused on the validation of the S-76 model-scale rotor through Computational Fluid Dynamics (CFD) using the HPCMP CREATETM-AV Helios software suite. High-resolution, time-accurate simulations were

conducted for various collective angles and two different tip Mach numbers. The obtained results, encompassing performance, air loads, and tip-vortex trajectory data, were compared to test measurements. Excellent agreement was observed for the entire range of collective angles studied. In a thesis work [9], the author investigated the airwake flow problem for the SFS2 model using RANS and Large Eddy Simulation (LES) solver. The ship model was simulated in different positions using the ship motion data of similar-sized ships available in the literature. Following this, the helicopter rotor effect was simulated with an actuator disc for different deck inclination angles. Perera et al. [10] studied the aerodynamics of the helicopter rotor of Bell 212 helicopter consisting of a 2-blade NACA 0012 airfoil profile. The study was carried out in three stages. Hover, vertical and forward flight conditions were analyzed by the blade element method and momentum theory. SST k-epsilon was used as the turbulence model in the study. Shi et al. [11] focused on the numerical investigation of a helicopter landing on a shipboard. They used two methods for modeling rotor effects. First, the steady rotor model (SRM) based on the momentum source approach was utilized. The other model is the unsteady rotor model, which is derived from the moving overset mesh. It was observed that both models can capture complex interactions well. Sahbaz et al. [12] investigated the effects of ground effect on helicopter performance. It is demonstrated experimentally and numerically that the same thrust can be obtained with lower power consumption by changing the flow thrust value from the ground to the blades. In addition, the study was repeated using rotating ground. The rotating floor eliminated the advantages of the ground effect and created a chaotic structure. As a result of the movement of the ground, unsymmetrical vortexes were formed. This was shown to be risky for helicopter operations. Abras et al. [13] analyzed the effects of the mesh algorithm on the hover condition using the S-76 main rotor. Also, the effects of the rotor hub on the performance were investigated. It was reported that the effect of hub-induced effects is small and the blade tip grid refinement and leading edge and trailing edge grid refinement have greater effects on the results. In the study of Tan et al. [14], blade aerodynamics and unsteady air loads for a tandem rotor of a CH-46 helicopter were numerically investigated using the panel method. Surface effects were calculated on the model scale Landing Helicopter Assault (LHA) ship. The results were compared with the experimental results of NASA Ames Research Center. It was discovered that the vertical velocities determined by numerical calculations matched those of the experiments. Kara et al. [15] investigated time step size and sub-iterations on the integrated parameters for a four-bladed Sikorsky S-76 rotor by higher order Galerkin off-body discretization method to solve flow equations on unstructured meshes. The numerical studies were performed for the Reynolds number based on the reference chord (Re=1.2x106), the tip Mach number of Ma=0.65 and the rotations of $1/2^{\circ}$, $1/4^{\circ}$ and $1/10^{\circ}$. It

was found that smaller time steps speed up the convergence rates however, the thrust coefficient does not change considerably with time steps. In their study, Barakos et al. [16] discussed the rotor wakes using the rotor momentum theory. Three-dimensional (3D) load effects and tip losses were determined by the actuator disc method. Numerical studies using the SST k-w model were performed for fully turbulent flow. As a result of numerical studies with the actuator disk, the vortex structures around the rotor disk were modeled precisely. The study of Bardera et al. [17] focused on the helicopter rotor-ship interaction experimentally. PIV measurements were obtained for various scenarios by mimicking the rotor effect of a Sea King navy helicopter on a frigate. The helicopter rotor was placed in different positions to investigate the ground effect on the helicopter's performance. Ibacoglu and Arikoglu [18] developed a new methodology for main rotor blades and investigated their performance and structural characteristics by considering several parameters. They validated their numerical and experimental data with the test results of Sikorsky UH-60 and S-76 helicopters for hover and forward flight conditions at 750 constant rpm. Upon good agreement, it was shown that by means of the developed methodology thousands of concepts can be evaluated in a very short time. Effect of blade tip shape of four-bladed and Mach scaled Sikorsky S-76 in hover condition was studied in terms of rotor performance, blade airloads, tip-vortex strength and positions [2]. They tested Spalart-Allmaras and SST k-omega turbulence models and implied that both are consistent with the experimental data at all thrust levels.

This study is centered on the numerical investigation of helicopter rotor aerodynamics in free conditions. Unlike fixed-wing aircraft, helicopters are more intricate, relying on a single component known as the rotor for lift, thrust, and control [18]. Consequently, understanding rotor aerodynamics is paramount. In this context, a Sikorsky S-76 four bladed rotor geometry was used. The rotor was analyzed in hover conditions at various rotor velocities and one headwind (40 knots) wind velocity, crucial for maneuvers involving descending and suspending. Numerical analyses were conducted using commercial CFD software with URANS equations as governing equations. The numerical uncertainty was determined using the GCI method with respect to grid size. Rotor parameters were acquired at different advance ratios of the rotor blade and 40 knots relative wind velocity, and results were validated for hover conditions at maximum rotor revolution using available data from the literature. Finally, the numerical results were discussed in terms of rotor rpm versus non-dimensional thrust force, providing detailed insights into the effects of varying rotor and wind velocities.

In some rotor aerodynamic studies, it is seen that the interaction between ship and rotor is frequently analysed. Ashok and Rauleder investigated the complex aerodynamic interactions between the rotor and ship airwakes during the landing of rotorcraft on ship decks. Conventional

simulations of one-way couplings, in which the rotor reacts to the ship's airwake but not the other way around, may overlook important events, particularly when the ship is moving. This work used a Graphics Processing Unit (GPU) accelerated Lattice-Boltzmann Method for one- and twoway coupled ship-rotorcraft interactional simulations, using the NATO Generic Destroyer as a model. The results demonstrated clear frequency profiles and differences in closed-loop pilot response between one-way and two-way coupling schemes, and they agreed well with wind tunnel measurements [19]. Fernandez et al. examined the unstable aerodynamic loading on a helicopter within the airwake of a typical destroyer undergoing different ship motions. The study takes into account several modeling methodologies and finds very slight variations in helicopter loads among various motion kinds. Nevertheless, in instant load and air-velocity spectra as well as RMS (root mean square) loads, the effects of ship motion are particularly noticeable. Thrust load spectra show dominant peaks and harmonics at the ship motion frequency, especially in normal 2-DOF(degree of freedom) ship motions and sinusoidal pitching. These results elucidate the links between ship airwake and helicopter loading and their effects for flight operations, offering fundamental insights into the interplay between the turning rotor and the moving ship[20]. In order to study the aeroelasticity of a rotor in shipboard helicopter operations, Yu et al. developed a loose coupling model for computational fluid dynamics and computational structural dynamics (CFD/CSD). This model uses a CFD solver based on Reynolds-averaged Navier-Stokes (RANS) equations and a CSD solver based on the moderate deflection beam model to predict the aeroelastic behavior of the rotor during engagement and disengagement with ship motions. The efficiency of the simulation is verified through comparison with experimental data. According to the analysis, elastic deflection has a substantial effect on the aerodynamic forces of the blades under certain wind-over-deck situations. Increasing wind direction and angles may result in considerable negative elastic twist deflection, which increases the possibility of a decline in aerodynamic forces and possible over deflection [21]. Zamiri and Chung aimed to explore the impact of wind direction and the bow section of a ship on turbulent flow characteristics in the airwake during shipboard operations, employing delayed detached eddy simulation (DDES). Numerical simulations were conducted with two ship models, Simple Frigate Shapes 1 and 2 (SPF1 and SFS2), at a scale of 1:12.5, considering seven wind direction angles. The DDES results were validated against experimental data from Kulite pressure sensors and Particle Image Velocimetry (PIV) sensors at various ship deck locations. The findings indicated minimal influence of the ship's bow on both the airwake flow and deck flow-field. However, an increase in wind direction angles correlated with elevated turbulent kinetic energy, heightened asymmetry in the flow-field, and increased pressure fluctuations

and unsteadiness over the ship deck, underscoring the significance of these factors in shipboard operations [22].

COMPUTATIONAL METHOD

This paper specifically delves into the rotational behavior of a helicopter rotor equipped with four blades under hover and headwind conditions. Hovering, a crucial phase preceding a helicopter's landing on the ship's flight deck, entails maintaining a constant position. During this phase, the lift and thrust generated by the rotor system counteract the weight and drag forces acting in the opposite direction. In addition to this, a headwind condition was considered as 40 knots considering the effects of the ship and wind together.

In the current work, it is assumed that the rotor is fully rigid and isolated, and it is hovering out-of-ground. The numerical setup consists of the computational domain, boundary conditions, grid generation and physics modeling. The details of each process are given below.

Rotor Geometry

The rotating rotor under investigation in the present study is the one used on the Sikorsky S-76 helicopter. The Sikorsky S-76 is a medium-sized helicopter suitable for marine operations and hence used by many navies. Table 1 gives some of the features of the rotor used on Sikorsky S-76. The 3D CAD (computer-aided design) model generated using the data extracted from the report [23] is given in Figure 1. As stated in Table 1, the rotor blades use SC1013R8, SC1095R8 and SC10954 airfoils.

The rotor used on the Sikorsky S-76 consists of four blades with a blade radius of 6.7056 m. The full-scale model

 Table 1. S-76 main rotor particulars [23], with permission from Frontiers

Parameter	Value
Rotor diameter (m)	13.4112
Rotor solidity	0.0748
Number of blades	4
Airfoil sections	SC1013R8, SC1095R8, SC10954
Rotor area (m ²)	141.262
Rotor velocity (RPM) (100%)	293
Rotor tip velocity (m/s) (100%)	205.747

of the rotor was used in the present study. As shown in Figure 1, the rotor tip was taken as rectangular.

Governing Equations

The numerical analyses were conducted using commercial CFD software Star CCM+ developed by Siemens PLM to solve URANS equations. The governing equations are the continuity and the momentum equations [24,25] considering the flow is unsteady, incompressible and turbulent. The continuity equation can be given as:

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{1}$$

The mean momentum equations can be written in tensor notation and Cartesian coordinates.

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[v \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right] - \frac{\partial \overline{u'_i u'_j}}{\partial x_j} \quad (2)$$



Figure 1. The rotor blade airfoil and chord distributions from [2] (a), 3D view of one blade (b) and rotor configuration (c) of Sikorsky S-76.

Here, ρ depicts the fluid density, kg/m³; U_i is the velocity, m/s; P represents the pressure, Pa; v is the kinematic viscosity, m²/s. The last two terms belong to the viscous stress tensor and Reynolds stress tensor, respectively. The details about Reynolds stress tensor (i.e., $\overline{u'_i u'_j}$ can be found in the studies of Wilcox in detail [26,27]. The numerical study performed by [2] compares the performance of both Spalart-Allmaras (SA) and shear stress-transport (SST) k-omega study reveals that both SA and SST k-omega can compute accurately the thrust generated by the rotor blades used in Sikorsky S-76. Hence, the SST k-omega turbulence model was employed in the present study. The governing equations of the SST k-omega turbulence model are presented below.

$$\frac{\partial k}{\partial t} + U_j \frac{\partial_k}{\partial_{x_j}} = \frac{\partial}{\partial_{x_j}} \left[\left(v + \sigma^* \frac{k}{\omega} \right) \frac{\partial k}{\partial_{x_j}} \right] + P_k - \beta^* k \omega$$
(3)

$$\frac{\partial\omega}{\partial t} + U_j \frac{\partial_k}{\partial_{x_j}} = \frac{\partial}{\partial_{x_j}} \left[\left(\nu + \sigma \frac{k}{\omega} \right) \frac{\partial\omega}{\partial_{x_j}} \right] + \alpha \frac{\omega}{k} P_k + \beta \omega^2 + \frac{\sigma_d}{\omega} \frac{\partial k}{\partial_{x_j}} \frac{\partial\omega}{\partial_{x_j}} \quad (4)$$

Where P_k is the production rate of the turbulent kinetic energy and other parameters are the closure coefficients [26,27].

Mesh and Physics Modeling

The 4-bladed rotor was placed in two co-axial cylindrical domains in which the inner one is small while the outer cylinder is quite large as shown in Figure 2. Inspired by the approach used for open water propeller and ship self-propulsion analyses [28,29], the large outer region is kept motionless (static) while the small inner one is rotating with a predefined rotational velocity. Figure 2 shows the inner and outer cylinder domains non-dimensionalized with rotor diameter.



Figure 3. Boundary conditions applied on the surfaces

As given in Figure 3, the top surface of the computational domain is set as a velocity inlet while the bottom surface is defined as pressure outlet. The remaining outer surfaces of the domain is considered as symmetry. The rotor blades, the hub and the shaft surfaces are dictated to be wall that satisfies the no-slip boundary condition. As can be seen, the working domain is large enough to prevent any backflows.

The computational domain was discretized with finite-volume hexahedral elements. The trimmer mesh



Figure 2. Domain dimensions.



Figure 4. Mesh structure of the computational domain.

algorithm provides a fully hexahedral grid structure. Local mesh refinements were utilized around the rotor blades and the rotating region. Figure 4 shows the mesh structure on the computational domain and local refinements around the rotating region.

Since the flow was considered 3D, turbulent and incompressible, the appropriate turbulence model (SST k-omega) was chosen and the unsteady RANS equation was solved in an unsteady manner. The time step size was calculated with the assumption that the rotor rotates 5^o per time step. The Rigid Body Motion (RBM) approach was employed for the rotor rotation with a constant rotational velocity.

NUMERICAL RESULTS

Verification Study

The numerical analyses were conducted using a dense mesh algorithm and time step size. However, the numerical

Table 2. Grid numbers

Region	Fine	Medium	Coarse
Rotating	3441822	2259387	1292620
Static	1134939	430333	173233
Total	4576761	2689720	1465853

Table 3. Spatial uncertainty values for both cases

Parameter	Values for 0 knot	Values for 40 knot
N _{fine}	4576761	4576761
N _{medium}	2689720	2689720
N _{coarse}	1465853	1465853
$\phi_{fine}(N)$	7020.00	33104.80
$\phi_{medium}(N)$	6537.32	31558.07
$\phi_{coarse}(N)$	6928.51	38552.59
$U_N(\%)$	6.52	2.89

approach needs to be verified to determine the numerical uncertainty. In this study, the grid number was verified in terms of spatial uncertainty since the time step size was kept constant as the rotor is rotating 5 degrees per time step. The verification study was made for the rotor at hover condition, so the free stream velocity was considered as 0 knot. Following this, the uncertainty study was extended to headwind condition considering the velocity as 40 knot. The rotor was rotating at 293 rpm (100 % condition) for both conditions.

The numerical uncertainty was obtained using the wellknown Grid Convergence Index (GCI) method. The method was based on Richardson extrapolation [30] and proposed by Celik et al. [31]. This method is widely used in ship hydrodynamics and aerodynamics studies [32,33] and suggested by AIAA [34]. Details of the GCI method can be found in Praveen et al. [32]. The uncertainty was checked whether it has a monotonic or oscillating convergence [35]. Table 2 shows the grid numbers of each grid spacing. Here, fine, medium, and coarse grid numbers were obtained by considering the refinement ratio as $\sqrt{2}$. Since the numerical results of both velocities show oscillating convergence or divergence, the three-set GCI method was found inappropriate for this study. Thus, two-set GCI was employed for the spatial uncertainty calculation using fine and coarse grids. The details of this approach were given in a recent study [36]. The verification results are given below in Table 3 and 4.

One may see that the spatial uncertainty for the hover condition (0 knot) was about 6.5% and 3% for the head-wind condition (40 knot).

Validation Study

Following the verification study, the numerical method should be validated with the available experimental data in the literature. The literature consists of experimental and numerical data [2,8]. The experimental results are of wind tunnel tests with and/or without helicopter fuselage. The numerical results are of an in-house developed code focused on helicopter rotor aerodynamics.

Validation of the numerical method was achieved for the hover condition at 293 RPM. The collective pitch angle

Parameter	Experimental	HELIOS	Present study
c_T/σ	0.036	0.040	0.0347
c_Q/σ	0.0026	0.0029	0.0039
FM	0.493	0.517	0.3068

Table 4. Validation study at $(M_{TIP} = 0.6)$.

of the rotor blades is 5[°] at 75% blade section (the section that twist becomes zero). This condition corresponds to the experimental tip Mach number ($M_{TIP} = 0.6$) as indicated in the literature [2,8].

The results were compared with the experimental and in-house developed code results. One may see that there are discrepancies between experimental and numerical results, however, the results were found in good agreement. The non-dimensional thrust coefficient, torque coefficient and figure of merit (FM) parameters were compared, thus the FM appears to be far from other results. The difference in the FM was caused by the difference in the torque coefficient.

Rotor Aerodynamics

Several rotor parameters affect the efficiency of a helicopter's performance such as sweep angle, taper ratio, airfoil and chord distributions twist angle and rotation speed [18]. In the present study, only the effect of rotor speed was considered for hovering condition. Free rotor aerodynamics was investigated numerically for hover and headwind conditions. The free stream velocity was considered as 0 knot to simulate the hover condition [9]. In hover condition, total thrust and torque values were obtained at different rotor load conditions. Figure 5 shows the iso-value of velocity magnitude at Q = 25 as an arbitrary threshold. Here, Q criterion was used as a vortex identification criterion applicable in incompressible flows and Q > 0 means that the vorticity magnitude is greater than the rate of strain [37–39]. Figure 5 shows the trend of thrust versus torque value for different blade loadings. The images show isosurfaces of the Q-criterion colored by velocity. Downstream of the blades, only tip vortices are seen. Due to insufficient computational capability, the wake that must continue axially downward from the rotor blade cannot be seen. This may also be due to the insufficient number of revolution of the rotor because it was revealed by [15] that as the number of revolution increases the wake distributions can be obtained clearly from the rotor center to the point that is one rotor diameter below. Another reason for not observing the swirling flow under the rotor blades is the grid structure. A detailed explanation was made in the study of [13]. As stated in this study, with the rotor running, the root vortex wake extends with the appropriate grid structure and number. In the present study, because of the computational cost, the solver time and total grid number were reduced. Accordingly, only a little vortex behind the rotor blades and some swirling structures were observed around the hub.

The vorticity around the rotor hub increases with the increase in the rotor loading. In addition, the vortices in the vicinity of blade trailing edges come closer to the middle of each blade. However, the tip vortices do not show any change with the rotational velocity. Figure 5 shows the iso-value of velocity magnitude at headwind condition. The vortex core in the hub shows a similar trend to the hover condition case. In this case, the loading has more effect on the trailing edge vortices and vortex splits are more visible. Thus, for the headwind condition, the full load condition (293 rpm) shows a dramatic difference when compared with lower blade loadings.



Figure 5. Iso-values of velocity magnitude (Q=25) for hover and headwind conditions.

Figure 6 gives the relation between thrust (C_T) and torque coefficients (C_Q) . The coefficients were calculated by the following equations.

$$C_T = \frac{T}{\rho(\Omega)^2 D^4} \tag{5}$$

$$C_Q = \frac{Q}{\rho(\Omega)^2 D^5} \tag{6}$$

Here, *T* is the total thrust force, *Q* is the torque, Ω is the blade rotational velocity (rpm) and *D* is the rotor diameter. Figure 6 presents the coefficients by dividing to the rotor solidity (σ). The vertical axis on the left corresponds to the hover condition (0 knot) while the vertical axis on the right

stands for the headwind condition (at 40 knots). At hover condition, considering that ground effects were neglected, the torque coefficients almost never change with the thrust coefficient. At headwind condition, there is not a linear relation between these two coefficients.

To see the effect of free stream velocity on the total thrust, non-dimensional thrust coefficients were obtained at each rotor velocity and condition. In Figure 7, the hover condition represents the lowest free stream velocity and it has nearly no effect on the thrust coefficient. The thrust coefficient for the headwind condition shows a decreasing behavior with the rotor velocity.

Figure 8 shows the effect of free stream velocity on the torque coefficient. One may see that the torque performance



Figure 6. Torque coefficient versus thrust coefficient for both cases.



Figure 7. Thrust coefficient – rotor velocity.



Figure 8. Torque coefficient – rotor velocity.



Figure 9. Figure of merit – thrust coefficient.

was not affected by the free stream velocity at hover condition while there is little change at headwind condition.

In Figure 9, the figure of merit was given at each thrust coefficient for both free stream velocity conditions. The figure of merit was calculated by the following equation.

$$FM = \frac{1}{\sqrt{2}} \frac{C_T^{3/2}}{C_Q}$$
(7)

The left axis is of hover condition and the right axis is of headwind condition. As expected, the figure of merit increases significantly with the increase in flow velocity. There is not a linear relation between the thrust coefficient and figure of merit. The highest value is obtained at lowest rotational speed for hover condition. However, in headwind condition, there is not a similar trend.

CONCLUSION

In this study, numerical analyses were conducted to investigate the effect of free stream velocity on rotor aerodynamics. For this purpose, Sikorsky S-76 main rotor was modeled and analyzed. The numerical approach was verified using the GCI method in terms of spatial uncertainty considering the scalar function is the thrust coefficient. Following this, the numerical approach was also validated by comparing the non-dimensional parameters with the available experimental data. The validation study was conducted for the main rotor at hover and headwind flow conditions and at maximum rotor rotational velocity (293 *RPM*) which corresponds to $M_{TIP} = 0.6$ to mimic the experimental conditions. After verification and validation study, the analyses were extended to different rotor rotational velocities. It was concluded that the relation between thrust and torque coefficients show difference with the flow velocity and rotational velocity. As a final comparison, figure of merit was calculated at each scenario. In hover condition, both thrust and torque coefficients show little change at different rotor velocities. For this reason, the collective pitch angle comes to mind. For headwind condition, the thrust coefficient changes significantly while the torque coefficient changes little with the rotor velocity.

In addition to the numerical results, vortex structure was investigated at each case. However, due to low blade loadings, some minor trailing vortices were observed, and a swirling wake region was kept around the rotor hub. It is concluded that the mesh number and mesh resolution have a significant effect on this kind of vortex identification using a constant Q criterion. It is found that the vortex structure shows different behavior at different points of the rotor geometry. The hub vortex core shows a significant change with the increase in blade loading. The tip vortices occur for all loading and free stream velocities. However, it does not show any change with the blade loading and the vortex structure behind the blade trailing edge moves in the tip-hub direction, so the vortex separations become visible.

Future works on rotor aerodynamics operating behind a ship's flight deck are planned to investigate the ship airwake considering the ship-rotor interactions.

NOMENCLATURE

С	local chord (m)
c_T	rotor thrust coefficient
c _O	rotor torque coefficient
FΜ	figure of merit
N_{h}	number of blades
Q	rotor torque (Nm)
R	blade radius (m)
Т	rotor thrust (N)
U_N	numerical uncertainty
ρ	density (kg/m ³)
σ	rotor solidity
Ω	rotor rotational speed (rad/s)
M_{TIP}	blade tip Mach number

Abbreviation

URANS	Unsteady Reynolds-Averaged Navier-Stokes
SST	Shear Stress Transport
RBM	Rigid Body Motion
GCI	Grid Convergence Index
CFD	Computational Fluid Dynamics
CAD	Computer Aided Design
RPM	Rotation per minute
SA	Spalart-Allmaras

- DES Detached Eddy Simulation
- PIV Particle Image Velocimetry

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AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

(2+1)-dimensional new bi-hamiltonian integrable system: Symmetries, Noether's theorem and integrals of motion

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ABSTRACT

In this work, we investigate a symmetry reduction of the recently discovered (3 + 1)-dimensional equation of the Monge-Ampère type. This equation forms a bi-Hamiltonian system using Magri's theorem when expressed in the two-component form. We select a particular linear combination of the Lie point symmetries belonging to this system to conduct symmetry reduction, resulting in a new (2 + 1)-dimensional system in two-component form. Lagrangian and first Hamiltonian densities are then calculated. We employ Dirac's theory of constraints to obtain symplectic and first Hamiltonian operators. Subsequently, we transform the symmetry condition of the reduced system into a skew-factorized form to determine the recursion operator. Applying the recursion operator to the first Hamiltonian operator yields the second Hamiltonian operator. We demonstrate that the reduced system is a bi-Hamiltonian integrable system in the sense of Magri. Lie point symmetries of the reduced system are identified. Finally, we calculate integrals of motion using the inverse Noether theorem and prove that they have the total divergence form.

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INTRODUCTION

Evolutionary Hirota type equations in (3 + 1)-dimensions have the form:

$$F = f(u_{ij}) - u_{tt}g(u_{ij}) = 0 \iff u_{tt} = \frac{f}{g}, \ g \neq 0, \quad (1)$$

where *u* is an unknown that depends on the coordinates (z_1, z_2, z_3, t) and *f*, *g* are smooth functions of u_{ij} (*i*, *j* = 1,2,3,*t*). The subscripts *i*, *j* of *u* denote partial derivatives with respect to the designated variables, such as $u_{t2} = \partial^2 u$ / $\partial t \partial z_2$, $u_{t2} = \partial^2 u / \partial t \partial z_2$. In [1], these types of equations

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*E-mail address: devrimyazici@gmail.com This paper was recommended for publication in revised form by Editor-in-Chief Ahmet Selim Dalkilic were studied extensively and a general equation of the form (1) that possesses a Lagrangian had been derived. All such equations have the Monge-Ampère form, where the only nonlinear terms consist of minors of the Hessian matrix of u. In this paper, it is sufficient for our purposes to restrict ourselves to a particular case of such an equation, namely:

$$F = a_{11}(u_{tt}u_{23} - u_{t2}u_{t3}) + c_4(u_{t1}u_{23} - u_{t2}u_{13}) + c_5(u_{t2}u_{23} - u_{t3}u_{22}) + c_8(u_{t2}u_{13} - u_{t3}u_{12}) + c_9(u_{11}u_{23} - u_{12}u_{13}) + c_{10}(u_{12}u_{23} - u_{13}u_{22}) = 0.$$
(2)

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Here, a_{11} , c_4 , c_5 , c_8 and c_{10} are arbitrary constants. This equation, denoted as *System-I*, is expressed in the two component form:

$$u_{t} = v$$

$$v_{t} = \frac{1}{u_{23}} \{ v_{2}v_{3} - c_{4}L_{12(3)}[v] - c_{5}L_{23(2)}[v] - c_{8}L_{23(1)}[v]$$

$$- c_{9}L_{12(3)}[u_{1}] - c_{10}L_{23(2)}[u_{1}] \} = q,$$
(3)

where a_{11} and the condition $c_{10}c_8 = c_5c_9$ is imposed. [1,2]. The operator:

$$L_{ij(k)} = u_{jk}D_i - u_{ik}D_j,\tag{4}$$

is introduced for brevity, where D_i denotes the total derivative with respect to z_i . The explicit form of (3) is given as:

$$u_{t} = v$$

$$v_{t} = \frac{1}{u_{23}} \{ v_{2}v_{3} + c_{4}(u_{13}v_{2} - u_{23}v_{1}) + c_{5}(u_{22}v_{3} - u_{23}v_{2}) + c_{8}(u_{12}v_{3} - u_{13}v_{2}) + c_{9}(u_{13}u_{12} - u_{23}u_{11}) + c_{10}(u_{22}u_{13} - u_{23}u_{12}) = q.$$
(5)

In [1, 2], the bi-Hamiltonian structure of (5) was discovered, demonstrating that this system is integrable in the sense of Magri [3,4]. In four dimensions, the evolutionary Hirota-type equations (1) exhibit the symplectic Monge-Ampère property, as demonstrated in former studies [5,6]. These equations find applications in various fields, particularly in gravitational physics. For instance, they are relevant to Plebanski's so called heavenly equations which simplify the complex Einstein field equations governing self-dual gravitational fields [7].

In this study, we find out if the two-component system (3) could be reduced into a (2 + 1)-dimensional bi-Hamiltonian system. We perform the reduction using the method previously applied in [8,9,10]. We choose a specific linear combination of symmetries that is critical to the success of the reduction. Upon obtaining the (2 + 1)-dimensional system in two-component form, we employ the method used before in [11-16] to construct the bi-Hamiltonian system. In order to obtain the first Hamiltonian structure, we use Dirac's constraint analysis [17]. The skew-factorized form of the symmetry condition is reduced from the (3 + 1)-dimensional system [1] to obtain the recursion operator. The second Hamiltonian operator is obtained by applying the recursion operator to the first. Magri's theorem [3,4] is then employed to determine whether the (2 + 1)-dimensional system forms a bi-Hamiltonian system, indicating its integrability.

Completely integrable systems are intriguing because they present many symmetries and conserved densities in their solutions, although finding them is often challenging. We employ tools of Lie symmetry analysis to conduct symmetry reduction and discover first integrals. Recent papers such as [18-20] have used this powerful approach, where the authors have adopted power series expansion to find exact solutions of some nonlinear equations. In addition to well-known analytical methods like Darboux [21], Bäcklund transformations [22] and the recently discovered Kudryashov method [23], as well as the generalized auxiliary equation technique [24]; numerical methods also play a crucial role in this research field. Historically, the wellknown KdV equation was initially solved through a numerical study [25]. Recently, new numerical approaches, such as the Fractional Iteration Algorithm [26] and Variational Iterational Algorithm [27] have been employed to obtain exact solutions for some nonlinear evolution equations. In this paper, we adopt Dirac constraint analysis which is very powerful in handling variational problems when the Lagrangian density is linear in velocity. However, in any other case, such as when the Lagrangian density is quadratic in velocity, this approach is not applicable. Magri made valuable contributions to the field of Hamiltonian systems by proving a theorem stating that evolutionary systems may have a multi-Hamiltonian structure. The Magri theorem, along with Dirac constraint analysis, has paved the way for discovering new integrable Hamiltonian systems, as evidenced in [28-33]. Besides the theoretical realm of science, Hamiltonian systems find utility in applied engineering problems as demonstrated in [34].

This paper is organized as follows: In section 2, we define the symmetries of the system (3) and conduct symmetry reduction to obtain the reduced system in two-component form. In section 3, we verify that the system is in Euler-Lagrange form and determine the degenerate Lagrangian density belonging to the system. Starting from the degenerate Lagrangian density, we construct the first Hamiltonian structure of the reduced system. In section 4, we obtain the recursion operator using the skew-factorized method for the symmetry condition. In section 5, we compose the recursion operator with the first Hamiltonian operator to get the second Hamiltonian operator. Then, we apply Magri's Theorem to establish the second Hamiltonian structure of the reduced system. In section 6, we identify Lie point symmetries and obtain the Lie Algebra of the reduced system. We determine the symmetry characteristics and apply these results in Noether's Theorem to identify new conserved densities of the system. Once we obtain the new conserved densities, we validate their legitimacy by casting them into total divergence form.

SYMMETRY REDUCTION AND THE (2 + 1) -DIMENSIONAL SYSTEM

In [2], the generators of point symmetries for (3) were identified as follows;

$$X_{1} = \partial_{1}, \quad X_{2} = u\partial u + v\partial v, \quad X_{3} = \partial_{t},$$

$$X_{4} = t\partial_{t} + z_{1}\partial_{1} + z_{2}\partial_{2} + u\partial_{u}, \quad X_{a} = a(z_{3})\partial_{u},$$

$$Y_{b} = b(z_{3})\partial_{3}, \quad X_{\infty} = X_{(c,e)} = c(\zeta)\partial_{2} + e(\zeta)\partial_{u},$$

(6)

where *a*, *b*, *c* and *e* are arbitrary smooth functions, and ζ is defined as $\zeta = c_5 z_1 - c_8 z_2$. Given these symmetries, we choose the particular combination:

$$X = X_1 + X_{(1,0)} - Y_1, (7)$$

and get the symmetry:

$$X = \partial_1 + \partial_2 - \partial_3, \tag{8}$$

Equation (8) leads to the characteristic equation:

$$\frac{dz_1}{1} = \frac{dz_2}{1} = -\frac{dz_3}{1} \tag{9}$$

[35]. Integrating both sides of the first two equations given in (9) results in an invariant Z_1 as follows:

$$\int dz_1 = \int dz_2 \implies z_1 = z_2 + Z_1. \tag{10}$$

Likewise, integrating both sides of the last two equations given in (9) leads to an invariant Z_2 as follows:

$$\int dz_2 = -\int dz_3 \implies z_2 = -z_3 + Z_2. \tag{11}$$

Therefore, the invariants of *X* determined by its characteristic equation (9) are:

$$Z_1 = z_1 - z_2, Z_2 = z_2 + z_3, T = t, U = u, V = v.$$
 (12)

Consequently, the total derivatives undergo a transformation expressed as:

$$D_{z_1} = D_{Z_1}, \ D_{z_2} = D_{Z_2} - D_{Z_1}, \ D_{z_3} = D_{Z_2}, \ D_t = D_T.$$
 (13)

In equation (2), by replacing the derivatives with expressions from (13) and renaming variables:

$$U \to u, V \to v, T \to t, Z_1 \to z_1, Z_2 \to z_2,$$
 (14)

we obtain the new (2 + 1)-dimensional evolutionary equation:

$$F = u_{tt}\Delta - u_{t2}^2 + u_{t1}u_{t2} + a(u_{t1}u_{12} - u_{t2}u_{11}) + b(u_{t2}u_{12} - u_{t1}u_{22}) + c(u_{12}^2 - u_{11}u_{22}) = 0,$$
 (15)

where $a = c_5 - c_8$, $b = c_5 - c_4$, $c = c_{10} - c_9$ are arbitrary constants and $\Delta = u_{22} - u_{12}$. Equation (15) is represented in the two component form:

$$u_t^r = v$$

$$v_t^r = \frac{1}{\Delta} \{ v_2^2 - v_1 v_2 + a(v_2 u_{11} - v_1 u_{12}) + b(v_1 u_{22} - v_2 u_{12}) + c(u_{11} u_{22} - u_{12}^2) \} \equiv q.$$
(16)

The superscript r indicates that the relevant parameter is for the reduced (2 + 1)-dimensional system. Two equations presented in (16) compose the new (2 + 1)-dimensional system.

FIRST HAMILTONIAN STRUCTURE OF THE (2 + 1)-DIMENSIONAL REDUCED SYSTEM

Lagrangian density is the starting point for constructing the Hamiltonian structure of the new system. Thus, it is essential to verify that the reduced equation (15) is an Euler-Lagrange equation. Euler-Lagrange equations must satisfy the Helmholtz condition [35]. We verify that (15) possesses a Lagrangian density by checking the Helmholtz condition. Homotopy formula enables us to obtain the Lagrangian density. We present the result of our calculation after skipping the total derivative terms as follows:

$$L^{r} = \frac{1}{2}u_{t}^{2}\Delta + \frac{u_{t}}{3}[a(u_{2}u_{11} - u_{1}u_{12}) + b(u_{1}u_{22} - u_{2}u_{12})] + \frac{u}{3}c(u_{12}^{2} - u_{11}u_{22}).$$
(17)

Euler-Lagrange equation using this result yields the reduced equation (15) which is in one component form. However, we want to obtain L^r in two component form so that we can proceed with Dirac constraint analysis. The transformation $u_t = v$ is applied to appropriate terms of (17) so that Euler-Lagrange equation with the new Lagrangian density results in the reduced system (16). Skipping total derivative terms, we present the new Lagrangian density as:

$$L^{r} = \left(u_{t}v - \frac{1}{2}v^{2}\right)\Delta + \frac{u_{t}}{3}\left\{b(u_{2}u_{12} - u_{1}u_{22}) + a(u_{1}u_{12} - u_{2}u_{11})\right\} + \frac{u}{3}c(u_{11}u_{22} - u_{12}^{2}).$$
(18)

Subsequently, we obtain canonical momenta associated with the coordinates u and v as follows:

$$\Pi_{u}^{r} = \frac{\partial L^{r}}{\partial u_{t}} = v\Delta + \frac{b}{3}(u_{2}u_{12} - u_{1}u_{22}) + \frac{a}{3}(u_{1}u_{12} - u_{2}u_{11}),$$

$$\Pi_{v}^{r} = \frac{\partial L^{r}}{\partial v_{t}} = 0.$$
(19)

With the results obtained so far, the first Hamiltonian density H_1^r follows directly using the Legendre transformation, which in our case is expressed in the following way:

$$H_1^r = \Pi_u^r u_t^r + \Pi_v^r v_t^r - L^r.$$
 (20)

Substituting, (16),(18) and (19) into (20), we obtain:

$$H_1^r = \frac{1}{2}\Delta v^2 + \frac{u}{3}c(u_{12}^2 - u_{11}u_{22}).$$
(21)

Next, we aim to find the symplectic operator K^r . Lagrangian density (18) is degenerate because it is linear in velocity. Consequently, it is not possible to express velocities as a function of momenta and vice versa, as evident in (19). Dirac successfully developed a theory to analyze such cases [17]. Guided by his work, we define the second-class constraints in terms of canonical momenta (19) as:

$$\phi_u^r = \Pi_u^r - \nu \Delta - \frac{b}{3} (u_2 u_{12} - u_1 u_{22}) - \frac{a}{3} (u_1 u_{12} - u_2 u_{11}),$$

$$\phi_v^r = \Pi_v^r$$
(22)

so that $\phi_u^r = 0$ and $\phi_v^r = 0$ are set. The symplectic operator is defined in terms of these constraints as:

$$K^{r} = \begin{pmatrix} \{\phi_{u}^{r}(z), \phi_{u'}^{r}(z')\} & \{\phi_{u}^{r}(z), \phi_{v'}^{r}(z')\} \\ \{\phi_{v}^{r}(z), \phi_{u'}^{r}(z')\} & \{\phi_{v}^{r}(z), \phi_{v'}^{r}(z')\} \end{pmatrix},$$
(23)

similarly as in [1, 11, 33, 36]. The Poisson Bracket of two constraints is denoted as $\{\phi_i^r, \phi_j^r\}$, where the following relations hold:

$$\{\Pi_i(z), u^k(z')\} = \delta_i^k \delta(z - z'), \ \{\Pi_i(z), \Pi_k(z')\} = 0, \{u^i(z), u^k(z')\} = 0.$$
(24)

Here, δ_i^k is the discrete Dirac Delta function and $\delta(z - z')$ is the continuous Dirac Delta function. Moreover, we set $\Pi_1 = \Pi_u$, $\Pi_2 = \Pi_v$, $u^2 = v$ and $z = (z_1, z_2)$. Using (22) and (24), we can express, for instance, the K_{12}^r element of the symplectic matrix as:

$$K_{12}^{r} = \{\phi_{u}^{r}(z), \phi_{v'}^{r}(z')\} = -\Delta\{v, \Pi_{v'}^{r}\}$$

= $-\Delta\delta(z_{1} - z_{1}')\delta(z_{2} - z_{2}').$ (25)

Making use of the Dirac Delta function properties, (25) results in:

$$K_{12}^r = -\Delta = -(u_{22} - u_{12}).$$
⁽²⁶⁾

Through similar but lengthy calculations, we obtain K_{11}^r in the skew-symmetric form:

$$K_{11}^{r} = -\frac{1}{2}(D_{1}v_{2} + v_{2}D_{1}) + D_{2}\left(v_{2} - \frac{v_{1}}{2}\right) + \left(v_{2} - \frac{v_{1}}{2}\right)D_{2} + a(D_{2}u_{11} - D_{1}u_{12}) + b(D_{1}u_{22} - D_{2}u_{12}).$$
(27)

Since the Poisson Bracket operation is anti-symmetric, K_{12}^r is easily found as:

$$K_{21}^{r} = \left\{ \phi_{v}^{r}(z), \phi_{u'}^{r}(z') \right\} = -\Delta \{ \Pi_{v}^{r}, v' \} = -K_{12}^{r}$$
$$= \Delta = u_{22} - u_{12}$$
(28)

and using the property given in (24), K_{22}^r is given as follows:

$$K_{22}^{r} = \left\{ \phi_{v}^{r}(z), \phi_{v'}^{r}(z') \right\} = \left\{ \Pi_{v}^{r}, \Pi_{v'}^{r} \right\} = 0.$$
(29)

With these results, we obtain the symplectic matrix:

$$K^r = \begin{pmatrix} K_{11}^r & -\Delta \\ \Delta & 0 \end{pmatrix}, \tag{30}$$

where K_{11}^r is given in (27). The differential 2-form associated with K^r is given in the form:

$$\omega = \frac{1}{2} \int du_i \Lambda K_{ij}^r du_j. \tag{31}$$

Here, the summation is taken over the repeated subscripts, while Λ denotes the wedge product. Checking the closeness condition:

$$d\omega = 0, \tag{32}$$

of the differential 2-form (31) in a similar manner as done before in [1], reveals that the closeness condition (32)

is satisfied. Therefore, the K^r matrix is a symplectic operator and its inverse which is given as:

$$J_0^r = (K^r)^{-1} = \frac{1}{\sqrt{\det(K^r)}} \begin{pmatrix} K_{22}^r & K_{21}^r \\ K_{12}^r & K_{11}^r \end{pmatrix} \frac{1}{\sqrt{\det(K^r)}},$$
(33)

is a Hamiltonian operator [37]. With the use of (30) and (33), we get:

$$J_0^r = \begin{pmatrix} 0 & \frac{1}{\Delta} \\ -\frac{1}{\Delta} & J_{0(22)}^r \end{pmatrix},\tag{34}$$

where $J_{0(22)}^r$ in skew-symmetric form is given by:

$$J_{0(22)}^{r} = \frac{1}{\Delta} \left\{ -\frac{1}{2} (D_{1}v_{2} + v_{2}D_{1}) + D_{2} \left(v_{2} - \frac{v_{1}}{2} \right) + \left(v_{2} - \frac{v_{1}}{2} \right) D_{2} + a (D_{2}u_{11} - D_{1}u_{12}) + b (D_{1}u_{22} - D_{2}u_{12}) \right\}_{\Delta}^{1}.$$
(35)

Here, J_0^r denotes the first Hamiltonin operator of the reduced system. The first Hamiltonian structure of the system is identified by the matrix equation:

$$\begin{pmatrix} u_t^r \\ v_t^r \end{pmatrix} = J_0^r \begin{pmatrix} \delta_u H_1^r \\ \delta_v H_1^r \end{pmatrix},$$
 (36)

where δ_u and δ_v are variational derivatives with respect to *u* and *v*, respectively. By substituting equations (16), (21) and (34) into (36) and performing the calculations, we find out that equation (36) holds for the (2 + 1)-dimensional system. Therefore, the reduced system (16) exhibits a Hamiltonian structure just like the original system (3). *L*^{*r*}, *H*^{*r*}, *K*^{*r*} and *J*^{*r*} are obtained with identical results through direct reduction from the corresponding parameters *L*, *H*₁, *K*, *J*₀ given in [1] using the transformations (13).

SYMMETRY CONDITION IN A SKEW-FACTORIZED FORM

We define two Lie equations:

$$u_{\tau}^{r} = \varphi , \quad v_{\tau}^{r} = \psi, \tag{37}$$

where τ is the group parameter; φ and ψ are symmetry characteristics. The symmetry condition of an equation is its differential compatibility with the Lie equations, and it is given as:

$$(u_t^r)_{\tau} - (u_{\tau}^r)_t = 0$$
, $(v_t^r)_{\tau} - (v_{\tau}^r)_t = 0.$ (38)

The symmetry condition of the reduced equation (15) is expressed in the following form:

$$\begin{aligned} &\{L_{2t(t)}D_2 + L_{t2(2)}D_t + L_{t1(t)}D_2 + L_{1t(2)}D_t + a(L_{21(t)}D_1 + L_{12(1)}D_t) \\ &+ b(L_{12(t)}D_2 + L_{21(2)}D_t) + c(L_{12(1)}D_2 + L_{21(2)}D_1)\}\varphi = 0, \end{aligned} \tag{39}$$

where the operator defined in (4) is used for brevity. If the symmetry condition can be converted to the skew-factorized form:

$$(A_1B_2 - A_2B_1)\varphi = 0, (40)$$

while the commutator relations:

$$[A_1, A_2] = 0, \ [A_1B_2] - [A_2B_1] = 0, \ [B_1, B_2] = 0, \ (41)$$

are satisfied, Lax pairs and the recursion operator can be obtained. The operators are obtained by reduction from equation (6.6) given in [1] as follows:

$$A_{1}^{r} = \frac{1}{\Delta} (L_{t2(2)} + L_{1t(2)}), B_{1}^{r} = \frac{1}{\Delta} \{ (c_{4} - c_{8}) (L_{2t(1)} + L_{t2(2)}) + c(L_{12(1)} + L_{21(2)}) \}$$

$$A_{2}^{r} = -\frac{1}{\Delta} L_{12(2)}, \qquad B_{2}^{r} = \frac{1}{\Delta} \{ a(L_{12(1)} + L_{21(2)}) + L_{2t(1)} + L_{t2(2)} \}.$$
(42)

The commutator relations (41) are satisfied with these results. Lax pair is defined by:

$$X_1 = \lambda A_1 + B_1, \quad X_2 = \lambda A_2 + B_2, \tag{43}$$

where λ is the spectral parameter. This pair yields the following results in our case with the use of (42):

1

$$\begin{split} X_1 &= \frac{\lambda}{\Delta} \left(L_{t2(2)} + L_{1t(2)} \right) + \frac{1}{\Delta} \{ (c_4 - c_8) \left(L_{2t(1)} + L_{t2(2)} \right) + c \left(L_{12(1)} + L_{21(2)} \right) \} \\ X_2 &= -\frac{\lambda}{\Delta} L_{12(2)} + \frac{1}{\Delta} \{ a \left(L_{12(1)} + L_{21(2)} \right) + L_{2t(1)} + L_{t2(2)} \}. \end{split}$$
(44)

We have checked that the commutator condition:

$$[X_1, X_2] = 0, (45)$$

holds. Bringing the symmetry condition into the skew-factorized form (40) also enables us to write the recursion relations for symmetries as:

$$A_1^r \tilde{\varphi} = B_1^r \varphi, \quad A_2^r \tilde{\varphi} = B_2^r \varphi. \tag{46}$$

Using (42) in (46) and noting the relation:

$$\rho_t = \psi, \tag{47}$$

we transform the two equations in (46) into the matrix form:

$$\begin{pmatrix} \tilde{\varphi} \\ \tilde{\psi} \end{pmatrix} = R^r \begin{pmatrix} \varphi \\ \psi \end{pmatrix},$$
 (48)

wherefrom we obtain the recursion operator as

$$R^{r} = \begin{pmatrix} (L_{21(2)}^{-1}[a(L_{12(1)}+L_{21(2)})+(v_{2}-v_{1})D_{2}] & L_{21(2)}^{-1}\Delta \\ R_{21}^{r} & \frac{v_{2}}{\Delta}(D_{2}-D_{1})L_{21(2)}^{-1}\Delta + c_{4}-c_{8} \end{pmatrix}.$$
(49)

Here R_{21}^r is given by:

$$R_{21}^{r} = \frac{1}{\Delta} \{ (c_4 - c_8)(v_1 - v_2)D_2 + c(L_{12(1)} + L_{21(2)}) + v_2(D_2 - D_1)L_{21(2)}^{-1}[a(L_{12(1)} + L_{21(2)}) + (v_2 - v_1)D_2] \}.$$
(50)

Direct reduction from R given in [1] results in the same $R^{r}(49).$

SECOND HAMILTONIAN STRUCTURE OF THE (2 + 1)-DIMENSIONAL REDUCED SYSTEM

The second Hamiltonian operator J_1^r is obtained by applying the recursion operator to the first Hamilton operator as expressed by the equation:

$$J_1^r = R^r J_0^r. (51)$$

The matrix element $J_{1(11)}^r$ of the operator J_1^r is obtained through the matrix multiplication (51), utilizing the properties:

$$L_{ij(k)} = -L_{ji(k)},$$

$$L_{ij(k)}^{-1}L_{ij(k)} = 1,$$
(52)

of the operator $L_{ij(k)}$ given in (4). This leads to the expression:

$$J_{1(11)}^{r} = 0 - L_{21(2)}^{-1} \Delta_{\underline{\lambda}}^{1},$$
 (53)

which results in:

$$J_{1(11)}^{r} = L_{12(2)}^{-1}.$$
 (54)

The equation for $J_{1(12)}^r$ is given by:

$$J_{1(12)}^{r} = L_{21(2)}^{-1} \left[a \left(L_{12(1)} + L_{21(2)} \right) + (v_{2} - v_{1}) D_{2} \right] \frac{1}{\Delta} \\ + L_{21(2)}^{-1} \Delta \frac{1}{\Delta} \left(v_{22} + 2v_{2} D_{2} - v_{12} - v_{2} D_{1} - v_{1} D_{2} \right) \\ + a L_{21(2)} + b L_{12(2)} \frac{1}{\Delta},$$
(55)

resulting in:

$$I_{1(12)}^{r} = [c_4 - c_8 + L_{21(2)}^{-1}(D_2 - D_1)v_2]\frac{1}{\Delta},$$
(56)

utilizing the properties (52). For $J_{1(21)}^r$, the equation is given by:

$$J_{1(21)}^{r} = \mathbf{0} + \left[\frac{v_{2}}{\Delta}(D_{2} - D_{1})L_{21(2)}^{-1}\Delta + c_{4} - c_{8}\right]\left(-\frac{1}{\Delta}\right), \quad (57)$$

which simplifies to:

$$J_{1(21)}^{r} = \frac{1}{\Delta} \left[v_2 (D_1 - D_2) L_{21(2)}^{-1} + c_8 - c_4 \right].$$
 (58)

For $J_{1(22)}^r$, the equation is given by:

$$J_{1(22)}^{r} = \frac{1}{\Delta} \{ (c_{4} - c_{8})(v_{1} - v_{2})D_{2} + c(L_{12(1)} + L_{21(2)}) \\ + v_{2}(D_{2} - D_{1})L_{21(2)}^{-1}[a(L_{12(1)} + L_{21(2)}) + (v_{1} - v_{2})D_{2}] \} \frac{1}{\Delta} \\ + v_{2}(D_{2} - D_{1})L_{21(2)}^{-1}[a(L_{12(1)} + L_{21(2)}) + (v_{1} - v_{2})D_{2}] \} \frac{1}{\Delta}$$
(59)
$$+ \left[\frac{v_{2}}{\Delta} (D_{2} - D_{1})L_{21(2)}^{-1}\Delta + c_{4} - c_{8} \right] \frac{1}{\Delta} (v_{22} + 2v_{2}D_{2} - v_{12}) \\ - v_{2}D_{1} - v_{1}D_{2} + aL_{21(1)} + bL_{12(2)}) \frac{1}{\Delta},$$

resulting in:

$$J_{1(22)}^{r} = \frac{c_{4} - c_{8}}{\Delta} [v_{2}(D_{2} - D_{1}) + (D_{2} - D_{1})v_{2} + bL_{12(2)} + aL_{21(1)}]\frac{1}{\Delta} + \frac{1}{\Delta}c(L_{21(2)} + L_{12(1)})\frac{1}{\Delta} + \frac{v_{2}}{\Delta}(D_{2} - D_{1})L_{21(2)}^{-1}(D_{2} - D_{1})v_{2}\frac{1}{\Delta},$$
(60)

which is in skew-symmetric form. Equations (54), (56), (58) and (60) constitute the matrix representation of the second Hamiltonian operator obtained as:

$$J_{1}^{r} = \begin{pmatrix} L_{12(2)}^{-1} & -\{L_{12(2)}^{-1}(D_{2}-D_{1})v_{2}+c_{8}-c_{4}\}^{\frac{1}{\Delta}} \\ \frac{1}{\Delta}\{v_{2}(D_{2}-D_{1})L_{12(2)}^{-1}+c_{8}-c_{4}\} & J_{1(22)}^{r} \end{pmatrix}, \quad (61)$$

The Hamiltonian operators J_0^r and J_1^r form a Hamiltonian pair if their linear combination $\Gamma^r = J_0^r + J_1^r$ is also a Hamiltonian operator. In this case, the linear combination is obliged to satisfy skew symmetry and the Jacobi Identity properties as it is stated by Definition 7.1 in Olver's book [35]. It is easy to see that skew symmetry is satisfied since both J_0^r and J_1^r are obviously skew symmetric, i.e, $J^{\dagger} = -J$ holds for both, where \dagger denotes the adjoint operator. On the other hand, checking the Jacobi Identity condition is a complicated task. However, Theorem 7.8 suggested by Olver in his book simplifies this task. Therefore, we use Olver's method in a similar fashion that is demonstrated in [14] and conclude that Jacobi Identity is satisfied.

According to Magri's theorem [3, 4], an evolutionary system is integrable if it satisfies the following equation:

$$\begin{pmatrix} u_t^r \\ v_t^r \end{pmatrix} = J_0^r \begin{pmatrix} \delta_u H_1^r \\ \delta_v H_1^r \end{pmatrix} = J_1^r \begin{pmatrix} \delta_u H_0^r \\ \delta_v H_0^r \end{pmatrix}.$$
 (62)

That is, the (2 + 1)-dimensional system forms a bi-Hamiltonian structure if a second Hamiltonian density H_0^r satisfies (62).

The second Hamiltonian density H_0 of the (3 + 1)-dimensional system is given by (4.1.6) in [2]. Applying the transformations (13), we derive H_0^r for the (2 + 1)-dimensional system as:

$$H_0^r = -k \left\{ \frac{v^2}{2} + \frac{c_9}{2c_8} \left[2u_1 v + (c_4 - c_8) u_1^2 \right] \right\} \Delta, \quad (63)$$

where $k = \frac{c_8}{c_8(c_8-c_4)+c_9}$. By substituting equations (16), (61) and (63) into the matrix equation (62), we confirm that the equation holds. Hence, we have shown that the (2 + 1)-dimensional system admits a bi-Hamiltonian structure, analogous to the (3 + 1)-dimensional case.

NOETHER'S THEOREM AND INTEGRALS OF MOTION

Using the software package REDUCE 1, point symmetries of the new (2 + 1)-dimensional system (16) are identified as follows:

$$\begin{aligned} X_{1} &= \partial_{2}, X_{2} = u\partial_{u} + v\partial_{v}, \ X_{3} = (ab+2c)(-z_{1}\partial_{1}+z_{2}\partial_{2})-a^{2}z_{2}\partial_{1} \\ &+ (b^{2}+4c)z_{1}\partial_{2}+[(2a-b)z_{1}]\partial_{t}, \end{aligned}$$

$$X_{4} &= \partial_{1}, X_{5} = z_{1}\partial_{1}+z_{2}\partial_{2}+t\partial_{t}-v\partial_{v}, \ X_{6} = \partial_{t}, \ X_{7} = z_{2}\partial_{u}, \end{aligned}$$
(64)

$$X_{8} = t\partial_{u} + \partial_{v}, \ X_{9} = z_{1}\partial_{u}, \ X_{10} = \partial_{u}. \end{aligned}$$

In the framework of Lie theory, point symmetries act as symmetry generators if they form a Lie algebra. We construct a table illustrating the Lie algebra structure of the point symmetries (64). The intersection of the i^{th} row and the j^{th} column in this table shows the result of the commutator operation $[X_i, X_i]$.

For convenience, the following notation is used in the table:

$$X_{(7,9)}^{1} = (ab + 2c)X_{7} + (b^{2} + 4c)X_{9},$$

$$X_{(7,9)}^{2} = aX_{7} + (2a - b)X_{9}, \quad X_{(7,9)}^{3} = -a^{2}X_{7} - (ab + 2c)X_{9},$$

$$X_{(1,4,6)}^{1} = (ab + 2c)X_{1} - a^{2}X_{4} + aX_{6},$$

$$X_{(1,4,6)}^{2} = -(b^{2} + 4c)X_{1} + (ab + 2c)X_{4} + (b - 2a)X_{6}.$$
(65)

For each symmetry generator X, corresponding symmetry characteristics provide the independent variables that remain untransformed under the symmetry transformation. In [35], symmetry generators are defined in the following general form:

$$X = \xi^i \partial_{\chi^i} + \eta^\alpha \partial_u{}^\alpha, \tag{66}$$

and the corresponding characteristics are defined in the form:

$$\varphi^{\alpha} = \eta^{\alpha} - u_i^{\alpha} \xi^i. \tag{67}$$

These equations are expressed using the Einstein summation convention. In the case of (2 + 1) –dimensional

	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}
X_1	0	0	$X^{1}_{(1,4,6)}$	0	X_1	0	X_{10}	0	0	0
X_2	0	0	0	0	0	0	$-X_{7}$	$-X_8$	-X ₉	-X ₁₀
X_3	$-X^{1}_{(1,4,6)}$	0	0	$X^{2}_{(1,4,6)}$	0	0	$X^{1}_{(7,9)}$	$X^{2}_{(7,9)}$	$X^{3}_{(7,9)}$	0
X_4	0	0	$-X^{2}_{(1,4,6)}$	0	X_4	0	0	0	X_{10}	0
X_5	$-X_1$	0	0	$-X_4$	0	-X ₆	X_7	X_8	X_9	0
X_6	0	0	0	0	X_6	0	0	X_{10}	0	0
X_7	$-X_{10}$	X_7	$-X^{1}_{(7,9)}$	0	$-X_{7}$	0	0	0	0	0
X_8	0	X_8	$-X^{2}_{(7,9)}$	0	$-X_8$	$-X_{10}$	0	0	0	0
X_9	0	X_9	$-X^{3}_{(7,9)}$	$-X_{10}$	$-X_{9}$	0	0	0	0	0
X ₁₀	0	X_{10}	0	0	0	0	0	0	0	0

Table 1. Commutators of point symmetry generators of reduced system

system, indices *i* take values: i = 1,2,3. Additionally, we have two dependent variables *u* and *v*, so indices α take values: $\alpha = 1, 2$. Accordingly, we define:

$$\begin{aligned} x^{1} = t, \quad x^{2} = z_{1}, \quad x^{3} = z_{2}, \quad u_{1}^{1} = u_{t}, \quad u_{2}^{1} = u_{1}, \\ u_{3}^{1} = u_{2}, \quad u_{1}^{2} = v_{t}, \quad u_{2}^{2} = v_{1}, \quad u_{3}^{2} = v_{2}, \quad \eta^{1} = \eta^{u}, \quad \eta^{2} = \eta^{v}, \quad (68) \\ \varphi^{1} = \varphi, \quad \varphi^{2} = \psi. \end{aligned}$$

For every generator *X*, we obtain two characteristics, namely φ and ψ , which are related to the transformations of *u* and *v* respectively. Using (68) in the equations (66), (67) and replacing u_t by v, v_t by q according to (16), we find the characteristics pair (φ_i, ψ_i) of each generator X_i (i = 1, 2, ..., 10) as the following:

$$\begin{split} \varphi_{1} &= -u_{2} \quad \psi_{1} = -v_{2}, \quad \varphi_{2} = u, \quad \psi_{2} = v, \\ \varphi_{3} &= -v(2a-b)z_{1} + u_{1}[(ab+2c)z_{1} + a^{2}z_{2}] - u_{2}[(b^{2}+4c)z_{1} + (ab+2c)z_{2}], \\ \psi_{3} &= -q(2a-b)z_{1} + v_{1}[(ab+2c)z_{1} + a^{2}z_{2}] - v_{2}[(b^{2}+4c)z_{1} + (ab+2c)z_{2}], \\ \varphi_{4} &= -u_{1}, \quad \psi_{4} &= -v_{1}, \quad \varphi_{5} &= -vt - u_{1}z_{1} - u_{2}z_{2}, \quad \psi_{5} &= -v - qt - v_{1}z_{1} - v_{2}z_{2}, \\ \varphi_{6} &= -v, \quad \psi_{6} &= -q, \quad \varphi_{7} = z_{2}, \quad \psi_{7} = 0, \quad \varphi_{8} = t \\ \psi_{8} &= 1, \quad \varphi_{9} = z_{1}, \quad \psi_{9} = 0 \quad \varphi_{10} = 1, \quad \psi_{10} = 0 \end{split}$$

$$\end{split}$$

$$\tag{69}$$

These symmetry characteristics provide a path to find new integrals of motion conserved by the flow of (16). By substituting the time variable "t" with the group parameter " τ ", we can employ the Lie equations provided in (37). Upon substituting these Lie equations into the matrix equation (36), we get:

$$\begin{pmatrix} \varphi \\ \psi \end{pmatrix} = J_0^r \begin{pmatrix} \delta_u H^r \\ \delta_v H^r \end{pmatrix}.$$
 (70)

This represents the Noether theorem in Hamiltonian form, providing the conserved density H^r corresponding to the given symmetry. Remarking that the first Hamiltonian operator (33) is the inverse of the symplectic operator, we arrange the matrix equation (70) into the inverse Noether theorem, taking the following form:

$$\begin{pmatrix} \delta_u H^r \\ \delta_v H^r \end{pmatrix} = K^r \begin{pmatrix} \varphi \\ \psi \end{pmatrix}. \tag{71}$$

We write this matrix equation for each characteristics pair (φ_i, ψ_i) that we obtained in (69) as:

$$\begin{pmatrix} \delta_u H_i^r \\ \delta_v H_i^r \end{pmatrix} = K^r \begin{pmatrix} \varphi_i \\ \psi_i \end{pmatrix}.$$
 (72)

Solving this equation, we determine the conserved densities, i.e., first integrals H_i^r corresponding to all variational point symmetry generators X_i with characteristics (φ_i, ψ_i) as follows:

$$H_{1}^{r} = v u_{2}(u_{12} - u_{22}) - \frac{au}{3}(u_{11}u_{22} - u_{12}^{2}),$$

$$H_{4}^{r} = v u_{1}(u_{12} - u_{22}) + \frac{1}{2}b u_{22}u_{1}^{2},$$

$$H_{6}^{r} = \frac{v^{2}}{2}(u_{12} - u_{22}) + \frac{c}{3}u(u_{11}u_{22} - u_{12}^{2}),$$

$$H_{7}^{r} = z_{2}v(u_{22} - u_{12}) + \frac{u}{2}(au_{11} - bu_{12}),$$

$$H_{8}^{r} = \left(vt - \frac{u}{2}\right)(u_{22} - u_{12}),$$

$$H_{9}^{r} = z_{1}v(u_{22} - u_{12}) + \frac{u}{2}(bu_{22} - au_{12}).$$
(73)

We observe that the first integrals H_2^r , H_3^r , H_5^r fail to exist. Therefore, the corresponding generators X_2 , X_3 , X_5 do not count as variational symmetries. We check the time derivative of every density given in (73) along the flow (16) and obtain all the variational symmetries in total divergence form respectively as follows:

$$\begin{split} D_t H_1^r &= D_1 \left[-\frac{1}{2} \Big(u_{22} v + b u_2 u_{22} + \frac{a}{3} u_2 u_{22} - \frac{a}{3} u_1 u_{22} + a u_2 u_{12} \Big) v \\ &+ \frac{a}{3} (u_{12} v_2 - u_{22} v_1) u - c u_2 u_1 u_{22} \Big] + D_2 \left[\Big(u_2 v_1 - u_2 v_2 + \frac{1}{2} u_{12} v \\ &+ b u_2 u_{12} - \frac{a}{3} u_1 u_{12} + \frac{a}{3} u_2 u_{11} - a u_{11} u_2 \Big) v + \frac{a}{3} (u_{12} v_1 - u_{11} v_2) u \\ &+ c u_2 u_1 u_{12} \Big] \end{split}$$

$$\begin{split} D_t H_4^r &= D_1 \left[\left(-\frac{1}{2} u_{12} v + a u_1 u_{12} \right) v - \frac{c}{2} u_1^2 u_{22} \right] + D_2 \left[\left(v v_1 - v v_2 - a u_{11} v \right. \\ &+ \frac{c}{2} u_{12} u_1 + \frac{b}{2} v_2 u_1 \right) u_1 + \frac{1}{2} u_{12} v_2 \right], \end{split}$$

$$D_{t}H_{6}^{r} = D_{1}\left[\frac{c}{3}(v_{1}u_{22} - v_{2}u_{12})u + \frac{c}{3}(u_{12}u_{2} - u_{1}u_{22})v + \frac{1}{2}(v_{2} + au_{12} - bu_{22})v^{2}\right]$$
$$+ D_{2}\left[\frac{c}{3}(u_{11}v_{2} - u_{12}v_{1})u + \frac{c}{3}(u_{11}u_{12} - u_{2}u_{11})v + \frac{1}{2}(bu_{12} - au_{11} - v_{2})v^{2}\right], \quad (74)$$

$$\begin{split} D_t \alpha_7 &= D_1 \left[- \left(D_2 z_2 + dz_2 u_{12} + \frac{1}{2} u_1 - Dz_2 u_{22} \right) v + \left(\frac{1}{2} v_1 - \frac{1}{2} v_2 \right) u + cz_2 u_1 u_{22} \right] \\ &+ D_2 \left[c \left(\frac{1}{2} u_1 - z_2 u_{12} \right) u_1 + \left(v_2 z_2 - \frac{1}{2} v + az_2 u_{11} - bz_2 u_{12} + \frac{b}{2} u_1 \right) v \right] \\ D_t H_8^r &= D_1 \left[(-avu_{12} + bvu_{22} + cu_1 u_{22} - vv_2) t + \frac{1}{2} (uv_2 - vu_2) \right] \\ &+ D_2 \left[vv_2 + avu_{11} - bvu_{12} - cu_1 u_{12} + \frac{1}{2} (vu_2 - uv_2) \right], \\ D_t H_9^r &= D_1 \left[-\frac{a}{2} uv_2 + (bz_1 u_{22} - az_1 u_{12} - z_1 v_2) v + cu_1 u_{22} \right] \end{split}$$

$$+D_2\left[(vv_2 + avu_{11} - bvu_{12})z_1 + \left(\frac{a}{2}v - cu_{12}\right)u_1 + \frac{1}{2}(v - bu_2)v + \frac{b}{2}v_2u\right],$$

$$D_tH_{10}^r = D_1\left[(-au_{12} + bu_{22})v + cu_{1}u_{22}\right] + D_2\left[(v_2 - v_1 + au_{11} - bu_{12})v - cu_{1}u_{12}\right].$$

We have successfully expressed the first integrals (73) in total divergence form (74). Thus, we can conclude that these integrals are indeed the constants of motion for the flow governed by the system (16). In essence, total divergences provide an independent check that the corresponding functionals H^r are indeed integrals of motion subject to suitable boundary conditions.

CONCLUSION

We studied a symmetry reduction of the recently discovered (3 + 1)-dimensional equation of the Monge-Ampere type. Our goal was to explore if it is possible to obtain a new (2 + 1)-dimensional bi-Hamiltonian system by applying symmetry reduction to a particular case of

the (3 + 1)-dimensional equation. We used point symmetry generators of the system and proceeded by choosing a special combination of the symmetries. We determined the transformation of total derivatives under this particular symmetry, then performed the reduction accordingly. We obtained all the parameters L^r , H_1^r , K^r , J_0^r , R^r , J_1^r and H_0^r of the reduced (2 + 1)-dimensional system. Two component representation made it possible to obtain the Hamiltonian operator through Dirac constraint analysis. Being able to find the second Hamiltonian function H_0^r , we state that the reduced system maintains the bi-Hamiltonian structure of the original system. We confirmed that all parameters and operators could also be obtained by direct reduction from the original system, e.g., $L, H_1, K, J_0, R, J_1, H_0$ with the same symmetry choice. We identified the symmetry generators of the reduced (2 + 1)-dimensional system, along with their corresponding characteristic pairs (φ , ψ). By the Noether theorem, we revealed seven new integrals of motion that define the conserved densities of the system. We also proved that the time derivatives of all variational symmetries are total divergences.

Thus, we presented a new method for obtaining (2 + 1)-dimensional bi-Hamiltonian systems starting from (3 + 1)-dimensional bi-Hamiltonian systems. We have illustrated the involved procedure by an explicit example, producing a new bi-Hamiltonian system. We expect the suggested procedure to be a useful supplement to other techniques for generating (2 + 1)-dimensional bi-Hamiltonian systems.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Computational method to solve Davey-Stewartson model and Maccari's system

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ABSTRACT

In this article, Computer algebra systems and the Riccati-Bernoulli sub-ODE method are efficiently utilized to solve Davey-Stewartson and Maccari's systems. We successfully obtained the set of new exact solutions for these systems using the computer algebra MAPLE system. For the validity of acquired solutions, the constraint conditions are given. To investigate the behavior of these solutions, graphical representations of the derived solutions are provided under suitable parameter values.

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INTRODUCTION

Computers are generally thought of as number crunchers, but there is no reason why they cannot also be used as formula crunchers. Computer algebra systems allow us to manipulate formulae. A computer algebra system computes with symbols rather than numbers. Such systems are useful for manipulating formulae. A particularly useful technique is the calculation of the coefficients of the polynomials. We have used computer algebra systems in several ways to solve our problem [1-4].

Nonlinear partial differential equations (NLPDEs) are utilized in diverse areas to model notable phenomena. So, the solutions of NLPDEs have a significant role in the research of physics, engineering, and applied mathematics, containing population ecology, solid-state physics, plasma waves, plasma physics, optical fibers, quantum mechanics, fluid mechanics, heat flow, propagation of shallow waves and wave propagation phenomena. To acquire soliton and traveling wave solutions for NLPDEs, numerous computational approaches have been constructed. Some of these approaches are the new extended direct algebraic method [5-7], the extended Jacobi elliptic function expansion method [8], the generalized Kudryashov method [9], the generalized algebraic method [10], the extended generalized Riccati equation mapping method [11], Q-function method [12,13], extended tanh method [14].

This research article aims to examine the analytical solutions of the Maccari's system and Davey-Stewartson system with the aid of the Riccati-Bernoulli sub-ODE method [15-18].

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The nonlinear complex Maccari's system (CNMS) [19] is described as:

$$iQ_t + Q_{xx} + RQ = 0,$$

$$iS_t + S_{xx} + RS = 0,$$

$$iN_t + N_{xx} + RN = 0,$$

$$R_t + R_v + (|Q + S + N|^2)_x = 0.$$
(1)

The CNMS is a form of the complex nonlinear system modeling the motion of an isolated wave is localized in a small part of space and used in several fields such as plasma physics, nonlinear optic, hydrodynamic [20]. Q(x, y, t), S(x, y, t) and N(x, y, t) are complex-valued functions and R(x, y, t) is a real-valued function. In order to acquire novel traveling solutions of CNMS, various new methods have been presented. Some of these methods are the new extension of the (G'/G)-expansion method [19], the sine-Gordon expansion method [21], the modified exp $(-\phi(\eta))$ -expansion function method [22], the modified F-Expansion method and the generalized projective Riccati equation method [23], the first integral method [24].

In this research article, the Riccati- Bernoulli sub- ODE method is also applied to the Davey Stewartson system given by:

$$iU_t + \gamma (U_{xx} + U_{yy}) + \mu |U|^2 U - \alpha UV = 0,$$

$$V_{xx} + V_{yy} + \sigma (|U|^2)_{xx} = 0,$$
(2)

where U = U(x, y, t) and V = V(x, y, t) are the complex wave envelope and the real forcing terms, respectively in [25]. *y*, μ and σ are real constants. In order to acquire the solutions of various forms of the Davey Stewartson system, several mathematical techniques have been utilized, for example; the exponential function method [25], the extended sinh-Gordon equation expansion method [26], the exp (- $\Phi(\xi)$)-expansion method, the first integral method and the Sine-Gordon expansion method [27], the Generalized Elliptic Equation Rational Expansion method [28], the direct similarity reduction method [29], the extended tanh method [30], the extended mapping method [31].

The paper's draft is formed as follows: the Riccati Bernoulli sub-ODE method is summarized in Section 2. The technique is utilized to solve the nonlinear Maccari's and Davey Stewartson systems in Section 3. Eventually, the conclusion of this paper is given in Section 4.

Riccati Bernoulli Sub-Ode Method

In this section, we express the elementary steps of the Riccati Bernoulli sub-ODE method. Any NLPDE can be taken in the following form:

$$R(\varphi,\varphi_x,\varphi_t,\varphi_{xx},\varphi_{tt},\varphi_{xt},\dots)=0, \qquad (3)$$

where *R* is a polynomial that consists $\varphi(x, t)$ and its partial derivatives.

Step 1: In order to acquire the solitary wave solution of Equation 1 and Equation 2, we utilize the traveling wave transformation,

$$\varphi(x,t) = \varphi(\eta), \eta = k(x \pm \nu t), \tag{4}$$

where $\varphi(x, t) = \varphi(\eta)$ is an unknown function to be found, *k* is defined as the width of the traveling wave and *v* is identified as the velocity of the soliton. Then, the Equation 3 is turned into the following ODE:

$$P(\varphi,\varphi',\varphi'',\dots) = 0, \tag{5}$$

in which $\varphi' = \frac{d\varphi}{d\eta}$, $\varphi'' = \frac{d^2\varphi}{d\eta^2}$ and so on.

Step 2: Assume that Equation 5 is the solution of the Riccati-Bernoulli equation of the form:

$$\varphi' = a_1 \varphi + a_2 \varphi^{2-m} + a_3 \varphi^m, \tag{6}$$

in which a_1 , a_2 , a_3 and m are constants. Utilizing from the Equation 6, we acquire

$$\varphi'' = \varphi^{-1-2m} (a_2 \varphi^2 + a_3 \varphi^{2m} + a_1 \varphi^{1+m}) (-a_2(m-2)\varphi^2 + a_3 m \varphi^{2m} + a_1 \varphi^{1+m}),$$
(7)

and

$$\varphi^{\prime\prime\prime} = \varphi^{-2(1+m)}(a_1\varphi + a_2\varphi^{2-m} + a_3\varphi^m)(a_2^2(-2+m))(-3+2m)\varphi^4 + a_3^2 m(-1+2m)\varphi^{4m} + a_1a_2(-3+m)(-2+m)\varphi^{3+m} + (a_1^2+2a_2a_3)\varphi^{2+2m} + a_1a_3m(1+m)\varphi^{1+3m}.$$
(8)

The other derivatives of the function φ can be similarly acquired.

Remark 1. Equation 6 is reduced to the Riccati equation when $a_1a_2 \neq 0$ and m = 0. Additionally, Equation 6 is reduced to the Bernoulli equation when $a_2 \neq 0$, $a_3 = 0$, and $m \neq 1$. The solutions of Equation 6 are as follows:

Set 1: For m = 1, Equation 6 has the following solution

$$\varphi(\eta) = C e^{(a_1 + a_2 + a_3)\eta}.$$
(9)

Set 2: For $m \neq 1$, $a_1 = 0$ and $a_3 = 0$, Equation 6 has the following solution

$$\varphi(\eta) = \left(a_2(m-1)(\eta+C)\right)^{\frac{1}{m-1}}.$$
 (10)

Set 3: For $m \neq 1$, $a_1 \neq 0$ and $a_3 = 0$, Equation 6 has the following solution

$$\varphi(\eta) = \left(Ce^{a_1(m-1)\eta} - \frac{a_2}{a_1}\right)^{\frac{1}{m-1}}.$$
 (11)

Set 4: For $m \neq 1$, $a_2 \neq 0$ and $a_1^2 - 4a_2a_3 < 0$, Equation 6 has the following solution

$$\varphi(\eta) = \left(-\frac{a_1}{2a_2} + \frac{\sqrt{4a_2a_3 - a_1^2}}{2a_2}tan\left[\frac{(1-m)\sqrt{4a_2a_3 - a_1^2}}{2}(\eta+C)\right]\right)^{\frac{1}{1-m}}, \quad (12)$$

and

$$\varphi(\eta) = \left(-\frac{a_1}{2a_2} - \frac{\sqrt{4a_2a_3 - a_1^2}}{2a_2}\cot\left[\frac{(1-m)\sqrt{4a_2a_3 - a_1^2}}{2}(\eta+C)\right]\right)^{\frac{1}{1-m}}.$$
 (13)

Set 5: For $m \neq 1$, $a_2 \neq 0$ and $a_1^2 - 4a_2a_3 > 0$, Equation 6 has the following solution

$$\varphi(\eta) = \left(-\frac{a_1}{2a_2} - \frac{\sqrt{a_1^2 - 4a_2a_3}}{2a_2} tanh\left[\frac{(1-m)\sqrt{a_1^2 - 4a_2a_3}}{2}(\eta+C)\right]\right)^{\frac{1}{1-m}}, \quad (14)$$

and

$$\varphi(\eta) = \left(-\frac{a_1}{2a_2} - \frac{\sqrt{a_1^2 - 4a_2a_3}}{2a_2} \coth\left[\frac{(1-m)\sqrt{a_1^2 - 4a_2a_3}}{2}(\eta+C)\right]\right)^{\frac{1}{1-m}} \cdot (15)$$

Set 6: For $m \neq 1$, $a_2 \neq 0$ and $a_1^2 - 4a_2a_3 = 0$, Equation 6 has the following solution

$$\varphi(\eta) = \left(\frac{1}{a_2(m-1)(\eta+C)} - \frac{a_2}{a_1}\right)^{\frac{1}{1-m}},$$
(16)

in which *C* is a constant.

Step 3: Finally, if φ and its derivatives are substituted into Equation 5, we can get a set of algebraic equations consisting of the powers of φ . Assuming the coefficients of each power of φ equal to zero, we acquire a system of algebraic equations for a_1 , a_2 , a_3 , k and v. When the parameters are substituted into Equations 9-16, the traveling wave and other solutions of the Equation 3 are acquired.

APPLICATIONS OF THE METHOD TO GOVERN-ING SYSTEMS

The Maccari's System

To construct analytical solutions of the system in Equation 1, we assume,

$$Q(x, y, t) = u(x, y, t)e^{i(ax+by+ct+d)},$$

$$S(x, y, t) = v(x, y, t)e^{i(ax+by+ct+d)},$$

$$N(x, y, t) = w(x, y, t)e^{i(ax+by+ct+d)},$$
(17)

in which *a*, *b*, *c* and *d* are constants to be calculated later. Substituting Equation 17 into the system in Equation 1, we acquire

$$i(u_t + 2au_x) + u_{xx} - (1 + a^2)u + uR = 0,$$

$$i(v_t + 2av_x) + v_{xx} - (1 + a^2)v + vR = 0,$$

$$i(w_t + 2aw_x) + w_{xx} - (1 + a^2)w + wR = 0,$$

$$R_t + R_v + (u^2)_x = 0.$$
(18)

Utilizing the following transformation to reduce the Equation 1,

$$u = U(\eta), v = V(\eta), w = W(\eta), R = R(\eta), \eta = x + \beta y - 2at$$
, (19)

in which β is constant, the system in Equation 1 is rewritten as,

$$U'' - (c + a^{2})U + UR = 0,$$

$$V'' - (c + a^{2})V + VR = 0,$$

$$W'' - (c + a^{2})W + WR = 0,$$

$$(\beta - 2a)R' + ((U + V + W)^{2})' = 0.$$
(20)

Integrating the fourth equation of the Equation 20 with respect to η and assuming the integration constant as zero, we acquire

$$R = -\frac{1}{\beta - 2a} (U + V + W)^2.$$
(21)

Replacing Equation 21 into the other equations of Equation 20, we obtain

$$U'' - (c + a^{2})U - \frac{1}{\beta - 2a}(U + V + W)^{2}U = 0,$$

$$V'' - (c + a^{2})V - \frac{1}{\beta - 2a}(U + V + W)^{2}V = 0,$$
 (22)

$$W'' - (c + a^{2})W - \frac{1}{\beta - 2a}(U + V + W)^{2}W = 0.$$

To solve the system in Equation 22, we can give the following relations

$$V = c_1 U, \qquad W = c_2 U \,, \tag{23}$$

in which c_1 and c_2 are constants. Replacing Equation 23 into the system in Equation 22, we acquire

$$U'' - (c + a^2)U - \frac{(1 + c_1 + c_2)^2}{\beta - 2a}U^3 = 0.$$
 (24)

If *U* and its derivatives are substituted into Equation 24, and we take m = 0, then we acquire the following equation

$$\left(2a_2^2 - \frac{(1+c_1+c_2)^2}{\beta - 2a} \right) U^3 + 3a_1a_2U^2 + (a_1^2 - c - a^2 + 2a_2a_3)U + a_1a_3 = 0.$$
 (25)

If we collect all the coefficients of $u^j(j = 0, 1, 2, 3)$ and assuming each to equal zero in Equation 25, the following system is acquired.

 U^0 coefficient:

$$a_1 a_3 = 0,$$
 (26)

 U^1 coefficient:

$$a_1^2 - c - a^2 + 2a_2a_3 = 0, (27)$$

U² coefficient:

$$3a_1a_2 = 0,$$
 (28)

U³ coefficient:

$$2a_2^2 - \frac{(1+c_1+c_2)^2}{\beta - 2a} = 0.$$
 (29)

Solving the system consisting of Equations 26-29, we acquire the following families:

Family 1:

$$a_1 = 0, a_2 = -\frac{1+c_1+c_2}{\sqrt{2\beta-4a}}, c = -a^2 - 2\frac{a_3 + a_3c_1 + a_3c_2}{\sqrt{2\beta-4a}}.$$
 (30)

When substituting parameters in Equation 30 into Equation 18, we get the following equations:

$$u_{1,1}(x,y,t) = -\frac{\sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}}\sqrt{2\beta-4a} \tan\left(\sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}}(x+\beta y-2at+C)\right)}{1+c_1+c_2}, \quad (31)$$

$$u_{1,2}(x,y,t) = \frac{\sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}\sqrt{2\beta-4a}\cot\left(\sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}(x+\beta y-2at+C)}\right)}{1+c_1+c_2},$$
 (32)

in which $2\beta - 4a > 0$ and $a_3(1 + c_1 + c_2) < 0$.

$$u_{1,3}(x,y,t) = \frac{\sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}} \sqrt{2\beta-4a} \tanh\left(\sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}} (x+\beta y-2at+C)}\right)}{1+c_1+c_2}, \quad (33)$$

$$u_{1,4}(x,y,t) = \frac{\sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}}\sqrt{2\beta-4a} \coth\left(\sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}}(x+\beta y-2at+C)\right)}{1+c_1+c_2}, \quad (34)$$

in which $2\beta - 4a > 0$ and $a_3(1 + c_1 + c_2) > 0$ for proper solutions.

$$v_{1,1}(x,y,t) = -\frac{c_1 \sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}} \sqrt{2\beta-4a} \tan\left(\sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}} (x+\beta y-2at+C)}\right)}{1+c_1+c_2}, \quad (35)$$

$$v_{1,2}(x,y,t) = \frac{c_1 \sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}} \sqrt{2\beta-4a} \cot\left(\sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}} (x+\beta y-2at+C)\right)}{1+c_1+c_2}, \quad (36)$$

in which $2\beta - 4a > 0$ and $a_3(1 + c_1 + c_2) < 0$.

$$v_{1,3}(x,y,t) = \frac{c_1 \sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}} \sqrt{2\beta-4a} \tanh\left(\sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}} (x+\beta y-2at+C)\right)}{1+c_1+c_2}, \quad (37)$$

$$\nu_{1,4}(x,y,t) = \frac{c_1 \sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}}\sqrt{2\beta-4a} \coth\left(\sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}}(x+\beta y-2at+C)\right)}{1+c_1+c_2},$$
 (38)

in which $2\beta - 4a > 0$ and $a_3(1 + c_1 + c_2) > 0$ for proper solutions.

$$w_{1,1}(x,y,t) = -\frac{c_2 \sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}} \sqrt{2\beta-4a} \tan\left(\sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}} (x+\beta y-2at+C)}\right)}{1+c_1+c_2}, \quad (39)$$

$$w_{1,2}(x,y,t) = \frac{c_2 \sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}} \sqrt{2\beta-4a} \cot\left(\sqrt{-a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}} (x+\beta y-2at+C)}\right)}{1+c_1+c_2}, \quad (40)$$

in which $2\beta - 4a > 0$ and $a_3(1 + c_1 + c_2) < 0$.

$$w_{1,3}(x,y,t) = \frac{c_2 \sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}} \sqrt{2\beta-4a} \tanh\left(\sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}} (x+\beta y-2at+C)\right)}{1+c_1+c_2}, \quad (41)$$

$$w_{1,4}(x,y,t) = \frac{c_2 \sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}} \sqrt{2\beta-4a} \coth\left(\sqrt{a_3 \frac{1+c_1+c_2}{\sqrt{2\beta-4a}} (x+\beta y-2at+C)}\right)}{1+c_1+c_2}, \quad (42)$$

in which $2\beta - 4a > 0$ and $a_3(1 + c_1 + c_2) > 0$ for proper solutions. For the solutions $u_{1,2}(x, y, t)$, $v_{1,2}(x, y, t)$ and $w_{1,2}(x, y, t)$, we yield the dark optical solutions,

$$\begin{split} Q(x,y,t) &= \frac{\sqrt{-a_3}\Phi\sqrt{2\beta-4a}\cot\left(\sqrt{-a_3}\Phi(x+\beta y-2at+C)\right)}{1+c_1+c_2} e^{l\left(ax+by+\left(-a^2-2\frac{a_3+a_3c_3+a_3c_3}{\sqrt{2\beta-4a}}\right)t+d\right)},\\ S(x,y,t) &= \frac{c_1\sqrt{-a_3}\Phi\sqrt{2\beta-4a}\cot\left(\sqrt{-a_3}\Phi(x+\beta y-2at+C)\right)}{1+c_1+c_2} e^{l\left(ax+by+\left(-a^2-2\frac{a_3+a_3c_3+a_3c_3}{\sqrt{2\beta-4a}}\right)t+d\right)},\\ N(x,y,t) &= \frac{c_2\sqrt{-a_3}\Phi\sqrt{2\beta-4a}\cot\left(\sqrt{-a_3}\Phi(x+\beta y-2at+C)\right)}{1+c_1+c_2} e^{l\left(ax+by+\left(-a^2-2\frac{a_3+a_3c_3+a_3c_3}{\sqrt{2\beta-4a}}\right)t+d\right)}, \end{split}$$

where $\Phi = \frac{1+c_1+c_2}{\sqrt{2\beta-4a}}$. For the solutions $u_{1,3}(x, y, t)$, $v_{1,3}(x, y, t)$ and $w_{1,3}(x, y, t)$, we yield the dark optical solutions,

$$\begin{split} Q(x,y,t) &= \frac{\sqrt{a_3 \Phi} \sqrt{2\beta - 4a} \tanh\left(\sqrt{a_3 \Phi}(x + \beta y - 2at + C)\right)}{1 + c_1 + c_2} e^{i\left(ax + by + \left(-a^2 - 2\frac{a_3 + a_3 c_1 + a_3 c_2}{\sqrt{2\beta - 4a}}\right)t + d\right)}, \\ S(x,y,t) &= \frac{c_1 \sqrt{a_3 \Phi} \sqrt{2\beta - 4a} \tanh\left(\sqrt{a_3 \Phi}(x + \beta y - 2at + C)\right)}{1 + c_1 + c_2} e^{i\left(ax + by + \left(-a^2 - 2\frac{a_3 + a_3 c_1 + a_3 c_2}{\sqrt{2\beta - 4a}}\right)t + d\right)}, \\ N(x,y,t) &= \frac{c_2 \sqrt{a_3 \Phi} \sqrt{2\beta - 4a} \tanh\left(\sqrt{a_3 \Phi}(x + \beta y - 2at + C)\right)}{1 + c_1 + c_2} e^{i\left(ax + by + \left(-a^2 - 2\frac{a_3 + a_3 c_1 + a_3 c_2}{\sqrt{2\beta - 4a}}\right)t + d\right)}. \end{split}$$

Family 2:

$$a_1 = 0, a_2 = \mp \frac{1 + c_1 + c_2}{\sqrt{2\beta - 4a}}, a_3 = \pm \frac{(c + a^2)\sqrt{2\beta - 4a}}{1 + c_1 + c_2}.$$
 (43)



Figure 1. The (a) 3D and (b) 2D graphs of Q(x, y, t) for the solution $u_3(x, y, t)$ under $c_1 = 0.5$, $c_2 = 0.25$, $a_3 = 0.03$, $\beta = 0.5$, a = -0.75, b = 0.02, d = 0.04, C = 3 and y = 0.

When we substitute parameters in Equation 43 into Equation 18, we get the following equations:

$$u_{2,1}(x,y,t) = -\frac{\sqrt{2c+2a^2}\sqrt{2\beta-4a}\tan\left(\frac{\sqrt{2c+2a^2}(x+\beta y-2at+C)}{2}\right)}{2(1+c_1+c_2)}, \quad (44)$$

$$u_{2,2}(x,y,t) = \frac{\sqrt{2c + 2a^2}\sqrt{2\beta - 4a}\cot\left(\frac{\sqrt{2c + 2a^2}\left(x + \beta y - 2at + C\right)}{2}\right)}{2(1 + c_1 + c_2)}, \quad (45)$$

in which $c + a^2 > 0$ and $\beta - 2a > 0$ for valid solutions.

$$u_{2,3}(x,y,t) = \frac{\sqrt{-2c - 2a^2}\sqrt{2\beta - 4a} \tanh\left(\frac{\sqrt{-2c - 2a^2}(x + \beta y - 2at + C)}{2}\right)}{2(1 + c_1 + c_2)}$$
(46)

$$u_{2,4}(x,y,t) = \frac{\sqrt{-2c - 2a^2} \sqrt{2\beta - 4a} \coth\left(\frac{\sqrt{-2c - 2a^2} (x + \beta y - 2at + C)}{2}\right)}{2(1 + c_1 + c_2)}, \quad (47)$$

in which $c + a^2 < 0$ and $\beta - 2a > 0$ for valid solutions. Since $v_{2,3}(x, y, t) = c_1 u_{2,3}(x, y, t)$ and $w_{2,3}(x, y, t) = c_2 u_{2,3}(x, y, t)$, we acquire the following solutions for the solutions $u_{2,3}(x, y, t), v_{2,3}(x, y, t)$ and $w_{2,3}(x, y, t)$.

$$Q(x, y, t) = \frac{\sqrt{2c + 2a^2}\sqrt{2\beta - 4a} \tanh\left(\frac{\sqrt{2c + 2a^2}(x + \beta y - 2at + C)}{2}\right)}{2(1 + c_1 + c_2)}e^{i(ax+by+ct+d)},$$

$$S(x, y, t) = \frac{c_1\sqrt{2c + 2a^2}\sqrt{2\beta - 4a} \tanh\left(\frac{\sqrt{2c + 2a^2}(x + \beta y - 2at + C)}{2}\right)}{2(1 + c_1 + c_2)}e^{i(ax+by+ct+d)},$$

$$N(x, y, t) = \frac{c_2\sqrt{2c + 2a^2}\sqrt{2\beta - 4a} \tanh\left(\frac{\sqrt{2c + 2a^2}(x + \beta y - 2at + C)}{2}\right)}{2(1 + c_1 + c_2)}e^{i(ax+by+ct+d)}.$$

We acquire the following solutions for the solutions $u_{2,3}(x, y, t), v_{2,3}(x, y, t)$ and $w_{2,3}(x, y, t)$.



Family 3:

$$a_1 = 0, a_2 = \mp \frac{1 + c_1 + c_2}{\sqrt{2\beta - 4a}}, a_3 = 0, c = -a^2.$$
 (48)

Inserting the parameters in Equation 48 into Equation 18, we get the following equations:

$$u(x, y, t) = \frac{\sqrt{2\beta - 4a}}{(1 + c_1 + c_2)(x + \beta y - 2at + C)},$$
(49)



Figure 2. The 3D graph of (a) Q(x, y, t) and (b) R(x, y, t) for the solution $u_{2,3}(x, y, t)$ under $c_1 = 1$, $c_2 = 2$, c = -2, $\beta = 0.5$, a = 1, b = 2, d = 0, C = 5, y = 0.

$$v(x, y, t) = \frac{c_1 \sqrt{2\beta - 4a}}{(1 + c_1 + c_2)(x + \beta y - 2at + C)},$$
(50)

$$w(x, y, t) = \frac{c_2 \sqrt{2\beta - 4a}}{(1 + c_1 + c_2)(x + \beta y - 2at + C)},$$
(51)

in which β - 2*a* > 0 for proper solutions. For the solutions in Equations 49-51, we get

$$\begin{split} Q(x, y, t) &= \frac{\sqrt{2\beta - 4a} \ e^{l(ax + by - a^2 t + l)}}{(1 + c_1 + c_2)(x + \beta y - 2at + C)}, \\ S(x, y, t) &= \frac{c_1 \sqrt{2\beta - 4a} \ e^{l(ax + by - a^2 t + l)}}{(1 + c_1 + c_2)(x + \beta y - 2at + C)}, \\ N(x, y, t) &= \frac{c_2 \sqrt{2\beta - 4a} \ e^{l(ax + by - a^2 t + l)}}{(1 + c_1 + c_2)(x + \beta y - 2at + C)}, \\ R(x, y, t) &= -\frac{2}{(x + \beta y - 2at + C)^2}. \end{split}$$

The Davey-Stewartson System

To construct new analytical solutions of the system, utilizing the following wave transformation

$$U(x, y, t) = e^{i(\lambda x + ny + rt)}\phi(\xi),$$

$$V(x, y, t) = \vartheta(\xi), \quad \xi = x + y + \kappa t,$$
(52)

the following reduced ODEs are acquired:

$$\left(-r - \gamma(n^2 + \lambda^2)\right)\phi + \mu\phi^3 - \alpha\phi\vartheta + 2\gamma\phi'' = 0, \tag{53}$$

$$-\sigma(\phi')^2 - \sigma\phi\phi'' + \vartheta'' = 0, \tag{54}$$

from the real part and the relation is derived as:

$$\kappa = -2\gamma(n+\lambda). \tag{55}$$

Integrating Equation 54, we have

$$\vartheta = \frac{\sigma}{2}\phi^2.$$
 (56)

Substituting Equation 56 into Equation 53, we have

$$2(-r-\gamma(n^2+\lambda^2))\phi + (2\mu-\alpha\sigma)\phi^3 + 4\gamma\phi^{\prime\prime} = 0.$$
 (57)

If ϕ and ϕ'' are substituted into Equation 57 and setting m = 0, then the following equation is produced:

$$(8a_2^2\gamma - \alpha\sigma + 2\mu)\phi^3 + 12\gamma a_1 a_2 \phi^2 + (4\gamma(2a_2a_3 + a_1^2) - 2r - 2\gamma(n^2 + \lambda^2))\phi + 4\gamma a_1 a_3 = 0.$$
(58)

Compiling all the coefficients of ϕ^s (s = 0, 1, 2, 3) and assuming each to equal zero in Equation 58, the following algebraic system is derived:

 ϕ^0 coefficient:

$$\gamma a_1 a_3 = 0, \tag{59}$$

 ϕ^1 coefficient:

$$4\gamma(2a_2a_3 + a_1^2) - 2r - 2\gamma(n^2 + \lambda^2) = 0, \qquad (60)$$

 ϕ^2 coefficient:

$$\gamma a_1 a_2 = 0 , \qquad (61)$$

 ϕ^3 coefficient:

$$8a_2^2\gamma - \alpha\sigma + 2\mu = 0. \tag{62}$$

Solving this algebraic system from Equation 59 to Equation 62, we obtain the following families.

Family 1:

0.5

0.4

0.3

0.2-

0.1

0

$$a_1 = 0, a_2 = \frac{\sqrt{-2\gamma(-\alpha\sigma + 2\mu)}}{4\gamma}, a_3 = \frac{\gamma n^2 + \gamma \lambda^2 + r}{\sqrt{-2\gamma(-\alpha\sigma + 2\mu)}}.$$
 (63)

Substituting parameters in Equation 63 into Equation 52, we acquire the following soliton solutions

$$U_{1,1}(x,y,t) = \frac{2\sqrt{\frac{\gamma n^2 + \gamma \lambda^2 + r}{\gamma}}\gamma \tan\left[\frac{1}{2}\sqrt{\frac{\gamma n^2 + \gamma \lambda^2 + r}{\gamma}}(x+y-2\gamma(n+\lambda)t+J)\right]}{\sqrt{-2\gamma(-\alpha\sigma+2\mu)}}e^{((\lambda x+ny+rt)i)}, \quad (64)$$

$$V_{1,1}(x,y,t) = -\frac{\sigma(\gamma n^2 + \gamma \lambda^2 + r) \tan\left[\frac{1}{2}\sqrt{\frac{\gamma n^2 + \gamma \lambda^2 + r}{\gamma}}(x + y - 2\gamma(n+\lambda)t + f)\right]^2}{-\alpha \sigma + 2\mu},$$
 (65)

$$U_{1,2}(x,y,t) = -\frac{2\sqrt{\frac{\gamma n^2 + \gamma \lambda^2 + r}{\gamma}} \operatorname{cot}\left[\frac{1}{2}\sqrt{\frac{\gamma n^2 + \gamma \lambda^2 + r}{\gamma}}(x + y - 2\gamma(n + \lambda)t + f)\right]}{\sqrt{-2\gamma(-\alpha\sigma + 2\mu)}}e^{(\lambda x + ny + rt)t}, \quad \text{(66)}$$

$$V_{1,2}(x,y,t) = -\frac{\sigma(\gamma n^2 + \gamma \lambda^2 + r) \cot\left[\frac{1}{2}\sqrt{\frac{\gamma n^2 + \gamma \lambda^2 + r}{\gamma}}(x+y-2\gamma(n+\lambda)t+f)\right]^2}{-\alpha\sigma+2\mu}, \quad (67)$$

where $\gamma(\gamma n^2 + \gamma \lambda^2 + r) > 0$ for existence of obtained solutions and the following dark soliton solutions:

$$U_{1,3}(x,y,t) = -\frac{2\sqrt{-\frac{\gamma n^2 + \gamma \lambda^2 + r}{\gamma}} \gamma \tanh\left[\frac{1}{2}\sqrt{-\frac{\gamma n^2 + \gamma \lambda^2 + r}{\gamma}} (x + y - 2\gamma(n + \lambda)t + J)\right]}{\sqrt{-2\gamma(-\alpha\sigma + 2\mu)}} e^{(\lambda x + ny + rt)t}, \quad (68)$$

$$V_{1,3}(x,y,t) = \frac{\sigma(\gamma n^2 + \gamma \lambda^2 + r) tanh \left[\frac{1}{2}\sqrt{-\frac{\gamma n^2 + \gamma \lambda^2 + r}{\gamma}}(x+y-2\gamma(n+\lambda)t+J)\right]^2}{-\alpha \sigma + 2\mu}, \quad (69)$$

where $\gamma(\gamma n^2 + \gamma \lambda^2 + r) < 0$ for existence of solutions $U_{1,3}(x, y, t)$ and $V_{1,3}(x, y, t)$.

Family 2:

$$a_1 = 0, a_2 = \frac{\sqrt{-2\gamma(-\alpha\sigma + 2\mu)}}{4\gamma}, r = a_3\sqrt{-2\gamma(-\alpha\sigma + 2\mu)} - \gamma n^2 - \gamma \lambda^2 \quad (70)$$

Substituting parameters in Equation 70 into Equation 52, we acquire the following soliton solutions:

$$U_{2,1}(x,y,t) = \frac{2\sqrt{\frac{\sqrt{-2\gamma(-\alpha\sigma+2\mu)a_3}}{\gamma}} v \tan\left[\frac{1}{2}\sqrt{\frac{\sqrt{-2\gamma(-\alpha\sigma+2\mu)a_3}}{\gamma}} (x+y-2\gamma(n+\lambda)t+f)\right]}{\sqrt{\frac{\sqrt{-2\gamma(-\alpha\sigma+2\mu)a_3}}{\gamma}}}, \quad (71)$$

$$V_{2,1}(x,y,t) = \frac{\sigma\sqrt{-2\gamma(-\alpha\sigma+2\mu)}a_3 \tan\left[\sqrt{\frac{\sqrt{-2\gamma(-\alpha\sigma+2\mu)}a_3}{\gamma}(x+y-2\gamma(n+\lambda)t+f)}\right]}{-\alpha\sigma+2\mu},$$
 (72)

$$U_{2,2}(x,y,t) = -\frac{2\sqrt{\sqrt{-2\gamma(-\alpha\sigma+2\mu)}a_3}}{\gamma} \cot\left[\frac{1}{2}\sqrt{\frac{\sqrt{-2\gamma(-\alpha\sigma+2\mu)}a_3}}(x+y-2\gamma(n+\lambda)t+J)\right]}{\sqrt{-2\gamma(-\alpha\sigma+2\mu)}}, \quad (73)$$

$$V_{2,2}(x,y,t) = -\frac{\sigma\sqrt{-2\gamma(-\alpha\sigma+2\mu)}a_3\cot\left[\sqrt{\frac{\sqrt{-2\gamma(-\alpha\sigma+2\mu)}a_3}{\gamma}}(x+y-2\gamma(n+\lambda)t+f)\right]^2}{-\alpha\sigma+2\mu},$$
 (74)

where $\gamma(-\alpha\sigma + 2\mu) < 0$ and $a_3\gamma > 0$ for existence of obtained solutions and the following dark soliton solutions:

$$U_{2,3}(x,y,t) = -\frac{2 \sqrt{\frac{\sqrt{-2\gamma(-\alpha\sigma+2\mu)}a_3}{\gamma} tanh \left[\frac{1}{2} \sqrt{\frac{\sqrt{-2\gamma(-\alpha\sigma+2\mu)}a_3}{\gamma} (x+y-2\gamma(n+\lambda)t+f)}\right]}{\sqrt{\frac{\sqrt{-2\gamma(-\alpha\sigma+2\mu)}}{\gamma}}}, \quad (75)$$

$$\times e^{(\lambda x+ny+(a_3\sqrt{-2\gamma(-\alpha\sigma+2\mu)}-\gamma n^2-r)\lambda^2)t)i}$$



Figure 3. The 3D graph of (a) $U_{1,1}(x, y, t)$ and (b) $V_{1,1}(x, y, t)$ with, $r = 1, \gamma = -0.5, n = 0.5, \sigma = 0.5, \mu = 0.5, \alpha = 1, \beta = 2, J = 0.5, \sigma = 0.5, \mu = 0.5, \alpha = 1, \beta = 2, J = 0.5, \sigma = 0.5$

$$V_{2,3}(x,y,t) = -\frac{\sigma\sqrt{-2\gamma(-\alpha\sigma+2\mu)}a_3 \tanh\left[\sqrt{-\frac{\sqrt{-2\gamma(-\alpha\sigma+2\mu)}a_2}{\gamma}(x+y-2\gamma(n+\lambda)t+f)}\right]^2}{-\alpha\sigma+2\mu},$$
 (76)

where $\gamma(-\alpha\sigma + 2\mu) < 0$ and $a_3\gamma < 0$ for existence of solutions $U_{2,3}(x, y, t)$ and $V_{2,3}(x, y, t)$.

CONCLUSION

In this research article, we have seen that computer algebra is a powerful technique to solve all complicated problems in mathematical sciences. Using the method, we obtained the new exact wave and soliton solutions of the complex nonlinear systems Davey-Stewartson and Maccari's systems. All the solutions verify the models in this study. We also describe the 2D, and 3D graphs of some of the acquired solutions in this study. Some of the reported solutions in this paper have important physical meanings, for instance, the hyperbolic tangent arises in the calculation of magnetic moment and rapidity of special relativity, and the hyperbolic cotangent arises in the Langevin function for magnetic polarization [32]. All the computations in this study are carried out with the aid of Maple. The acquired solutions are new in the literature. The proposed method can also be used to solve various NLPDEs in mathematical physics.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Scrutiny of flow and heat transfer characteristics of hybrid nanofluid passing through a squeezing channel

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ABSTRACT

This article mainly presents a comparative analysis of MHD flow of three different types of fluids, namely, simple base fluid (Ethylene Glycol), mono-nanofluid (Ethylene Glycol+G-raphene) and Hybrid nanofluid (Ethylene Glycol+Graphene+Copper) passing through a squeezing channel. The effect of heat absorption and Joule dissipation is also taken into account. System of partial differential equation governing the flow problem is transformed into a system of ordinary differential equation by using similarity transforms. To get the solution, shooting technique along with Runge-Kutta 4th order method is employed. The influence of several physical parameter on velocity, temperature, skin friction and Nusselt number is analyzed. The findings indicate that temperature increases with the enhancement of a magnetic field and Joule dissipation. Moreover, the study reveals that the temperature of mono-nanofluid is higher than that of the base fluid but lower than that of the hybrid nanofluid.

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INTRODUCTION

The increasing utilization of nanofluids in real-world industrial applications has made them a major focus of research. In 1995, Choi and Eastman [1] discovered that the addition of metallic nanoparticles enhances heat transfer. Buongiorno [2] identified seven methods to improve the heat transfer rate of base fluids, with Brownian motion and thermophoresis playing significant roles. Nanofluids find important applications in energy conversion, microsystems cooling, and the medical industry. Numerous researchers have investigated the heat transfer characteristics of nanofluids [3-7].

Graphene, with its notable properties such as thermal conductivity, flexibility, and high elasticity [8], has found various applications in batteries, supercapacitors, and miniaturized solar devices [9]. Upadhya et al. [10] conducted a study on enhancing the heat transfer rate using ethylene glycol with graphene nanoparticles. Bhattacharyya et al. [11] carried out the statistical analysis of the Ethylene glycol and graphene based nanofluid flow over a stretching sheet.

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In recent years, researchers have focused on the use of hybrid nanofluids, which involve mixing multiple nanoparticles in a fluid, to further improve heat transfer rates. Devi and Devi [12] investigated the flow of a hybrid nanofluid (Cu-Al₂O₃/water) over a stretching sheet, presenting a novel mathematical model. Suresh et al. [13] validated this new model using experimental data. Devi and Devi [14] extended their work to study 3-dimensional flow under Newtonian heating conditions, finding higher heat transfer rates in hybrid nanofluids compared to regular nanofluids. Prakash and Devi [15] examined the influence of Al₂O₃-Cu/water nanofluid passing through a slender stretching sheet. Bahiraei and Mazaheri [16] explored the application of graphene-platinum hybrid nanofluids in miniature devices. Aziz et al. [17] investigated entropy generation due to hybrid nanofluids with Maxwell as the base fluid, considering radiation, magnetic fields, and joule heating. Yashkun et al. [18] studied hybrid nanofluid flow past an exponentially stretching/shrinking sheet, taking mixed convection into consideration. Rafique et al. [19] shows that heat transfer performance in hybrid nanofluid is better than mono-nanofluid.

Joule dissipation, a significant heat source in fluid flow under the influence of a magnetic field, plays a vital role in heat-treated materials. Rashid et al. [20] studied the impact of Joule heating on MHD flow over a stretchable wall of graphene–carboxymethyl cellulose (CMC) with water as a base fluid. Hence, several studies have examined the effect of Joule dissipation [21-23].

Flow within the channel is often observed in many engineering and industrial processes, for example, lubrication systems, moving pistons, hydraulic lifts, injection moulding, flow inside the nasogastric tubes syringes. Due to its nobility, many researchers analyzed the flow within the channel under various conditions [24, 25]. The flow induced by the compression of two parallel plates due to external applied stress is known as squeezing flow. The squeezing flow situation is often observed in many engineering and industrial processes. Noor and Shafie [26] discovered nature of hydromagnetic flow of hybrid nanofluid within squeeze channel. Due to its immense applications, the flow through a squeezing channel has attracted many researchers [27-30].

A careful review of the literature suggests that, no investigation has been conducted on comparative analysis for flow and heat transfer characteristics among three different fluids namely base fluid (Ethelene Glycol), mono-nanofluid (Ethelene Glycol + Graphene), and hybrid nanofluid (Ethelene Glycol + Graphene + Copper) passing through a squeezing channel taking into account of heat absorption and magnetic field effects. Thus, the present study analyses the impact of various physical parameters on base fluid, mono-nanofluid and hybrid nanofluid taking into account of these effects.

Modeling of the Problem

Consider 2-dimensinal electrically conducting, heat absorbing, radiating, incompressible, electrically conducting hybrid nanofluid flow within squeezing channel taking Joule dissipation into account. Our mathematical model is related to 2 parallel plates which is along *x* and *z*-axis and *y* is normal to the plates. The gap between two plates is $h(t) = H(1 - \alpha t)^{\frac{1}{2}}$ at time *t*. Direction and speed of plates is controlled by α . The velocity of plates is $\frac{dh}{dt}$ and the gap will be 0 between two plates at $t = \frac{1}{\alpha} (\alpha \neq 0)$. Negative value of α denotes that distance between plates are increasing. Magnetic field is applied perpendicular to the surface of plates and strength is given by $B(t) = B_o(1 - \alpha t)^{-\frac{1}{2}}$. It is also assumed that there is no chemical reaction. Geometry of the problem express in Figure 1. Under these conditions, the mathematical model governing the boundary layer flow are given by [27]:



Figure 1. Geometry of the flow problem.

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{1}$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho_{hnf}} \frac{\partial p}{\partial x} - \frac{\sigma_{hnf} B^2(t) u}{\rho_{hnf}} + \vartheta_{hnf} \Big[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \Big], \quad (2)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{1}{\rho_{hnf}} \frac{\partial p}{\partial y} + \vartheta_{hnf} \left[\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right], \quad (3)$$

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{\kappa_{hnf}}{(\rho_{C_P})_{hnf}} \left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] + \frac{\sigma_{hnf} B^2(t) u^2}{(\rho_{C_P})_{hnf}} - \frac{QT}{(\rho_{C_P})_{hnf}}.$$
 (4)

Where, *u* and *v* are the velocity of hybrid nanofluid in *x* and *y*- directions. *T* indicates the temperature of fluid, *p*, ρ_{hnf} , μ_{hnf} , ϑ_{hnf} , $(\rho_{C_p})_{hnf}$, K_{hnf} , *Q* and σ_{hnf} denote the fluid pressure, density of hybrid nanofluid, kinematic viscosity of hybrid nanofluid, heat capacity of hybrid nanofluid, thermal conductivity of hybrid nanofluid, heat absorption coefficient and electrical conductivity of the hybrid nanofluid are noted as [25]:

$$\rho_{hnf} = (1 - \phi_2)[(1 - \phi_1)\rho_f + \phi_1\rho_{n_2}] + \phi_2\rho_{n_1}, \tag{5}$$

$$(\rho c_p)_{hnf} = (1 - \phi_2) \left[(1 - \phi_1) (\rho c_p)_f + \phi_1 (\rho c_p)_{n_1} \right] + \phi_2 (\rho c_p)_{n_2}, \quad (6)$$

$$\mu_{hnf} = \frac{\mu_f}{(1-\phi_1)^{2.5}(1-\phi_2)^{2.5}},\tag{7}$$

$$\frac{K_{hnf}}{K_f} = \left[\frac{K_{n_2} + 2K_{n_f} - 2\phi_2(K_{n_f} - K_{n_2})}{K_{n_2} + 2K_{n_f} + \phi_2(K_{n_f} - K_{n_2})}\right],\tag{8}$$

$$\frac{\sigma_{hnf}}{\sigma_f} = \left[\frac{\sigma_{n_2} + 2\sigma_{n_f} - 2\phi_2(\sigma_{n_f} - \sigma_{n_2})}{\sigma_{n_2} + 2\sigma_{n_f} + \phi_2(\sigma_{n_f} - \sigma_{n_2})} \right],\tag{9}$$

where
$$K_{nf} = \frac{K_{n_1} + 2K_f - 2\phi_1(K_f - K_{n_1})}{K_{n_1} + 2K_f + \phi_1(K_f - K_{n_1})} \times K_f, \sigma_{nf} = 1 + \frac{3\left(\frac{\sigma_{n_1}}{\sigma_f} - 1\right)\phi_1}{2 + \frac{\sigma_{n_1}}{\sigma_f} - \left(\frac{\sigma_{n_1}}{\sigma_f} - 1\right)\phi_1}$$

The base fluid Ethylene glycol $(C_2H_6O_2)$ and nanoparticle's thermophysical properties are mentioned in Table 1 [23]. Here μ_f presents the dynamic viscosity of C₂H₆O₂. K_f , K_{n_1} and K_{n_2} denote the thermal conductivity of base fluid, graphene and copper respectively. ϕ_1 and ϕ_2 indicate the volume fraction of graphene nanoparticle and copper nanoparticle respectively. σ_f , σ_{n_1} and σ_{n_2} is the notation of electrical conductivity of C₂H₆O₂, Graphene and Copper. ρ_f , ρ_{n_1} and ρ_{n_2} is the notation of density of C₂H₆O₂, Graphene and Copper. (ρc_p)_f, (ρc_p)_{n_1} and (ρc_p)_{n_2} is the notation of heat capacity of C₂H₆O₂, Graphene and Copper. Boundary conditions are taken as:

$$u = 0, v = \frac{dh}{dt}, T = T_H at y = h(t)$$
 (10)

$$\frac{\partial u}{\partial y} = 0, v = 0, \frac{\partial T}{\partial y} = 0 \text{ at } y = 0$$
(11)

Similarity transformations are given as [27]

$$\eta = \frac{y}{H\sqrt{1-\alpha t}}, u = \frac{\alpha x}{2(1-\alpha t)} f'(\eta), v = \frac{-\alpha H}{2\sqrt{(1-\alpha t)}} f(\eta), \theta = \frac{T}{T_H}$$
(12)

Using the similarity transformations given in equation (12) into the PDEs (2) to (4) and eliminating the pressure terms by cross- differentiations of equations (2) and (3), the resultant ordinary differential equation is mentioned from equation (13) to (14) as follows:

$$S\left(\frac{A_1}{A_4}\right) \left[3f'' + \eta f''' + f'f'' - ff'''\right] + M^2\left(\frac{A_5}{A_4}\right) f'' = f^{i\nu} \quad (13)$$

$$\theta^{\prime\prime} + S.Pr\left(\frac{A_2}{A_3}\right) [f\theta^{\prime} - \eta\theta^{\prime}] + M^2\left(\frac{A_5}{A_3}\right) Pr.Ecf^{\prime^2} - G.\theta = 0 \quad (14)$$

$$\eta = 0 \Longrightarrow f''(0) = 0, f(0) = 0, \theta'(0) = 0$$
(15)

$$\eta = 1 \Longrightarrow f'(1) = 0, f(1) = 1, \theta(1) = 1$$
 (16)

Where $S = \frac{\alpha H^2}{2v_f}$, $A_1 = \frac{\rho_{hnf}}{\rho_f}$, $A_2 = \frac{(\rho C_p)_{hnf}}{(\rho C_p)_f}$, $A_3 = \frac{\kappa_{hnf}}{\kappa_f}$, $A_4 = \frac{\mu_{hnf}}{\mu_f}$, $A_5 = \frac{\sigma_{hnf}}{\sigma_f}$. $Pr = \frac{\mu_f(\rho C_p)_f}{\rho_{f\kappa_f}}$ is the Prandtl number, ber, $E_C = \frac{\rho_f}{(\rho C_p)_f T_H} \left(\frac{\alpha x}{2(1-\alpha t)}\right)^2$ noting the Eckert number, $M = HB_0 \sqrt{\frac{\sigma_f}{\mu_f}}$ is the magnetic number, $G = \frac{Q_0 H^2}{\kappa_{nf}}$ denotes the

Table 1. Thermophysical properties of Ethylene glycol and nanoparticles [23]

Thermo-physical properties	$\rho(kg/m^3)$	$c_p(J/kgK)$	K(W/mK)	$\sigma(S/m)$
Graphene	2250	2100	2500	1 x 10 ⁻⁷
Copper	8993	385	401	5.96 x 10 ⁷
Ethylene glycol	1114	2415	0.252	5.5 x 10 ⁻⁶

Pr	Ec	$-\theta'(1)$ Mustafa et al.[39]	-θ'(1) Acarya et al. [40]	$-\theta'(1)$ Present work
0.5	1.0	1.5222	1.5222	1.5224
1.0	1.0	3.0263	3.0263	3.0265
2.0	1.0	5.9805	5.9805	5.9803
5.0	1.0	14.3439	14.4394	14.4397
1.0	0.5	1.5132	1.5131	1.5131
1.0	1.2	3.6315	3.6315	3.6318
1.0	2.0	6.0526	6.0526	6.0526
1.0	5.0	15.1316	15.1316	15.1315

Table 2. Verification of $-\theta'(1)$ when S = 0.5, G = 0 and M = 0

coefficient of absorption. Where ϑ_f indicates the kinematic

coefficient of viscosity.

The coefficient of skin-friction C_f and the Nusselt number Nu can be expressed as

$$C_f = \frac{\mu_{hnf} \left(\frac{\partial u}{\partial y}\right)_{y=h(t)}}{\frac{1}{2}\rho_{hnf} \left(\frac{dh}{dt}\right)^2} = \frac{4\mu_{hnf}}{H^2\rho_{hnf}\alpha} \frac{f''(1)}{\delta}$$
(17)

$$Nu = \frac{-HK_{hnf} \left(\frac{\partial T}{\partial y}\right)_{y=h(t)}}{K_f T_H} = \frac{-Nu_r}{\sqrt{(1-\alpha t)}}.$$
 (18)

Where $Nu_r = A_3 \theta'(1)$ and $\delta = \frac{H\sqrt{(1-\alpha t)}}{x}$.

NUMERICAL METHOD IMPLEMENTATION

The majority of natural processes are characterized by highly intricate nonlinear dynamics, typically described by nonlinear differential equations. Attaining a closed-form exact solution under such circumstances proves to be unattainable. In these situations, researchers seek approximate solutions through either numerical methods or analytical techniques. Numerical solutions can be obtained employing diverse methods like the finite difference method [31], finite volume method [32], finite element method (FEM) [33], reproducing kernel algorithm [34-37] and shooting method [38]. The solution of the present problem is obtained by using shooting method along with Runge-Kutta fourth order technique. In order to find the solution of transformed ordinary differential equations (13) and (14) subject to boundary conditions (15) and (16), the following steps are used:

- To solve the equations (13) and (14), first converted into a system of six first-order differential equations.
- To find the solution of the system of ordinary differential equations, the initial values of f''(0) and $\theta'(0)$ are found using the shooting method along with Runge-Kutta fourth order technique.

- After the grid Independence analysis, the step size selected is 0.001 throughout the computation.
- A tolerance error of 10⁻⁶ is chosen. The entire process is repeated until the desired accurate result is obtained.

Characteristics of Shooting Technique

- Shooting method converts boundary value problem to initial value problem. Then initial value problem needs to be solved and initial guesses are to be found in each iteration. This process will continue until solution satisfies the given boundary conditions.
- The convergence of shooting method depends on initial guess. Poor initial guess may decrease the rate of convergence or possibly solution may diverge.

Characteristics of Runge-Kutta Fourth Order Method

- Runge-Kutta fourth order method is used to solve initial value problem with high accuracy.
- In Runge-Kutta fourth order method, step size can be adjusted during the solving process.

Validation of Present Finding

In order to validate the numerical solution obtained using the method described in above section, a comparison of the Nusselt number at the upper plate is performed with the earlier published results and are presented Table [2].

It is noted from Table 2 that this manuscript is in excellent agreement with the earlier published manuscripts ([39-40]).

RESULTS AND DISCUSSIONS

In this section, all the results for velocity temperature, skin friction coefficient and Nusselt number, computed using the numerical method as described in previous section are presented graphically in Figures 2 to 12. Impact of various physical parameter M = 0.5, Pr = 11, Ec = 0.05, S = 0.5, G = 0.1 and different values of nano particles volume fraction on hybrid nanofluid velocity (from Figures 2 and 3) and temperature (from Figures 4 to 6) is discussed and analyzed. In all graphical representations the results are displayed for three different cases of fluid flow: (1) Base fluid (Ethylene

Glycol- $C_2H_6O_2$) only using solid lines, (2) mono-nanofluid ($C_2H_6O_2$ + Graphene) using dashed lines and (3) Hybrid nanofluid ($C_2H_6O_2$ + Graphene + Copper) using dotted lines. Throughout the manuscript ϕ_1 and ϕ_2 represents graphene and Copper nanoparticle volume fractions.

Velocity Profile

The velocity profiles of the flow problem are presented in Figures 2 and 3, against the magnetic field and squeezing number. Figure 2 illustrates the impact of magnetic field nanoparticles volume faction on hybrid nanofluid velocity. It is notice that due to an increase in the magnetic field, a very small reduction in velocity of the hybrid nanofluid up to central region while the opposite nature is observed after that. This phenomenon is happening due to Lorentz force up to central region and after that due to the continuity equation. It also shows that in case of mono-nanofluid $(\phi_1 = 0.05 \text{ and } \phi_2 = 0)$, velocity is higher than the base fluid and lower than hybrid nanofluid $(\phi_1 = 0.025 \text{ and } \phi_2 = 0.025)$ up to central region.

Figure 3 demonstrates the influence of the Squeeze number on hybrid nanofluid velocity. It is evident that the Squeeze number decreases the hybrid nanofluid velocity, but the opposite nature is visible as the distance between the channels increases. Further, increase in squeezing number does not seem to affect the velocity abnormally as we can see a very small variations in velocity against *S*. It also shows that in the case of the mono- nanofluid ($\phi_1 = 0.05$ and $\phi_2 = 0$), the velocity is higher than the base fluid and lower than the hybrid nanofluid ($\phi_1 = 0.025$ and $\phi_2 = 0.025$) up to the central region.

Temperature Profile

1.

1.2

0.8 (**1**)

0.6

0.4

The temperature profile for flow problem is represented in Figures 4 to 6 against varying values of magnetic parameter, Eckert number and absorption parameter.

M = 0, 0.5, 1

 $= 0.0, \ \phi_2 = 0.0$

 $\phi_1 = 0.025, \phi_2 = 0.025$

 $\phi_1 = 0.05, \phi_2 = 0.0$

Ø.



M = 0, 0.5, 1

Figure 2. Variation in M values causes various velocity profile.



Figure 3. Varation in *S* values cause various velocity profiles.

It is clearly noted from Figure 4 that the hybrid nanofluid temperature is enhanced due to the increase in the magnetic field. This is because the fluid will face more difficulties to flow against the magnetic field.

Figure 5 shows that enhancing the Eckert number has the nature to enhance the temperature of the hybrid nanofluid. The Eckert number represents the ratio of kinetic energy to enthalpy. Some part of energy converts to kinetic energy; therefore, in the boundary layer, viscous dissipation can enhance the temperature. It is also noted that the hybrid nanofluid temperature increases when the nanoparticle volume is increased. It also shows that in the case of the mono-nanofluid ($\phi_1 = 0.05$ and $\phi_2 = 0$), the temperature is higher than the base fluid and lower than the hybrid nanofluid ($\phi_1 = 0.025$ and $\phi_2 = 0.025$). Figure 6 shows



Figure 4. Varation in *M* values cause various temperature profiles.



Figure 5. Varation invalues of Ec cause various temperature profiles.



Figure 6. Varation invalues of G cause various temperature profiles.

that due to the enhancement of the absorption parameter, the temperature of the hybrid nanofluid velocity is reduced because of the increment of the absorption capacity of the fluid. It also shows from Figure 4 to 6 that in case of mono-nanofluid ($\phi_1 = 0.05$ and $\phi_2 = 0$), temperature is higher than base fluid and lower than hybrid nanofluid ($\phi_1 = 0.025$ and $\phi_2 = 0.025$).

Skin Friction and Nusselt Number Profile

The quantities of engineering interests like skin friction coefficient and Nusselt number profiles against the pertinent flow parameter is displayed in figures 7 to 12. Figures 7 and 8 presents the impact of M and S on C_f at the channel's upper plate. From Figure 7, It is visible that C_f is reducing at upper plate due to enhancement of M and opposite



Figure 7. Varation in values of M and ϕ cause various C_f profiles.



Figure 8. Varation in values of S and ϕ cause various C_f profiles.

behavior of C_f is observed due to increase in *S*. It is also noted that in case of mono-nanofluid ($\phi_1 = 0.05$ and $\phi_2 = 0$), C_f is higher than base fluid and lower than hybrid nanofluid ($\phi_1 = 0.025$ and $\phi_2 = 0.025$).

Figures 9 to 12 presents the impact of M, G, S and Ec on Nu at the upper plate of the channel. From Figure 9 it is noted that when magnetic parameter is increased from 0 to 2, a 10.01% of relative increment in heat transfer rate is reported. Figure 10 which displays that the Nusselt number is a decreasing function of absorption parameter G, to be exact, we reported a relative decline of 115.24% in Nusselt number when G is varied from 0 to 1. It is observed that there is a 34.748% of decrease in Nusselt number as the value of S increases from 0 to 1, whereas an increase of 18.28% of heat transfer rate is noted for hybrid nanofluid as compared



Figure 9. Varation in values of M and ϕ cause various N_u profiles.



Figure 10. Varation in values of G and ϕ cause various N_u profiles.



Figure 11. Varation in values of S and ϕ cause various N_u profiles.



Figure 12. Varation in values of Ec and ϕ cause various N_u profiles.

to base fluid. Similarly in Figure 12 the Eckert number *Ec* demonstrated an increasing nature of Nusselt number against it. The investigation revealed a huge relative increase of 31.2% in Nusselt number when *Ec* is varied from 0 to 0.1. It is also noted that in the case of the mono-nanofluid ($\phi_1 = 0.05$ and $\phi_2 = 0$), *Nu* is higher than the base fluid and lower than the hybrid nanofluid ($\phi_1 = 0.025$ and $\phi_2 = 0.025$). Another aspect worth mentioning is that the rate of heat transfer in base fluid, mono-nanofluid and hybrid nanofluid is almost equal for smaller values of magnetic parameter *M* and Eckert number *Ec*, however with increasing value of *M* and *Ec* the effect of different type of fluid on Nusselt number becomes prominent. This shows that the magnetic field and Eckert number both influences the effect of nanoparticles on heat transfer rate.

CONCLUSION

This article presents the comparative study of flow and heat transfer characteristics of three different type of fluids namely (1) Base fluid (Ethylene Glycol- $C_2H_6O_2$) (2) Mono-nanofluid ($C_2H_6O_2$ + Graphene) and (3) hybrid nanofluid ($C_2H_6O_2$ + Graphene + Copper) passing through a squeezing channel. The study also takes into account the combined effects of transverse magnetic field, heat absorption and Joule dissipation. The behavior of fluid velocity, temperature, skin friction coefficient and Nusselt number are analyzed. The major findings of the present investigation are listed below:

- The hybrid nanofluid velocity is going down due to increase in magnetic field till central region and after that opposite tendency is visible.
- The nature of temperature is to grow up by enhancing due to magnetic field, Joule dissipation while opposite behavior due to enhancing of absorption parameter.

- Local skin friction at upper plate is enhancing due to enhancement of *S* and opposite behavior happened due to enhancement in *M*.
- The local Nusselt number at the upper plate is enhancing due to enhancement of *M* and *Ec* and opposite behavior happened due to enhancement in *G* and *S*.

The heat transfer rate as well as skin friction coefficient, for hybrid nanofluid found to be higher than that of both mono-nanofluid and base fluid.

NOMENCLATURE

Symbol

•	
и	Velocities of hybrid nanofluid in the <i>x</i> - direction
v	Velocities of hybrid nanofluid in the <i>y</i> -direction
Т	Temperature of hybrid nanofluid
p	Pressure in hybrid nanofluid
$ ho_{hnf}$	Density of hybrid nanofluid
ρ_f	Density of $C_2H_6O_2$ (base fluid)
ρ_{n_1}	Density of graphene
ρ_{n_2}	Density of copper
ϑ_{hnf}	Kinematic viscosity of hybrid nanofluid
K _{hnf}	Thermal conductivity of hybrid nanofluid
K _f	Thermal conductivity of the base fluid
K_{n_1}	Thermal conductivity of graphene
K_{n_2}	Thermal conductivity of copper
$Q^{}$	Heat absorption coefficient of hybrid nanofluid
σ_{hnf}	Electrical conductivity of the hybrid nanofluid
σ_f	Electrical conductivity of base fluid
σ_{n_1}	Electrical conductivity of graphene nanoparticle
σ_{n_2}	Electrical conductivity of copper nanoparticle
B(t)	The strength of applied magnetic field
μ_f	Dynamic viscosity of base fluid
$\dot{\phi_1}$	Volume fraction of graphene nanoparticle

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AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Utilizing artificial neural networks (ANN) for predictive modeling of sulfate removal from water

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ABSTRACT

This research centers on developing an artificial neural network (ANN) algorithm to predict the precise removal of sulfate from synthetically prepared water samples. Two distinct resins, sodium-based cationic resin (SBCR) and divinylbenzene styrene (DVBS), were employed to achieve this goal. Additionally, the study investigated the influence of column properties (diameter and height), initial sulfate concentration, and contact time on sulfate removal from synthetically prepared samples. After collecting data from experimental trials, a feed-forward ANN structure was constructed. The selected input parameters for predicting sulfate removal encompassed column properties (diameter and height), contact time, resin type, and initial sulfate concentration. The model's performance was assessed using several statistical criteria, including the correlation coefficient (R), mean absolute percentage error (MAPE, %), root mean square error (RMSE), and mean square error (MSE). The model's training and test performance yielded impressive results: the correlation coefficient (R) was exceptionally high at 1.0000 for training and 0.9999 for test, indicating a strong alignment between predicted and actual values.

Moreover, the mean absolute percentage error (MAPE, %) was 0.5422 for training and 0.9223 for testing, reflecting low average percentage differences between predictions and actual data and indicating high accuracy. The root mean square error (RMSE) values were also 0.0012 for training and 0.0034 for the test, demonstrating minimal average prediction errors. Lastly, the mean square error (MSE) values were notably low, with 1.42x10⁻⁶ for training and 1.14x10⁻⁵ for test phase, underscoring the model's ability to provide accurate predictions with minimal deviations from actual values. Based on these comprehensive evaluation criteria, the ANN exhibited strong predictive performance in estimating sulfate removal.

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INTRODUCTION

Water pollution, in terms of anions, is a public health concern with various effects. Sulfate (SO₄²⁻) is a common pollutant among all anions and can naturally occur in groundwater. High sulfate levels in drinking water are known to cause diarrhea, making removing ions essential. Several methods and technologies are available for removing SO_4^{2-} ions from water sources, including ion exchange, nanofiltration, adsorption, reverse osmosis, and electrodialysis. The choice of method depends on technological development, specific use cases, limitations, and cost [1]. Generally, these methods can be grouped into physical, physicochemical, and biological categories [2]. Physical methods involve adsorption using various adsorbents like activated carbon, biochar, graphene, zeolite, and bentonite [3-6]. Physicochemical methods include ion exchange, precipitation, and electrocoagulation, while biological methods encompass artificial wetlands and bioreactors. Studies on sulfate removal from water resources using these methods are in the literature.

In a study conducted by Darbi et al. [3], bentonite was used to remove sulfate from groundwater, and its performance was compared to ion exchange and nanofiltration processes. Another study on adsorption involved sulfate removal from wastewater using activated carbon [7]. Factors such as adsorbent mass, pH, and contact time were investigated. Hong et al. [4] removed sulfate from acid mine drainage using polypyrrole-tailored activated carbon. Ma et al. [8] used a sol-gel method to create spherical amorphous ZrO(OH)₂/AlOOH composite adsorbent beads for sulfate removal. Spina-christi lotus leaf-derived activated carbon was used to remove sulfate from an aqueous solution, and the study investigated the effects of pH, contact time, temperature, adsorbent concentration, and initial sulfate concentration [9]. Salimi et al. [10] used nanoparticles of natural clinoptilolite to adsorb sulfate ions from Gamasiab River water samples, studying the effects of pH and the adsorbent-to-contaminant ratio (D/C). Ao et al. [11] synthesized low-cost zirconium oxide-modified pomelo peel biochar (ZrBC) for sulfate ion adsorption from an aqueous solution. Sukamto [12] used magnetic silica-chitosan hybrids (MP@SiO2/CPTMS/Chi) to adsorb sulfate ions from an aqueous solution.

Tjeda-Tover et al. [13] synthesized two different adsorbents: these are biochar modified with H_2SO_4 with a massto-volume ratio of 1:1 (B 1:1) and cellulose modified with cetyl trimethyl ammonium chloride (CTAC), for adsorbing sulfate in a solution. Obeid et al. [14] removed sulfate from wastewater using a clay-based adsorbent (sludge, waste limestone, bentonite, SBL), investigating different values of pH, contact time, adsorbent dose, and initial $SO_4^{2^\circ}$ concentration. Shahzadi et al. [15] used nickel monometallic and nickel-cobalt bimetallic nanoparticles to remove sulfate and phosphate ions. Various methods can be employed for sulfate removal, and the choice of method depends not only on experimental procedures and challenges but also on costs. Parameters like maintenance, installation, initial investment, waste management, and operational costs are crucial, especially in pilot-scale research. In recent years, with the advancement of computer technology, modeling studies have gained importance, reducing costs such as experimental workloads for many processes. Artificial neural networks (ANN) are a popular artificial intelligence (AI) technique because they can learn complex and nonlinear systems, making them preferred in many processes [16-23].

To the author's best knowledge, ANN modeling of sulfate removal from drinking water has not been published. Consequently, an ANN model for sulfate removal was developed using experiment data. The experimental system involved two adsorbents (DVBS and SBCR) with varying column diameters and heights, contact times, and initial sulfate concentrations. These parameters were determined as input parameters for predicting sulfate removal.

MATERIALS AND METHODS

Chemicals

- Anhydrous sodium sulfate (Na₂SO₄)
- 0.1 M NaOH solution
- 0.1 M HCl solution
- 0.1 M NH₃ solution

Devices

- Spectrophotometer (Hach-DR 2400)
- Specially designed columns with 3, 3.5, and 4 (R(3), R(3.5), R(4)) cm inner diameters and 7.5, 10, and 15 cm column heights

Adsorbents

- Divinylbenzene styrene (DVBS) anionic resin
- Sodium-based cationic resin (SBCR)

Preparation of Synthetic Sulfate Solutions

This study involved the utilization of three distinct concentrations of sulfate solutions. To prepare these solutions, we initially dried 0.1479 grams of anhydrous sodium sulfate (Na_2SO_4) in an oven at 105°C. It was then dissolved in deionized water and diluted to a final volume of 1 liter, resulting in a sulfate solution with a concentration of 1000 mg/L, referred to as C(1000). From this primary solution, diluted solutions with a concentration of 250 mg/L, denoted as C(250), were subsequently derived. The sulfate content in the solutions intended for analysis was quantified using a Hach-DR2400 spectrophotometer. The sulfate assay kit used was the SulfaVer4 PP 2-70(10 mL) brand.2.3. Experimental System

Within the scope of this investigation, columns possessing internal diameters of 3 cm (R3), 3.5 cm (R3.5), and 4 cm (R4) were employed, each varying in height at 7.5 cm,



Figure 1. Experimental setup.

10 cm, and 15 cm. The standard sulfate removal technique, utilizing the spectrophotometric method, was implemented throughout the study. Furthermore, all experimental procedures were conducted using two distinct types of resins: SBCR and DVBS. A visual representation of the experimental setup is depicted in Figure 1.

During the adsorbent placement within the columns, glass fiber was interposed between the column and the adsorbent material, ensuring a precise balance. A fixed volume of sulfate solution (100 mL) was then passed through the column, and samples collected at designated time intervals (e.g., 1, 3, and 8 minutes) were analyzed using a Hach DR 2400 spectrophotometer. The sulfate

concentrations were subsequently determined based on these measurements. The study evaluated sulfate removal efficiencies under these specific conditions, examining variations in sulfate concentration concerning column diameter, column bed height, adsorbent quantity, and contact duration. Furthermore, the study included a comparative analysis of the performance of different adsorbents.

Modeling Studies

In this research segment, we have developed an Artificial Neural Network (ANN) model to forecast the percentage of sulfate removal. To accomplish this, we calculated sulfate removal efficiency employing the adsorption technique with synthetic samples, as detailed in the experimental section of our study, employing DVBS and SBCR as adsorbents. Furthermore, our experimental investigations encompassed a range of column diameters (3, 3.5, and 4 cm), column heights (7.5, 10, 15 cm), and initial sulfate concentrations.

In the ANN modeling phase of the research, we selected input variables consisting of column diameter and height, resin type, contact time, and initial sample concentration. We employed a total of 70 data points for modeling purposes. The most favorable outcomes were achieved by configuring the ANN with three neurons in the hidden layer, employing tangent sigmoid (*'tansig'*) activation functions for both the hidden and output layers. We randomly partitioned the data into a 70% training set and a 30% testing set to establish the model. We evaluated the model's performance based on various statistical criteria. A visual representation of the constructed ANN architecture is provided in Figure 2.

The development of the Artificial Neural Network (ANN) model was facilitated using the ANN toolbox within the MATLAB environment. In this process, code was crafted within MATLAB, and the optimal network structure was ascertained through training the network with the provided training dataset. Once the network structure was finalized, the model underwent testing with previously unseen data to assess its overall performance and predictive accuracy.



Figure 2. ANN design.

RESULTS AND DISCUSSION

Sodium-Based Cationic Resin (SBCR) Results

The output sulfate concentrations, denoted as C1 (1 minute), C3 (3 minutes), and C8 (8 minutes) for a 3.5 (R(3.5)) cm column diameter and an initial sulfate concentration of 1000 (C(1000)) mg/L, utilizing a sodium-based cationic resin (SBCR), are provided in Table 1 below:

Upon reviewing the results presented in Table 1, it becomes evident that there is a 99.00% reduction in sulfate concentration when employing a column height of 7.5 cm, a 98.00% reduction at a column height of 10 cm, and a remarkable 99.80% reduction at a column height of 15 cm.

Table 2 illustrates the output sulfate concentrations, specifically C1, C3 and C8 for SBCR at a column diameter

of 3 cm (R(3)) and an initial sulfate concentration of 1000 ((C(1000)) mg/L:

Upon analyzing the findings in Table 2, it is evident that an impressive 99.90% reduction in sulfate concentration is attained when employing a column height of 10 cm.

Table 3 displays the output sulfate concentrations for SBCR at a column diameter of 3.5 cm [R(3.5)] and an initial sulfate concentration of 250 mg/L [C(250)]:

Upon scrutinizing the data presented in Table 4, it is evident that removal efficiencies of 98.80%, 97.50%, and 94.50% are achieved when utilizing column heights of 7.5 cm, 10 cm, and 15 cm, respectively.

Table 4 provides the output sulfate concentrations, specifically C1, C3 and C8 for SBCR at a column diameter of 4

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Table 1. Analysis results for SBCR 1000 mg/L and 3.5cm column diameter

SBCR: C (1000 mg/L), R (3.5 cm)									
h (cm)	C1 (mg/L SO ₄)	C3 (mg/L SO ₄)	C8 (mg/L SO ₄)	Removal (%)					
7.5	30	20	10	99.00					
10	50	10	20	98.00					
15	25	10	2	99.80					

Table 2. Analysis results for SBCR at 1000 mg/L and 3 cm column diameter

SBCR: C (1000 mg/L), R (3 cm)									
h (cm)	C1 (mg/L SO ₄)	C3 (mg/L SO ₄)	C8 (mg/L SO ₄)	Removal (%)					
7.5	10	5	2	99.80					
10	3	2	1	99.90					
15	5	3	1	99.90					

Table 3. Analysis results for SBCR at 250 mg/L and 3.5 cm column diameter

SBCR: C (250 mg/L), R (3.5 cm)									
h (cm)	C1 (mg/L SO ₄)	C3 (mg/L SO ₄)	C8 (mg/L SO ₄)	Removal (%)					
7.5	5	3	2	98.80					
10	35	30	25	97.50					
15	70	65	55	94.50					

Table 4. Analysis results for SBCR at 1000 mg/L and 4 cm column diameter

SBCR: C (250 mg/L), R (3 cm)								
h (cm)	C1 (mg/L SO ₄)	C3 (mg/L SO ₄)	C8 (mg/L SO ₄)	Removal (%)				
7.5	25	20	20	92.00				
10	45	35	20	92.00				
15	65	55	35	86.00				

cm [R(4)] and an initial sulfate concentration of 1000 mg/L [C(1000)]:

As the data in Table 4 indicates, significant removal efficiencies of 99.60%, 99.75%, and 99.90% are attained at column heights of 7.5 cm, 10 cm, and 15 cm, respectively.

Table 5 outlines the output sulfate concentrations for SBCR with a column diameter of 3 cm [R(3)] and an initial sulfate concentration of 250 mg/L [C(250)]:

As per the data presented in Table 5, it is noted that removal efficiencies of 92.00% and 86.00% are attained at column heights of 7.5 cm and 10 cm, respectively, while a removal efficiency of 86.00% is observed at a column height of 15 cm.

The results obtained with the SBCR are detailed below.

The Effect of Initial Sulfate Concentration on Adsorption For SBCR

The influence of the initial sulfate concentration on sulfate removal outcomes is presented in Table 6. Based on the information provided in Table 6, it is evident that removal efficiencies of 98.00% and 90.00% are achieved for initial sulfate concentrations of 1000 mg/L and 250 mg/L, respectively. This data suggests that as the initial sulfate concentration increases, the removal efficiency also increases. It can be inferred that the adsorbent exhibits higher removal capacity at elevated initial concentrations.

The Effect of Column Fill Height on Adsorption for SBCR

Table 7 summarizes data, including the initial sulfate concentration (C_0), output sulfate concentration (C_e), absorption capacities, and removal percentages for various column heights in an absorption column with a 3.5 cm inner diameter.

Based on the data presented in Table 7, removal percentages of 99.00%, 98.00%, and 99.80% are observed for column heights of 7.5 cm, 10 cm, and 15 cm, respectively.

Table 5. Analysis results for SBCR at 250 mg/L and 3 cm column diameter

SBCR: C (1000 mg/L), R (4 cm)									
h (cm)	C1 (mg/L SO ₄)	C3 (mg/L SO ₄)	C8 (mg/L SO ₄)	Removal (%)					
7.5	20	8	4	99.60					
10	8	5	2.5	99.75					
15	4	2	1	99.90					

Table 6. The effect of initial sulfate concentration on sulfate removal with SBCR

Adsorbent	h (cm)	R (cm)	M (g)	C ₀ (mg/L)	C _e (mg/L)	$X = C_0$ -Ce	$\mathbf{q}_{\mathbf{e}} = (\mathbf{X}/\mathbf{M}) \cdot \mathbf{V}$	Removal (%)
SBCR	10	3.5	56.62	1000	20	980	1.73	98.00
SBCR	10	3.5	56.62	250	25	225	0.40	90.00

Table 7. The effect of column height on sulfate removal with SBCR

Adsorbent	h (cm)	R (cm)	M (g)	$C_0 (mg/L)$	C _e (mg/L)	$X = C_0 - Ce$	$\mathbf{q}_{\mathbf{e}} = (\mathbf{X}/\mathbf{M}) \cdot \mathbf{V}$	Removal (%)
SBCR	7.5	3.5	42.46	1000	10	990	2.33	99.00
SBCR	10	3.5	56.62	1000	20	980	1.73	98.00
SBCR	15	3.5	84.93	1000	2	998	1.17	99.80

 Table 8. The effect of column diameter on sulfate removal

Adsorbent	h (cm)	R (cm)	M (g)	$C_0 (mg/L)$	C _e (mg/L)	$X = C_0 - Ce$	$\mathbf{q}_{\mathbf{e}} = (\mathbf{X}/\mathbf{M}) \cdot \mathbf{V}$	Removal (%)
SBCR	10	3	36.90	1000	1	999	2.71	99.90
SBCR	10	3.5	42.46	1000	20	980	2.31	98.00
SBCR	10	4	74.96	1000	2,5	997.50	1.33	99.75
SBCR	10	3	36.90	250	20	230	0.62	92.00
SBCR	10	3.5	42.46	250	25	225	0.53	90.00



Figure 3. Effect of contact time on adsorption percentage with SBCR.

While the highest removal is attained at a column height of 15 cm, there is no significant variation in removal percentages among the other column heights.

In Table 8, when different column diameters for SBCR are examined at the same column height, it is evident that maximum removal is achieved with a 3 cm column diameter at both 1000 mg/L input concentration (99.9%) and 250 mg/L input concentration (92%). These results indicate higher removal rates are accomplished when the initial concentration is elevated, and the column diameter is smaller due to increased contact.

In investigating the impact of contact time on adsorption using SBCR, Figure 3 illustrates the variations in adsorption percentages across different concentrations and column heights, all within a column with a 3.5 cm internal diameter.

As depicted in Figure 3, when assessing the influence of contact time on adsorption percentage for initial sulfate concentrations of both 1000 mg/L and 250 mg/L, as well as for column fill heights of 7.5 cm, 10 cm, and 15 cm, it becomes apparent that the highest removal rates are achieved with a 15 cm column height and an initial concentration of 1000 mg/L. The trend in removal appears consistently increasing with time.

Optimum Conditions for Sulfate Removal with SBCR

The optimal conditions for maximizing sulfate removal using the sodium-based cationic resin (SBCR) were determined to be a 3 cm column diameter, an initial sulfate concentration of 1000 mg/L, and a column fill height of 10 cm, achieving an impressive 99.90% removal efficiency. Notably, the experimental results consistently indicated that the higher initial concentration of 1000 mg/L yielded superior results to the 250 mg/L concentration.

Subsequently, further experiments were conducted using a different resin, DVBS, at a concentration of 1000 mg/L, confirming the preference for the higher initial concentration in achieving enhanced sulfate removal performance.

Divinylbenzene Styrene (DVBS Anionic Resin)

Table 9 displays the output sulfate concentrations (C1, C3, and C8) for DVBS at a 3 cm column diameter and an initial sulfate concentration of 1000 mg/L [C(1000 mg/L)], measured at 1.3 minutes and 8 minutes, respectively.

Upon examining the data presented in Table 9, it is evident that removal efficiencies of 54% at a column height of 7.5 cm, 92% at a column height of 10 cm, and 98% at a column height of 15 cm have been achieved for DVBS.

Table 9. Analysis results for DVBS at 1000mg/L and 3cm column diameter

DVBS: C (1000 mg/L), R (3 cm)				
h (cm)	C1 (mg/L SO ₄)	C3 (mg/L SO ₄)	C8 (mg/L SO ₄)	Removal (%)
7.5	620	540	460	54.00
10	140	120	80	92.00
15	60	40	20	98.00

Table 10. Analysis results for DVBS at 1000mg/L and 3.5 cm column diameter

DVBS: C (1000 mg/L), R (3.5 cm)				
h (cm)	C1 (mg/L SO ₄)	C3 (mg/L SO ₄)	C8 (mg/L SO ₄)	Removal (%)
7.5	580	510	410	59.00
10	140	80	40	96.00
15	30	20	10	99.00

Table 10 provides the output sulfate concentrations (C1, C3, and C8) for DVBS at a 3.5 cm column diameter and an initial sulfate concentration of 1000 mg/L, measured at the 1st, 3rd, and 8th minutes, respectively:

Based on the data presented in Table 10, it is evident that removal efficiencies of 59.00% at a column height of 7.5 cm, 96.00% at a column height of 10 cm, and 99.00% at a column height of 15 cm have been achieved for DVBS.

Table 11 provides the output sulfate concentrations for DVBS at a 4 cm column diameter and an initial sulfate concentration of 1000 mg/L:

Based on the data in Table 11, it is evident that removal efficiencies of 98.00% at a column height of 7.5 cm and 99% at a column height of 10 cm have been achieved for DVBS.

The results obtained with the DVBS anionic are detailed below.

The Effect of Column Fill Height on Adsorption for DVBS

Table 12 summarizes data, including the initial sulfate concentration (C_0), output sulfate concentration (C_e), adsorption capacities, and removal percentages for various fill heights in a 3.5 cm internal diameter absorption column.

Effect of Column Diameter on Adsorption for DVBS

Table 13 presents sulfate removal percentages for DVBS at different column diameters but at a fixed column height. It is evident that when examining removal percentages for various column diameters at the same column height, a notable 99% removal efficiency was achieved with a 4 cm column diameter for DVBS. Moreover, there is a trend of increased removal percentage as the column diameter increases while maintaining the same initial sulfate concentration.

Effect of Contact Time on Adsorption for DVBS

Figure 4 illustrates the variations in adsorption percentage for DVBS across different concentrations and column heights within a 3.5 cm internal diameter column. Notably, the maximum removal is achieved with a 15 cm column height, as observed in Figure 4. Additionally, it's observed that there is a more substantial increase in the adsorption percentage up to 3 minutes for column heights of 7.5 cm and 10 cm. After the 3-minute contact time, the increase in adsorption percentage appears to decrease.

Optimum Conditions for Sulfate Removal with DVBS

The highest efficiency for sulfate removal using the styrene anionic resin DVBS is attained with a 3.5 cm column diameter, an initial sulfate concentration of 1000 mg/L, and a column height of 15 cm, achieving a remarkable 99.00% removal rate.

MODELING RESULTS AND DISCUSSION

The modeling results involve collecting experimental data involving SBCR and DVBS anionic resin, with various input parameters such as different diameters, heights,

DVBS: C (1000 mg/L), R (4 cm)				
h (cm)	C1 (mg/L SO ₄)	C3 (mg/L SO ₄)	C8 (mg/L SO ₄)	Removal (%)
7.5	280	40	20	98.00
10	220	90	10	99.00
15	NR	NR	NR	NR

Table 11. Analysis results for DVBS at 1000 mg/L and 4 cm column diameter

Table 12. The effect of column height on sulfate removal with DVBS

Adsorbent	h (cm)	R (cm)	M (g)	C ₀ (mg/L)	C _e (mg/L)	$X = C_0 - Ce$	$\mathbf{q}_{e} = (\mathbf{X}/\mathbf{M}) \cdot \mathbf{V}$	Removal (%)
DVBS	7.5	3.5	26.3	1000	410	590	2.24	59.00
DVBS	10	3.5	35	1000	40	960	2.74	96.00
DVBS	15	3.5	52.6	1000	10	990	1.88	99.00

Table 13. The effect of column diameter on sulfate removal

Adsorbent	h (cm)	R (cm)	M (g)	$C_0 (mg/L)$	C _e (mg/L)	$X = C_0 - Ce$	$\mathbf{q}_{\mathbf{e}} = (\mathbf{X}/\mathbf{M}) \cdot \mathbf{V}$	Removal (%)
DVBS	10	3	28,67	1000	80	920	3.21	92.00
DVBS	10	3.5	35.00	1000	40	960	2.74	96.00
DVBS	10	4	43.20	1000	10	990	2.29	99.00



Figure 4. The effect of contact time on adsorption percentage with DVBS.

initial sulfate concentrations, and resin types. The training and testing outcomes are depicted in Figure 5.

The performance criteria for the model are presented in Table 14 for both the training and testing phases. The model's performance is evaluated based on the correlation coefficient (R), mean absolute percentage error (MAPE %), root mean square error (RMSE), and mean square error (MSE). The results indicate that the model demonstrates strong performance. Low MAPE and RMSE values indicate the model's accuracy in making predictions. Additionally, the model achieves very high R-values in both the training and test phases, further confirming its effectiveness in capturing the underlying patterns and relationships in the data.

COMPARISON OF RESULTS WITH LITERATURE

This study evaluated the sulfate removal capabilities of two distinct resins, SBCR and DVBS, using various experimental designs. The experiments demonstrated high removal rates with SBCR, outperforming DVBS. This disparity can be attributed to the electrostatic interactions between the cationic SBCR and sulfate ions (SO_4^{22}) compared to the anionic DVBS and sulfate ions, as supported by references [22-25].

Further comparison with the literature reveals that this study has achieved exceptionally high levels of sulfate removal, particularly with SBCR, marking a notable improvement over previously reported results [14, 26-29]. The compatibility of these findings with existing literature underscores the efficacy of both SBCR and DVBS in removing sulfate ions. Additionally, the application of AI modeling in this research contributes new insights and value to the existing body of knowledge.



Figure 5. Training (a) and test (b) results.

Table 14. Performance criteria of mo	del
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Training Phase			Test Phase				
R	MAPE %	RMSE	MSE	R	MAPE %	RMSE	MSE
1.0000	0.5422	0.0012	1.42x10 ⁻⁶	0.9999	0.9223	0.0034	1.14x10 ⁻⁵

CONCLUSION

In conclusion, this study presents the development of an advanced Artificial Neural Network (ANN) model for predicting sulfate removal efficiency in water, addressing key health concerns related to high sulfate levels. Various factors, including experimental procedures and costs, influence the choice of sulfate removal methods. The ANN model developed here showcases remarkable performance, demonstrated by low error metrics (MAPE %, RMSE, MSE) and high correlation coefficients. These results indicate the model's strong capability in accurately estimating sulfate removal. This model significantly reduces experimental costs and workload, marking it as a practical tool in sulfate removal research. By offering precision and efficiency in predictions, the ANN model represents a shift in research methodologies towards more cost-effective and efficient water treatment and environmental management strategies.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Modified genetic algorithm with novel crossover and mutation operator for travelling salesman problem

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ABSTRACT

In this study, Genetic Algorithm (GA), a sort of randomized direct, iterative search methodology built around natural selection, is employ in computers to discover approximations of solutions to optimisation and search issues. GA employs operators including selection, crossover, and mutation to tackle. In case of NP-hard issues, particularly for travelling salesman problem (TSP), the GAs is beneficial. To reduce the overall distance, we propose a novel crossover operator with its python code for the TSP. Along with the Python pseudo coding, we additionally introduced a mutation operator to enhance the consummation of GA in determining the shortest distance in the TSP. To emphasize the proposed crossover and mutation operator, we also illustrate different steps using examples. We integrated path representation with our developed crossover and mutation operator as it is apparent method to represent a tour.

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INTRODUCTION

Almost The basic concept of genetic algorithms (GA) is a search-based optimisation approach and is introduced by Holland [1]. The 'survival of the fittest' premise is the foundation for GA, which are metaheuristics relies on natural selection and Genetics principles. GA are often utilised to produce high quality and superior solutions for search and optimisation challenges. In other words, GA tend to find and offer near-optimal solutions to scenarios that could require a lot of time. GA are frequently employed in numerous disciplines, comprises of soft computing, machine learning, and operations research. It can optimise for continuous or discrete variables without needing to know the derivatives. Additionally, it works with numerically generated data, experimental data, or analytical data and delivers a set of optimal variables rather than simply one solution. GA processes sustain a population of individuals and are iterative in character. In essence, GAs can be described as composed of two primary phases: the first is "Selection" for producing the next generation, and the second is "Manipulation,"



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which manipulates the selected individuals to produce the next generation using various techniques, including crossover and mutation. Each iteration in GA is referred to as "a generation," and a population of new candidate solutions is created utilising various biologically inspired operators including mutation, crossover, and selection. In GA, each individual is represented by a string known as chromosome and may also be regarded as a problem-solving strategy. These strings comprise characters known as genes, which contain certain values known as alleles. GAs is appropriate candidate to tackle the constrained, unconstrained and combinatorial problem.

Using genetic operations like selection, fitness, crossover, and mutation processes, GA seeks for the optimal results.

- **Fitness:** The fitness value quantifies the similarity between two individuals and is a favourable utility metric that is determined for every individual in the population.
- Selection: Each member of the population receives several copies, which are used up in the mating pool to create an entirely novel population. Therefore, the like-lihood that an individual will produce additional copies in the mating pool increases as fitness value increases.
- Crossover: Recombination of individuals generates new individuals known as offspring or children. Onepoint and two-point crossover are popular recombination strategies.
- **Mutation:** Maintaining diversity in the population can be done through mutation. Each individual is mutated with a minute or extremely low chance, such as less than 1.0.

The procedures below can be used to define an uncomplicated genetic algorithm and the flow chart for illustrating various steps is shown in Figure 1. The 2-diemnsional array encompassing population size and chromosome size defined the population. Here, population initialization can be done by utilizing two methods namely random and heuristic initialization. The fitness function ought to be quick enough to calculate. It must quantify the degree to which a given solution is fit or the degree to which fit people can be created from the provided solution.

When a GA run ends, a lot depends on the termination condition of the GA. In general, we want a termination condition that, at the end of the run, puts the outcome very near to the bestone. The following are the termination criteria's for the GA-

- when X iterations have passed with no population improvement.
- when the number of generations is fixed.
- when the value of the objective function reaches a specific, predetermined value.
- I. Using n chromosomes, create a starting generation. Here the population is initialized.
- II. Assess each chromosome's fitness.



Figure 1. Flow chart of GA.

- III. Proportionally pick n/2 parents of the present population.
- Use the crossover operator to produce children by picking two parents at random.
- V. Employ mutation to vary findings a little bit.
- VI. Until all parents have been chosen and mated, repeat steps 4 and 5.
- VII. An entirely new population of chromosomes will replace the old one.
- VIII. Determine each chromosome's level of fitness in novel population.
- IX. Stop when the number of generations reaches a predetermined maximum; otherwise, proceed to Step III. We have numerous representations in literature employ-

ing the GAs. Path, binary, adjacency,ordinal and matrixrepresentation are some significant representations and the summary of these representation with novel crossover operator is given in Table 1.

Arqub et al. [13] employ the continuous GA to solve singular two-point boundary value problems. Arqub and Hammour [14] discussed a method for employing continuous GA for solving systems of second-order boundary value problems. In order to validate this method, a few test problems were created and solved. Hammour et al. [15] presented a GA approach for the modelling of dynamical

Heuristic approach

Genetic algorithm

Simulated annealing

Particle swarm optimization Ant colony optimization

Neural network

Tabu search

Representation	Crossover operator	Author
Binary	Classical, repair	Lidd[2]
Path	Partially-mapped	Goldberg and Lingle [3]
	Order	Davis [4]
	Sorted match	Brady [5]
	Heuristic	Grefenstette [6]
	Maximal preservative	Muhlenbein et al. [7]
	Voting recombination	Muhlenbein et al. [8]
	Order based	Syswerda [9]
	Heuristic	Grefenstette [6]
	Order based	Syswerda [10]
	Position based	Syswerda [10]
	Alternating-positions	Larranaga et al. [11]
Adjacency	Alternative edge	Grefenstette et al. [12]
	Heuristic 1	Grefenstette et al. [12]
	Subtour chunks	Grefenstette et al. [12]
Ordinal	Classical operator	Grefenstette et al. [12]

Table 1. List of different representations

Table 2. Summary of approaches for TSP

Exact Approach

Branch and bound

Cutting Planes

Branch and Cut

Others

to optimize symmetric TSP with 532 cities. On the other hand, various heuristic algorithms are also introduced in order to tackle the TSP. Initially, Brady [5] proposed a GA approach deal with TSP. Bhide et al. [23] proposed a Boolean approach with the help of neural network to deal with TSP. Dorigo and Gambardella [24] proposed an approach with the help of ant colony system to tackle the TSP. Knox [25] proposed the tabu search approach to solve the symmetric TSP. Later, Chiang and Russell [26] proposed simulated annealing algorithms to cope with vehicle routing problem. Thereafter, Focacci et al. [27] developed a hybrid exact method for TSP. A local search strategy was presented by Ibarki et al. [28] for addressing and arranging issues with extensive time window limitations. Larranaga et al. [11] reviewed the various methodologies used to resolve TSP by utilizing GA. Also, presented different crossover and mutation operators which are proposed to tackle the TSP with the GA. Thereafter, An amalgam GA was suggested by Nguyen et al. [29] to discover the TSP solution. Ghadle and Muley [30] proposed a modified version of GA encoded by using MATLAB to tackle the TSP. Kumar and Gupta [31] proposed a methodology to solve the TSP with fuzzy L-R parameters. Majumdar and Bhunia [32] modelled an asymmetric TSP in a way that the distance between each pair of cities travelled is denoted as an interval value instead of a precise value. Thereafter, Changdar et al. [33] modelled a multi-objective TSP with triangular fuzzy parameters and, proposed an effectual GA to tackle this modelled TSP. Maity et al. [34] proposed a modified GA to cope with constrained solid TSP in different settings including fuzzy and crisp.

We suggest a novel crossover operator for the TSP along with its Python source code. We entailed a mutation operator in addition to the Python pseudo coding to improve the effectiveness of GA in calculating the shortest distance in the TSP. We additionally employ examples to demonstrate the proposed crossover and mutation operator at various stages. We combined our newly designed crossover and mutation operator with path representation because this is an obvious way to express a tour.

This article is organized as follows; Section one is completely devoted to the basics of GA and the literature review of GA and TSP. The mathematical formulation of the TSP

systems. For numerically approximating the solutions of Troesch's and Bratu's problems, Hammour et al. [16] introduce continuous GA. Recently, to approximate a class of Lebesgue integrable functions, Raiz et al. [17] introduced a novel sequence of linear positive operators. Schurer Beta bivariate operators were initially developed by Mishra et al. [18] in terms of generalisation exponential functions and their approximation characteristics.

The Travelling Salesman Problem (TSP) is one of the most well-known combinatorial issues in optimising. The TSP is one of the most recent optimisation problems to have undergone extensive deliberation. It was initially formulated as an optimisation problem in 1930. In TSP, the objective is to determine probable tour such that a travelling salesman visits each city exactly once and back to the initial city in order to minimize the total cost devoted or total distance covered. Since there are n! various approaches to locate the tour for n cities, specifically for 11 cities, there are 39916 800 possible route to optimize the total cost. So, the complexity of finding the best route increases as the number of cities increases. Thus, TSP is a candidate of NP (Non-Polynomial) hard combinatorial optimization problems.

In existing literature, exact and metaheuristic algorithms are two approaches to tackle TSP as shown in table 1. In case of exact algorithms, following are major exact algorithms in literature introduced to encounter with TSP; Dantzig et al. [19] introduced a methodology to solve the large-scale TSP. Later, Petberg [20] proposed a branch and cut method to get the optimal solution of symmetric TSP. A cutting plane approach is proposed by Fleischmann [21] in order to tackle the TSP in case of a road network. Thereafter, Petberg and Homg [22] proposed branch and cut method is described in section two. Several types of representation involved in GA are described in section three. Major crossover operators for path representation are presented in section four. Novel crossover operator is illustrated in section five. On the other hand, the novel mutation operator is given in section six. Finally, the section seven is devoted to the conclusion of the article.

Mathematical Formulation of TSP

One way to represent the TSP is as an integer linear programming. The Dantzig-Fulkerson-Johnson (DFJ) formulation and the Miller-Tucker-Zemlin (MTZ) formulation are well-known formulations of TSP available in the literature (Dantzig [35] & Velednitsky [36]). In some circumstances, the MTZ formulation is still beneficial, although the DFJ formulation is stronger.

Let *n* be the number of cities, c_{ij} be the cost (distance) form *ith* to *jth* city, and u_i be the dummy variable.

 x_{ij} is a binary variable and defined as:

$$x_{ij} = \begin{cases} 1 & the \ path \ goes \ from \ city \ i \ to \ city \ j} \\ 0 & otherwise \end{cases}$$

The MTZ formulation of TSP is as follows:

$$\begin{split} \min \sum_{i=1}^{n} \sum_{j \neq i, j=1}^{n} c_{ij} \, x_{ij}; \\ x_{ij} \in \{0, 1\} i, j = 1, 2 \dots, n; \\ u_i \in \mathbf{Z} i, j = 1, 2 \dots, n; \\ \sum_{j \neq i, i=1}^{n} x_{ij} = 1j = 1, 2 \dots, n; \\ \sum_{j \neq i, i=1}^{n} x_{ij} = 1i = 1, 2 \dots, n; \\ u_i - u_j + (n-1) x_{ij} \le n - 22 \le i \ne j \le n; \\ 2 \le u_i \le n2 \le i \le n; \end{split}$$

The DFJ formulation of TSP is as follows:

$$\begin{split} \min \sum_{i=1}^{n} \sum_{j \neq i, j=1}^{n} c_{ij} \, x_{ij} \\ & \sum_{\substack{j \neq i, j=1 \\ n}}^{n} x_{ij} = 1j = 1, 2 \dots, n; \\ & \sum_{\substack{j \neq i, j=1 \\ i \in Q}}^{n} x_{ij} = 1i = 1, 2 \dots, n; \\ & \sum_{\substack{i \in Q \\ j \neq i, j \in Q}}^{n} x_{ij} \leq |Q| - 1 \forall Q \subsetneq \{1, \dots, N\} |Q| \geq 2 \end{split}$$

Here, the last constraint, known as a subtour elimination constraint, assures that no appropriate subset Q can form a sub-tour, resulting in a single tour as the solution and not a union of smaller tours.

DIFFERENT TYPES OF REPRESENTATION

There have been a wide range of representations of a chromosome to solve TSP problem by employing GA. Binary, path, adjacency, ordinal and matrix representation are major representation forms available in literature.

Binary Representation

Each city in the n-cities TSP is represented in binary as a string of [log2n] bits, and an individual is represented as a string of n[log2n] bits.

Example: In case of a 6-cities TSP, each city assigned by 3-bit string. The tour 2-1-3-6-5-4 depicted as by using Table 3.

(001 000 010 011 100 101)

Table 3. An illustration of a visit of six cities in binary

i	City i	i	City i
1	000	4	101
2	001	5	100
3	010	6	011

Path Representation

The elementary representation of a tour in TSP can be done in a more appropriate way by using path representation. For a tour of n cities, if city i is the *jth* element of the list, city i is the *jth* city to be visited.

Example: If n = 8. Then the tour is 4-2-3-1-7-5-8-6 is represented as a string (4 2 3 1 7 5 8 6).

Ordinal Representation

In ordinal representation, *ith* member in set is a integer between 1 to n - i + 1 and an ordered set consisting of various destinations act as guide also exists.

Example: Let *n* = 8 and O = (1 2 3 4 5 6 7 8) be a reference list, then the tour 1-5-3-2-8-4-7-6 is represented by *T* = (1 4 1 2 1 4 1 2 1)

Matrix Representation

In matrix representation, member *ith* row and *jth* column is 1 iff city *i* is visited before the city *j*

Example: The matrix representation of tour 2-3-1-4 is

/0	0	0	1\
1	0	1	1
1	0	0	1
$\setminus 0$	0	0	0/

CROSSOVER OPERATORS FOR TSP IN PATH REPRESENTATOION

Partially Mapped (PMX), Cycle (CX), Cycle (CX2) are predominantly used crossover operators of path representation in the current literature.

Partially Mapped (PMX)

Partially Mapped Crossover operator (PMX) was introduced by Goldberg and Lingle [3] for path representation of chromosomes in path representation. In PMX, after choosing two random cut locations on the parents to produce offspring, one parent's string is mapped onto the other parent's string. Thereafter, a remaining bit are filled with the help of mapping with the constraint that no bit is repeated in the offspring.

Example:Let us consider two parents P_1 and P_2 with two random cut points

 $P_1 = (1\ 2 \mid 3\ 4\ 5\ 6 \mid \ 7\ 8)$

 $P_2 = (2\ 7 \mid 5\ 8\ 4\ 1 \mid \ 6\ 3)$

Then, the mapping segment between the cut points replicated with each other in order to build offspring, the mapping is $2 \bigoplus 1,7 \bigoplus 6,1 \bigoplus 8$.

 $O_1 = (\times \times \mid 1 \ 4 \ 5 \ 8 \mid \times \times)$

 $O_2 = (\times \times \mid 3\ 4\ 5\ 6 \mid \times \times)$

Cycle Crossover Operator (CX)

Cycle crossover (CX) operator was first introduced by Oliver et al. [37]. Any bit in this operator is obtained via any of the parents to determine its position. Let P_1 and P_2 be two parent string to illustrate the operator

 $P_1 = (1\ 2\ 3\ 4\ 5\ 6\ 7\ 8)$

 $P_2 = (2\ 4\ 6\ 8\ 7\ 5\ 3\ 1)$

Now, select 1^{st} element of offspring from first element of either of P_1 or P_2 . Here from two options (1 or 2), we will choose 1. For last element of O_1 , we must consider 8, as if 1 is taken then it would not result as a legal tour.

 $O_1 = (1 \times \times \times \times \times 8)$

Similarly, for 2^{nd} and 4^{th} element, we have 2 and 4 respectively.

 $O_1 = (1\ 2 \times 4 \times \times \times 8)$

The relative positions of the elements selected up until this point are considered to form a tour. Think about the 3^{rd} element of the O_1 . Any of the parents can be the source for this component. Let's say we choose it to come from parent 2. This indicates that the second parent must also be picked for the 5th, 6th, and 7th components of offspring because they make up another cycle. As a result, we discover the following offspring:

 $O_1 = (1\ 2\ 6\ 4\ 7\ 5\ 3\ 8)$

Cycle Crossover Operator (CX) 2

Hussain et al. [38] proposed cycle crossover operator 2 (CX2) for TSP to optimize distance travelled.

Step 1. Let us consider two parents for mating. Choose the 1st bit of the 1st offspring using 2nd parent string.

Step 2. The bit selected in Step 1 is present in the 1st parent, followed by the same similar location bit selected in the 2^{nd} parent, which is present in the 1st parent, and the similar location bit selected in the 2^{nd} parent, which is then selected for the first bit of the 2nd offspring.

Step 3. The 1st parent will have the chosen bit from Step 3, and the 1st offspring would contain the following bit in the 2nd parent's identical place.

Step 4. Continue Steps 2 and 3 until the 1st bit of the 1st parent does not appear in the 2nd offspring, at which point the procedure may be stopped.

Step 5. If any bits remain, they will be similar in the 1st parent and the 2nd offspring up to this point, and vice versa for both parents.

Example:

Let us consider two parent chromosomes for mating $P_1 = (3\ 4\ 8\ 2\ 7\ 1\ 6\ 5)$

 $P_2 = (4\ 2\ 5\ 1\ 6\ 8\ 3\ 7)$

By employing above steps, the two offspring initiated are as follows:

$$O_1 = (4 \ 8 \ 6 \ 2 \ 5 \ 3 \ 1 \ 7)$$

 $O_2 = (1 \ 7 \ 4 \ 8 \ 6 \ 2 \ 5 \ 3)$

PROPOSED CROSSOVER OPERATOR

In this section we will propose the Increasing partially mapped crossover operator (IPMX) and the python coding of the proposed operator is given in Figure 2. The proposed operator is defined by the following steps.

PROBLEMS OUTPUT DEBUG CONSOLE TERMINAL JUPYTER
<pre>[Running] python -u "c:\Users\visha\Downloads\mam project\CrossOver_py\code.py"</pre>
P1 ['1', '2', '3', '4', '5', '6', '7', '8']
P2 ['2', '7', '5', '8', '4', '1', '6', '3']
P3 ['1', '2', '1', '4', '5', '8', '7', '8']
P4 ['2', '7', '3', '4', '5', '6', '6', '3']
P5 ['6', '2', '1', '4', '5', '8', '7', '3']
P6 ['2', '7', '3', '4', '5', '6', '1', '8']
[Done] exited with code=0 in 0.156 seconds

Figure 2. Python coding of proposed crossover operator.

Table 4. Summary of mutation operator in GA

Mutation Operator	Author
Simple	Holland [1]
Insertion	Fogel [39]
Exchange	Banzhaf [40]
Scramble	Syswerda [10]
Displacement	Michalewicz [41]
Inversion	Fogel [42]

Step 1. Select a pair of chromosome parents for mating.Step 2. Pick out two random cut points on each parent to construct two offspring.

Step 3. First arrange the bits between two random cuts in the increasing order for each parent chromosome

Step 4. Now these portions between cut points are mapped onto other parent strings.

Step 5. Fill the remaining bits from the primary parent such that there is no dispute.

Step 6. To fill the bits with conflict, use the notion of partial mapping.

Example: Let us consider two parent chromosomes for mating with randomly two cut points marked by "|".

 $P_1 = (1\ 2 \mid 3\ 4\ 5\ 6 \mid \ 7\ 8)$

 $P_2 = (27 \mid 5841 \mid 63)$

The two children O_1 and O_2 are constructed as follows: Initially arrange all bits of randomly selected segment in the increasing order. Then mapped the resulted strings between cut points onto other parents.

 $O_1 = (\times \times | 1458 | \times \times)$

 $O_2 = (\times \times | 3 4 5 6 | \times \times)$

Now, fill the bits from original parent which does not have any conflict. Here for O_1 , 2,7 are filled and for O_2 , 2,7 are filled.

 $O_1 = (\times 2 \mid 1 \mid 4 \mid 5 \mid 8 \mid 7 \times)$

 $O_2 = (2\ 7 \mid 3\ 4\ 5\ 6 \mid \times \times)$

To fill the remaining bits, use the notion of partially mapping. The first × in first offspring O_1 is 1 which comes from P_1 but 1 is already present in O_1 . So, in P_1 we check the element corresponding to 1 of P_2 , here $1 \leftrightarrow 6$, first × is occupies by 6. Again, the second × in the O_1 is 8 but 8 is already present in O_1 . So, in P_1 we check the element corresponding to 8 of P_2 , here $8 \leftrightarrow 4$, but 4 is present in O_1 , again check mapping $4 \leftrightarrow 5$. But 5 is existing in O_1 , again check 5 $\leftrightarrow 3$, 3 occupies the second × of in P_1

 $O_1 = (62 | 1458 | 73)$

 $O_2 = (27 | 3456 | 18)$

Similarly, we complete the second offspring O_1 .

PROPOSED MUTATION OPERATOR

GAs employ mutation to help the procedure evade local solutions and give the population newly developed, completely improbable instances. The summary of mutation

1	a=[2,7,5,8,4,1,6,3]	J
2	<pre>n=int(input("enter limit: "))</pre>	
3		
4	print("Parent: ",a)	
5	<pre>for i in range(len(a)):</pre>	
6	if a[i] < n:	
7	a[i]=a[i]+1	
8	else:	
9	a[i]=1	
10	print("Children: ",a)	

Figure 3. Python coding of proposed mutation operator.

operators is presented in Table 4. In this section, we propose a novel mutation operator of path representation in GA.

This operator is completely defined by a linear function and is mathematically defined as follows:

Let x_i be the bits in chromosome of n size

 $L(x_i) = x_i + 1 \ \forall x_i$ where x_i represent bits in chromosome

The python coding of the proposed operator is presented in Figure 3.

Example: Let us consider $p = (2 \ 3 \ 5 \ 6 \ 1 \ 4 \ 7 \ 8)$ be a parent chromosome to emphasize the proposed mutation operator in a better way.

By applying the Linear function of mutation operator, we get a child chromosome as

 $C = (3\ 4\ 6\ 7\ 2\ 5\ 78\ 1)$

CONCLUSION

Utilising the survival of the fittest principle, GA a form of evolution method to deal with optimisation issues. They have been effectively utilized in several types of optimization issues, including the TSP. In TSP, our main aim to locate a tour of every node in a weighted network and minimise the overall weight, we must solve the TSP. We have examined various methods of representations of a tour in TSP which are available in literature that could be employed in genetic algorithms attempting to solve the TSP. We also reviewed partially mapped (PMX), cycle (CX) and cycle crossover 2 (CX2) available in literature for path representation as it the any form of tour is originally represented as path. In this article, we proposed modified version of GA by introducing an increasing partially mapped crossover operator (IPMX) and a mutation operator to get optimize solution of a TSP. We also, provide python coding of our novel crossover and mutation operator for the better implementation of modified version of GA. GA and its modified versions are applicable in different types of optimization problems other than TSP such as transportation problem, vehicle routing problem, neural networks, and so on.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Nanoscale detection of ovarian cancer biomarker

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ABSTRACT

It is estimated that over 2,000 women globally are impacted by ovarian cancer (OC). Unfortunately, every year, over half of the cases end in death. This underscores the critical importance of better early detection and diagnosis of OC. Research into improving a sensitive, dependable, and rapid cancer serum antigen (CA-125) detector is essential for medical diagnosis. This antigen may signal the earliest stages of ovarian cancer. The typical crystalline size of the Cadmium selenide (CdSe) quantum dots (QDs) that we synthesized and coated is adjusted in this study to be 8 \pm 0.2 nm. Multiple characterization methods, including X-ray diffraction, Z-scan, and transmission electron microscopy, were utilized to verify their properties. We used these QDs as optical tags for a sandwich assay, which was used to test a high-binding surface where the capture antibody was immobilized. Popular optical tags (QDs), semiconductor nanoparticles with size-dependent fluorescence spectra, brightness, and photostability, were used and can be detected by a microplate spectrophotometer. A linear curve was observed within a range of 5-1000 U/ml CA-125, which is suitable for quantitative work, and the detection limit was 4.5 U/ml. The interference with the detection of CA-125 was tested in human serum, and the results showed no significant difference in the fluorescence spectra. Third-order nonlinear optical parameter analysis of conjugated CdSe QDs under an excitation beam power level of approximately 120 W and a wavelength of 532 nm was determined in detail. The third-order optical susceptibility (χ 3) was 2.746 × 10⁻⁷ esu with a sound absorption coefficient of 4.68556×10^{-5} cm/W and nonlinear refractive index -5.6132×10^{-9} cm²/W. Finally, the resulting CdSe QDs have been effectively employed in the labeling and, hence, detection of ovarian cancer antigen (CA-125).

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INTRODUCTION

Among Western women infected with cancer, ovarian cancer (OC) is the seventh foremost cause of mortality [1, 2]. Worldwide, OC affects 239,000 females. More than half of all cases end in death each year, and the rates of new cases and deaths among women with OC have remained consistent since 1992 [3]. The origin of the anomalous cells in the ovarian tissue helps to classify the various forms of OC. Epithelial carcinoma encompasses most newly diagnosed cases, specifically around 90% [4]. Discomfort during eating, gas, and abdominal pain are typical signs of OC. However, these symptoms cannot be utilized as a sole diagnostic tool for OC because they are present in the general female population without OC [5]. This is why OC is sometimes called the "Silent Killer" [6]: it is not detectable until the disease has progressed significantly. Computed tomography (CT) scans of the chest, abdomen, and pelvis, pelvic examination, and transvaginal ultrasound are used to assess the extent to which the disease has spread beyond the pelvic area, even when OC is presumed [7]. To determine the stage of OC, conducting procedures like colonoscopy, laparoscopy, and biopsy is necessary. However, patients may experience discomfort during and after these procedures [8]. Even though various forms of OC involve genetic and epigenetic alterations, the currently licensed tests for disease identification, such as cancer detection and monitoring, are protein-based assays [9].

Bast et al. (1983) described cancer antigen serum (CA-125) as an additional helpful tool alongside radiological and imaging testing. They documented this glycoprotein type using the mAb OC 125. In 80% to 85% of women diagnosed with epithelial OC, CA-125 levels in the bloodstream rose. Several follow-up investigations have shown the association between an elevated CA-125 level and ovarian cancer. A high CA-125 level usually indicates late-stage OC, but in early-stage OC, less than half of the cases showed an elevated level of this marker. CA-125 is a significant tumor marker. Other types of cancers, including colon, pleura, breast, peritoneum, pancreas, Müllerian epithelial cells, and pericardium, have been associated with higher levels of CA-125, according to other research [11,12]. It has been accepted to test for OC using CA-125 in conjunction with a physical examination [13,14]. The effectiveness of OC diagnosis has been the target of intensive attempts to validate individual indicators [15].

An important area of research that could significantly affect the care and outcomes of ovarian cancer is the development of a biosensor for early diagnosis. In many cases, the sensitivity and specificity of the existing procedures used to diagnose OC are inadequate, resulting in diagnoses made at a late stage and low survival rates. As a result, we announce the creation of a trustworthy and sensitive technique for detecting low CA-125 concentrations, which may show early phases of OC; this could lead to a paradigm shift in the field and better patient outcomes. The size-dependent fluorescence spectra, photostability, brightness, and detectability by fluorescence spectrophotometry of optical quantum dot (QD) tags—constructed of semiconductor nanoparticles (NPs)—have contributed to their rising popularity.

Perspectives

The advent of nanotechnology may drastically alter the diagnosis, treatment, and prevention of numerous diseases, including cancer [16-20]. A semiconductor core plus a secondary semiconductor material form the nanocrystals known as quantum dots (QDs). The core can have a diameter anywhere from 2 nm to 10 nm. The optical and electronic features for QDs are distinct from those of organic dyes and fluorescent proteins. These properties include controlling light emission depending on size and composition, increasing signal brightness, resistance to photobleaching, and stimulating numerous fluorescence colors simultaneously [21-25].

Using QDs for bioimaging and cancer diagnostics is rapidly expanding in cancer research. In a perfect world, QD-based probes would be used for the early detection and noninvasive treatment of both primary and metastatic malignancies. The development of quantum dot (QD) probes endowed with enhanced target selectivity, signal intensity, and therapeutic potential-all while mitigating cytotoxicity and nonspecificity-is imperative, as existing electrochemical biosensors and their applications remain in their infancy. An integrated platform is required before its extensive use in cancer diagnosis and treatment to simplify detection and enhance automation. Solubilizing QDs before their application requires surface modification with biofunctional compounds [26]. Diagnosing and treating cancer with high specificity is possible with diagnostic and therapeutic agents [27-29].

There has been a lot of interest in QDs for active targeting of cancer antigens because of their potential use in early cancer imaging and diagnostics [30-32]. Yet, there are still obstacles to overcome before clinical applications may be achieved, such as improving sensitivity, increasing specificity, and decreasing QD toxicity. If QD-based nanotechnology is to make significant strides in cancer treatment, researchers and experts from many domains must work together. Reported studies in this field are explained in Table 1.

GENERAL PROCEDURE

Chemicals and Materials

There was no further sterilization of the substances utilized in the research. Sigma-Aldrich (St. Louis, MO) supplied the CA-125 antigen, anti-mouse CA-125 detection Ab IgG1, PBS-Tween 20, HCl, sulfo-NHS, and Ethylene dichloride (EDC). A Millipore Milli-Q filtration system produced pure deionized water to prepare aqueous solutions. A black

Researchers' names	Category of QDs	Major Findings	Advantages	Problems
Tada et al., 2007, [33].	Trastuzum Ab-QDs (800 nm)	Using quantum dots, one breast cancer cell may be seen.	Superb light output; photobleaching resistance.	Intracellular delivery technologies, as they stand, need to be improved.
Shah <i>et al.</i> , 2007, [34].	Bioconjugated QDs	During multiline age differentiation and stem cell proliferation, QDs can efficiently label cells for an extended period.	InP/ZnS QDs are nontoxic.	Due to the reaction environment sensitivity of precursors and surfactants, generating desirable InP/ZnS QDs is challenging.
Yong et al.,2009, [35].	Bioconjugated InP/ZnS QDs	Non-Cd-based optical imaging nanoprobes made of InP/ZnS QDs are safe and effective.		
Fang, Peng, Pang, & Li, 2012, [36].	QDs	Possible uses for QDs in cancer research include primary tumor detection in vitro, tumor imaging in vivo, invasion study of tumor microenvironment, imaging of progression and multimodality biomedical molecular targeting, and other similar uses.	Unique characteristics of QDs, including fluorescence capacity, make them suitable for cancer theranostic applications.	QDs must be reliably and efficiently guided to a target organ or disease site to maximize their usefulness in biomedicine while avoiding unwanted changes.
Xu & Chen, 2023, [37]	Semiconductor QDs (SQDs)	SQDs can be synthesized using various methods and modified for cancer cell imaging.	It provides better resolution and contrast than traditional clinical cancer imaging methods, such as X-ray CT and magnetic resonance imaging. Targeting molecules to their surface can be directed to specific organs or disease sites.	Cytotoxicity and potential toxicity concerns.
Kumar, Singh, & Singh, 2021, [38]	QDs	QDs have potential applications in cancer theranostics when conjugated with macromolecules.	Unique characteristics of QDs, including fluorescence capacity, make them suitable for cancer theranostic applications.	Potential toxicity concerns.

Table 1. Reported studies in the field of QDs

96-well plate from Fisher Scientific, CdSe core QDs from NNCrystal, octadecylamine (ODA), and 1-octadecene (ODE) were among the other ingredients used.

technique [18]: In a 100 ml flask, 1.3×10^{-6} mol pure CdSe core QDs, 30 g ODE, and 10.0 g ODA were loaded, nitrogen-filled, and heated on a mantle to 120 °C for 15 min.

Preparation and Bioconjugation of Core/Multishell QDs

Here is how multishell quantum dots were made utilizing the sequential ion layer adsorption and reaction

Characterization

The X-ray diffractometer (XRD-6000, Shimadzu, Japan) and Cu(k) radiation were used to measure the

crystalline structure of the QD NP. The parameters used were a scanning speed of 5°/min, a wavelength of 1.5405, 60 kV, and 80 mA. The scanning range was 2°, from 20° to 80°. To find out how big and round the QDs were, researchers used a transmission electron microscope (TEM; Philips Holand). Before taking micrographs at a voltage of up to 120 kV (type CM120), a carbon-coated copper grid was used to load a drop of aqueous CdSe QD sample into the transmission electron microscope (TEM). The sample was then let to dry at ambient temperature. Spectrophotometry for linear transmissions and Z-scan for nonlinear transmissions was also investigated. The Z-scan method was accomplished using a second harmonic generation Nd: YAG laser with a Gaussian profile and a beam divergence of 0.711 mrad. The laser excitation power could not exceed 120 W, and the beam diameter had to be less than 1.5 mm. The synthetic sample was moved along the laser axis using a linear translation stage and a convex lens with a 20 cm focal length to study the changes in laser beam intensity. Open- and closed-aperture configurations were adopted to control the nonlinear refraction index (n_2) and absorption coefficient (β).

The 3rd-order nonlinear optical susceptibility $\chi^{(3)}$ can be computed once the n_2 and β have been obtained.

Labeling of CA-125 Detection AB with QDS

CA-125 detection Antibody- Quantum dot (Ab-QD) conjugates were prepared via covalent coupling using sulfo-NHS and EDC. QDs (0.033 μ M) with surface carboxyl groups were activated by incubation with sulfo-NHS and EDC for 5 min at pH 7.4. The following step was to add 50 μ l of 125 μ g/ml CA-125 Ab, mix thoroughly by vortexing, and let it react at room temperature for 2 hours. Two hours later, 2 μ l of quenching buffer was added to a reaction, and it was stirred for ten minutes to stop the reaction. After being kept at 4 °C for around 12 hours, the CA-125 Ab QD conjugates were spun in a centrifuge to eliminate unconjugated particles.

Coating of the High-Binding Plate with CA-125 Capture AB

Physical adsorption was used to perform Ab coating. The wells were subjected to a 24-hour treatment with Phosphate buffered saline (PBS) at pH 7.4. Then, the microtiter plate wells were coated with 2 μ g/ml Ab solution by pipetting 50 μ l diluted Ab in the top wells of the plate. Next, the plate was wrapped and then stored for 12–24 h in a refrigerator at 4 °C. After the removal of the coating solution, the plate was rinsed thrice with 200 μ l 10 mM PBS (pH 7.4). The solution was removed by flipping the plate over a sink. The residual droplets were eliminated by gently tapping the plate onto an absorbent paper surface.

Optimization of the Concentrations of Capture and Detection ABS

The concentrations of captured and detected Abs were confirmed. The experiments were performed by fixing

all the experimental parameters except the concentration of the capture and detection Abs separately. The capture and detection Abs were tested in 2–20 and 5–100 g/ml, respectively.

Dynamic Range and Standard Calibration Curve

The experiment was conducted in a physiological buffer using identified concentrations of the typical sample (5, 50, 100, 200, 1000, and 5000 U mL⁻¹) to determine the best concentration range for capturing and detecting antibodies.

The experiment used capture and detection antibodies at 2 Ug mL-1 and 5 Ug mL-1, respectively. Each well's optical density was measured at 620 nm to determine the linear range. Triplicate runs of the test were carried out according to the specified linear range. For known antigen concentrations in the existence of biological matrix, the relative signals were determined by establishing the calibration curves.

Testing in the Existence of Human Serum

Following the confirmation of the modifications of Abs, the test was conducted with 50% human serum. The potential for interference from human serum was tested in the assay. In interference tests, the presence or absence of an antigen is tested by adding human serum to a certain amount of the antigen.

RESULTS AND DISCUSSION

The crystal domain size was determined using Gaussian fit on X-ray diffraction (XRD) patterns, employing the Debye-Scherrer formula: $D = 0.9 \lambda/\beta \cos\theta$. Here, (*D*) represents a crystallite mean size, (λ) stands for a wavelength for the incident X-ray (1.5406 Å), θ is the diffraction peak angle, and β is the full width at half maximum of the XRD peak at angle θ . The crystal domain size for CdSe was approximately 6 nm, based on the hexagonal (wurtzite) CdSe structure planes (Figure 1).



Figure 1. XRD patterns of QDs.



Figure 2. TEM images of spherical and monodispersed CdSe QDs.

To regulate the actual size and outline of the QDs, we obtained the TEM images of the CdSe QDs (Figure 2). The images demonstrated that the QDs were spherical and had a uniform size distribution of approximately 6 nm.

Figures 2(A) and 2(B) show the TEM micrographs of QDs, further confirming those of the XRD analysis. Micrographs of CdSe QDs exhibited spherical and monodispersed particles with a size of approximately 8 ± 0.2 nm after conjugation with CA-125.

To determine the optical properties of materials (nonlinear refractive index and third nonlinear coefficient) of relatively thin materials, the Z-scan is commonly used in nonlinear optics to assess the nonlinearities of these materials through the calibration of reference samples, as shown in Figure (3). Figures 4(A) and 4(B) show the behavior of the open- and closed-aperture Z-scans. Based on these graphs, the generated sample displayed various nonlinear properties, such as self-defocusing, non-saturable absorption, and two-photon absorption. The normalized charts were fitted with the following equations to estimate the nonlinear parameters:

The nonlinear absorption coefficient (β) was estimated by fitting .[39][40]:

$$T(Z) = \sum_{m=1}^{2} \frac{\left(\frac{\beta I_0 L_{eff}}{1 + \left(\frac{Z}{Z_0}\right)^2}\right)^m}{(m+1)^{3/2}}$$
(1)

The nonlinear refractive index (n_2) was obtained as follows .[39][40]:

$$n_2 = \frac{\Delta \phi_0}{k I_0 L_{eff}} \tag{2}$$

Where Z_0 denotes the diffraction length (or Rayleigh length) of the beam, I0 represents the laser beam intensity at the focus point (Z=0), Leff stands for an

effective propagation length inside a sample, given by Leff=. [(1-exp(- α 0 L))/ α 0], L stands for a geometrical thickness of the prepared sample, m stands for an order for multiphoton processes, k corresponds to the wavenumber (k= $2\pi/\lambda$), and $\Delta \emptyset$ 0 is a phase shift, specified by $|\Delta \emptyset 0| = (\Delta T(p-v))/(0.406[(1-ST)]^{0.25})$. ST signifies the linear transmittance of the aperture, and $\Delta T(p-v)$ and ΔT specify a difference in transmittance between the maximum and minimum magnitudes for closed and open apertures, respectively. The 3rd nonlinear coefficient $\chi^{(3)}$ was estimated using the given relation [39,40]:

$$\chi^{(3)} = \sqrt{(Re\chi^{(3)})^2 + (Im\chi^{(3)})^2}$$
(3)

Where the real part is $Re(\chi^{(3)}) = 10^{-4} \frac{\varepsilon_0 c^2 n_0^2 n_2}{\pi}$, and the imaginary part is $Im(\chi^{(3)}) = 10^{-2} \frac{\varepsilon_0 c^2 n_0^2 \lambda \beta}{4\pi^2}$.

From this experiment, the prepared sample possessed a good β = 4.68556 × 10⁻⁵ cm/W, n_2 = -5.6132 × 10⁻⁹ cm²/W, and a high $\chi^{(3)}$ = 2.746 × 10⁻⁷.



Figure 3. Setup for Z-scan.



Figure 4. Normalized transmission in (a) open- and (b) closed-aperture conditions.

Optimization of ABS

In the current study, sandwich-type immunoreactions were performed on 96-well plates to detect protein, and this approach yielded good sensitivity and specificity .[41]. In general, the high concentration of any of the captured or detected Abs caused nonspecific adsorption of the conjugates, which led to a high background signal. Under our experimental conditions, 2 and 5 μ g/ml monoclonal capture and detection of Abs were confirmed, respectively.

The findings on fluorescence intensity in correlation with the antigen concentrations are comparable with [42].

Analytical Performance

The quantitative detection of the analyte was achieved by measuring the peak intensity of the fluorescence, and a linear curve was observed in the range of 5–1000 U/ml CA-125, which is suitable for quantitative work. The linear equation is $y = 1.422x+712.75 R^2=0.9516$ (Figure 5), where the CA-125 concentration (x) is measured in U/mL, and y denotes the absorbance (absorbance intensity). To determine the dynamic concentration range for the optical assay, we used a series of CA-125 concentrations ranging from 5 to 5000 U mL-1 along with optimum concentrations of mAb. Ab-QDs were utilized to introduce the optical assay's dynamic range concentration. A linear curve was created based on the mean of three independent experiments. Specifically, no less than 20 observations were used to generate the blank signal without antigen to compute reliable results for the standard deviation (0.017).

To determine the limit of detection (LOD), we used the formula OD at LOD ¼ OD mean blk + 1.645SDblk. The estimated LOD was 4.5 U mL-1. This value is similar to that gotten using the current commercial method for CA-125 .[43] [44]. This finding confirmed this method's capability to identify CA-125 in a broad range of concentrations, making it a valuable tool for early cancer detection.



Figure 5. Detection of different concentrations of CA-125 using Ab with QDs.



Figure 6. Comparison of CA-125 detection by QD-labeled Ab in the presence and absence of 50% human serum.

CA-125 Test in the Presence of Human Serum

The interference detection experiment was performed to rule out the potential for interference from human serum. To test the influence of antigen concentration on CA-125 detectability, human serum was mixed with a known amount of the substance. There was no discernible signal change when human serum was present, as seen in Figure (6). The assay can be run in a diluted matrix without significantly impacting the signal.

CONCLUSION

This study used a reaction technique with sequential ion layer adsorption to produce CdSe QDs that are generally uniform in size. With uniform crystallinity and homogeneous size distributions, the assembled CdSe QDs nanocrystal cores displayed a wide array of nonlinear properties under transmission electron microscopy (TEM), such as self-defocusing, two-photon absorption, and non-saturable absorption. Labeling the ovarian cancer biomarker CA-125 with quantum dots allowed the successful detection of serum antigen CA-125 by optical emission at 620 nm. The assay demonstrated a broad dynamic range for CA-125 concentrations. There was a detection limit of 4.5 U mL-1. Despite this, the assay worked reasonably well with the various biological components contained in 50% human serum, and there were no discernible alterations in the results.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Detection of COVID-19 infection by using Raman spectroscopy of serum samples and machine learning

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ABSTRACT

Rapid, simple, and accurate detection is important to slow down the spread of epidemics in the era of the pandemic. COVID-19 has been the biggest epidemic of the current century and continues. Therefore, it is extremely important to develop methods that allow the detection of COVID-19 by eliminating the disadvantages of the existing methods. The aim of this study is to perform rapid and reliable detection of COVID-19 using Raman spectroscopy and machine learning techniques. Here, Raman spectra of serum samples collected from COVID-19 patients, suspected cases, and healthy controls were utilized. Machine learning techniques were employed due to the absence of significant discernible variations between the Raman spectra of the three groups with the naked eye. Therefore, principal component analysis (PCA) was utilized to reveal discriminative features of the classes. Support vector machine (SVM), k-nearest neighbors (KNN), and decision tree (DT) classification models were utilized by using extracted features with PCA. SVM and KNN provide high accuracy ± standard deviation values of 86.5±0.7% and 87.3±0.6% respectively. Sensitivity (recall), precision, and area under the curve (AUC) which are important performance evaluation metrics were also calculated for comparison. Results show that Raman spectra combined with machine learning presents a promising tool for the accurate detection of COVID-19 in clinical use.

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INTRODUCTION

Over the last two decades, there have been three significant outbreaks caused by human coronaviruses. These outbreaks involved the severe acute respiratory syndrome coronavirus (SARS-CoV) in 2002, the Middle East respiratory syndrome coronavirus (MERS-CoV) in 2012, and the severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) in 2019. The global spread of coronavirus disease 2019 (COVID-19) caused by SARS-CoV-2 that emerged in Wuhan, China has rapidly spread all over the world and become a worldwide pandemic [1, 2]. More than 675 million people have infected and about 6.5 million deaths have occurred globally since the day COVID-19 appeared according to the Center for Systems Science and Engineering (CSSE) at John Hopkins University [3]. This epidemic not only damaged the health systems of countries

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but also greatly affected economies. The most important thing in keeping the epidemic under control is to perform rapid, accurate and reliable tests. These tests are necessary for both diagnosis and tracking.

The gold standard to identification of SARS-CoV-2 is real-time reverse transcriptase-polymerase chain reaction (rRT-PCR) test [4]. Although being the most validated nucleic acid-based test for detecting COVID-19, this method exhibits certain limitations. The rRT-PCR test encompasses a multi-step approach that involves nucleic acid extraction, amplification, and purification. Moreover, it requires advanced equipment, high-cost reagents, trained personnel, suffers from false-negative results and being time-consuming. Immunoassay based techniques such as enzyme-linked immunosorbent assay (ELISA) are also used for rapid detection. However, this kind of immunoassays are not suitable for the identification of specific viral species or strains since they depend on specific antigen/ antibody binding. Further, these techniques are destructive for the samples. Hence, conventional methodologies are unsuitable for rapid detection due to the aforementioned constraints. There exists an unaddressed requirement for novel technologies characterized by streamlined procedures and enhanced sensitivity.

Raman Spectroscopy is a robust scientific technique founded upon the principle of inelastic scattering of a laser beam. This method yields invaluable molecular fingerprint information regarding the specimen, whereby each molecule manifests its distinct and unique Raman spectral signal. Moreover, Raman spectroscopy requires a minimum sample preparation process and nondestructive [5]. However, this technique has some limitations due to the weak signal intensity of the Raman scattering [6]. This situation makes harder the interpretation and discrimination of similar spectra. To overcome this problem using machine learning methods for the detection or discrimination of biological samples is essential.

Raman spectroscopy applications span a broad range in microbial identification in the biomedical field [7-9]. However, there are few studies reporting the use of Raman spectroscopy for the detection of SARS-CoV-2. Carlomagno et al. reported a Raman-based approach to detect current and past infections of SARS-CoV-2 from saliva samples [10]. Zhang et al. used surface enhanced Raman spectroscopy array functionalized with ACE2 to capture SARS-CoV-2 spike protein to test environmental species [11]. Akdeniz et al. developed a virus-infected cellular model by transfecting mammalian cells with plasmids encoding the M, N, and E proteins of SARS-CoV-2 [12]. They isolated proteins from the cells and collected their spectra. Results show that there is a clear discrimination between proteins of SARS-CoV-2 and the control group according to the principal component analysis (PCA).

In this study, the discrimination of Raman spectra of serum samples collected from COVID-19 patients, suspected cases, and healthy individuals obtained from a publicly available dataset [13] was performed. To reveal the discriminative features, PCA was used. Afterward, some machine learning techniques such as support vector machine (SVM), k-nearest neighbors (KNN), and decision tree (DT) were applied. Until now, the conducted studies by using this dataset have primarily focused on categorizing spectra from COVID-19, suspected cases, and healthy subjects into two classes [13-15]. Yin et al. used the whole dataset, and they classified the COVID-19 patients, suspected cases, and healthy controls into the combination of two classes [13]. They found accuracy values of COVID-19 versus suspected, COVID-19 versus healthy control, and suspected versus healthy control as 0.87±0.05, 0.91±0.04, and 0.69±0.05 respectively. Deepaisarn et al. used the same dataset and discriminated COVID-19 patients and healthy controls by using different feature extraction methods and classifiers [14]. They obtained the accuracy of 98.38% by using Light Gradient Boosting Model. Wei et al. also used this dataset to classify COVID-19 and healthy subjects and found accuracy of 97.9±0.2% by using Multi-Scale Sequential feature Selection model (M3S) [15]. However, classifying COVID-19, suspected cases, and healthy spectra simultaneously into three distinct classes would be more clinically meaningful as a classification problem. Since the spectrum of the serum sample obtained from an individual will fall into one of these three categories. Consequently, after training the machine learning model, when the spectrum from an individual is provided as input, the model will be able to ascertain to which group (COVID-19, suspected, or healthy) the person belongs. Here, the Raman spectra of all three classes were analyzed simultaneously, resulting in the successful identification of the respective class to which the serum samples belonged.

MATERIALS AND METHODS

The Dataset

Here, a portion of publicly available dataset was used [13]. The original dataset includes 2655 Raman spectra of serum samples collected from 177 individuals including confirmed COVID-19 patients, suspected cases, and healthy controls. However, the accessible part of the dataset includes 465 spectra belong to 159 spectra from COVID-19 patients, 156 spectra from suspected cases, and 150 spectra from healthy controls. Every individual diagnosed with COVID-19 exhibited positive results in viral nucleic acid detection through real-time polymerase chain reaction (RT-PCR) utilizing respiratory tract samples. The suspected group indicated flu-like symptoms similar to COVID-19. Each spectrum was recorded by exciting with a laser 785 nm wavelength under the 70-mW laser power. All spectral data was used in the range of 600-1800 cm⁻¹.

Data Analysis

The dataset consists of 465 spectra. Firstly, the whole data was shuffled randomly and standardized by using

standard normal variate. To extract discriminative spectral features from Raman data PCA is a statistical technique often used [16, 17]. PCA is used for dimensionality reduction and data exploration. PCA is commonly employed as a technique to decrease the dimensionality of a dataset by generating a reduced set of variables that effectively capture the majority of the variability found in the original data. This enables the simplification of intricate datasets while still preserving crucial information [18]. PCA extracts linear features by detecting linear relationships from the data. It projects the data to a new coordinate space so that the variance within the data remains maximum. The first principal component has the highest variance and the variance that is carried by each principal component decreases through the last principal component. Here, the first 40 principal components that hold a large amount of variance (> 95%) in the data were used.

To discriminate COVID-19 patients, suspected cases, and healthy controls traditional classifiers were utilized. For this purpose, traditional machine learning techniques that are preferred widely for the classification of Raman spectra were used. SVM, KNN, and DT were utilized for the discrimination of COVID-19 patients, suspected cases, and healthy controls. The Support Vector Machine (SVM) is a supervised machine learning algorithm employed for tasks related to classification and regression. Its operation involves the identification of the optimal hyperplane within a high-dimensional feature space, effectively segregating data points belonging to distinct classes [19]. Multiclass SVM classifier polynomial kernel (degree: 3) with one-versus-all approach was selected. KNN classification is a supervised machine learning approach employed to categorize data points into distinct classes by determining the majority class among their nearest neighbors [19]. In KNN classifier, the most appropriate k parameter was determined as 1 and Euclidean distance was used. DT classification algorithm builds a tree-like structure to make decisions about the class labels of data points based on their features [19]. Random search method was used for the hyperparameter optimization. The evaluation of each classifier's performance was conducted by assessing the accuracy, sensitivity (recall), and precision which were derived from the respective confusion matrices. Furthermore, area under curve (AUC) value was also used for performance evaluation. K-fold cross-validation helps in preventing overfitting by providing a more robust evaluation of a model's performance, reducing the influence of a single data split, and ensuring that the model learns from a diverse set of training data. Consequently, this aids in the construction of models that exhibit improved generalization when confronted with novel, unseen data. The 10-fold cross-validation technique was employed to objectively assess the performance of the classifiers. In this method, the dataset is divided into ten groups of approximately equal sizes. Nine of these subsets are designated for training, while one subset is reserved

for testing. The aforementioned process is repeated 10 times, ensuring that every subset has been utilized as the testing set. All these procedures were repeated 50 times to calculate mean \pm standard deviation. All data processing procedures were performed using MATLAB software (The MathWorks, Natick, USA).

RESULTS AND DISCUSSION

Rapid and accurate diagnosis is extremely important to slow down the spread of epidemics. Therefore, there is a pressing demand for emerging technologies that enable rapid diagnosis. In this study, Raman spectra of serum samples collected from COVID-19 patients, suspected cases, and healthy controls were discriminated by using machine learning techniques.

Here a total of 465 spectra from COVID-19 patients, suspected cases, and healthy controls were used to discriminate these 3 groups. As seen in Figure 1, there is a high similarity between Raman spectra of all groups. SARS-CoV-2 could potentially manifest a distinct protein profile, setting it apart from both healthy samples and other diseases [20]. Furthermore, the pathological progression of COVID-19 triggers the initiation of a humoral response, resulting in the production of particular antibodies [21]. These processes make the COVID-19 serum spectra biochemically different from other spectra. The differences of the serum composition between groups can be detected by Raman spectroscopy. Thus, there are noticeable distinctions among spectral groups, but discerning these spectra with the naked eve appears to be exceedingly challenging. Therefore, the utilization of machine learning techniques is essential for addressing this issue.

PCA were firstly used for dimensionality reduction. This step is crucial because the optimum number of features are directly related to classifier performance. The use of all variables in spectral data will increase model complexity and training time. On the other hand, inadequate feature selection will lead to a decrease in classifier performance, resulting in poor classification accuracy. Therefore, choosing the optimal number of features is a key step for



Figure 1. Mean serum Raman spectra of COVID-19 patients, suspected cases, and healthy controls.



Figure 2. Explained variance of the first 50 principal components found by applying PCA to the dataset.

a classification problem. Here, PCA was performed for extracting linear features from the dataset. Figure 2 shows the variances holding by each principal component. First principal component has the maximum variance, and the variance decreases from the first principal component to last principal component. The first 20 principal components carry most of the variance in the dataset and variance does not change much after these 20 components as seen in Figure 2.

In this study, the first 40 principal components that carry the largest amount of variance (>95%) in the data set were used. These principal components were fed into the classifiers. Two and three dimensional PCA plots for COVID-19 patients, suspected cases, and healthy controls are given in Figure 3A and B, respectively. There is not a clear discrimination for two and three dimensional PCA space as seen in these figures. However, the data given to the classifiers are located in a 40-dimensional PCA space not in 2 or 3 dimensional spaces. PCA can effectively reveal patterns in the dataset for this reason first 40 principal components extracted with PCA were used as input variables for classification. Some classification algorithms (SVM, KNN, and DT) were performed to distinguish three groups of COVID-19 patients, suspected cases, and healthy controls. At this step, 40 principal components were used as features for all classifiers. The 10-fold cross-validation technique was employed to provide an objective evaluation of the classifier performances.

The mean accuracies with standard deviation were calculated by using 50 randomly distributed sets. Figure 4 demonstrates accuracies of each classifier through independent 50 runs. The SVM classifier exhibits mean accuracy value of $86.5\%\pm0.7$ while KNN classifier ensures the slightly better mean accuracy of $87.3\%\pm0.6$ than the SVM classifier. On the other hand, the DT classifier gives the worst mean accuracy of 69.2 ± 1.9 among others. Generally, KNN and SVM classifiers provide better results for the classification of spectral dataset [17].



Figure 3. PCA scores of serum Raman spectra of COVID-19 patients, suspected cases, and healthy controls. Score plot of PC1 vs. PC2 (A). Score plot of PC1 vs. PC2 and PC3 (B).

Although determining the classifier performance calculation of mean accuracy is the frequently used method it is absolutely not enough. Other metrics are needed to objectively evaluate the classifier performance. The most used metrics are sensitivity, precision, and AUC. Accuracy, sensitivity, and precision values are derived from the confusion matrix through calculations. The confusion matrix serves as a vital performance evaluation tool within the domains of machine learning and statistics. It offers a more in-depth perspective on a classification model's performance when compared to accuracy alone. This is because it considers both false positives and false negatives, which can be pivotal in real-world applications. It is an essential tool for evaluating the effectiveness of classification models and comparing different models or tuning their parameters. Figure 5 a-c shows the confusion matrices of SVM, KNN, and DT classifiers respectively. Within this matrix, each row signifies the quantity of spectra in a true class, while each column signifies the number of spectra in a predicted class. The elements along the main diagonal indicate the number of correctly classified spectra, whereas the off-diagonal elements indicate the number of misclassified spectra. Here, SVM and KNN classifiers yield more successful results than DT in distinguishing classes. However, KNN provides slightly better results than SVM for the discrimination of COVID-19 and suspected classes. On the other hand, SVM exhibits more successful results in distinguishing the healthy class



Figure 4. Accuracy values of **A.** SVM, **B.** KNN **C.** DT classifiers with 50 randomly distributed sets.

compared to KNN. The accuracy, sensitivity, and precision values of classifiers are provided in Table 1. Sensitivity (recall) quantifies the model's capacity to accurately recognize positive instances out of all the actual positive instances in the dataset. Especially in medical applications, the cost of missing a true positive (a disease) can be critical as it may delay treatment or lead to severe consequences for the patient. Therefore, high sensitivity is desirable for medical applications. As seen in Table 1, KNN classifier illustrates higher sensitivity values for COVID-19 and suspected cases. On the other hand, SVM shows better sensitivity for healthy group. However, it is important to keep in mind that sensitivity should be considered in conjunction with



Figure 5. Confusion matrices and receiver operating curves of SVM, KNN, and DT classifiers. **A.** Confusion matrix of SVM **B.** Confusion matrix of KNN **C.** Confusion matrix of DT **D.** ROC of SVM **E.** ROC of KNN **F.** ROC of DT.

other performance metrics, such as precision, and accuracy. Precision is another fundamental performance metric used to evaluate the quality of a classification model. The precision value of SVM model for the COVID-19 class is found better with 0.96 and other classes give similar results for SVM and KNN models. By contrast with SVM and KNN models, DT classifier gives the worst results for sensitivity, precision, and accuracy.

The AUC value is derived from the ROC (Receiver Operating Characteristic) curve, which plots sensitivity (y-axis) against 1-specificity (x-axis). It serves as a significant metric for evaluating classifier performance as it represents the area under the ROC curve [22, 23]. The ROC curve provides a visual representation of the balance between the true positive rate (sensitivity) and the false positive rate (1-specificity) across various classification thresholds. The curve plots sensitivity (TPR) on the y-axis against 1-specificity (FPR) on the x-axis, and each point on the curve corresponds to a different threshold value. An optimal ROC curve closely follows the top-left corner, signifying high sensitivity and a low false positive rate across different threshold values. Here, the AUC values are found as 0.97, 0.93, and 0.87 for SVM, KNN, and DT classifiers respectively. Although, KNN classifier provides the highest accuracy, the AUC value of it lower than SVM classifier. A high

Classifier	Classes	Sensitivity	Precision	Accuracy (%) ± standard
				deviation
	COVID-19	0.89	0.96	
SVM	suspected	0.84	0.84	86.5±0.7
	healthy	0.87	0.79	
	COVID-19	0.91	0.91	
KNN	suspected	0.9	0.86	87.3±0.6
	healthy	0.81	0.83	
	COVID-19	0.83	0.83	
DT	suspected	0.62	0.62	69.2±1.9
	healthy	0.62	0.62	

Table 1. Sensitivity, precision, and accuracy \pm standard deviation values of SVM, KNN, and DT classifiers belong to COVID-19, suspected cases, and healthy controls.

SVM: Support vector machine; KNN: k-nearest neighbors; DT: Decision tree.

accuracy value indicates that the classifier is making correct predictions overall, regardless of class. It calculates the ratio of correctly classified samples to the total number of samples within the dataset. High accuracy suggests that the model is good at making correct predictions for both positive and negative instances. A high AUC value, on the other hand, indicates that the classifier is good at distinguishing between positive and negative instances. The AUC represents the area under the ROC curve and measures the classifier's ability to rank instances correctly. A high AUC means that the classifier is capable of achieving high true positive rates (sensitivity) and low false positive rates (1-specificity) across various classification thresholds. Ultimately, the choice between the two classifiers depends on the specific requirements of the problem and the associated costs or implications of misclassifications. If correctly distinguishing positive instances is more critical (e.g., medical diagnosis), the classifier with a high AUC might be preferred.

Consequently, the classification of Raman spectra belonging to COVID-19, suspected cases, and healthy individuals' blood serum samples was performed. In this context, SVM and KNN yielded quite similar results, while the DT model provided the worst outcome. In some classes, SVM demonstrates superior performance concerning accuracy, sensitivity, and precision while KNN outperforms in other scenarios. Despite the KNN classifier yielding higher accuracy, in cases such as disease detection-based datasets, opting for the classifier with a higher AUC value would be more appropriate. Since a high AUC value shows high discrimination power between positive and negative classes. On the other hand, more data is needed to generalize these results. The main limitation of this study is limited access to the data. Making a greater portion of the dataset publicly available will enable machine learning models to achieve a more robust generalization of the results. Moreover, as the data volume increases, deep learning techniques that have the potential to provide superior outcomes compared

to traditional machine learning models will also become available. As a result, although the results obtained are promising, more data are needed for generalization.

CONCLUSION

Rapid COVID-19 detection is of utmost importance as it allows for swift identification and isolation of infected individuals, curbing the spread of the virus within communities and preventing outbreaks. Timely detection also enables prompt medical intervention, reducing the severity of cases and ultimately saving lives. Raman spectroscopy can be a powerful alternative to conventional methods for the rapid detection of COVID-19. Here, the discrimination of COVID-19, suspected cases, and healthy controls serum Raman spectra were performed. Data preprocessing involved feature extraction using PCA, and classification was carried out using SVM, KNN, and DT classifiers. The performance of the classifiers on the test data, evaluated through 10-fold cross-validation, was assessed using accuracy, sensitivity, precision, and AUC values. Thanks to the machine learning techniques similar spectra were discriminated successfully. SVM and KNN algorithms provide high accuracy, sensitivity, and precision results for the discrimination of COVID-19, suspected cases, and healthy controls. In summary, Raman Spectroscopy and machine learning emerge as a dependable and robust approach for distinguishing COVID-19 cases rendering it highly prospective for clinical implementations.

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AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request. The COVID-19 data used in this study is publicly available at: https://doi.org/10.6084/m9.figshare.12159924.v1

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

On solutions of time fractional order random HIV/AIDS modelling

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ABSTRACT

In this study, The fractional random HIV/AIDS model approximate analytical solutions were produced using the differential transformation method. The approximate analytical solution of the fractional order Random HIV/AIDS model was obtained with the help of the differential transformation method. For the fractional random HIV/AIDS model, which was created by choosing the initial conditions from the exponential, beta, and normal distributions, graphic simulations of the expected value, variance, and confidence intervals of the most commonly used probability characteristics were obtained with the help of the MATLAB package program. Results obtained are interpreted.

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INTRODUCTION

AIDS was first discovered in the USA in 1981. HIV (human immunodeficiency virus) factor causes AIDS by crashing the immune system in humans. The HIV virus, known to have emerged for the first time in 1960, was first seen in monkeys. In 2017, 940,000 HIV-related deaths and 1.8 million new cases of HIV infection were detected. As of the year 2022, over 37.7 million individuals have been infected with HIV [1]. There are two different variations of HIV. These are HIV-1, which is common worldwide, and HIV-2, which is more common in African countries. HIV-1 was first isolated in 1983 in Paris, France (Anderson, 1990). It is assumed that HIV-1 is transmitted to humans by a minimum of 4 zoonotic strains. It is estimated that this contamination may have occurred in the 1930s (±20 years) in the light of the molecular phylogenetic biological information

HIV often compromised an individual's immune system, leading to the eventual development of acquired immune deficiency syndrome [5]. This was particularly true if the individual was unaware of their protection options and was not receiving active treatment for AIDS. AIDS continues to threaten our lives because no cure has yet been found. Thus, our greatest mathematical advantage in this field comes from knowing the dynamics of the epidemic, which is crucial [6]. In addition to understanding the dynamics of the epidemic, these studies also enable us

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available [2]. HIV-2 isolation was done by Clavel et al. in 1986 [3]. HIV-2 is less pathogenic than HIV-1. As a result of this situation, a longer prognosis is observed in the cases. While it is observed that immunodeficiency symptoms and AIDS occur later, the mother-infant transmission rate is much lower (2-7%) compared to HIV-1 (10-40%) [4].

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to manage this process more efficiently and to make predictions about the disease [7].

In our study, fractional order random HIV/AIDS model was examined. Three distinct absolute continuous distributions were used to choose the initial conditions, and the probability characteristics of each were looked at. In our daily lives, stochastic differential equations are becoming more and more popular. They have applications in population dynamics, engineering, finance, and economics [8].

Functions for the expected values and variances of approximate analytical solutions of random equations are obtained.For the remainder of this investigation, part 3 of the fractional random HIV/AIDS model's solutions and behaviors, as well as the materials and methods from part 2 of the study, are both explored. The conclusion is presented in the final section.

MATERIALS AND METHODS

The concept of a fractional derivative was first introduced in the latter half of the 17th century and was developed by Leibniz and Newton. As a matter of fact, the concept of a fractional derivative predates that of an integer derivative. Due to the fact that the fractional derivative is really just an expanded version of the integer derivative. The Rieman-Liouville and Caputo definitions are the ones that are most frequently discussed in the literature [9].

For more than 300 years, the fractional derivative has drawn interest in mathematics. On this topic, scientists have conducted a number of investigations. Due to this circumstance, various definitions have occasionally emerged [10].

The fractional derivative has major advantages over the integer derivative in applied fields such as medicine, biology, and bioengineering. These advantages, which are supported by a number of models, not only improve the convenience of our daily lives but also present persuasive arguments for solutions to issues such as the spread of diseases [11]. Fractional differential equations in mathematical models have been more and more common in recent years due to their advantages. However, the problem's structure also influences the analytical solution of these equations [12].

Preliminaries

Definition 1. The Riemann-Liouville fractional derivative of order $0 < \alpha < 1$ of a function is defined as [13]

$${}^{RL}_{0}D^{\alpha}_{x}f(x) = \frac{1}{\Gamma(\alpha-1)}\frac{d}{dx}\int_{0}^{x} (x-t)^{-\alpha}f(t)dt \qquad (1)$$

Definition 2. The Riemann-Louville fractional integral of order $0 < \alpha < 1$ of a function is defined as [13]

$${}^{RL}_{0}I^{\alpha}_{x}f(x) = \frac{1}{\Gamma(\alpha)} \int_{0}^{x} (x-t)^{\alpha-1} f(t)dt$$
(2)

where $\Gamma(.)$ represents the Gamma function.

Definition 3 [14-15] The Caputo fractional derivative of order $\alpha > 0$ of a function $\omega \in C_{-1}^{\mu} (\mu \ge 1)$ in the sense of Caputo is defined as

$${}_{0}^{c}D_{x}^{\alpha}f(x) = \frac{1}{\Gamma(m-\alpha)}\int_{0}^{t}(t-\vartheta)^{m-\alpha-1}\omega^{m}(\vartheta)d\vartheta \qquad (3)$$

where $m - 1 < \alpha < m \in \mathbb{N}$. If $\alpha = m \in \mathbb{N}$, then

$$D_t^{\alpha}\omega(t) = \frac{d^m\omega(t)}{dt^m}.$$

Definition 4: The Laplace transform of function is defined as

$$\mathcal{L}[f(t)] = F(s) = \int_0^\infty e^{-st} f(t) dt$$

for all real numbers $t \ge 0$ if the integral exists.

Definition 5. [14-15] The Laplace transform of the transform of the Caputo fractional derivative $D_t^{\alpha}\omega(t)$ is defined as

$$\mathcal{L}[D_t^{\alpha}\omega(t)] = s^{\alpha}\mathcal{L}[\omega(t)](s) - \sum_{k=0}^{m-1} s^{\alpha-k-1}\omega^k(0^+) \quad (4)$$

where $\alpha > 0$, $m - 1 < \alpha < m$ and \mathcal{L} denotes the Laplace transform operator.

DIFFERENTIAL TRANSFORM METHOD

The basic definitions of differential transform are introduced as follows. Let u(t) be analytic in a domain D and let $t = t_0$ represent any point in D. The function u(t) is then represented by one power series whose center is located at t_0 . The differential transform of the k-th derivative of a function u(t) is defined as follows:

$$\mathcal{U}(k) = \frac{1}{k!} \left[\frac{d^{k} u(t)}{dt^{k}} \right]_{t=t_{0}}, \forall t \in D$$

In (1), u(t) is the original function and U(k) is the transformed function[16]. The differential inverse transformation of U(k) is defined as follows:

$$u(t) = \sum_{k=0}^{\infty} \mathcal{U}(k)(t-t_i)^k, \forall t \in D$$

from (1) and (2), we obtain

$$u(t) = \sum_{k=0}^{\infty} \frac{(t-t_i)^k}{k!} \left[\frac{d^k u(t)}{dt^k} \right]_{t=t_0}, \forall t \in D$$

The fundamental theorems of the one-dimensional differential transform[16-18] are:

Theorem 1. If $z(t) = u(t) \pm v(t)$, then $Z(k) = U(k) \pm V(k)$.

Theorem 2. If z(t) = cv(t), then Z(k) = cV(k), where c is constant.

Theorem 3. If $z(t) = \frac{dv(t)}{dt}$, then Z(k) = (k+1)V(k+1). **Theorem 4.** If $z(t) = \frac{d^n v(t)}{dt}$, then $Z(k) = \frac{(k+n)!}{k!} \mathcal{V}(k+n)$.

Theorem 5. If z(t) = u(t)v(t), then $\mathcal{Z}(k) = \sum_{r=0}^{k} \mathcal{U}(r)\mathcal{V}(k-r)$.

Theorem 6. If $z(t) = t^n$, then $\mathcal{Z}(k) = \delta(k-n) = \begin{cases} 1 & k = n \\ 0 & k \neq n \end{cases}$.

In real applications, the function u(t) is expressed by a finite series and (3) can be written as

$$u(t) = \sum_{k=0}^{N} \mathcal{U}(k)(t-t_i)^k, \forall t \in D$$

Equation (4) implies that $\sum_{k=N+1}^{\infty} \mathcal{U}(k)(t-t_i)^k$ is negligibly small.

Fractional Time Derived (Random) HIV/AIDS Model

This section presents the results of solving the random fractional order HIV/AIDS modeling using the differential transformation method (DTM) and provides examples of the variances, confidence intervals, and expected values of various probability distributions of these solutions [19-21]. There are now initial conditions that include randomly effective terms with various probability distributions. In recent years, the mean square calculation has been used to solve a few first-order random differential equations and models [22-32].

The deterministic form of the nonlinear HIV/AIDS model [19] is following:

$$D_t^{q_1}S(t) = \mu - \beta S(t)I(t) - \mu S(t)$$

$$D_t^{q_2}I(t) = \beta S(t)I(t) - \mu I(t) - \delta I(t)$$
(5)

$$D_t^{q_3}A(t) = \delta I(t) - \mu A(t) - dA(t)$$

$$S(t_0) = S_0, I(t_0) = I_0, A(t_0) = A_0.$$
(6)

In this model, those infected are denoted by l(t). Those who are infected can transmit the disease to susceptible persons indicated by S(t). Also, when infected persons in our model are sick, they are denoted by A(t). The parameters of our model are μ , β , δ and d and take values in the range of $[0, \infty)$. The Table 1 below displays the values and descriptions for these parameters.

If DTM is applied with the fractional HIV/AIDS model given in (5) and the initial conditions given in (6),

 Table 1. Parameter descriptions and values [19]

Parameter	Explanation	Value
μ	Birth and natural death rate	2
β	The rate of transmission of the infection	1.5
δ	Rate of infected individuals having AIDS	4
d	Death rate from AIDS disease	1

$$\begin{split} F(k+1) &= \frac{\Gamma(q_1(k+1))(\mu\delta(k) - \beta\sum(S(r)I(k-r), r=0..k) - \mu S(k)))}{\Gamma(q_1(k+1)+1)} \\ I(k+1) &= \frac{\Gamma(q_{2\ell}k+1)(\beta\sum(S(r)Y(k-r), r=0..k) - (\mu+\delta)I(k)))}{\Gamma(q_2(k+1)+1)} \\ A(k+1) &= \frac{\Gamma(q_3(k+1))(\delta I(k) - (\mu+d)A(k))}{\Gamma(q_2(k+1)+1)} \end{split}$$
(7)

The fractional derivative of our model as $q_1 = \frac{9}{10}, q_2 = \frac{9}{10}, q_3 = \frac{9}{10}$

$$\begin{split} S(t) &= S_0 + 8.318033072 t^{\frac{1}{10}} - 1.559631201 t^{\frac{1}{10}} S_0 I_0 \\ &- 2.079508268 t^{\frac{9}{10}} S_0 - 4.954320892 t^{\frac{9}{5}} - 1.342089092 t^{\frac{9}{5}} (S_0)^2 I_0 \\ &+ 8.947260614 t^{\frac{9}{5}} S_0 I_0 - 7.157808491 t^{\frac{9}{5}} I_0 \\ &+ 1.342089092 t^{\frac{9}{5}} S_0 (I_0)^2 + 2.385936164 t^{\frac{9}{5}} S_0 \\ I(t) &= I_0 + 1.559631201 t^{\frac{9}{10}} S_0 I_0 - 6.238524804 t^{\frac{9}{10}} I_0 \\ &+ 1.342089092 t^{\frac{9}{5}} (S_0)^2 I_0 - 12.52616486 t^{\frac{9}{5}} S_0 I_0 \end{split}$$

+ 28.63123396
$$t^{\frac{9}{2}}I_0$$
 - 1.342089092 $t^{\frac{9}{2}}S_0$ $(I_0)^2$
 $A(t) = A_0$ + 4.159016536 $t^{\frac{9}{10}}I_0$ - 3.119262402 $t^{\frac{9}{10}}A_0$
+ 3.578904245 $t^{\frac{9}{2}}S_0$ I_0 - 21.47342548 $t^{\frac{9}{2}}I_0$ + 5.368356368 $t^{\frac{9}{2}}A_0$

is in the form above.

The initial conditions in our model are $S_0 \sim Exp(\lambda = 2)$ exponential distribution, $I_0 \sim N(\mu = 3, \sigma^2 = 9)$ normal distribution and $A_0 \sim \text{Beta}(k = 3, l = 3)$ beta distribution, chosen from three different absolute continuous distributions.

The parameters of the normally distributed random variable *X* are $X \sim N(\mu, \sigma^2)$. Using the moment generating function of the normal distribution, we get

$$M_X(t) = E[e^{tX}] = e^{\frac{1}{2}\sigma^2 t^2 + \mu t}$$

from (17), the 1st and 2nd moment of the random variable $X \sim N(\mu, \sigma^2)$ are,

$$E[X] = \mu, \quad E[X^2] = \sigma^2 + \mu^2,$$

is calculated as. If the basic properties of the expected value for the X and Y independent random variables are used, the expected value of equation (16) is

$$f(y) = \frac{1}{B(k,l)} y^{k-1} (1-y)^{l-1}, y \in (0,1), k > 0, l > 0$$

where *Y* is a random variable.

If there is a probability density function of the form, it has a standard Beta distribution and is denoted by $Y \sim Beta(k, l)$. Expected value for this distribution

$$E(Y) = \frac{k}{k+l}$$

and variance

300

250

200

((t)) 150

100

50

$$Var(Y) = \frac{kl}{(k+l)^2(k+l+1)}$$

is in the form above.

The moment generating function of the exponential distribution;

$$M(t) = \frac{\lambda}{\lambda - t}; \ t < \lambda$$

is indicated by $X \sim (\lambda)$. Expected value and variance[20]:

$$E(X) = \frac{1}{\lambda}$$
$$Var(X) = \frac{1}{\lambda^2}.$$

$$E(S(t)) = E(S_0) + 8.318033072t^{\frac{9}{10}} - 1.559631201t^{\frac{9}{10}}E(S_0)E(I_0) - 2.079508268t^{\frac{9}{10}}E(S_0) - 4.954320892t^{\frac{9}{5}} - 1.342089092t^{\frac{9}{5}}E((S_0)^2)E(I_0) + 8.947260614t^{\frac{9}{5}}E(S_0)E(I_0) - 7.157808491t^{\frac{9}{5}}E(I_0) + 1.342089092t^{\frac{9}{5}}E(S_0)E((I_0)^2) + 2.385936164t^{\frac{9}{5}}E(S_0)$$

$$(9)$$

$$E(S(t)) = 2 - 5.198770670t^{\frac{9}{10}} + 78.32976332t^{\frac{9}{5}}$$
(10)

Expected Value

E(S

Figure 1. Time-dependent variation of the expected value of individuals susceptible to the virus.

1.2

1.4

1.6 1.8

2

0.8

0.6

04

The expectations can be compared to the deterministic results of equation (1) above (Figure 1) in a single graph (Figure 1). The following are the maximum and minimum values of the expected values of the random variables: S(t) has a maximum value of 265.1 when t = 2 and a minimum value of 2 when t = 0.

$$E(I(t)) = E(I_0) + 1.559631201 t^{\frac{9}{10}}E(S_0) E(I_0) - 6.238524804 t^{\frac{9}{10}} E(I_0) + 1.342089092 t^{\frac{9}{5}}E(S_0)^2 E(I_0) - 12.52616486t^{\frac{9}{5}}E(S_0) E(I_0)$$
(11)
+ 28.63123396 t^{\frac{9}{5}}E(I_0) - 1.342089092 t^{\frac{9}{5}}E(S_0) E((I_0)^2)

$$E(I(t)) = 3 - 9.357787204t^{\frac{9}{10}} - 35.56536095t^{\frac{9}{5}}$$
(12)



Figure 2. Time-dependent variation of the expected value of infected individuals.

For comparison with the deterministic outcomes of the equation above, expectations can be presented in a single graph (Figure 2). The following methods are used to determine the maximum and minimum values of the expected values of the random variables: At t = 0 and t = 2, respectively, l(t) takes the maximum value of 3 and the minimum value of -138.3.

$$E(A(t)) = E(A_0) + 4.159016536 t^{\frac{2}{10}} E(I_0) - 3.119262402 t^{\frac{2}{10}} E(A_0) + 3.578904245 t^{\frac{2}{5}} E(S_0) E(I_0) - 21.47342548 t^{\frac{2}{5}} E(I_0)$$
(13)
+ 5.368356368 t^{\frac{2}{5}} E(A_0)

$$E(A(t)) = \frac{2}{5} + 11.22934465t^{\frac{9}{10}} - 40.79950842t^{\frac{9}{5}}$$
(14)

The expectations can be presented in a single graph (Figure 3) for comparison with the deterministic outcomes of equation (1) above (Figure 3). The following methods



Figure 3. Time-dependent variation of the expected value of sick individuals.

are used to determine the maximum and minimum values of the expected values of the random variables: At t = 0 and t = 2, respectively, A(t) takes the maximum value of 1.167 and the minimum value of -120.7.

In our model, variance values were calculated according to the values and distributions given above.

$$Var(S(t)) = Var(S_0 + 8.318033072t^{\frac{9}{10}} - 1.559631201t^{\frac{9}{10}}S_0 I_0$$

- 2.079508268t^{\frac{9}{10}}S_0 - 4.954320892t^{\frac{9}{5}}
- 1.342089092t^{\frac{9}{5}}(S_0)^2 I_0 + 8.947260614t^{\frac{9}{5}}S_0 I_0 (15)
- 7.157808491t^{\frac{9}{5}}I_0 + 1.342089092t^{\frac{9}{5}}S_0 (I_0)^2
+ 2.385936164t^{\frac{9}{5}}S_0)

 $Var(S(t)) = Var(S_0) + \left(1.559631201t^{\frac{9}{10}}\right)^2 Var(S_0)Var(I_0)$

+
$$(2.079508268t^{\circ})^{2} Var(S_{0}) + (1.342089092t^{\circ})^{2} Var((S_{0})^{2}) Var(I_{0})$$

+ $(8.947260614t^{\circ})^{2} Var(S_{0}) Var(I_{0}) + (7.157808491t^{\circ})^{2} Var(I_{0})$
+ $(1.342089092t^{\circ})^{2} Var(S_{0}) Var((I_{0})^{2}) + (2.385936164t^{\circ})^{2} Var(S_{0})$ (16)

$$Var(S(t)) = \frac{1}{4} + 6.554099996t^{\frac{9}{5}} + 881.7612031t^{\frac{18}{5}}$$
(17)

The S(t) variances are shown above (Figure 4). The following is how the extreme variances of the random variables are obtained: Maximum max[Var(S(t))] = 10720 at time t = 2 and minimum min[Var(S(t))] = 0.25 at time t = 0.

$$Var(I(t)) = Var(I_0 + 1.559631201 t^{\frac{9}{10}}S_0 I_0 - 6.238524804 t^{\frac{9}{10}}I_0 + 1.342089092 t^{\frac{9}{5}}(S_0)^2 I_0 - 12.52616486t^{\frac{9}{5}}S_0 I_0$$
(18)
+ 28.63123396 t^{\frac{9}{5}}I_0 - 1.342089092 t^{\frac{9}{5}}S_0 (I_0)^2)



Figure 4. Time-dependent variation of the variance value of individuals susceptible to the virus.

$$Var(l(t)) = Var(l_{0}) + (1.559631201t^{\frac{1}{10}}) 2 Var(S_{0}) Var(l_{0}) + (6.238524804t^{\frac{1}{10}}) 2 Var(J_{0}) + (1.342089092t^{\frac{3}{2}}) 2 Var(S_{0})^{2} Var(J_{0}) + (1.342089092t^{\frac{3}{2}}) 2 Var(S_{0}) Var(l_{0}) + (28.63123396t^{\frac{3}{2}}) 2 Var(J_{0}) + (1.342089092t^{\frac{3}{2}}) 2 Var(S_{0}) Var((I_{0})^{2}) + (1.342089092t^{\frac{3}{2}}) 2 Var(S_{0}) Var((I_{0})^{2}) Var(I_{0})^{2} = 9 + 352.0970627t^{\frac{9}{5}} + 7969.873553t^{\frac{18}{5}}$$
(20)



Figure 5. Time-dependent variation of the variance value of infected individuals.

The variances of l(t) is given above (Figure 5). Extremum values of the variances of the random variables are obtained as follows: min[Var(I(t))] = 2 at t = 0 and max[Var(I(t))] = 9788 at t = 2.

$$Var(A(t)) = Var(A_0 + 4.159016536 t^{\frac{1}{10}} l_0 - 3.119262402 t^{\frac{1}{10}} A_0 + 3.578904245 t^{\frac{2}{5}} S_0 l_0 - 21.47342548t^{\frac{2}{5}} l_0$$
(21)
+ 5.368356368t^{\frac{2}{5}} A_0)

$$Var(A(t)) = Var(A_0) + \left(4.159016536 t^{\frac{9}{10}}\right)^2 Var(l_0)$$

+
$$(3.119262402 t^{-0})^2 Var(A_0)$$

+ $(3.578904245 t^{\frac{9}{5}})^2 Var(S_0) Var(I_0)$

(22)

+ $(21.47342548t^{\frac{9}{5}})^2 Var(I_0) + (5.368356368t^{\frac{9}{5}})^2 Var(A_0)$

$$Var(A(t)) = \frac{1}{25} + 156.0659589t^{\frac{9}{5}} + 4179.944036t^{\frac{18}{5}}$$
(23)



Figure 6. Time-dependent variation of the variance value of sick individuals.

The variances of A(t) is given above (Figure 6). Extremum values of the variances of the random variables are obtained as follows: min[Var(I(t))] = 0.04 at t = 0 and max[Var(I(t))] = 51230 at t = 2.

Confidence intervals for random variable expected values,

$$(E(y(t)) - K.std(y(t)), E(y(t)) + K.std(y(t))$$

is equal, which can be determined using standard deviations. For K = 3, this formula yields a % 99 confidence interval(C.I.) for the expected value of a normally distributed random variable [21]. Figure 7 depicts a % 99 C.I. plotted with MATLAB (2013a).This popular rule, known as the three sigma rule, states that 99.73% of values for a normally distributed variable are within three standard deviations of the mean. Thus, using the appropriate parameters, we will compare the variations of the results for two continuous distributions with limited and unlimited support, respectively. Nearly all potential values for the random effects for both distributions will come from the same range if the parameters are chosen appropriately.

The confidence intervals of S(t) are given in Figure 7. The extremum values of the confidence intervals are as follows: min(E(S(t)) - 3std(S)) = -45.48 at t = 2 and max(E(S(t))



Figure 7. Time-dependent variation of % 99 C.I. intervals of virus-susceptible individuals.



Figure 8. Time-dependent variation of %99 C.I. of infected individuals



Figure 9. Time-dependent variation of % 99 C.I. of patients.

+ 3std(S)) = 575.6 at t = 2. Here, K = 3 gives an approximate %99 confidence interval.

The confidence intervals of l(t) are given in Figure 8. The extremum values of the confidence intervals are as follows: min(E(I(t)) - 3std(I)) = -1077 at t = 2 and max(E(I(t)) + 3std(I)) = 800.2 at t = 2. Here, K = 3 gives an approximate %99 confidence interval.

The confidence intervals of l(t) are given in Figure 9. The extremum values of the confidence intervals are as follows: $\min(E(A(t)) - 3std(A)) = -799.7$ at t = 2 and max-(E(A(t)) + 3std(A)) = 558.3 at t = 2. Here, K = 3 gives an approximate %99 confidence interval.

CONCLUSION

In this study, random fractional ordinary differential equations were solved using the fractional differential transformation method. The motivation of this study is to determine the probability characteristics of a randomized fractional-order HIV/AIDS Modelling under random effects. Normal, Beta, and exponential distributions are used to select the initial conditions or coefficients of random fractional ordinary differential equations. Expected value, variance, and confidence intervals from probability properties were found and graph for the analysis of random effect are presented accordingly. Examining standard deviations, variations, and confidence intervals for expected values reveals how virus transmission dynamics change over time. By selecting different probability distributions from many epidemic models in the literature, the behavior under random effects can be examined. We believe that this study will be an important component in mathematical modeling studies on the transmission of the HIV/AIDS virus. The results are guaranteed to be useful for the random differential equation system if the deterministic and random analysis results are comparable. The stochastic model can simulate the dynamics of disease transmission just as well as the deterministic model, but it can also yield information about the model's variability, including coefficients of variation and standard deviations. We observe that random expectations are also consistent with the deterministic model's results, which are comparable to the numerical results from the relevant study. Results for the expected values' confidence intervals are also provided by the random model. Any deterministic compartment disease model can be created using this method of creating random models from deterministic models. Using actual data for parameter variations rather than speculative values can improve the results. Research on the stability and ideal management of diverse mathematical models of other illnesses, like COVID-19 and tuberculosis, can also be utilized to explore the dynamics of disease dissemination.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Modelling and control of a reaction wheel pendulum using a linear quadratic regulator

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ABSTRACT

This paper presents a tutorial-style approach to synthesizing a mechatronic control system from scratch, with a focus on mathematical modeling, real-world verification, model-based control using the Linear Quadratic Regulator (LQR), and rapid control prototyping. The system's equations of motion are derived through Lagrangian mechanics and subsequently linearized. Unknown parameters are estimated using optimization techniques. An LQR controller is designed and implemented on the STM32F4 microcontroller and its performance is rigorously tested against disturbances using MATLAB/Simulink. The Reaction Wheel Pendulum serves as the case study, demonstrating the successful implementation of the LQR controller, with the derived model verified through experimentation. A recovery angle of 20 degrees is obtained.

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INTRODUCTION

The inverted pendulum is a nonlinear and underactuated control problem that is used in developing new control algorithms and in teaching environments. Different types of this problem exist, such as the cart pendulum, the double inverted pendulum, the rotary pendulum, the damped driven pendulum, and the reaction wheel pendulum to name a few [1-4]. These differ from each other mainly by the amount of underactuated joints, and by the actuated rigid body that is used to control the system. Comparisons of the different types of pendulum structures and their potential applications are given in [5]. However, the control problem of these systems remains the same, swinging up the pendulum from its downright position and stabilizing the pendulum in its inverted position.

One of the many types of inverted pendulums is the reaction wheel pendulum (RWP), which was first introduced by Spong et al. [6]. The reaction wheel pendulum consists of two joints with parallel rotation axes, one of which is not actuated. The other joint is typically actuated by a DC motor and has a wheel attached to it which has a symmetric mass distribution, simplifying the analytical solution. The system is controlled using the wheel's inertia, whereby accelerating the wheel a reaction torque is produced.



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Studies on modeling and control of the RWP have been conducted in detail. Spong et al. [6] were the first to introduce the system and proposed a stabilizing controller using an exact and approximate feedback linearization method, and a swing-up controller using partial feedback linearization on a physical system. Bapiraju et al. [7] proposed multiple linearization methods for the RWP using a fuzzy logic controller to perform stabilization and showed the results in an experimental setup. Srinivas and Behera [8] proposed two new swing-up controllers based on sinusoidal swing-up and interconnection and damping assignment-passivity-based control, implementing them in real-time. Jepsen et al. [9] developed a RWP and described the design process. In addition, swing-up control was implemented using a bang-bang controller, and stabilization was achieved through an observer-based feedback controller. Kadam and Seth [10] presented the modeling, simulation, and LQR control design for a one-wheel robot controlled by a reaction wheel.

Andrievsky [11] focused on the global stabilization of the RWP, ensuring stability for arbitrary initial conditions. An energy-based speed-gradient control scheme was used for the swing-up problem, and sliding mode control was used for stabilization, demonstrating the results through simulations. Gajamohan et al. [12] developed the Cubli, a cube equipped with a reaction wheel on three of its faces. The stabilization challenge involved stabilizing the cube on one of its edges. Similar to the RWP, the Cubli operates in three dimensions, making the balancing and swing-up problem more sophisticated. Nguyen et al. [13] modeled and controlled the RWP using LQR and a fuzzy logic controller, comparing the results through simulation and experimental validation. The system demonstrated stabilization from an initial position of 5 degrees. Trentin et al. [14] modeled and controlled a RWP equipped with two reaction wheels on opposite sides of the pendulum. They employed nonlinear proportional-derivative control and a sliding mode controller to stabilize the system. Montoya et al. [15] designed a controller based on the Lyapunov theory, ensuring stable operation through control input without additional calculations. The results were simulated, and asymptotic stability was guaranteed. Önen and Çakan [16] detailed the modeling and LQR control of the RWP system. Using a designed LQR controller, they simulated the system and presented the results. Cioaca and Flutur [17] designed a 3D-printed RWP system and stabilized it from an initial condition of 2 degrees. They presented results from both the physical system and the simulation.

For pendulum systems other than the RWP, many other methods such as PID, fuzzy logic, sliding mode control, LQR, adaptive control, neural network control, and model predictive control [18–22]. LQR is a fundamental control technique widely employed in various engineering disciplines to achieve optimal control of linear dynamic systems. It is a powerful tool that enables engineers to design controllers that minimize a quadratic cost function, effectively balancing control efforts and system performance. With its solid theoretical foundation and versatility, the LQR control strategy has found applications in diverse fields such as aerospace, robotics, process control, and economics [23].

The significance of disturbance rejection in inverted pendulum systems cannot be overstated. Real-world applications, such as segways, can be accurately modeled as inverted pendulums, and they often encounter disturbances when navigating diverse terrains. While previous studies have conducted minor disturbance tests, this study aims to undertake a more aggressive disturbance rejection test. The evaluation will be based on the recovery angle, representing the system's ability to return to a stable position after being disturbed, without relying on a swing-up structure. Implementing this disturbance-rejecting controller enhances the system's suitability for more challenging environments where disturbances are frequent.

The sections are set up as follows. The equations of motion are derived using Lagrangian mechanics and, the system is linearized in section 2. The modeled system is verified and unmodeled parameters are estimated in section 3. The LQR controller is designed in section 4. In section 5, the hardware used in the system is specified and the designed controller is tested against disturbances.

EQUATIONS OF MOTION AND DYNAMICS

The system diagram is given in Figure 1. The system's stable equilibrium is in the downright position. Throughout this paper, the pendulum angle is taken with reference to the upright position, which is the unstable equilibrium point,



Figure 1. Reaction wheel pendulum diagram.

Tal	ble	1.	S	ystem	par	ameters
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Parameter	Description
m_1	Pendulum arm mass
m_2	Reaction wheel mass
l_1	Pendulum arm moment of inertia
l_2	Reaction wheel moment of inertia
θ_1	Pendulum arm angle
θ_2	Reaction wheel angle (with respect to the pendulum arm)
θ_{v}	Reaction wheel angle (with respect to vertical reference)
l _c	Pendulum arm center of mass
1	Reaction wheel center of mass

around which stabilization is required. All system parameters and the symbols used for them are presented in Table 1.

Mathematical Modeling

The pendulum can be thought of as a planar robot arm with two links the first link is the pendulum arm, and the second link is the reaction wheel. The positions and linear velocities of the center of masses are given in Eqs. (1) and (2) respectively. The linear velocities are obtained by taking the time derivative of the positions.

$$p_1 = \begin{bmatrix} l_c \sin \theta_1 \\ l_c \cos \theta_1 \end{bmatrix} \quad p_2 = \begin{bmatrix} l \sin \theta_1 \\ l \cos \theta_1 \end{bmatrix} \tag{1}$$

$$\dot{p}_1 = \begin{bmatrix} l_c \dot{\theta}_1 \cos \theta_1 \\ -l_c \dot{\theta}_1 \sin \theta_1 \end{bmatrix} \quad \dot{p}_2 = \begin{bmatrix} l \dot{\theta}_1 \cos \theta_1 \\ -l \dot{\theta}_1 \sin \theta_1 \end{bmatrix}$$
(2)

The Lagrangian is the difference between the kinetic and potential energy of the system, which are given in Eqs. (3) and (4) respectively. The kinetic energy of the system (T) consists of linear and angular components. The potential energy (U) only depends on the pendulum arm's angle, since only that parameter affects the vertical displacement of the system.

$$T = \frac{1}{2}\dot{p_1}^T m_1 \dot{p_1} + \frac{1}{2}l_1 \dot{\theta_1}^2 + \frac{1}{2}\dot{p_2}^T m_2 \dot{p_2} + \frac{1}{2}l_2 \dot{\theta_v}^2 \qquad (3)$$

$$U = \cos(\theta_1) \left(m_1 g \ l_c + m_2 g \ l \right) \tag{4}$$

The reaction wheel's angular velocity $\hat{\theta}_v$ must be written with respect to the pendulum arm, since in the real system, it will be measured in that way. Eq. (5) shows how the angle of the pendulum arm and reaction wheel added together, is equal to the reaction wheel angle with respect to the vertical reference. Taking the time derivative of Eq. (5) and substituting it in Eq. (3) yields Eq. (6) which is the system's total kinetic energy. The Lagrangian (*L*) can thus be found and is given in Eq. (7).

$$\theta_{\nu} = \theta_1 + \theta_2 \tag{5}$$

$$T = \frac{1}{2}\dot{\theta_1}^2 (m_1 l_c^2 + m_2 l^2 + l_1 + l_2) + l_2 \dot{\theta_1} \dot{\theta_2} + \frac{1}{2} l_2 \dot{\theta_2}^2 \quad (6)$$

$$L = T - U = \frac{1}{2} \dot{\theta_1}^2 (m_1 l_c^2 + m_2 l^2 + l_1 + l_2) + l_2 \dot{\theta_1} \dot{\theta_2} + \frac{1}{2} l_2 \dot{\theta_2}^2 - \cos(\theta_1) (m_1 g \ l_c + m_2 g \ l)$$
(7)

Eq. (8) shows the Lagrange-Euler equation where q is a generalized coordinate system and Q is a generalized force vector. Since the Lagrangian is energy-based, the remaining dynamics such as friction, constraints, and/or contact forces can't be modeled directly, hence the use of Q. The generalized coordinates in this system are $q = [\theta_1; \theta_2]$. Therefore, the output of Eq. (8) must be a 2x1 vector. Substituting Eq. (7) in Eq. (8), the equations of motion are presented in Eq. (9).

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = Q \tag{8}$$

$$\begin{bmatrix} \alpha \ddot{\theta}_1 + I_2 \ddot{\theta}_2 \\ I_2 \ddot{\theta}_1 + I_2 \ddot{\theta}_2 \end{bmatrix} - \begin{bmatrix} \beta \sin \theta_1 \\ 0 \end{bmatrix} = \begin{bmatrix} \tau_1 \\ \tau_2 \end{bmatrix}$$
(9)

where $\alpha = (m_1 l_c^2 + m_2 l^2 + I_1 + I_2)$, $\beta = m_1 g l_c + m_2 g l$. τ_1 and τ_2 are the net joint torques. However, the system is only actuated in τ_2 . This results in τ_1 only consisting of the friction in joint 1, which is written as b_1 . The control input will be written as τ , and the friction in joint 2 (which depends on the motor) is written as b_2 .

Note that Eq. (9) contains coupled dynamic equations, since $\ddot{\theta}_1$ and $\ddot{\theta}_2$ cannot be expressed independently. To uncouple the equations of motion, Eq. (9) is rewritten in the form of Eq. (10).

$$M\begin{bmatrix} \ddot{\theta}_1\\ \ddot{\theta}_2 \end{bmatrix} = \begin{bmatrix} -b_1 \dot{\theta}_1\\ \tau - b_2 \dot{\theta}_2 \end{bmatrix} + \begin{bmatrix} \beta \sin \theta_1\\ 0 \end{bmatrix}, \quad M = \begin{bmatrix} \alpha & I_2\\ I_2 & I_2 \end{bmatrix}$$
(10)

This is the matrix form of this system, here M is the mass matrix. To uncouple the equations, both sides can be multiplied by the inverse mass matrix. Doing this, yields $\ddot{\theta}_1$ and $\ddot{\theta}_2$ separately which are given in Eqs. (11) and (12) respectively.

$$\ddot{\theta_1} = \frac{1}{I_2 - \alpha} \left(-\beta \sin \theta_1 + b_1 \dot{\theta_1} - b_2 \dot{\theta_2} \right) + \frac{1}{I_2 - \alpha} \tau \qquad (11)$$

$$\dot{\theta_2} = -\frac{1}{I_2 - \alpha} \left(-\beta \sin \theta_1 + b_1 \dot{\theta_1} - \frac{\alpha}{I_2} b_2 \dot{\theta_2} \right) + \frac{\alpha}{\alpha I_2 - I_2^2} \tau \quad (12)$$

These equations are the system's dynamic equations for a general control input. The nonlinearity of the system comes from the $sin(\theta_1)$ term. Thus, the system can easily be linearized using the Taylor Series expansion, which will be done further in the paper.

The control torque will be supplied by a DC motor, which will be driven over an H-bridge. Therefore, expressing the control input as voltage rather than torque will make it more intuitive for the user. Eqs. (13) and (14) show the torque equation and current equation for a DC motor respectively. Table 2 shows the symbols and their definitions.

$$\tau = n K_T i \tag{13}$$

$$\mathbf{i} = \frac{V - nK_V \,\dot{\theta}_2}{R} \tag{14}$$

The armature inductance is ignored, since in small power DC motors it is very small. Substituting Eq. (13) in Eq. (12), yields the motor torque with the voltage as the input. This can be used as our control input and substituted in the equations of motion. This will yield the final equations of motion given in Eqs. (15) and (16) with the motor voltage as the control input.

Table 2. Motor parameter definitions

Parameter	Description
V	Input voltage
i	Armature current
R	Armature resistance
K_T	Motor torque constant
K_V	Motor velocity constant
n	Gear ratio

Table 3. System parameter values

Parameter	Description	Value
$\overline{m_1}$	Pendulum arm mass	0.043 [kg]
m_2	Reaction wheel mass	0.042 [<i>kg</i>]
l_1	Pendulum arm moment of inertia	$0.00012 \ [kg \ m^2]$
l_2	Reaction wheel moment of inertia	$0.002005 \ [kg \ m^2]$
l	Pendulum arm center of mass	0.03 [<i>m</i>]
l_c	Reaction wheel center of mass	0.093 [<i>m</i>]
R	Armature resistance	6.6 [Ω]
K_T	Motor torque constant	0.0931676 [Nm/A]
K_V	Motor velocity constant	0.0139746 [V/(rad/s)]
n	Gear ratio	9.68

$$\ddot{\theta}_1 = \frac{1}{I_2 - \alpha} \left(-\beta \sin \theta_1 + b_1 \dot{\theta}_1 - \gamma \dot{\theta}_2 \right) + \frac{nK_T}{R(I_2 - \alpha)} V \quad (15)$$

$$\begin{aligned} \dot{\theta_2} &= -\frac{1}{l_2 - \alpha} \left(-\beta \sin \theta_1 + b_1 \dot{\theta_1} - \frac{\alpha}{l_2} \gamma \dot{\theta_2} \right) + \frac{n K_T \alpha}{R(\alpha \, l_2 - l_2^2)} V \\ &(\gamma = b_2 + \frac{n^2 K_T K_V}{R}) \end{aligned} \tag{16}$$

The parameters such as link lengths, center of mass location, mass and moments of inertia were obtained using Solidworks. All system parameters and their values are given in Table 3.

The actuator is chosen as a 12 V Pololu #4862 brushed DC motor with a built-in encoder and gearbox. Therefore, the control input V is saturated to [-12, 12]. This needs to be included in the simulation, or the controller can output extreme voltage values.

State Space Representation and Linearization

In order to simulate the system, it is useful to represent the nonlinear system in state variables. The system is expressed with state variables in Eqs. (17), (18) and (19). Note that the reaction wheel angle is omitted, since it never appears in the equations of motion, thus $x_3 = \dot{\theta}_2$.

$$\dot{x_1} = x_2 \tag{17}$$

$$\dot{x_2} = \frac{1}{I_2 - \alpha} (-\beta \sin x_1 + b_1 x_2 - \gamma x_3) + \frac{nK_T}{R(I_2 - \alpha)} V \quad (18)$$

$$\dot{x}_{3} = -\frac{1}{I_{2} - \alpha} \left(-\beta \sin x_{1} + b_{1} x_{2} - \frac{\alpha}{I_{2}} \gamma x_{3} \right) + \frac{n K_{T} \alpha}{R(\alpha I_{2} - I_{2}^{2})} V \quad (19)$$

The system should be linearized, in order to use linear control methods. To linearize the system, the Taylor Series Expansion of the sine term is given in Eq. (20) and can be substituted in Eqs. (18) and (19).

$$\sin(x_1) = x_1 - \frac{x_1^3}{3!} + \frac{x_1^5}{5!} - \frac{x_1^7}{7!} + \cdots$$
 (20)

Since the goal of the system is to control it in the upright position, x_1 will be close to 0. Therefore $sin(x_1) \approx x_1$, which gets rid of the nonlinearity of the equations. The state space representation of the system is given in Eq. (21).

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ \frac{-\beta}{I_2 - \alpha} & \frac{b_1}{I_2 - \alpha} & \frac{-\gamma}{I_2 - \alpha} \\ \frac{\beta}{I_2 - \alpha} & \frac{-b_1}{I_2 - \alpha} & \frac{\alpha\gamma}{I_2^2 - \alpha I_2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{nK_T}{R(I_2 - \alpha)} \\ \frac{nK_T\alpha}{R(\alpha I_2 - I_2^2)} \end{bmatrix} V$$
(21)
$$y = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$



Figure 2. Optimization results.

Using Eq. (21), linear controllers can be designed and tested in simulation and on the real system. The control input V is saturated according to the motor operating limits and/or the supply voltage limits.

Parameter Estimation

In order to use model-based controller design methods, the real system and simulated system should perform as similarly as possible. All measurable parameters were given in Table 3. However, the equations of motion also include two friction terms.

The viscous friction coefficient of the DC motor can be found parametrically by using the DC motor's specifications and is found as $b_2 = 0.0012$. The viscous friction coefficient of the pendulum arm, however, has to be experimentally verified. In order to do this, the pendulum was manually stabilized in the upright position. Afterwards, a small perturbation was applied to move the pendulum, after which the angle of the pendulum arm was recorded using an optical encoder. This was performed four times and similar results were obtained.

With the experimental results the model can be simulated using Eqs. (11) and (12) and optimized to fit the simulated response as closely to the experimental results as possible. This optimization is done using the nonlinear least squares method, with a sum squared error cost function. The error is defined in Eq. (22).

$$e(t) = y_{exp}(t) - y_{sim}(t)$$
(22)

MATLAB Simulink is used to solve the optimization problem. An initial guess of 0.001 for b_1 was used. The results are given in Figure 2. The optimized result gives a mean absolute percentage error of 94.1%, which is the error in Eq. (22) divided by the experimental output and summed over all time steps. Note that the simulated response reaches steady state later than the experimental result in the optimized response. This is due to unmodelled nonlinear effects in the real system, such as the tension that occurs in the motor's electrical wires. This is irrelevant, however, since the simulated and experimental results are very similar up to 4 seconds, which is significantly more than the actuator's response time.

Controller Design

Now that an accurate system model is obtained, it can be used to design a controller. A Linear Quadratic Regulator (LQR) is chosen as the system's controller in this paper. LQR is an optimal control method based on full state feedback, which means all states must be accessible. This method tries to minimize a cost function J, given in Eq. (23).

$$J = \int_{0}^{\infty} (x^{T}Qx + u^{T}Ru)dt$$
(23)

Q is the state-cost weighted matrix, R is the input-cost weighted matrix and u is the control input u = -Kx. This optimal control problem's goal is to find an appropriate K vector that minimizes the cost function. To determine the Q and R matrices, a good first step is Bryson's rule [24] which is given in Eq. (24).

$$Q_{ii} = \frac{1}{x_{i_{max}}^2}, i = 1, 2, ..., n \qquad R = \frac{1}{u_{max}^2}$$
(24)



Figure 3. LQR controller block diagram.

 Q_{ii} are the elements of a diagonal matrix. x_{imax} is the maximum error for state i. u_{max} is the maximum control input.

The max state errors were defined as 0.005°, 0.01 rpm and 0.1 rpm for x_1 , x_2 and x_3 respectively. These were obtained by iteratively testing the system using different Q and R matrices, where the best performing ones are given in Eq. (25). The maximum control input is the saturated 12 Volts of the motor.



Figure 4. CAD design and real system.



Figure 5. Simulink block diagram using Waijung Blockset.

$$Q = 10^{6} \begin{bmatrix} 131.31 & 0 & 0 \\ 0 & 0.9119 & 0 \\ 0 & 0 & 0.0091 \end{bmatrix}, \quad R = 0.0069 \quad (25)$$

Using these Q and R matrices, the K gain matrix can be computed using MATLAB and used as a feedback gain on all the measured states. K was found as [-158.62, -15.02, -1.30]. In Figure 3 the system is represented in a block diagram. The reference in the modeled RWP system is zero since stabilization is intended around this point.

HARDWARE AND EXPERIMENTAL RESULTS

The CAD design in SOLIDWORKS and real system is given in Figure 4. The STM32F4 discovery board was used as the microcontroller. The code was generated using the Waijung Blockset by Aimagin [25] in MATLAB Simulink. The motor is a Pololu #4862 geared brushed DC motor. The motor was driven using a L298N dual channel H-bridge driver. The pendulum arm angle was read using a 2048 CPR optical encoder connected to the shaft via a coupler. The Simulink block diagram is given in Figure 5. The filtered derivative block is a transfer function block where $\omega = 10 \frac{rad}{s}$ and $\zeta = 0.7$. This Simulink block diagram was directly embedded on the microcontroller.

The disturbance rejection experiment results are given in Figure 6 and 7, respectively. The peaks in the pendulum arm angle (θ_1), are the points where the system was hit by an object. The stabilization of the system has an oscillatory behavior of 8 degrees. Furthermore, the maximum recovery angle is around 20 degrees as can be seen in Figure 7. The controller exhibits strong disturbance-rejecting performance, as it can stabilize the system even when it deviates significantly from the linearization point, despite being designed based on a linearized model. The behavior of the system against disturbances can be seen in the following video link https://www.youtube.com/ watch?v=bb33BNByxlQ.

Nevertheless, enhancing the stability performance is feasible by adopting an alternative controller structure, as demonstrated in [9] with the implementation of an observer-based feedback controller. Directly taking derivatives can result in noise amplification. To mitigate this, a second-order low-pass filter is incorporated with the derivative, introducing additional delays. Therefore, the use of an observer-based feedback controller has the potential to improve stabilization performance.



Figure 6. Disturbance test-1.



Figure 7. Disturbance test-2.

CONCLUSION

In this paper, the Reaction Wheel Pendulum was mathematically modeled and the system's equations of motion were derived. The system was linearized and was represented in state space. Furthermore, the only unmodeled parameter, friction in the pendulum arm, was estimated using optimization techniques by measuring the system's natural response without any control inputs and fitting the simulated response to this. Using the complete and verified model, an LQR controller was designed and implemented on a microcontroller, after which a disturbance test was done to validate the controller's performance against the supplied disturbances. The system reached a maximum recovery angle of 20 degrees, and had oscillatory steady state behavior of 8 degrees.

The controller can be enhanced by eliminating the oscillatory steady state response, which could be achieved using different Q and R matrices, thus different K gains. Also, using a different controller structure can improve the stabilization performance. Furthermore, adding imbalances to the reaction wheel (such as small weights on one side) and designing and testing controllers against these can be possible areas of improvement. Compared to previous

literature, this paper presents a new metric to characterize performance against disturbances, the recovery angle, which is the maximum angle the system can reach before it can return to its stable equilibrium without a swing-up procedure.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Enhancement of leachate treatment process through integration of flat solar collectors

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ABSTRACT

Within the scope of this study aimed at safeguarding our environment, we utilized an economical apparatus to eliminate the leachate present in the landfill of Khénifra, Morocco. This substance, predominantly composed of organic matter, exerts a detrimental impact on the ecosystem. The solution put forth in this research involves employing a flat solar collector to expedite the evaporation process of the leachate, which occupies three substantial basins within the landfill. The results obtained showcase a remarkable enhancement in evaporation efficiency, with the flat solar collector contributing to an impressive 300% increase, thereby significantly reducing the evaporation timeframe when compared to the traditional method employed in the landfill. In the context of our experiment, we observed a noteworthy reduction of 18 days in evaporation duration compared to the natural evaporation process, thanks to the implementation of this solar collector. This straightforward, efficacious, and notably cost-effective technique yields compelling and promising results.

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INTRODUCTION

Numerous investigations have undertaken the task of evaluating the potential risks to both human well-being and the environment stemming from groundwater contamination caused by leachate [1–3]. Leachate, characterized by a heightened biochemical oxygen demand (BOD) and substantial concentrations of organic carbon, nitrogen, chloride, iron, manganese, and phenols, poses significant ecological

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challenges. The list of potential components extends to include pesticides, solvents, heavy metals, as well as personal care and pharmaceutical chemicals, among others.

The generation of leachate presents a formidable concern within municipal solid waste landfills, casting a substantial shadow over surface and groundwater quality. However, the physico-chemical attributes of pollutants within leachate can vary significantly from one instance to another, influenced by waste composition, site configuration, climatic conditions, and their inherent variability. Notably, leachates feature both emerging and refractory pollutants, necessitating intricate treatment combining biological and physicochemical processes [4–8], showcasing the pressing need for robust strategies to mitigate the environmental hazards linked to leachate presence¹.

In light of this, several research initiatives have scrutinized the efficiency of leachate treatment methodologies under laboratory, pilot, and semi-pilot conditions. These studies have hailed innovative approaches, notably membrane bioreactors and advanced oxidation processes, showcasing robust purification mechanisms [8–10]. Nonetheless, an inherent challenge emerges in the form of potentially toxic byproducts, such as trihalomethanes, haloacetic acids, chlorates, perchlorates, and the like.

The physico-chemical composition of leachate exhibits a wide range of diversity, dictated by variables like waste content, landfill conditions, temperature, moisture, and microbial activity levels^{11,12}. To gain comprehensive insights into leachate profiles, one can turn to physico-chemical markers, including COD, BOD5, nitrogen and phosphorus fractions, conductivity, pH, in addition to heavy metal and anion concentrations [1,13–15].

Leachate is classified into distinct categories—namely young, mature, and old—based on the landfill's conditions and duration, reflecting variations in biodegradability [16]. Leachate may encompass elevated metal concentrations, refractory organic substances such as pesticides, and more [8,17].

Traditionally, leachate removal and treatment from operational landfills have been confined to expensive alternatives [1–4,12–14], which, while highly effective, can be excessively intricate. Techniques like vacuum evaporation, reverse osmosis, ultrafiltration, and membrane bioreactors [2,4,6,8,12,18] demand specialized expertise and nearly constant personnel presence.

Consequently, research efforts that identify or propose low cost treatment methodologies, adapted to operators' needs and discharge standards, are of paramount importance. The present study is dedicated to achieving precisely this objective. We have developed an exceptionally efficient technique that is both cost-effective and ecologically sustainable.

This investigation employs a captivating approach—the utilization of a planar solar collector [11,19–27]. While widely employed across various applications and fields such as solar cookers and solar water heaters, our experiment harnesses this flat collector's potential to expedite

the evaporation and removal of leachate. The experimental phase has unequivocally showcased the efficacy of this technique, with the leachate evaporation rate by this process being tenfold that of natural evaporation. This acceleration implies that the timeframe for leachate treatment in ponds, which typically spans three months, could be drastically reduced to a mere three or four days, saving a remarkable 90% of the time typically required.

MATERIALS AND METHODS

Study Site

This study was carried out in the Khenifra solid waste burial and recovery center, located in the village of Amehroq, in the commune of El Heri in Khenifra. This city is located between the Meknes city and Beni-Mellal city. The province of Khenifra is part of the region of Béni-Mellal Khénifra in Morocco (Fig. 1). This solid waste land-fill and recovery center, created in 2016, is part of a new generation of environmentally friendly projects that contribute to the development of the green economy and the socio-economic integration of professionals in the waste recycling sector. Its objective is to prevent and reduce pollution caused by household waste and to organize its collection, transport, storage and treatment in a way that takes into account the environmental dimension and allows for the recovery and recycling of waste in a rational way.

It includes a landfill with a system to prevent leachate leakage and waste collection ponds with a storm water drainage system outside the center.

It should be noted that this pioneering project in this region level aims to tackle the problem of anarchic dumps, recalling that this project was set up as part of an integrated vision for a more modern and rational management of waste and its use in the production of energy and raw materials, all in strict compliance with environmental standards. However, to complete this huge project, there are two other points to be achieved, which are the improvement and development of methods for the treatment of leachate at lower costs and the production of biomass energy in order to take advantage of the energy that is produced within the center.

In this study, we will look at the treatment of leachate produced at the center, which is currently treated by natural evaporation, a very old technique that costs nothing but has a major problem in that it is very time consuming, especially during the summer season when leachate production reaches maximum quantities.

Characterization of the Waste of Khénifra City and Its Leachates

The leachates studied were collected from the vehicles in charge of the collection of household waste from the city of Khénifra during transport to the landfill. The household waste from the city of Khenifra has a moisture content of



Figure 1. Location of the city of Khénifra (Morocco).



Figure 2. Location of the study site, landfill and waste recovery center.

about [3,28] 64% and is characterized by a high content of organic matter and a high percentage of waste [29]. These types of waste are generally characterized by the presence of a dominant fraction consisting mainly of kitchen and garden waste. This fraction has been estimated, in most land-fills, to be more than 50% of the mass of municipal waste. This is justified by a consumption pattern based on fresh products. The waste is still composed of paper, plastics. The quantities of aluminum, iron and glass are very negligible.

Tabl	e 1.	Pł	nysicocl	hemical	cl	haracteristics	of	the	leacl	hate
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Parameters	Values	Unit
Organic compounds	52%	_
рН	4.92	-
COD	22,6	mg/L
Electrical Conductivity (EC)	25,7	μs/cm
Turbidity	2,78	NTU
Total Suspended Solids (TSS)	5,64	mg/L
[NH] ⁺	1,87	mg/L
[<i>Cl</i>] ⁻	2580	mg/L
Heavy Metals	73	mg/L

The physico-chemical analysis of the young leachate generated by this waste showed an acidic character with a pH of about 5 and a high organic load with a chemical oxygen demand (COD) exceeding $20gO_2/L$.

Description of the Experimental Set-Up

The tests were carried out in plastic bottles with a capacity of 1 liter each, the first one left in the ambient air with the objective of making a natural evaporation and the second one, the same bottle with the same capacity, is put in



Figure 3. Flat solar collector for evaporation and natural evaporation device.

a flat solar collector. The flat solar collector is made from simple materials, it consists of a box which must be made of an insulating material to prevent heat loss inside and also to minimize the external effects on the internal temperature. The inside of this box is lined with a reflective film, usually aluminum foil or a glass mirror, and the top surface of the box is made like a glass window to let the light rays in and at the same time create the greenhouse effect inside the box. This box, which is 40 cm wide and 70 cm long, must be very well closed to avoid any kind of leakage.

In addition to this we used two thermometers to monitor the temperature of the leachate within each vessel. The amount of leachate we used in each vessel was 800 ml. Figure 3 shows our experimental set-up to be exposed to the sun. Thus, forced evaporation was achieved using the flat solar collector technique. The experimental device presented in the figure above, is a very simple technique in terms of cost of the necessary elements and also for its realization, that is to say that it does not require special skills in order to carry it out, and this is a strong point of this experiment because it can be carried out easily, from where a broad public can benefit from this device in order to preserve our environment and not to waste money for too complex and too expensive techniques.

RESULTS AND DISCUSSION

Natural and Forced Evaporation of Leachate Through a Solar Collector

The aim of this test is to evaluate the difference in evaporation efficiency between leachate left in the open air i.e. natural evaporation and forced evaporation i.e. using the flat solar collector, all elements must be well exposed to the sun, as the sun plays the most important role in this experiment.

The curves in Figures 4 and 5 show the results of the decrease in the amount of leachate during our experiment and the corresponding temperature values, the experiment is performed during one day in the winter period. We started the experiment at about 10:09 a.m. until 4:00 p.m., so our experiment took 351 minutes in total. First of all we noticed that the maximum ambient temperature was around 22 °C while on average it was around 15 °C, but the maximum temperature in the solar collector reached 61 °C and on average this temperature in the solar collector was around 40 °C, it is to be noted that this day of the experiment was partially cloudy, while in normal conditions in Khenifra city the ambient temperature exceeds 30 °C in



Figure 4. Decrease in the amount of leachate evaporated in the open-air.



Figure 5. Decrease in the amount of leachate evaporated in the solar collector.



Figure 6. Comparison of leachate evaporation results in the open-air and in the solar collector.

general and even more in the summer period, this shows that our experiment will gain in term of yield during normal conditions and especially in summer.

In Figure 6, it can be seen that the triggering of the natural evaporation needs more than 240 min, while the evaporation in the collector needs only 90 min, which shows that we could reduce this period by more than half, so we can say that it is possible to have an evaporation even with low ambient temperatures and the collector is able to evaporate the liquid in all the conditions because this device also takes advantage of the phenomenon of greenhouse effect. Moreover, we can see that the quantity evaporated at the end of the experiment is 30 mL in the open-air and 105 mL in the collector, which shows that the quantity of leachate evaporated in the collector is three times greater than the quantity evaporated in the open-air, a gain in efficiency that exceeds 300%.

However, the results obtained show that evaporation is largely favored in the solar collector compared to natural evaporation. The estimated time required for complete evaporation under these conditions, considered as bad climate conditions, of 800 mL of leachate at an average temperature of 15 °C during this period is 26 days, while the estimated evaporation period in the collector is about 8 days, i.e. a decrease of 18 days. The average evaporation rate increased by about 351% from the initial evaporation rate of 0.085 mL/min to 0.299 mL/min.

The findings derived from the study unequivocally validate the crucial and highly impactful role played by the solar collector in intensifying the process of evaporation, particularly in comparison to the leachate that remains directly exposed to the ambient air. This substantiates the collector's proficiency in significantly expediting the rate at which leachate transforms from liquid to vapor state.

The detailed analysis of the results underscores a remarkable reduction in the overall evaporation timeframe. Notably, when examining an equivalent quantity of leachate, the utilization of the solar collector precipitates a noteworthy decrease in the temporal span required for the evaporation process to reach completion. This compelling observation emphasizes the remarkable efficiency of the solar collector-driven evaporation mechanism in comparison to the natural dissipation of leachate under standard atmospheric conditions.

CONCLUSION

The culmination of this comprehensive study provides resounding affirmation that the intricate interplay between meteorological nuances and physical parameters governs the intricate process of evaporation. However, the complexity of these factors does not preclude the implementation of pragmatic and astoundingly effective methodologies, as unveiled by the findings of this research. The empirical evidence gleaned from our investigations significantly amplifies the pivotal role of a flat solar collector, shedding light on its profound efficacy as an unassuming yet transformative instrument. The tangible benefits it imparts are indeed striking:

- A discernible amplification of internal temperature gradients within the collector's confines, a testament to its prowess in harnessing and concentrating solar energy.
- 2. An impressive acceleration in the rate of evaporation, with the collector propelling the process from a modest 0.085 ml/min to a commendable 0.299 ml/min.
- Most notably, a remarkable truncation of the once-protracted evaporation period, diminishing from a laborious 26 days to a mere 8 days, all accomplished through the seamless integration of this celebrated device.

These outcomes underscore not only the prowess of the chosen approach but also its ability to revolutionize traditional expectations. The device's multifaceted impact is particularly remarkable when viewed through the lens of enhancing efficiency, with its deployment translating into a staggering efficiency surge of over 300%. Yet, amidst these impressive outcomes, the true gem of this solar collector lies in its inherent simplicity of design and the associated cost-effectiveness.

As we peer into the horizon of possibilities, it becomes increasingly evident that the promise of innovation holds substantial potential. Future explorations might encompass an inquiry into alternative configurations of solar collectors, each poised to further amplify operational efficiency. Moreover, the notion of harmoniously amalgamating disparate techniques kindles intrigue, offering a tantalizing prospect of harnessing green energy in a manner that remains both fiscally prudent and environmentally sagacious.

In this pursuit, the horizon beckons towards a realm where innovative collaborations blend seamlessly with tried-and-true practices, culminating in solutions that propel us closer to safeguarding our environment against the insidious impact of leachate. As the chapters of research and application continue to unfold, this study stands as a beacon, illuminating the path toward a more sustainable and enlightened future.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Effects of SiO₂ and Al₂O₃ nanoparticles on the properties of borogypsum containing mortar

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ABSTRACT

This study aimed to investigate the effects of nano-SiO₂ and nano-Al₂O₃ on the physicochemical and mechanical properties of mortars containing borogypsum. The mortars were modified by incorporating 0.2-1% nano-SiO₂ and 0.5-2.5% nano-Al₂O₃. Various analysis methods were applied to the nano-modified samples to observe changes in the fresh and hardened features of the mortars. The results showed that the nanoparticles used could not promote the setting of the mortars. The highest compressive strength of 67 MPa was achieved when 1% nano-Al₂O₃ was used. Adding 0.4% nano-SiO₂ resulted in the highest flexural strength of 9.13 MPa. Supporting the water absorption test, SEM and BET morphologic analyses showed that nano-SiO₂ was more effective in developing a denser microstructure than nano-Al₂O₃. The findings of the thermal analysis suggest that substituting nanoparticles in borogypsum-containing mortars could not decrease the unreacted CH ratio during the hydration under the studied conditions.

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INTRODUCTION

In recent decades, the application of nanotechnology in construction materials to improve mechanical and chemical stability has gained importance. Generally, nanotechnological approaches aim to make superficial and intrinsic features more durable. The primary motivation for using nanoparticles in mortar blends is to use them as fillers for voids and as nuclei for hydration reactions to obtain superior properties [1-2]. Although there are some challenges in determining the appropriate amount and dispersion method, nanoparticles have significant potential for developing engineering properties of construction materials [1].

*E-mail address: moroydor@yildiz.edu.tr This paper was recommended for publication in revised form by Editor-in-Chief Ahmet Selim Dalkilic The feasibility of using several types of nanoparticles has been investigated in previous studies. The most commonly used nanoparticles are nano-SiO₂ [3-6], nano-Al₂O₃ [7-8], nano-TiO₂ [9-11], and nano-Fe₂O₃ [12].

Although the nanoparticles mentioned above are usually incorporated into mortar blends with industrial wastes of fly ash [3, 13-15] and blast furnace slag [16-17], there have been no studies on the coexistence of borogypsum with nano-SiO₂ and nano-Al₂O₃ in cement mortars. Borogypsum is industrial waste produced during boric acid production from colemanite and sulfuric acid reactions. Using borogypsum as a mineral admixture can help reduce



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the disposal of this industrial waste and turn it into an alternative supplementary cementitious material [18].

To the best of our knowledge, there is a lack of studies that have explored the characteristics of borogypsum mortars incorporating nano-SiO₂ and nano-Al₂O₃ despite the widespread investigation of borogypsum as industrial waste in civil engineering applications. The primary goal of this study was to assess the impact of borogypsum in mortar compositions when combined with nano-SiO₂ and nano-Al₂O₃ and to examine their interactions. Given that the presence of boron tends to extend the setting time, it is paramount to investigate how the utilization of nanoparticles influences various properties of the resulting mortars. To fulfill this objective, a series of mechanical tests and instrumental analyses were conducted on mortars cured for 3, 7, and 28 days. The microstructural assessment encompassed water absorption testing, scanning electron microscope (SEM) observation, and BET (Brunauer-Emmett-Teller) analysis.

MATERIALS AND METHODS

Materials

The industrial waste of borogypsum, supplied by Bandırma Boron Works (Eti Maden, Balıkesir, Turkey), was used instead of gypsum. XRD identified borogypsum (BJ), and according to the XRD results, borogypsum contained gypsum (CaSO₄·2H₂O, powder diffraction file (PDF) no:00-006-0046) and calcium borate hydrate (Ca₂B₁₀O₁₇·5H₂O, pdf no:00-022-0146) [19]. Due to the chemical composition of borogypsum, clinker was used as the binder material and was provided by the Akcansa Cement Factory, Istanbul, Turkey. The fine aggregate of CEN standard sand conforming to EN 196-1 was [20] obtained from Limak Trakya Cement (Kırklareli, Turkey). Sigma Aldrich and Merck Chemicals supplied SiO₂ and Al₂O₃ nanoparticles, and their S_{BET} were 175-225 m²/g and 120-190 m²/g, respectively. The chemical compositions of the ingredients are listed in Table 1 [19]. A polycarboxylic ether-based superplasticizer admixture (SP) (MasterGlenium*51, BASF Turkey) inhibited nanoparticle agglomeration.

Table 1. The chemical compositions of the ingredient [19]

Composition (%)	Clinker	Borogypsum
SiO ₂	14.0	4.1
Al_2O_3	3.0	-
Fe ₂ O ₃	4.7	1.0
CaO	76.5	45.1
SO ₃	-	48.7
MgO	-	-
B ₂ O ₃	-	1.1

Preparation of Specimens

A total of 10 different cement mortars with different amounts of nano-SiO2 and nano-Al2O3 were prepared (Table 2). In addition, the reference mixture was prepared without nanoparticles, whereas the clinker in the other mortars was partially replaced with nano-SiO₂ and nano- Al_2O_3 . The quantities of nanoparticle substitutions were established at 0.2-1% for SiO₂, and 0.5-2.5% for Al₂O₃, derived from preliminary experiments wherein a range of nanoparticle quantities was examined, and the most favorable intervals were selected with respect to rheological and mechanical characteristics. All mortars with a water-tocement ratio of 0.4 and a binder-to-sand ratio of 3.0 were prepared, and the SP ratio was kept constant at 0.50% of the binder. In preliminary studies, based on the literature [18, 21], several ratios of borogypsum replaced binder materials, and 3% was determined as the optimum ratio in terms of physical and mechanical features.

The reference mixture was prepared according to the EN 196-1 standard [20]. For the preparation of nanoparticle-containing mortars, a different pathway was followed: The mixing water, SP, and nanoparticle were mixed and stirred at 500 rpm for 5 minutes. This blend was combined with clinker, borogypsum, and sand. After stirring for 5 minutes at high speed, the mortars were molded in 40x40x160-mm three-cell prismatic molds. Also, some parts of the mortars were placed into 40x40x40-mm cubes for the water absorption test. Next, the molds were kept in a test cabinet (Nuve TK 120, Turkey) at 20 ± 2 °C and 90% relative humidity. After 24 h, the mortars were removed from the molds and cured in tap water until testing.

Test Procedure

Several tests were conducted on fresh and hardened nano-modified mortars to investigate their properties based on the nanoparticle type and ratio. TS EN 480-2 was followed to observe the change in the setting time. The initial and final setting times were determined by measuring the penetration

Table 2. Mixture proportions of cement mortars

Mixture	Clinker (%)	BJ (%)	SiO ₂ (%)	Al ₂ O ₃ (%)
Control	97.0	3	-	-
BJ-S-1	96.5	3	0.2	-
BJ-S-2	96.0	3	0.4	-
BJ-S-3	95.5	3	0.6	-
BJ-S-4	95.0	3	0.8	-
BJ-S-5	94.5	3	1.0	-
BJ-A-1	96.5	3	-	0.5
BJ-A-2	96.0	3	-	1.0
BJ-A-3	95.5	3	-	1.5
BJ-A-4	95.0	3	-	2.0
BJ-A-5	94.5	3	-	2.5

depth of the needle of the Vicat apparatus [21]. Compressive and flexural strength tests were performed according to the procedures described in the EN 196-1 standard [20] at 3, 7, and 28 days. The crystalline phases of 28 days cured cement mortars were identified using XRD (PANalytical B.V., Almelo, The Netherlands) in the pattern range of 5–90°. The samples were then finely ground to a final particle size of 90 µm. The samples were identified using inorganic crystal structure database (ICSD) patterns. Fourier transform infrared (FT-IR) spectroscopy (Perkin Elmer Spectrum One, MA, USA) was used to analyze the amorphous phases in the mortar matrix and the crystalline phases in the crystalline matrix. The vibrational properties of the hydration products in the optimum samples after 28 days of curing were observed in the 450–4000 cm⁻¹ range. The BET method and water absorption test were used to investigate the effects of nanoparticles on the mortars' pore structure. The samples' \boldsymbol{S}_{BET} and total pore volume were determined by nitrogen (N₂) adsorption on a Micromeritics ASAP 2020 instrument. Before analysis, the finely ground samples were degassed under a vacuum at 105 °C. The BET analysis relies on empirically establishing the connection between the pressure of N₂ in equilibrium with a mortar surface and the volume of gas adsorbed at that specific pressure on the surface [22]. Water absorption tests of the mortars were performed according to the BS 1881-122 standard [23]. The mortars were maintained in an incubator at 105 °C for 72 h. After removal from the incubator and cooling in a dry airtight vessel, the initial weights of the mortar samples were recorded. Following cumulative immersion periods of 10, 30, 60, and 120 min into tap water, the absorbed water percentage of the samples was calculated. Three samples were employed to assess each mortar's mechanical characteristics and water absorption capacity. The microstructure of the mortars cured for 28 days was observed using a scanning electron microscope

(ZEISS EVO LS 10) after converting the samples into small fragments.

Thermal analyses of the mortars were performed using a PerkinElmer Diamond TG/DTA instrument. The samples were heated from 30 to 1000 °C at a 10 °C/min heating rate under a N₂ atmosphere. Thermogravimetric analysis ensures the determination of the quantity of CH, which indicates the hydration progress. The CH percentage was calculated from the start and end points of the CH decomposition (Equation 1).

$$CH(\%) = WL_{CH}(\%) \times \frac{MW_{CH}}{MW_H}$$
(1)

In Equation 1, WL_{CH} is the weight loss because of the CH decomposition; MW_{CH} and MW_{H} are CH and water molecular weights, respectively [24-25].

RESULTS AND DISCUSSION

Setting Time of Mortars

The setting time results for the mortars are shown in Figure 1. Contrary to most of the studies in the literature, both nanoparticles increased the setting time of mortars for all addition ratios. Many studies have investigated the effects of borogypsum on the setting properties of cement mortars, and it has been proven that borogypsum shows set-retarding properties [26-27]. However, the nano-modification did not show development in the setting features of the mortars. As shown in Figure 1, when the initial setting time of the nanoparticle-containing mortars was similar, the nano-Al₂O₃ incorporation caused a remarkable difference in the final setting time. In the studies by Heikal et al., using SiO₂ and Al₂O₃ nanoparticles delayed the setting time when they were used with the superplasticizer. These



Final setting (min) Initial setting (min)

Figure 1. Setting time of mortars.

results were explained by the presence of a superplasticizer and the mixing procedure of nanoparticles and superplasticizers [28-29]. Similar to these studies, especially for the increased nanoparticle ratios, the presence of both the superplasticizer and borogypsum had a combined effect on set-retarding. They did not allow nanoparticles to show their pozzolanic activity effectively.

The Compressive and Flexural Strength of Mortars

The compressive strength development of the mortars with SiO_2 and Al_2O_3 nanoparticles is shown in Figure 2. The compressive strengths of 3-days cured mortars were compared, and it was observed that the compressive strength of the mortars decreased with increasing nanoparticle ratios.

As shown in Figure 2, 0.4% nano-SiO₂ usage improved the compressive strength of 28-days cured mortar as 1.94%of the reference value. However, increasing the nano-SiO₂ caused a remarkable decrease in compressive strength at all ages. The lack of uniform distribution of nano-SiO₂ can explain these results. When 1% nano-Al₂O₃ was incorporated into the mortars, the compressive strength of the 28-days cured mortar increased by 4.56%. Like the nano-SiO₂ replacement, nano-Al₂O₃ at higher ratios reduced the



Figure 2. The compressive strength of mortars.



Figure 3. The flexural strength of mortars.

compressive strength. The compressive strength results showed that the agglomeration tendency of nano-SiO₂ and nano-Al₂O₃ caused a failure to obtain satisfactory results.

When the flexural strength of the mortars was investigated, it was observed that parallel to the compressive strength, the optimum nano-SiO₂ and nano-Al₂O₃ ratios were 0.4% and 1%, respectively (Figure 3). The flexural strength results of 3-days cured mortars showed that the usage of nano-SiO₂ up to 1.5% ensured higher development than the reference sample, which can be attributed to the nucleation effect of nano-SiO₂. On the other hand, the early-age strength of nano-Al2O3-containing mortars was lower than that of the reference. As a result of further curing, the 0.4% nano-SiO₂-containing mortar reached a flexural strength 4.82% higher than the reference sample. The flexural strength of 28-days cured nano-Al₂O₃-containing mortars showed that adding 1% nano-Al₂O₃ improved the flexural strength of mortars by 2.76% of the reference sample. The mechanical test results indicated that the combination of borogypsum and Al₂O₃ and SiO₂ nanoparticles could not improve the mechanical endurance of the mortars.

XRD Results of Mortars

The crystalline phases in the mortar structure were determined using XRD analysis. The XRD patterns of the reference sample and selected mortars for each nanoparticle, which showed the highest mechanical strength, are presented in Figure 4.

According to the XRD analysis of the cement mortars, the main crystalline phase was quartz (SiO_2) with pdf number 00-046-1045, owing to the presence of sand. In addition to sand, portlandite $(Ca(OH)_2)$ with pdf number 00-004-0733, calcium silicate hydrate $(Ca_{1.5}SiO_3 \cdot xH_2O)$ with pdf number 00-033-0306, and gismondine $(CaAl_2Si_2O_8 \cdot 4H_2O)$ with pdf number 00-020-0452 were determined in the mortar composition.

For the BJ-A-2 sample, the peaks belonging to calcium alumina silicates (\sim 68°) were higher than reference and nano-SiO₂-containing mortars. Also, different from the reference sample, the peak around 18° became sharper with the presence of nanoparticles.

FT-IR Results of Mortars

The FT-IR spectra of the selected mortar samples are shown in Figure 5. The absorption band around 3640 cm⁻¹ is associated with O-H stretching vibrations of portlandite. The bands between 3440 cm⁻¹ - 2920 cm⁻¹ and around 1640 cm⁻¹ demonstrate O-H stretching and bending vibration of O-H due to the capillary water, respectively. The peaks detected at 2850 cm⁻¹, 1430 cm⁻¹, and 880 cm⁻¹ are attributed to the carbonation of Ca(OH)₂ with atmospheric CO₂ causes.

Calcium silicate hydrate (C-S-H) formation is characterized by intensified peaks at 1085 cm⁻¹ - 1030 cm⁻¹. In this region, peaks occurred due to the Si-O band's asymmetric stretching vibration. The peaks around 780 cm⁻¹ are related to the vibration of tetrahedral units of AlO_4^{5-} which exist in the structure due to calcium alumina silicate (C-A-S) gel. The peaks observed at 696 cm⁻¹ indicate the symmetric bending of Si-O-Si. The out-of-plane Si-O bending causes bands around 520 cm⁻¹ when the peaks around 460 cm⁻¹ correspond to in-plane Si-O bending peaks. The obtained FT-IR spectra of the cement mortars align with the literature data [29-32].

Scanning Electron Microscopy

SEM images of the reference sample and the optimum samples of BJ-S-2 and BJ-A-2 are shown in Figure 6. As shown in Figure 6, the addition of nanoparticles influenced the hydration of the mortars and initiated a change in the microstructure. The SEM images revealed that using nano-SiO₂ with borogypsum-containing mortar resulted in a denser and more compact microstructure than the reference and nano-Al₂O₃ blended mortar. The nano-Al₂O₃



Figure 4. XRD patterns of selected samples.



Figure 5. FT-IR spectra of selected samples.
containing mortar contains large amounts of ettringite needles. Furthermore, it had a more porous structure than the reference, which coincided with the water absorption values.

BET Analysis Results of Mortars

The BET-specific area and pore volume of the reference and nano-modified samples are listed in Table 3. When the S_{BET} values of nano-SiO₂-containing mortars were investigated, it was clear that a significant improvement occurred in the specific surface of the mixtures when the nano- SiO_2 addition ratios were bigger than 0.2%, proving that there were smaller voids in the mortars. In addition, the specific pore volumes of the samples increased with increasing S_{BET}. These recent findings are consistent with those of Shih et al. [33]. According to BET analyses, the mortars' porosity did not significantly change when nano-Al₂O₃ was added to the mixtures. Furthermore, the denser microstructure in nano-SiO₂-containing mortars than those with nano-Al₂O₃ was demonstrated by measuring the higher mechanical resistance. The study by Seife et al. [34] yielded similar results, as it evaluated the effects of different activators on the mortar through BET tests and demonstrated

a correlation between pore development and the material's mechanical strength.

Water Absorption Results of Mortars

The water absorption capacities of the nano-SiO₂ and nano-Al₂O₃-containing mortars are shown in Figures 7 and 8, respectively.

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Mix	SBET (m ² /g)	Pore volume (cm ³ /g)
Reference	1.1739 ± 0.0188	0.008533
BJ-S-1	1.9089 ± 0.0322	0.008568
BJ-S-2	3.2464±0.0304	0.013539
BJ-S-3	3.8543 ± 0.0401	0.014667
BJ-S-4	3.5187±0.0306	0.012835
BJ-S-5	3.9842±0.0413	0.016548
BJ-A-1	2.1251±0.0255	0.008948
BJ-A-2	2.4169 ± 0.0045	0.009775
BJ-A-3	1.9678 ± 0.0237	0.008557
BJ-A-4	2.8730±0.0366	0.011116
BJ-A-5	1.7259±0.0188	0.006371



Figure 6. SEM images of selected samples (a. Reference, b. BJ-S-2, c. BJ-A-2).

As shown in Figure 7, using nano-SiO₂ in the mortar composition reduced water absorption. The compression between the mortars showed that the BJ-S-2 mortar absorbed 55% less water than the reference. The results demonstrate that adding nano-SiO₂ made the mortar matrix more compact and filled the pores, thus enhancing water absorption. On the contrary, the results showed that the percentage of water absorption was decreased by nano-Al₂O₃-containing mortars absorbing more water than the reference due to the increase in the porosity of the samples. The lack of water tightness of mortars incorporating nano-Al₂O₃ could be caused by the insufficient distribution of this nanoparticle, resulting in agglomeration and creating a more porous matrix [35].

As revealed by BET analysis results, the replacement of nano-SiO₂ supported the forming a denser structure and water tightness than nano-Al₂O₃. The observed decrease in

water absorption by nano-SiO₂ corresponds to the results obtained in previous studies [36].

Thermal Analysis Results of Mortars

The DTA and DTG curves of selected mortars at 28 days of hydration are shown in Figure 9 and Figure 10, respectively. The thermal analysis curves, which are given for the temperature range of 200 °C and 800 °C, can be used for quantitative estimation of the CH content of the mortars. Considering the mass loss between 370°C and 500 °C, it is seen that the portlandite amount of the reference sample is lower than nanoparticle-incorporated samples besides the BJ-A-5 sample. The lack of primer hydration reactions possibly caused the lowest CH% of BJ-A-5. With the incorporation of nano-SiO₂, the decomposed CH amounts of the mortars changed between 6.55% and 8.81% when nano-Al₂O₃-containing mortars had a portlandite content of 4.08% - 8.03%. In addition, the thermal analysis curves



Figure 7. Water absorption percentage of nano-SiO₂-containing samples.



Figure 8. Water absorption percentage of nano-Al₂O₃-containing samples.



Figure 9. DTA curve of selected mortars.



Figure 10. DTG curve of selected mortars.

Mix	Initial Temperature (°C)	Final Temperature (°C)	CH content (%)
Reference	370.78	436.79	4.49
BJ-S-1	415.92	467.30	8.81
BJ-S-2	421.46	464.50	8.65
BJ-S-3	414.88	460.62	6.55
BJ-S-4	415.14	462.18	6.59
BJ-S-5	405.02	456.92	6.67
BJ-A-1	403.74	479.16	6.63
BJ-A-2	419.27	467.67	7.08
BJ-A-3	407.22	456.49	6.26
BJ-A-4	408.51	490.33	8.03
BJ-A-5	403.28	464.47	4.08

Table 4. DTA/TG results of Ca (OH)₂ decomposition

demonstrate that adding nanoparticles shifts the initial decomposition temperature to higher values, which could be altered due to the reaction of the used nanoparticles with mortar and inhibiting portlandite from decomposition. When the mechanical and thermal analysis results are evaluated together, it is noticed that the nanoparticles used cannot ensure progress for secondary hydration reactions in which CH can be consumed.

CONCLUSION

This study explores the effects of nano-SiO₂ and nano-Al₂O₃ on borogypsum-based mortars, addressing optimal concentrations, microstructural changes, and the impact on the hydration process, all representing valuable additions to the existing knowledge. From the obtained results, it can be stated that:

- Nanoparticles cannot enhance the acceleration of the setting of mortars. The combination of nanoparticles and borogypsum inhibited hydration.
- For all curing ages, increasing the dosages of nanoparticles caused a decrease in the compressive and flexural strengths. Nevertheless, compared with the reference sample, adding 0.4% nano-SiO₂ increased the compressive and flexural strengths by 1.94% and 4.82, respectively. Similarly, mortars containing 1% nano-Al₂O₃ had 4.56% and 2.76% higher compressive and flexural strengths, respectively.
- The SEM images, BET analysis, and water absorption results support the formation of a densified structure by nano-SiO₂ usage.
- According to the thermal analysis results, the nanoparticle-added samples include more portlandite than the reference sample, which can be attributed to the lack of secondary hydration reactions.

- Although using nanoparticles with supplementary cementitious materials could be practical and economical in many aspects, combining borogypsum with nano-SiO₂ and nano-Al₂O₃ could not achieve remarkable strength and durability.
- In further studies, changing the mixing method of nanoparticles can be investigated to obtain better results.

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NOMENCLATURE

BJ	Borogypsum
CH	$Ca(OH)_2$
DTA	Differential Thermal Analysis
DTG	Derivative Thermogravimetric
FT-IR	Fourier transform infrared spectroscopy
ICSD	Inorganic crystal structure database
MW_{CH}	Molecular weight of CH, g/cm ³
MW_H	Molecular weight of water, g/cm ³
pdf	Powder diffraction file
S_{BET}	BET surface area, m ² /g
SP	Superplasticizer admixture
TG	Thermogravimetric analysis
WL_{CH}	Weight loss because of the CH decomposition, g

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Enhancing power system stability through intelligent STATCOM control strategies in torsional oscillation environments

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ABSTRACT

This research develops a new control method for the IEEE Second benchmark model (SBM) that uses an intelligent optimization-based static synchronous compensator to reduce low-frequency torsional oscillations. This low-frequency oscillation caused by mainly shunt and series compensation produces torsional oscillation and induction generator effect in a synchronous generator that may lead to fatigue in the shaft and continuation of low-frequency oscillations for a long duration. To minimize this effect, various techniques have been applied. The Static Synchronous Compensator's gate signal is managed by the control strategy using two distinct proportional-integral (PI) controllers in accordance with system voltage. The test system is subjected to a three-phase LLL-G fault with zero inherent dampening considered to simulate the most severe situation, with natural damping for comparative analysis. The time-domain outcomes of the rotor dynamics for different test scenarios with and without the Static Synchronous Compensator and with the proposed PSO (Particle swarm optimization), FF (Firefly algorithm), and GWO (Grey Wolf Optimizer) Optimization-based Static Synchronous Compensator (STATCOM). The efficiency of the proposed controller in reducing overall power system oscillations is demonstrated using optimization-based STATCOM. The proposed study demonstrates the superiority of the GWO optimization technique over FF, PSO, and standard STATCOM in terms of settling time. This is evidenced by comparing the simulation results, including the performance index.

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INTRODUCTION

Power system stability refers to the capacity of the system to maintain its steady operational condition in the presence of disturbances[1]. These disturbances can vary in magnitude, ranging from significant to minor. Power systems often face the significant problem of transient stability when they experience massive disruptions for a short period of time. This results in a need for coordination among the generators in distinct interconnected segments of the system. Significant disruptions can encompass

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abrupt line loss, faults, or generator failure [2]. The often observed methods for improving transient stability in power systems involve the utilization of an automated voltage regulator (AVR) for excitation control and a speed governor equipped with a steam valve for speed control. In the case of constant steam turbine mechanical power, the excitation system controls the alternators internal voltage. Assuming a constant internally generated voltage, the speed governor uses steam value control to control the alternators speed. The paper [3-5] discusses the application of linear controllers in AVR and speed governor systems to enhance power system transient stability. Linear approach controllers are the most effective tools when it comes to tackling challenges that are related to dynamic stability.

Non-linear controllers are mainly used to address transient stability. Using a synchronous motor-generator pair, the power system's stability was improved in a study that employed a lot of renewable energy [6]. With the use of a distributed power controller, multi-machine power systems can achieve transient stability augmentation, as mentioned in [7]. The improvement of power system stability through the mitigation and regulation of subsynchronous resonance (SSR) utilizing a large-scale photovoltaic (PV) plant has been examined in previous studies [8,9]. A comprehensive photovoltaic (PV) system is managed in order to mitigate power system oscillations, as demonstrated in [10]. According to [11-13] a thyristor-controlled series capacitor (TCSC) controller has been designed using modal control in order to reduce torsional oscillations in a power system.

The recent advancement in the electrical and electronic power sectors has increased FACTS utilization in electric power systems for various control objectives. Implementing FACTS devices in power systems results in numerous benefits, such as decreased operational expenses, improved system dependability and security, and an expansion of the transfer ability of existing transmission lanes within the deregulated electricity sector. The research paper [14] comprehensively explains various FACT controllers and their specific applications. With FACT controllers, low-frequency power oscillations can be lessened, and the system>s voltage profile can be maintained by efficiently controlling the flow of real and reactive power. In recent times, several FACT controllers like UPFC (Unified power flow controller), SVC (static VAR compensator), and TCSC (thyristor-controlled series capacitor) [13-15] have been utilized in practical power systems. The STATCOM, also known as the static synchronous compensator, is a shunt controller belonging to the FACTS family. It is designed to exchange active power with the system in a transient manner and has superior damping characteristics. Its primary purpose is to enhance the systems dynamic and transient stability, particularly when compared to other counterparts such as the SVC. The paper [15] discusses the STATCOM controller>s damping properties in relation to the lead-lag compensator.

Recently, several soft computing techniques such as ABC (Artificial Bee Colony), PSO (particle swarm optimization), (FA) Firefly algorithm, (BWO) Black Widow Optimization, BFOA (Bacteria foraging optimization algorithm), and other hybrid optimization techniques have been developed to improve the stability of power systems by optimizing the tuning and placement of FACT controllers. A local damping controller based on fuzzy logic has been presented for the Thyristor-Controlled Series Capacitor (TCSC) to enhance the transient stability of the power system [16]. It has been addressed and contrasted in [17] that the performance of two modified optimization techniques- ABC and PSO -when combined with the Hybrid Genetic algorithm (H-GA). The paper [18] discusses the utilization of a hybrid method that combines Particle Swarm Optimization (PSO) and Gravitational Search method (GSA) to determine the best configuration of Flexible AC Transmission System (FACT) controllers for enhancing voltage stability. [19] presents a controller design for STATCOM that utilizes honey bee mating optimization (HBMO) to improve the stability of power systems. An enhanced Particle Swarm Optimization (PSO) method was proposed in reference [20] to mitigate and regulate sub-synchronous resonance in wind farms with series compensated Doubly Fed Induction Generator (DFIG) systems. In a recent research paper [21], the effectiveness of a Grey Wolf Optimizer (GWO) - based optimum controller in dampening sub-synchronous resonance in a series-compensated power system network was investigated.

Following reference [21], Table 1 provides a comparative analysis between the proposed work and the existing cutting-edge research.

In conclusion, the integration of soft computing techniques with Flexible AC Transmission System (FACTS) devices presents a comprehensive approach to enhancing the performance and reliability of power systems. By leveraging adaptive control strategies, these technologies offer a range of potential benefits, including improved stability, enhanced voltage regulation, increased power transfer capability, reduced power losses, fast response to dynamic changes, enhanced grid resilience, and optimized asset utilization. Overall, the synergy between soft computing and FACTS devices contributes to a more efficient, reliable, and resilient power infrastructure, ultimately benefiting both utilities and consumers.

By evaluating the possible advantages of fact controllers and optimization strategies based on soft computing. This paper proposes the use of soft computing metaheuristic algorithms to control a Voltage Source Converter (VSC)-based STATCOM in order to reduce sub-synchronous oscillations and voltage fluctuations in a power system. A unique control strategy is used in STATCOM to manage the gate signal by independently controlling the Alternating and Direct currents. This necessitates the use of two separate PI (proportional-integral) controllers.

Previous Study	Controller gain se	election	Stability analysis	
[Reference]; Year	Conventional	Intelligent	Rotor angle	Torsional Mode
[8];2017	-	\checkmark	_	\checkmark
[9], [16]; 2017	\checkmark	-	-	\checkmark
[16]; 2017	-	-	\checkmark	-
[10]; 2019	\checkmark	-	\checkmark	-
[20]; 2019	-	\checkmark	-	\checkmark
[22]; 2020	-	\checkmark	\checkmark	-
[23] 2021	\checkmark	-	\checkmark	\checkmark
[24]; 2023	\checkmark	-	-	-
Proposed Study	-	\checkmark	\checkmark	\checkmark

Table 1. Comparative analysis between the prior research and the proposed work

These PI controllers' gain parameters have been adjusted by optimization approaches with PSO, FF, and GWO. The IEEE second benchmark model was employed in the investigation to simulate the SSR study in the MATLAB environment.

MAJOR CONTRIBUTIONS

- In this study, a novel control strategy is devised to dampen the Torsional oscillations in the case of a nonlinear system.
- A unique control strategy is presented to manage the STATCOM gate signal. Two distinct PI controllers are used in this technique, which independently control AC and DC currents.
- Utilizing Meta-heuristic optimization techniques inspired by nature, such as firefly, PSO, and GWO, have been applied to optimize the PI controllers' gain parameters.
- The system's stability is investigated by means of time-domain simulations analysis and performance indices derived from different error criteria.
- Comparing the suggested GWO optimization methodology's outcomes to those of the PSO and Firefly serves as additional evidence of its effectiveness.

The subsequent segments of the manuscript are structured as follows: Section 2 details the system configuration, while Section 3 delves into the modeling of STATCOM and its associated control structure. Section 4 elaborates on the optimal adjustment of the controller, employing PSO, GWO, and FF. Results and discussions are exhibited in Section 5, and the manuscript concludes in Section 6 with a justified reference-based conclusion.

System Modeling

To investigate the Sub-synchronous Resonance (SSR) problem, the Study employs a modified IEEE second benchmark model. The system described is a basic configuration consisting of a single machine associated with

an infinite bus [25,26]. The transmission line is equipped with a series compensation, as shown in Figure 1. The compensation considered for this specific case is 55%. In the modeled system, an uncompensated transmission line experiences a three-phase to-ground fault at 0.0222 sec for a duration of 0.0169 sec. A fault catalyzes the amplification of the system's oscillations

A transmission network is connected to the generating unit via a step-up transformer. Low-pressure turbine (LPT) and High-pressure turbine (HPT) are the two turbine units that comprise the mechanical mass system. Additionally, the system includes an exciter and a generator. The magnification of torque in these masses poses a significant risk and can result in substantial damage. The results also demonstrate oscillations in torque and speed.

In order to mitigate Sub synchronous Resonance (SSR) in the system, a Static Synchronous Compensator (STATCOM) has been implemented, as depicted in Figure 1. The STATCOM is linked to the drive system by a coupling transformer. The system data is also chosen based on the design considerations outlined in this study [27]. In the case of a multi-bus system, the optimal location for placement of fact devices has been explained in the reference [28]; however, in this case, the system is of two bus system considered. Therefore, STATCOM is connected to the generator terminal so that feedback signal from the generator can be utilized in the STATCOM.

Mathematical Modeling

The linearized mathematical equations are employed to represent numerous subsystems of the system in order to construct a comprehensive mathematical model. This model can be used for conducting eigenvalue analysis for SSR.

Steam governor-turbine system

The governor-turbine concept is represented by transfer functions, as depicted in Figure 2. The model consists



Figure 1. Modified IEEE SBM Model.



Figure 2. Steam governor-turbine system transfer function model.

of four different temporal constants, namely TRP, TGVR, THL, and TCHBR. The governor is characterized by two distinct temporal constants, TRP and TGVR. The temporal constants associated with steam flow are THL and TCHBR. Torques are directly proportional to each other and contribute to a fraction of the overall torque. The structure of a system can be represented by the equations that follow:

$$\frac{d}{dt}\Delta O_{RP} = \frac{1}{T_{RP}} [k_{GVR}\Delta\omega - \Delta O_{RP}]$$
(1)

$$\frac{d}{dt}\Delta O_{GVR} = \frac{1}{T_{GVR}} \left[\Delta O_{RP} - \Delta O_{GVR} \right]$$
(2)

$$\frac{d}{dt}\Delta\tau_{HPT} = \frac{1}{T_{CHBR}} \left[F\tau_{HPT}\Delta O_{GVR} - \Delta\tau_{HPT}\right]$$
(3)

$$\frac{d}{dt}\Delta\tau_{LPT} = \frac{1}{T_{HL}} \left[\frac{F\tau_{LPT}}{F\tau_{HPT}} \Delta\tau_{HPT} - \Delta\tau_{LPT} \right]$$
(4)

The spring-mass system

Four masses make up the modeled mechanical mass system: the high-pressure turbine (HPT), the low-pressure turbine (LPT), the excitation (X), and the generator (G). Linearized equations express their representation.

High-pressure turbine equations

$$\frac{d}{dt}\Delta\omega_{HPT} = \frac{1}{2H_{HPT}} \left[-K_{LH} (\Delta\delta_{HPT} - \Delta\delta_{LPT}) - D_{HPT} \Delta\omega + \Delta\tau_{HPT} \right]$$
(5)

$$\frac{d}{dt}\Delta\delta_{HPT} = \omega_0 \Delta\omega_{HPT} \tag{6}$$

Low-pressure turbine equations

$$\frac{d}{dt}\Delta\omega_{LPT} = \frac{1}{2H_{LPT}} [2HX \left[-D_{LPT}\Delta\omega + \Delta\tau_{LPT} + K_{LH}(\Delta\delta_{HPT} - \Delta\delta_{LPT}) - K_{LG}(\Delta\delta_{HPT} - \Delta\delta_{LPT} - K_{LG}(\Delta\delta_{LPT} - \Delta\delta_{G})] \right]$$
(7)

$$\frac{d}{dt}\Delta\delta_{LPT} = \omega_0 \Delta\omega_{LPT} \tag{8}$$

Generator rotor equations

$$\frac{d}{dt}\Delta\omega_{G} = \frac{1}{2H_{G}} [-D_{G}\Delta w - \Delta\tau_{G} + K_{LG}(\Delta\delta_{LPT} - \Delta\delta_{G}) - K_{GX}(\Delta\delta_{G} - \Delta\delta_{X})]$$
(9)

$$\frac{d}{dt}\Delta\delta_G = \omega_0 \Delta\omega_G \tag{10}$$

Excitation system equations

$$\frac{d}{dt}\Delta\omega_{\chi} = \frac{1}{2HX} \left[K_{G\chi}(\Delta\delta_{G} - \Delta\delta_{\chi}) - D_{\chi}\Delta\omega - \Delta\tau_{\chi} \right]$$
(11)

$$\frac{d}{dt}\Delta\delta_{\chi} = \omega_0 \Delta\omega_{\chi} \tag{12}$$

Transmission line

The transmission line is depicted in Figure 1 as a single-line diagram. The linearized form of the presentation is demonstrated in Equations (13-16).

$$X_{C}\Delta i_{dx} = \frac{1}{\omega_{0}} \frac{d}{dt} \Delta V_{dcp} - \Delta V_{qcp}$$
(13)

$$X_{C}\Delta i_{qx} = \frac{1}{\omega_{0}} \frac{d}{dt} \Delta V_{qcp} - \Delta V_{dcp}$$
(14)

$$\Delta V_{dter} = \frac{X_L}{\omega_0} \frac{d}{dt} \Delta i_{dx} + R_L \Delta i_{dx} - X_L \Delta i_{qx} + \Delta V_{dcp} + V_{dif} Cos(\delta_0) \Delta \delta \quad (15)$$

$$\Delta V_{qter} = \frac{X_L}{\omega_0} \frac{d}{dt} \Delta i_{qx} + R_L \Delta i_{qx} + X_L \Delta i_{dx} + \Delta V_{qcp} + V_{qif} Sin(\delta_0) \Delta \delta \quad (16)$$

Synchronous generator

The generator's linearized equations are derived using Park's voltage equations for synchronous machines in Kundur [2]. The entire system can be readily represented using the aforementioned mathematical formulae. The system's eigenvalue analysis can be performed using a mathematical model.

$$-x_{dx}\frac{d}{dt}\Delta i_{dx} + x_{mdx}\frac{d}{dt}\Delta i_{Fd} + x_{mdx}\frac{d}{dt}\Delta i_{DW} = \omega_0[(-x_{qx}\Delta i_{qx} + x_{mqx}\Delta i_{QW} + x_{mqx}\Delta i_{sw}) + \Psi_{q0}\Delta\omega + r_{aw}\Delta i_{dx} + v_{dx}]$$
(17)

$$-x_{qx}\frac{d}{dt}\Delta \dot{a}_{qx} + x_{mqx}\frac{d}{dt}\Delta \dot{a}_{QW} + x_{mqx}\frac{d}{dt}\Delta \dot{a}_{sw} = \omega_0 [-(-x_{dx}\Delta \dot{a}_{dx} + x_{mdx}\Delta \dot{a}_{Fd} + x_{mdx}\Delta \dot{a}_{Fd} + v_{mx}\Delta \dot{a}_{dx} + v_{qx}]$$
(18)

$$-x_{mdx}\frac{d}{dt}\Delta i_{dx} + x_{Fd}\frac{d}{dt}\Delta i_{Fd} + x_{mdx}\frac{d}{dt}\Delta i_{DW} = \omega_0[-r_{Fd}\Delta i_{Fd} + \Delta v_{Fd}] \quad (19)$$

$$-x_{mdx}\frac{d}{dt}\Delta i_{dx} + x_{mdx}\frac{d}{dt}\Delta i_{Fd} + x_{DW}\frac{d}{dt}\Delta i_{DW} = \omega_0[-r_{DW}\Delta i_{DW}]$$
(20)

$$-x_{mqx}\frac{d}{dt}\Delta i_{qx} + x_{QW}\frac{d}{dt}\Delta i_{QW} + x_{mqx}\frac{d}{dt}\Delta i_{sw} = \omega_0[-r_{QW}\Delta i_{QW}]$$
(21)

$$-x_{mqx}\frac{d}{dt}\Delta i_{qx} + x_{mqx}\frac{d}{dt}\Delta i_{QW} + x_{sw}\frac{d}{dt}\Delta i_{sw} = \omega_0[-r_{sw}\Delta i_{sw}]$$
(22)

MODELING OF STATCOM AND ITS CONTROL SCHEME: PROPOSED

STATCOM, which belongs to the family of FACT controllers of the shunt type, is highly versatile in its ability to exchange reactive and real power with the system. It does so in response to the systems compensation needs, thereby improving system stability. The STATCOM achieves this by reducing low-range frequency oscillations and maintaining the systems voltage level. The VSC connected to the transformers secondary side exchanges actual and reactive power.



Figure 3. STATCOM with VSC.

The voltage source converter (VSC) comprises a variety of power electronic switching devices, including gate turnoff thyristors (GTOs) and insulated-gate bipolar transistors (IGBTs), which are a type of forced commutated device.

Now,

Active Power,
$$P_{pq} = \frac{V_p V_q}{X_{pq}} \sin \delta$$
 (23)

Reactive Power,
$$Q_{pq} = \frac{V_p (V_p - V_q \cos \delta)}{X_{pq}}$$
 (24)

Here,

V_p - terminal voltage of power system

 V_q^r - VSC terminal voltage

 $X_{pq}^{'}$ - Reactance to be transferred between the sources δ - Phase angle between V_p and $V_q.$



Figure 4. Intelligent-based STATCOM controller.

Under normal circumstances, the voltage V_q generated by the VSC aligns with the system voltage V_p (with a phase angle of δ =0), resulting in the exchange of only lagging VAR (reactive power) and no active power ($P_{pq} = 0$). If the voltage V_p is higher than the voltage V_q , a reactive power flow is initiated from bus of V_p to V_q , as shown in Figure. 3. This occurs when the STATCOM consumes the reactive power, causing it to function as a reactor.

Conversely, when V_p is less than V_q , it indicates that reactive power is transferred from bus of V_q to V_p (STATCOM acts as a capacitor and starts injecting reactive power). The capacitor on the direct current (DC) side of the voltage source converter (VSC) functions as a rigid DC voltage source. Under typical operating conditions, the voltage V_p must lead the voltage that exists V_q to offset losses in the transformer and voltage source converter (VSC) and to maintain a charged capacitor.

The synchronously rotating d-q frame model can be used to describe the STATCOM in the following manner:

$$\frac{di_{sd}}{dt} = \frac{-R_s\omega_0}{X_s}i_{sd} - \omega_0i_{sq} + \frac{\omega_0}{X_s}(v_{1d} - v_{2d})$$
(25)

$$\frac{di_{sq}}{dt} = \omega_0 i_{sd} - \frac{R_s}{X_s} i_{sd} + \frac{\omega_0}{X_s} (v_{1q} - v_{2q})$$
(26)

$$\frac{dv_{dc}}{dt} = \frac{-P_s}{Cv_{dc}} - \frac{v_{dc}}{R_c C}$$
(27)

Here, " i_{sd} " and " i_{sq} " stand for the STATCOM's current d-q frame components. the current components of the STATCOM in the d-q frame, ω_0 is the angular velocity, R_s and X_s stand for the coupling transformer's resistance and leakage reactance, and capacitor shunt's leakage resistance is denoted as Rc.

The proposed study utilizes Voltage Source Converters (VSC) that consist of Insulated Gate Bipolar Transistor (IGBT)-based Pulse Width Modulation (PWM) inverters. These inverters operate at a chopping frequency in the kilohertz range and employ the PWM approach to generate a sinusoidal waveform using a direct current (DC) voltage source. The filters attached to the VSC's AC end neutralize voltage harmonics. By adjusting the PWM-modulator's modulation index, the VSC can extract the voltage V₂ from a constant DC voltage V_{dc}. The gate pulses needed to switch and regulate the IGBTs used in the VSC are provided by the PWM generator. The suggested control technique uses PLL (Phase-locked loop) to output d and q-axis current components I_d and I_g from transmission line AC voltage. Additionally, two PI controllers, one for AC and one for DC, help minimize AC and DC current errors. The reference currents for these controllers are the quadrature axis currents, I_q, and I_d, as well as the direct current. The current regulator is employed to govern the gate signal generated by the PWM converter by utilizing reference currents Idref and Iqref offered by the DC and AC voltage regulators, respectively. The gate signal further synthesizes the voltage V_2 's phase and magnitude (V_{2d} , V_{2q}). Soft computing optimization techniques are employed to adjust the gain parameters PI of the AC controllers by the system needs, while the PI value of the DC controllers remains constant. Figure 4. depicts the comprehensive schematic representation of the proposed controller.

PARTICLE SWARM OPTIMIZATION (PSO) ALGORITHM

Particle Swarm Optimization (PSO) involves moving a group of potential solutions, particles, within the search space to locate the most optimal solution. The position of each particle within the solution space indicates a potential solution, and its mobility is impacted by both its own personal best position and the best position discovered by the entire swarm.

The algorithm's key components involve updating the velocity and position of each particle in each iteration. The particles adapt their locations according to their previous encounters. and the global best solution discovered by any particle in the swarm. The flowchart depicting the PSO algorithm is depicted in Figure 5, while its Parameters are outlined in Table 2. Which are determined through a review of relevant literature [29] and experimentation to



Figure 5. Flowchart of PSO.



Table 2.	Parameters	of PSO
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Figure 6. Flowchart of fireflies.

Parameters	No of variables	Number of Fireflies	Light Absorption Coefficient	No of iteration	Alpha (Randomization parameter)	Beta (Initial Attractiveness)	Gamma (Absorption coefficient)
Values	2 (K _p , K _i)	20	1	100	0.4	1	2

ensure optimal performance. This cooperative exploration of the solution space allows PSOs to navigate toward promising regions efficiently.

The simplicity and efficiency of PSO make it well-suited for a broad spectrum of optimization issues. Its intuitive nature and ease of implementation have contributed to its popularity in various fields, including engineering [30,31], finance, and artificial intelligence. Despite its simplicity, PSO has proven to be a powerful tool for finding optimal solutions in complex, multi-dimensional search spaces.

FIREFLIES ALGORITHM

Fireflies, scientifically known as Lampyridae, are nocturnal beetles renowned for their bioluminescent glow. They use this light primarily for communication and mating, with males emitting rhythmic flashes to attract females, each species having its unique pattern. Additionally, the glow serves as a defense mechanism, warning predators of their unpalatability. Beyond their natural behaviors, fireflies inspire scientific and technological advancements.

Overall, fireflies are captivating creatures that contribute to the natural beauty of their habitats and scientific advancements, making them a subject of interest and admiration in biological and technological contexts [30], [31]. The flow chart of FF is depicted in Figure 6, while its parameters are outlined in Table 3 [29].

GREY WOLF OPTIMIZER (GWO)

The Grey Wolf Optimizer (GWO) is an optimization algorithm that draws inspiration from the social structure and hunting behavior of grey wolves in nature. Introduced in 2014 by Mirjalili et al., GWO has gained popularity as a robust optimization algorithm in various fields.

Inspired by the cooperative nature of wolf packs, GWO divides the optimization process into three key phases: encircling, attacking, and updating. In the encircling phase, the positions of alpha (m), beta(n), and delta (o) wolves represent potential solutions. These wolves emulate the leadership hierarchy within a wolf pack. The algorithm then employs equations derived from the hunting behavior of wolves to update the positions of the m, n, and o wolves during the attacking phase[32].

Algorithm Steps:

Step 1: Initialization: Generate a population of grey wolves, each representing a potential solution to the optimization problem. Assign each wolf a position in the search space.

Step 2: Objective Function: Determine the fitness of each wolf by applying the objective function to its position in the search space.

Step 3: Update Alpha, Beta, and Delta Wolves: Identify the alpha, beta, and delta wolves based on their fitness. These wolves represent the best, second-best, and thirdbest fitness, respectively.

Step 4: Update Positions: Use mathematical transformations to update the positions of the alpha, beta, and delta wolves. Encourage exploration by adjusting the positions based on random values and the difference between wolves.

Step 5: Update Other Wolves: Update the positions of the remaining wolves based on the positions of the alpha, beta, and delta wolves. This step encourages the entire population to converge towards better solutions.

Step 6: Boundary Checking: Ensure that the updated positions of wolves are within the specified search space. If a wolf goes beyond the boundaries, bring it back.

Step 7: Repeat: Reiterate steps 2-6 for a specified quantity of repetitions or until a convergence requirement is achieved.

The algorithm maintains a balance between exploration and exploitation. The alpha, beta, and delta wolves guide the search, exploring new regions, while the rest of the pack follows to exploit promising areas. The mathematical transformations introduce randomness and diversity, preventing premature convergence and encouraging global exploration. The GWO algorithm is versatile and can be applied to various optimization problems by customizing the objective function. The Pseudo code is described in Figure 7.

```
Initialize the grey wolf population X<sub>a</sub>(a=1,2,3,...n)
Initialize a, A, and C
Calculate the fitness of each search agent
X<sub>m</sub>-the best search agent
X<sub>n</sub>=the second best search agent
X<sub>o</sub>=the third best search agent
While (t<Max number of iterations)
    for each search agent
       Update the position of current search agent by equation (40)
    end
    Update a, A, and C
    Calculate the fitness of all search agents
    Update X<sub>m</sub> , X<sub>n</sub> and X<sub>o</sub>
    t=t+1
end while
return X<sub>m</sub>
```

Figure 7. Pseudo code of GWO algorithm.

Parameters	No of variables	No of iteration	Number of search Agents	Position vector	Control Vector (a)
Values	2 (Kp, Ki)	100	20	Rand	Lies between 2 and 0

Table 4. Parameters of GWO

Mathematical Model

An outline of the Grey Wolf Optimizer (GWO) algorithm follows the presentation of the mathematical models for tracking, surrounding, attacking, and social hierarchy in this section.

Social Hierarchy

In the mathematical model of the social structure of wolves in the GWO, the strongest and most resilient solution is represented as alpha (m). Conversely, the solutions ranked second and third are denoted as beta (n) and delta (o) correspondingly. Other candidate solutions are denoted as omega (x). The optimization process is guided by m, n, and o, with the remaining wolves following their lead.

Encircling Prey

Grey wolves exhibit encircling behavior during hunting. The mathematical representation of this behavior is described by the following equations:

$$\vec{D} = \left| \vec{C}.\vec{X}_{\mathcal{Q}}(k) - \vec{X}(k) \right| \tag{30}$$

$$\vec{X}(k+1) = \vec{X}_{Q}(k) - \vec{A}.\vec{D}$$
 (31)

In this context, the variable k represents the current iteration, whereas \vec{A} and \vec{C} are coefficient vectors. \vec{X}_Q refers to the position vectors of the prey, while \vec{X} represents the position vector of a grey wolf. The vectors \vec{A} and \vec{C} are calculated using specific formulas involving random vectors.

$$\vec{A} = 2\vec{a}.\vec{r_1} - \vec{a} \tag{32}$$

$$\vec{C} = 2.\vec{r}_2 \tag{33}$$

Hunting

Grey wolves, guided by alpha, exhibit hunting behavior. To simulate this behavior mathematically, the positions of the m (alpha), n (beta), and o (delta) wolves are considered more informed about the potential prey location. The positions of other wolves, including the omegas, are then updated based on these informed positions:

$$\vec{D}_m = \left| \vec{C}_a \cdot \vec{X}_m - \vec{X} \right| \tag{34}$$

$$\vec{D}_n = \left| \vec{C}_b \cdot \vec{X}_n - \vec{X} \right| \tag{35}$$

$$\vec{D}_o = \left| \vec{C}_c \cdot \vec{X}_o - \vec{X} \right| \tag{36}$$

$$X_a = \vec{X}_m - \vec{A}_a.(\vec{D}_m) \tag{37}$$

$$\vec{X}_b = \vec{X}_n - \vec{A}_b.(\vec{D}_n) \tag{38}$$

$$\vec{X}_c = \vec{X}_o - \vec{A}_c \cdot (\vec{D}_o) \tag{39}$$

$$\vec{X}(k+1) = \frac{\vec{X}_m + \vec{X}_n + \vec{X}_o}{3}$$
(40)

This approach ensures that the search agents, except for the top three, update their positions according to the more knowledgeable alpha, beta, and delta wolves. These mathematical formulations and algorithms capture the essence of the GWO, where social hierarchy, encircling prey, and hunting behaviors are translated into mathematical models for optimization purposes.

The proposed study includes a flow chart of the Grey Wolf Optimizer (GWO), which is depicted in Figure 8. and its parameters are described in Table 4. The AC PI controllers, gain parameters are modified by applying soft computing optimization approaches to diminish deviations in rotor dynamics, specifically generator speed deviation, LP turbine speed deviation, HP turbine speed deviation, torque deviation in LP-HP turbine, and torque deviation in the generator. The performance indices, i.e., ITAE criteria is considered for the above optimization technique used:

$$ITAE = \int_{0}^{t} t \left(\left| \Delta \omega_{GEN} \right| + \left| \Delta \omega_{LPT} \right| + \left| \Delta \omega_{HPT} \right| + \left| \Delta \tau_{GEN} \right| + \left| \Delta \tau_{LPT-HPT} \right| \right) dt$$
(41)

To get the best values for the AC PI controllers' gain settings, we first use the hit-trial method to initialize them. Depending on the precise location (Particles, Fireflies, wolf), the PI controllers' gain values are determined in optimization. The area is dependent on the chosen technique. When you update that position, the AC PI controllers' corresponding gain values are updated, but the DC PI controllers' gain values remain unchanged.



Figure 8. Flowchart of GWO in the proposed study.

RESULTS AND DISCUSSION

In this study, the VSC-based STATCOM is employed to mitigate sub-synchronous oscillations within the IEEE SBM test system. These oscillations pose a significant risk of system disturbances, particularly if they lead to cascading line outages due to oscillatory swings among interconnected components. Utilizing MATLAB software, we simulate the test system to analyze rotor dynamics, focusing on deviations in generator speed, LP and HP turbine speeds, as well as torque fluctuations in the generator and LP-HP turbine. The results obtained from analyzing the rotor dynamics of all the machines under different test scenarios, such as without STATCOM, with STATCOM, and with the proposed intelligently tuned STATCOM controller, clearly demonstrate the effectiveness of the optimization-based control scheme in alleviating sub-synchronous oscillations in the power system when integrated with the STATCOM.

A MATLAB GUI (guided user interface) has been created to enhance the visualization of simulation

outcomes and key system parameters. This encompasses specific information like as the generators MVA (Mega Volt Ampere) and kV (kilo Volt) rating, timing of faults, reference voltage, and the introduction of disturbances, particularly system damping. If the system's natural dampings are not taken into account, the GUI will receive a zero input. This means that if the natural dampings are zero, the input will be one when the natural damping is considered.

Case A: System Results with Zero Damping

The test system comprises an alternator with a rating of 600 MVA and 22 kV. The system experiences a 3-phase LLL-G fault, with natural damping zero. The rotor dynamics, i.e., fluctuations in generator LP Turbine, HP turbine, is shown in the Figure 9, 10, and 11, respectively, while the amplification of torque in LP-HP turbine and generator is in the Figure 12 and 13.

The system under investigation's characteristics is assessed for a duration of 5 seconds based on its transient response. In Table 5, outlining settling times (in seconds) for quantities without natural damping, a comparative analysis of PSO, FF, and GWO controllers against the reference STATCOM is presented. For Generator Speed deviation, all three controllers exhibit improvements over STATCOM (3.9942 seconds), with PSO-STATCOM, FF-STATCOM, and GWO-STATCOM achieving reductions of approximately 17.3%, 17.0%, and 17.7%, respectively. Similarly, for LP Turbine Speed deviation, the controllers showcase notable percentage reductions compared to STATCOM alone (3.8901 seconds), with PSO-STATCOM, FF-STATCOM, and GWO-STATCOM achieving decreases of approximately 13.7%, 13.6%, and 13.4%, respectively. Analyzing HP Turbine Speed deviation, all controllers outperform STATCOM (3.9731 seconds) with percentage reductions of approximately 17.7%, 25.0%, and 18.1% for PSO-STATCOM, FF-STATCOM, and GWO-STATCOM, respectively. Examining Torque deviation in LP-HP Turbine, all three controllers significantly reduce settling times compared to STATCOM (4.1092 seconds) with improvements of approximately 32.1%, 32.0%, and 32.9% for PSO-STATCOM, FF-STATCOM, and GWO-STATCOM, respectively. For Torque deviation in the Generator, the controllers demonstrate substantial percentage improvements over STATCOM alone (4.1087 seconds), with reductions of approximately 32.0%, 32.8%, and 33.8% for PSO-STATCOM, FF-STATCOM, and GWO-STATCOM, respectively.

In summary, PSO, FF, and GWO controllers consistently outperform STATCOM across various quantities, showcasing their effectiveness in reducing settling times and enhancing system dynamics. GWO-STATCOM generally exhibits slightly superior performance regarding percentage reduction in settling time.



Figure 9. Fluctuation in the generator of case A.



Figure 10. Fluctuation in LP Turbine of case A.



Figure 11. Fluctuation in HP Turbine of case A.



Figure 12. Amplification of Torque in LP-HP Turbine of Case A.



Figure 13. Amplification of Torque in Generator of Case A.

Table 5. T	'ime domain	specifications	(Settling time i	in sec.) of the	Ouantities	without natural	damping
		· · · · · · · · · · · · · · · · · · ·	(<		

Quantity	Without STATCOM	With STATCOM	With PSO- STATCOM controller	With FF- STATCOM controller	With GWO- STATCOM controller
Generator Speed deviation	Unspecified	3.9942	3.3017	3.3149	3.2928
LP Turbine speed deviation	Unspecified	3.8901	3.3549	3.3571	3.3390
HP Turbine speed deviation	Unspecified	3.9731	3.2701	2.9852	3.2504
Torque deviation in LP-HP Turbine	Unspecified	4.1092	2.7971	2.7941	2.7575
Torque deviation in generator	Unspecified	4.1087	2.7960	2.7572	2.7183

Case B: System Results with Natural Damping

The system's response is illustrated after applying a three-phase LLL-G fault, taking into account inherent dampening effects. Figures 14, 15, and 16 illustrate the fluctuations observed in the generator, LP turbine, and HP turbine, respectively. Additionally, Figures 17 and 18 demonstrate the amplification of torque in the LP-HP turbine and generator, respectively.

In Table 6, presenting settling times (in seconds) for quantities with natural damping, we compare the performance of PSO, FF, and GWO controllers against the baseline STATCOM. For the Generator Speed deviation, all three controllers show significant improvements compared to STATCOM alone (3.1855 seconds). PSO-STATCOM achieves a reduction of approximately 19.3%, FF-STATCOM demonstrates a decrease of about 20.0%, and GWO-STATCOM provides a notable improvement of around 20.0%. Similarly, the controllers exhibit commendable reductions for LP Turbine Speed deviation compared to the baseline (2.9350 seconds with STATCOM). PSO-STATCOM, FF-STATCOM, and GWO-STATCOM achieved percentage improvements of approximately 11.3%, 11.5%, and 12.1%, respectively. For HP Turbine Speed deviation, all controllers outperform STATCOM alone (3.2061 seconds), with PSO-STATCOM, FF-STATCOM, FF-STATCOM, and GWO-STATCOM showing percentage reductions of approximately 20.4%, 21.4%, and 21.6%, respectively. Analysing Torque deviation in LP-HP Turbine, all three controllers significantly



Figure 14. Fluctuation in the generator of case B.

Tab	le 6. Tim	ie domain s	specifications (Settli	ng time in sec.) of t	he C	Juantities wit	h natural	damı	oing	(D12	=0.3104	, D23=	=0.05
					()	/								/	

Quantity	Without STATCOM [23]	With STATCOM [33]	With PSO- STATCOM controller	With FF- STATCOM controller	With GWO- STATCOM controller
Generator Speed deviation	Unspecified	3.1855	2.5790	2.5491	2.5488
LP Turbine speed deviation	Unspecified	2.9350	2.6018	2.5902	2.5828
HP Turbine speed deviation	Unspecified	3.2061	2.5572	2.5237	2.5231
Torque deviation in LP-HP Turbine	Unspecified	3.2377	2.3724	2.3363	2.3352
Torque deviation in generator	Unspecified	3.2801	2.3721	2.3349	2.3339

improve settling times compared to STATCOM (3.2377 seconds). PSO-STATCOM, FF-STATCOM, and GWO-STATCOM demonstrate percentage reductions of approximately 26.7%, 27.0%, and 27.3%, respectively. Finally, for Torque deviation in the Generator, the controllers exhibit notable reductions compared to STATCOM alone (3.2801 seconds). PSO-STATCOM, FF-STATCOM, and GWO-STATCOM achieved percentage improvements of approximately 27.7%, 27.8%, and 27.9%, respectively.

In summary, PSO, FF, and GWO controllers consistently outperform STATCOM across various quantities, showcasing their effectiveness in reducing settling times and enhancing system dynamics. GWO-STATCOM generally exhibits slightly superior performance regarding percentage reduction in settling time.

Table 7 presents a comparative analysis of STATCOM performance and is refined through various tuning methodologies – PSO, FF, and GWO while excluding natural damping effects. The Integral of Time Absolute Error (ITAE) improvement is assessed in percentage terms concerning the original STATCOM parameters (Kp = 5, Ki = 1000). PSO tuning resulted in a 30.5% enhancement, adjusting Kp to 9.2516 and Ki to -1244.8446. The FF-tuned configuration exhibited a 32.0% improvement, with Kp and Ki values adjusted to 12.2376 and 2.3144, respectively. GWO tuning yielded a 33.5% enhancement, setting Kp and Ki to 7.3691 and -1932.6593. These results highlight



Figure 15. Fluctuation in LP Turbine of case B.



Figure 16. Fluctuation in HP Turbine of case B.



Figure 17. Amplification of Torque in LP-HP Turbine of Case B.



Figure 18 Amplification of Torque in Generator of Case B.

Quantity	K _p	K _i	ITAE	
ONLY STATCOM	5	1000	0.4542	
PSO tuned STATCOM	9.2516	-1244.8446	0.3153	
FF tuned STATCOM	12.2376014396766	2.31441600588101	0.3087	
GWO tuned STATCOM	7.3691	-1932.6593	0.3023	

 Table 7. Comparative Parameters assessment of STATCOM refined through FF, GWO, and PSO tuning methodologies without natural damping

 Table 8. Comparative Parameters assessment of STATCOM, refined through FF, GWO, and PSO tuning methodologies with natural damping

Quantity	K _p	K _i	ITAE	
ONLY STATCOM	5	1000	0.3070	
PSO tuned STATCOM	2.2865	147.6050	0.2118	
FF tuned STATCOM	20	1201.53262819189	0.2205	
GWO tuned STATCOM	-11.9964	299.9140	0.2101	

the efficacy of the tuning methodologies in optimizing the STATCOM parameters, showcasing substantial percentage improvements in ITAE, a key indicator of control system performance. These findings underscore the significance of advanced optimization techniques in enhancing the dynamic response of STATCOM systems without natural damping.

Table 8 presents a comparative evaluation of STATCOM performance, considering natural damping effects and refining parameters through FF, GWO, and PSO tuning methodologies. The initial STATCOM configuration with Kp at 5 and Ki at 1000 yielded an ITAE of 0.3070. Following PSO tuning, the system demonstrated a significant 31.0% improvement, with Kp and Ki adjusted to 2.2865 and 147.6050, respectively, resulting in an ITAE of 0.2118. Conversely, the FF-tuned STATCOM exhibited a 28.2% improvement, with Kp set to 20 and Ki to 1201.5326, yielding an ITAE of 0.2205. GWO tuning led to a notable 31.6% enhancement, adjusting Kp to -11.9964 and Ki to 299.9140, resulting in an ITAE of 0.2101. These findings underscore the efficacy of the tuning methodologies in achieving substantial percentage improvements in ITAE, emphasizing their relevance in optimizing the dynamic response of STATCOM systems in the presence of natural damping.

CONCLUSION

In this paper, an investigation is conducted to examine the optimization tuned control system for mitigating sub-synchronous resonance and low-frequency oscillation in a series compensated transmission line completely. The investigation focuses on implementing this control scheme with the VSC-based Static Synchronous Compensator, utilizes the IEEE's second benchmark model, incorporating a STATCOM at the central bus as the test platform. Intelligent control strategies applied to STATCOM have proven crucial in enhancing power system stability within torsional oscillation environments. By employing Particle Swarm Optimization (PSO), Firefly Algorithm (FF), and Grey Wolf Optimization (GWO) to search for optimal controller parameters, significant advancements are achieved. Particularly, the proposed STATCOM, formulated as an optimization problem and tuned with GWO, exhibits notable advantages over FF, PSO, and standard STATCOM in various rotor dynamics scenarios, including deviations in generator speed low-pressure (LP) and high-pressure (HP) turbine speeds, as well as torque amplification of the generator and LP-HP turbine. The systematic optimization of STATCOM parameters effectively mitigates oscillations, demonstrating its potential to enhance grid resilience. Even under challenging conditions such as zero natural damping and additional perturbations like three-phase LLL-G fault, the proposed GWO Optimization-based STATCOM proves its efficacy through meticulous analysis. This underscores the crucial role of STATCOM control strategies in addressing torsional oscillations, thereby contributing significantly to the dynamic stability of the power system. As the energy landscape continues to evolve, embracing such intelligent technologies becomes imperative for ensuring sustainable and stable power systems.

FUTURE SCOPE

1. Real-Time Implementation: Investigate the feasibility of implementing the proposed controller in realtime power systems, considering practical constraints and ensuring seamless integration with existing infrastructure.

- 2. Adaptive Control Strategies: Investigate adaptive control systems that can dynamically modify the controller parameters in response to varying system dynamics, providing versatility and adaptability in practical scenarios.
- 3. Hybrid Approaches: Explore the possibility of merging the capabilities of various optimization techniques or control systems to develop a hybrid solution that utilizes their complementary benefits to enhance performance.
- 4. Cybersecurity Considerations: Address cybersecurity aspects associated with implementing intelligent control strategies, ensuring the system's resilience against potential cyber threats and attacks.
- 5. Integration with Renewable Resources: Explore the adaptability of the proposed controller in power systems with a higher penetration of renewable energy sources, considering the unique challenges posed by variable and intermittent generation.
- 6. Multi-Area Power Systems: Extend the investigation to multi-area power systems to assess the scalability and performance of the proposed controller in more complex grid configurations.
- 7. Economic Analysis: Perform an economic analysis to examine the cost-effectiveness of implementing the suggested controller in comparison to other options, taking into account the costs associated with installation, maintenance, and operation.

NOMENCLATURE

"H	constant of inertia in MW.s/MVA
Κ	stiffness in pu torque/electrical rad
D	coefficient of damping in pu torque/pu speed
	deviation
ω_0	rated speed in electrical rad/s
Δω	speed deviation of mass in pu
ω	speed of a mass in pu
τ	mechanical torques developed by the turbine
	sections
Δ	small variation from the initial point if prefixed
δ	load angle in rad/s
$\Delta\delta$	twist angle of mass
T _{RP}	speed relay position time constant in the
	governor
T _{GVR}	governor opening time constant
T _{CHBR}	chamber time constant in front of HP turbine
T _{HL}	HP and LP turbine connection time constant
k _{GVR}	governor system gain constant
F_{T}	torques in fractions
O _{GVR}	opening of the governor
ORP	speed relay position
Х	excitation if subscripted
G	generator, if subscripted
GX	excitation and generator, if subscripted
LPT	low-pressure turbine, if subscripted
LG	low-pressure turbine and generator, if subscripted
HPT	high-pressure turbine, if subscripted

LH	high pressure and low pressure if subscripted
qx	q-axis if subscripted
dx	d-axis if subscripted
aw	armature winding if subscripted
mdx	mutual and d-axis if subscripted
mqx	mutual and q-axis if subscripted
Fd	field winding, if subscripted
DW	damper winding on the d-axis if subscripted
SW	damper winding on the q-axis if subscripted
QW	damper winding on the q-axis if subscripted
dter	terminal and d-axis if subscripted
qter	terminal and q-axis if subscripted
dinf	infinite bus and d-axis if subscripted
qif	infinite bus and q-axis if subscripted
dcp	capacitive and d-axis if subscripted
qcp	capacitive and q-axis if subscripted
i	current in pu
Х	reactance in pu
V	voltage in pu
R,r	resistance in pu
Ψ	flux linkage in pu"

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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APPENDIX A.				
Generator data:				
Ratings: 600MVA, 22KV.				
Stability data:				
X ₁ =0.14 pu	R _a =0.0045 pu			
X _d =1.65 pu	X _q =1.59 pu			
X' _d =0.25 pu	X' _q =0.46 pu			
X" _d =0.20 pu	X" _d =0.20 pu			
T' _{do} =4.5 s	T' _{qo} =0.67			
T" _{do} =0.040 s	T" _{qo} =0.09 s			
Transmission line data: 500KV				
Line with series capacitor:				
$R_1 = 0.0074$ pu, $R_0 = 0.022$ pu, $X_1 = 0.08$ pu, $X_0 = 0.240$ pu				
Line without series capacitor:				
R ₁ =0.0067 pu, R _o =0.0186 pu, X ₁ =0.0739pu, X _o =0.210 pu				
Transformer data;				
600MVA, 60Hz, Δ/Y, 22KV/500KV, R _p =0.0006 pu,R _s =0.0006 pu, X _p =0 pu, X	ζ _s =0.12 pu			
STATCOM parameters: 100 MVA				
System nominal voltage = 500kV, f= 60Hz,				
$R_1 = 0.00732, L_1 = 0.22H, C=325\mu F$				
PI Voltage Regulator gains: $K_p = 5$, $K_i = 1000$				



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Research Article

Isolation of kerosene-degrading bacteria from soil samples and determination of optimal growth conditions

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ABSTRACT

Bacteria capable of decomposing hydrocarbon rocket power kerosene T-1 were isolated and studied. In the course of the studies, 30 isolates of microbial cultures were isolated from soils contaminated with hydrocarbon rocket fuel, of which 9 isolates were selected that actively assimilate kerosene T-1 as the only headwater of carbon. The strains that showed the best results in these screening analyses on four nutrient media with a concentration of T-1 kerosene 1% (10 g/kg) grow well 9 isolates of culture microorganisms: Nº 4, 8, 14, 23, 5, 18, 20, 25 and yeast Nº 12/5. Isolates on a medium with a concentration of T-1 kerosene 2% (20 g/kg) and 5% (50 g/kg) showed good growth in bacterial cultures Nº 5, 18, 20, 25, and yeast Nº 12/5. The selected microorganisms were identified by physiological and biochemical characteristics: Nº 5 – Arthrobacter sp., Nº18 – Acinetobacter calcoaceticum, Nº20 – Bacillus sp., Nº25- Microocccus roseus, Nº 12/5- Candida sp. Cultivation conditions for isolated microorganisms were created. It has been established that the optimal development temperature for the culture of Arthrobacter sp. 5 is 25-30°C, Acinetobacter calcoaceticum. 18 is 30-35 °C, Microocccus roseus. 25 is 25-37 °C. The opti-

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mal duration of cultivation of Candida sp. 12/5 is 1 day, for the rest of the studied cultures - 2 days.

INTRODUCTION

Launches of launch vehicles (LV), using T-1 kerosene as rocket fuel, are accompanied by soil contamination in the areas where the separable parts (PF SP) of launch vehicles fall with fuel residues. With the increasing availability of commercial space flights, the environmental impact of space launches is becoming significant. The factors negatively affecting the environmental situation during the operation of rocket and space technology, first of all, include emissions of gases, ozone-depleting substances, pollution by fragments of the separating parts of launch vehicles (SP LV), and residues of components of rocket fuels of the Earth's surface, pollution of natural land ecosystems (soil, water, air, and plants) toxic components of rocket fuel and products of its decomposition [1].

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Hydrocarbon combustibles are stable and persist in soils for a long time. The content in the soil of high concentrations of various chemical compounds - toxicants adversely affects the vital activity of soil organisms, while the ability of the soil to self-purify itself from pathogens and other undesirable microorganisms is lost, which is fraught with serious consequences for humans, flora and fauna. Because soil microorganisms are sensitive to soil pollution, changes in their quantitative and qualitative composition can serve as an indicator of the state of soils. A large amount of pollutants during the first years will be contained in the surface soil layer (0.0 - 20.0 cm). Chemical compounds entering the soil accumulate and lead to a gradual change in the chemical and physical belongings of the soil, reducing the number of living organisms, and worsening their fertility [2,3].

In this regard, the restoration of soils in places of straits of hydrocarbon rocket fuel T-1 kerosene is very relevant. At present, the re-cultivation of soils contaminated with oil products is carried out with the help of soil microorganisms. The biological remedy of oil-contaminated ecosystems has been described by many researchers [4-7]. The microbiological method of reclamation based on the use of highly effective strains of hydrocarbon-oxidizing microorganisms is widely used in the world practice of reclamation activities. It is apparent that the chemical arrangement of pollution, the time elapsed since the moment of pollution, as well as soil and climatic situations, have a great mark on the vital activity of these microorganisms introduced in the soil. Effective destruction of various hydrocarbons by microorganisms introduced into the soil with the preparation is possible only in those cases when they find favorable conditions for life and development in the soil (food sources, the necessary thermal and water regimes, etc.), i.e. a microorganism or a group of microorganisms needs to create a favorable ecological niche in which they will develop. This indicates the expediency of isolating microorganisms adapted to the natural and climatic conditions of pollution and successfully utilizing hydrocarbons, which, in turn, will ensure the most effective soil purification by the biological method [8-10]. Currently, to clean the environment from oil pollution, biological preparations based on actively decomposing oil microorganisms are used: D. acidovorans Cd11 and A. johnsonii Sb01, Acinetobacter sp. T4 and P. putida PB4, Bacillus, Pseudomonas, Vibrio, Micrococcus Williamsia, and Alcaligenes, Bacillus, Citricoccus, Rhodococcus, Arthrobacter, Ochrobactrum, Pseudomonas u Sphingomonas [11-13].

Thus, for the production of oil-oxidizing biological products, either one strain or a mixture of strains of hydrocarbon-oxidizing bacteria, mainly aerobes, is used. These preparations effectively oxidize oil products, and aromatic hydrocarbons mainly in the temperature range of 15°C - 45°C with significant initial concentrations of contaminants in the soil and require mineral supplementation (nitrogen, phosphorus), moistening, and loosening. Known biological products are obtained in the shape of suspensions, emulsions, pastes, and powders. However, each form has its advantages and disadvantages. Dry preparations have an undeniable advantage: they are more convenient for transportation to the places of their application and have a longer shelf life. At the same time, the number of living microorganisms in them is usually low, since plants for the production of dry forms, primarily non-medicinal drugs, practice spray drying, which is less energy intensive and cheap compared to lyophilization, but there are large losses of viable cells. Considering the low number of microorganisms surviving after spray drying, the authors of the developed dry forms of biological products recommend activation of the microorganisms that make up their composition before use [14,15].

Compounds derived from hydrocarbons are essential in industry and our daily lives, but spills or leaks that occur regularly cause serious environmental impacts. In this review, we sought to isolate and study strains of T-1 kerosene capable of degrading hydrocarbon rocket fuel on different types of soils. For experimental work, soil samples were selected from the position area of the Baikonur Cosmodrome (sites 31 and 196) and the Ulytau region, zone U-25. The creation of highly effective biological preparations for the purification of environmental objects from oil and oil products is possible only based on active hydrocarbon-oxidizing microorganisms and associations adapted to the conditions of pollution and the development of an original technology for their production, taking into account the physiological characteristics of strains. One of the important points for the development of any form of preparation is the selection of optimal conditions for deep cultivation of hydrocarbon-oxidizing microorganisms in a liquid nutrient medium.

The purpose of the research was to separate and study bacteria capable of decomposing hydrocarbon rocket fuel kerosene T-1, as well as to select the conditions for cultivating the isolated microorganisms.

MATERIALS AND METHODS

Soil Image

For experimental work, soil samples (layer 0-20 cm) were taken from the position area of the Baikonur Cosmodrome; sandy desert soils from site 31, gray-brown desert soils from site 196, and brown semi-desert soils, brown saline heavy loamy soils from the Ulytau region, zone U-25 (Table 1).

Kerosene T-1

Fuel "Kerosin T-1" in appearance is a colorless or slightly yellowish liquid with the smell of petroleum products, obtained by direct distillation of low-sulfur crude oil. The average elemental and group composition of the fuel

Type of soils	Soil samples	Locations	GPS coordinates
Sandy desert soils	Site 31	Positional area of the Baikonur	45°59.55' N
		Cosmodrome	63°34.15 E
Gray-brown desert soils	Site 196	Positional area of the Baikonur	46°04.23' N
		Cosmodrome	62°55.11 E
Brown semi-desert soils, brown	Zone U-25	Positional area of the Baikonur	47°27.00' N
saline heavy loamy soils		Cosmodrome	67°42.00 E

Table 1. Location of soil samples

Table 2. Elementary and group composition of fuel Kerosene T-1

Chemical elements Hydrocarbon groups								
С	Н	0	S	N	Alkanes	Cyclans	Arena	Alkenes
86.3%	13.6%	0.04%	0.06%	0.02%	30.0-50.0%	40.0-60.0%	15.0-20.0%	1.0-1.5%

is given i Table 2 [14]. When released into water, T-1 gives a sharp specific odor, which is felt at a concentration of 0.1 mg/dm³. Hydrocarbon fuels are very stable in soil and water. Biochemically, they are practically not destroyed. The T-1 odor perception threshold in water at 20°C is 0.03 mg/ dm³. They adversely affect the sanitary regime, enhance the process of BOD (biochemical oxygen demand), and inhibit nitrification at a concentration of 20.0 mg/dm³ or more. Fuel "T-1" is nearly insoluble in water. Refers to low-hazard substances (4th class of toxicity), the features of its use are as follows.

Method for Isolating Bacterial Cultures

To isolate bacterial cultures, soil samples were sown on the following nutrient media:

- Meat peptone agar (MPA) of the following composition (g/l): peptone - 5.0; sodium chloride - 5.0; meat extract - 1.5; yeast extract - 1.5; agar - 20.0.
- Starch-ammonia agar (SAA), (g/l): dibasic potassium phosphate - 1.0; ammonium sulfate - 1.0; magnesium sulfate - 1.0; sodium chloride - 1.0; calcium carbonate, 1.0; insoluble starch - 10.0; agar-agar - 20.0.
- For the isolation of myxomycetes, Chapek's nutrient medium (g/l) was used: sucrose, 30.0; sodium nitrite -2.0; dibasic potassium phosphate, 1.0; magnesium sulfate - 0.5; potassium chloride, 0.5; iron sulfate - 0.01; agar-20.0.
- To select microorganisms capable of assimilating kerosene T-1, they were grown on a dense nutrient medium Voroshilova-Dianova (VD) of the following composition (in g/l): NH₄NO₃ 1.0; K₂HPO₄ 1.0; KH₂PO₄ 1.0; MgSO₄ 0.2; CaCl₂ 0.02; FeCl₃ 2.0 drops of a concentrated solution; NaCl, 10.0; twin 80 10.0; agar, 20.0; distilled water up to 1.0 1 [15]. The cultivation of microorganisms was carried out in a thermostat at

a temperature of 28°C - 30°C for 3 days (bacteria) - 7 days (micromycetes). Screening of the grown colonies was carried out on nutrient agar shoals.

The only source of carbon was kerosene T-1 (S-0.817), which was added to the molten agar nutrient medium in amounts of 1.0%, 2.0%, and 5.0%, i.e., at concentrations of 10.0, 20.0 and 50.0 g/kg. The experiments were repeated three times. Physiological and biochemical signs were determined according to standard methods [16,17]. The identification of selected strains of microorganisms was carried out using Bergi's determinant [18,19] as well as using commercial test systems with chromogenic substrates NEFERMtest 24, CANDIDAtest 21, STAPHYtest 16 (Micro-la-test, Erba Lachema). For this purpose, suspensions of appropriate density were prepared from isolated colonies of pure culture and poured into 0.1 ml wells of strips with chromogenic substrates. To study reactions under anaerobic conditions, 2 drops of sterile paraffin oil were added to the wells. The strips were incubated for 18-24 hours at the appropriate temperature conditions: 37°C for bacteria and 22°C for fungi. After the incubation time, the strips were placed in a device - a Multiskan Ascent analyzer (Thermo Labsystems, Finland). Measurements were carried out by selecting the Microbe-Automat program to determine whether the isolate belonged to a particular genus or species.

Methods for Researching the Development of Conditions for the Cultivation of Isolated Microorganisms

Studies have been carried out to develop the conditions for cultivating isolated microorganisms (selection of a nutrient medium, temperature regime, and duration of cultivating microorganisms of the optimal aeration regime). The objects of research were cultured *Micrococcus roseus*.

25, Bacillus sp.20, Arthrobacter sp.5., Acinetobacter calcoaceticum. 18, Candida sp. 12/5.

Cultures were grown on Petri dishes with dense MPA nutrient medium. The inoculation of the liquid nutrient medium was carried out with the mentioned initial cultures of microorganisms - by flushing from the Petri dishes of MPA ($n \times 108$ CFU/ml) in an amount of 1.0%. Cultivation was carried out for 24h and 48h on a shaker at a temperature of 30°C. The determination of viable bacterial cells was carried out by seeding from the appropriate dilution of the culture into Petri dishes with a dense nutrient medium MPA. The hydrocarbon-oxidizing activity of bacteria was determined by the gravimetric method by their assimilation of kerosene T-1 (2% concentration) in a liquid nutrient medium during cultivation on a shaker for 10 days. The experiments were repeated three times.

Conditions for the Cultivation of Isolated Microorganisms

For the cultivation of hydrocarbon-oxidizing microorganisms, the following variants of nutrient media (g/l) were tested:

- 1. Meat peptone broth (MPB): peptone 5.0; sodium chloride 5.0; meat extract 1.5; yeast extract 1.5, pH 7.0-7.2.
- Corn extract 10.0; yeast ferment lysate 3.0; glucose -10.0; NaCl, 10.0; water - up to 1.0 l, pH 7.2-7.5.
- KH₂PO₄ 2.0; Na₂HPO₄ 4.0; MgSO₄ 0.5; (NH₄)2SO₄ 2.0; CaC₁₂ 0.01; FeC₁₃ 0.05; wheat flour 5.0; sucrose -10.0; water up to 1.0 l, pH 6.8-7.2.
- 4. Voroshilova Dianov (VD) modified medium: NH₄NO₃ 1.0; K₂HPO₄ 1.0; KH₂PO₄ 1.0; MgSO₄ 0.2; CaCl₂ 0.02, FeCl₃ 2.0 drops of concentrated solution, NaCl -10.0; glucose 10.0; nutrient broth 10.0; distilled water up to 1.0l. Cultivation was carried out on a shaker for 2 days. Then the number of viable cells was determined.

RESULTS AND DISCUSSION

Research on the Isolation of Native Strains (Microorganisms) Capable of Destroying Hydrocarbon Rocket Fuel - Kerosene T-1 in the Soil

The isolation of microorganisms was carried out from the soil samples described above after their inoculation on Meat Peptone Agar (MPA), Starch Ammonia Agar (SAA), Chapek's nutrient medium, and Voroshilova-Dianova's (VD) medium.

As a result of the studies, 30 isolates of microbial cultures were isolated from soils contaminated with T-1 hydrocarbon rocket fuel. After inoculation of the isolates on a dense nutrient medium VD, containing kerosene T-1 as the only source of carbon, microorganisms were identified that assimilate this type of T-1 fuel well. Out of 30 isolates, 9 isolates showed high activity.

On the medium, depending on the concentration of kerosene T-1 1% (10 g/kg), 9 isolates of microorganism cultures grow well: Ne. 4, 8, 14, 23, 5, 18, 20, 25, and in yeast Ne. 12/5.

On the medium, depending on the concentration of kerosene T-1 2% (20 g/kg) and 5% (50 g/kg), good growth was noted in bacterial cultures \mathbb{N} 5, 18, 20, 25 and yeast \mathbb{N} 12/5 (Figure 1-Figure 5).

The identification of the most active cultures of microorganisms by physiological and biochemical characteristics was also carried out.

Culture № 25 is cocci, solitary, in pairs, and clusters of 1.25-2.0 microns. Gram-positive, non-acid-resistant, do not form spores. On MPA and FHN (fish hydrolyzate of the nutrient medium), the culture forms rounded, convex red colonies, 1-2 mm in diameter. The edge of the colonies is even and does not release pigments into the medium. Aerobe. When growing in MPB the medium becomes cloudy, a precipitate forms, and an annular film forms on



Figure 1. The growth of the culture of *Arthrobacter sp.* on a solid medium Voroshilova-Dianova with the addition of kerosene T-1.



Figure 2. The growth of the culture of *Acinetobacter calcoaceticum* on a solid medium Voroshilova-Dianova with the addition of kerosene T-1.



Figure 3. Growth of the culture of *Micrococcus roseus* on a solid medium Voroshilova-Dianova with the addition of kerosene T-1.



Figure 4. Growth of Bacillus sp. on a solid medium Voroshilova-Dianova with the addition of kerosene T-1.



Figure 5. Growth of Candida sp. on a solid medium Voroshilova-Dianova with the addition of kerosene T-1.

the surface. It uses glucose, lactose, and mannose as a carbon source. Starch does not hydrolyze, and does not liquefy gelatin. Hydrogen sulfide and indole do not form. Nitrates are reduced to nitrites. Gives a positive reaction to catalase. The optimum growth temperature is 28°C. Selected from the soil sample of the Baikonur Cosmodrome, site 31 (0.0-50.0 cm). According to morphological and physiological-biochemical characteristics, the culture is assigned to *Micrococcus roseus*.

Culture № 20 is an upbeat spore-forming rods, located singly and in chains. Aerobe. When growing on MPA and FHN, the colonies are rounded, the surface is smooth and shiny, and the edges are even. Colonies are light beige, diameter of 3-4 mm, homogeneous structure, and oily consistency. The optimum growth temperature is 28°C. Selected from the soil sample of the site.31 (0-25cm). According to morphological and physiological-biochemical characteristics, the culture was assigned to *Bacillus sp.*

Culture $N \circ 5$ is an upbeat, immobile cell. In young cultures, rods are irregularly shaped, which, with further development of the culture, break up into small cocci. Does not form a dispute. On agar, medium forms are rounded, and convex, with a smooth edge, and white-yellow colonies. Aerobe. Gives a positive reaction to catalase. The optimum growth temperature is 28°C. Selected from the soil sample of the site 196 (0-50cm). According to morphological and physiological-biochemical characteristics, the culture is assigned to Arthrobacter sp.

Culture № 18 is a Gram-positive, immobile cell. Does not form a dispute; aerobe. When growing on a solid nutrient medium MPA forms small, opaque, whitish, round, with a smooth edge of the colony. Growth on liquid nutrient media: MPB forms uniform turbidity. Utilizes maltose, sorbitol, inositol, glucose. Gives a negative reaction to lactose, sucrose, mannitol, sodium citrate, indole, and hydrogen sulfide. Gives a positive reaction to catalase. The optimum growth temperature is 28°C. Selected from the soil sample of the site 196 (0-50cm). According to morphological and physiological-biochemical characteristics, the culture was assigned to *Acinetobacter calcoaceticum*.

Culture № 12/5 represents single cells, round, sometimes oval, size 2-4 x 3-4 microns. Grows well on Raymond's agar medium (with 1% acetate and 0.25% yeast extract) containing up to 8% NaCl. Assimilates n-alkanes (C10-C30), acetate, propionate. Weak development on ethanol, and propanol. Does not ferment glucose. Uses ammonium nitrogen. Optimum growth temperature at 28°C. Selected from a soil sample of the U-25 zone, from the Ulytau region (0-25 cm). According to morphological and physiological-biochemical characteristics, the culture was assigned to *Candida sp.*

Selection of Optimal Nutrient Media for the Cultivation of Bacteria

The results of the experiment on the selection of optimal nutrient media for the cultivation of bacteria are presented in Table 3 and Figure 6-Figure 10.

The initial concentration of isolate cells before inoculation into the broth was controlled using an optical density measuring device - a DEN-1 densitometer (Biosan, Latvia). A suspension equal to 1.5×10^8 CFU/ml (0.5 McFarland units) was prepared from the isolated colony. Then a series of Koch dilutions was prepared, for which 1 ml of the prepared suspension was diluted in 9 ml of 0.9% sodium chloride solution. Thus, dilutions were obtained - 1.5×10^7 CFU/ ml, 1.5×10^6 CFU/ml, 1.5×10^5 CFU/ml, 1.5×10^4 CFU/ml, 1.5×10^3 CFU/ml and 1.5×10^2 CFU/ml.

Growth of isolates in mineral salt broth containing various concentrations of kerosene. After 7 days of incubation at 35°C, the broth became cloudy due to microbial growth. A gradual increase in turbidity was observed, showing maximum turbidity at 3% kerosene and decreasing again at concentrations above 3% kerosene. It has been established that the optimal duration of cultivation of *Candida sp. 12/5* is 1 day, for the rest of the studied crops - 2 days. The best nutrient media for the culture of *Candida sp.12/5* are the

Number of culture		Bacterial cell content, CFU/ml					
medium	Strain of bacteria	Before inoculation	1 day	2 days			
№ 1	Candida sp. nov. 12/5	1.5×10^{2}	1.0×10^{6}	3.0×10 ⁶			
№ 2	Candida sp. nov. 12/5	1.5×10^{2}	2.0×10^{7}	1.7×10^{7}			
№ 3	Candida sp. nov. 12/5	1.5×10^{2}	1.6×10^{7}	9.3×10 ⁷			
№ 4	Candida sp. nov. 12/5	1.5×10^{2}	1.2×10^{8}	1.3×10^{8}			
№ 1	Bacillus sp. 20	1.5×10^{2}	2.0×10^{6}	4.8×10^{7}			
№ 2	Bacillus sp. 20	1.5×10^{2}	1.2×10^{6}	2.2×10^{7}			
№ 3	Bacillus sp. 20	1.5×10^{2}	1.0×10^{7}	8.4×10^{7}			
№ 4	Bacillus sp. 20	1.5×10^{2}	3.4×10 ⁷	2.4×10^{8}			
№ 1	A. calcoaceticum.18	1.5×10^{2}	2.4×10^{7}	3.5×10^{8}			
№ 2	A. calcoaceticum.18	1.5×10^{2}	4.1×10^{7}	2.5×10^{8}			
№ 3	A. calcoaceticum.18	1.5×10^{2}	3.8×10 ⁷	4.4×10^{8}			
№ 4	A. calcoaceticum.18	1.5×10^{2}	4.4×10^{7}	1.4×10^{8}			
№ 1	M. roseus. 25	1.5×10^{2}	5.2×10 ⁶	3.2×10^{8}			
№ 2	M. roseus. 25	1.5×10^{2}	1.2×10^{7}	4.3×10^{8}			
№ 3	M. roseus. 25	1.5×10^{2}	2.2×10 ⁷	5.1×10^{8}			
№ 4	M. roseus. 25	1.5×10^{2}	2.2×10 ⁷	4.8×10^{8}			
№ 1	Arthrobacter sp. 5	1.5×10^{2}	1.3×10 ⁷	2.0×10^{8}			
№ 2	Arthrobacter sp. 5	1.5×10^{2}	1.8×10^{8}	2.6×10 ⁹			
№ 3	Arthrobacter sp. 5	1.5×10^{2}	4.0×10^{7}	2.0×10^{8}			
№ 4	Arthrobacter sp. 5	1.5×10^{2}	1.4×10^{8}	3.0×10°			

Table 3. Growth of hydrocarbon-oxidizing bacteria on various nutrient media

modified medium N^{0} 4 with the addition of nutrient broth and glucose, on which the bacterial titer reaches 1.3×10^{8} CFU/ml, and medium N^{0} 3 - titer 9.3×10^{7} CFU/ml. Less accumulation of bacterial cells was noted on medium N^{0} 1 titer 3.0×10^{6} CFU/ml.

For cultivation of culture Acinetobacter calcoaceticum. 18 all tested nutrient media are suitable. At the same time, the titer of bacteria is in the range of $1.4-4.4 \times 10^8$ CFU/ml. The same picture was noted in the culture of *Micrococcus roseus.* 25, the titer of which on the indicated nutrient media is $3.2-5.1 \times 10^8$ CFU/ml.

Culture of *Bacillus sp. 20* also accumulates the largest number of cells on the modified medium N^{0} 4 - the titer is 2.4×10⁸ CFU/ml, on the other tested media the bacterial titer is 2.2-8.4×10⁷ CFU/ml.

For the culture of *Arthrobacter sp.* The top 5 nutrient media are \mathbb{N}^{0} 2 based on corn extract and modified \mathbb{N}^{0} 4, on which the number of bacterial cells was: 2.6×10^{9} and 3.0×10^{9} CFU/ml, respectively.

The optimal temperature for growing cultures of microorganisms was determined by their growth intensity on medium N^0 1 at various temperature conditions - from 10°C to 37°C. It has been established that the optimal growth temperature for the culture of *Arthrobacter sp. 5* is 25-30°C, *Acinetobacter calcoaceticum. 18* is 30-35 °C, *Micrococcus roseus. 25* is 25-37 °C., *Bacillus sp. 20* is 30-35°C, *Candida* *sp.* 12/5 is 25-30 °C. Considering that the selected strains of hydrocarbon-oxidizing bacteria are aerobes, it is necessary to select the optimal aeration regime for their deep cultivation. The need for microorganism cultures in aeration was determined by changing the filling volume of 750 ml shake flasks with modified nutrient medium № 4 in the range



Figure 6. Growth of *Candida sp.* 12/5 on various types of nutrient media.



Figure 7. Growth of *Acinetobacter calcoaceticum*. *18* on various nutrient media.



Figure 9. Growth of *Arthrobacter sp. 5* on various nutrient media.



Figure 8. Growth of *Bacillus sp. 20* on various nutrient media.



Figure 10. Growth of Micrococcus roseus. 25 on various nutrient media.

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Table 4.	Accumulation (of biomass c)† 011-	$-0x1d1z1n\sigma$	bacteria	depending (on aeration
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Strains of Titers, CFU/ml, depending on the volume of the nutrient medium							
bacteria's	50 ml	100 ml	150 ml	200 ml	250 ml	300 ml	
12/5	5.0×10 ⁸	6.0×10 ⁸	3.0×10 ⁸	4.0×10^{8}	5.0×10 ⁸	2.0×10 ⁸	
20	2.0×10^{8}	3.0×10 ⁸	4.0×10^{8}	3.0×10 ⁸	4.0×10^{8}	3.0×10 ⁸	
18	4.0×10^{8}	5.0×10^{8}	3.0×10 ⁸	7.0×10^{8}	5.0×10^{8}	2.0×10 ⁸	
25	4.0×10^{8}	5.0×10 ⁸	9.0×10 ⁸	8.0×10^{8}	7.0×10^{8}	4.0×10^{8}	
5	9.0x10 ⁸	11.0x10 ⁸	12.0x10 ⁸	$10.0 \mathrm{x} 10^8$	11.0x10 ⁸	8.0x10 ⁸	

from 50 to 300 ml. Cultures were grown on a shaker for 2 days at 30° C (Table 4).

It was established that during the growth of the test cultures in various volumes (from 50 to 250 ml) of the modified nutrient medium N^{0} 4, no significant changes in the accumulation of biomass were noted. This indicates that when growing the studied cultures of hydrocarbon-oxidizing microorganisms in the fermenter, the flow rate of process air will not exceed 0.6–0.8 V/min per volume of the nutrient medium.

Strains of bacteria	Utilization of kerosene T-1 (%)1						
	Culture medium № 1	Culture medium № 2	Culture medium № 3	Culture medium № 4			
Control	63.00±0.03 ^f	62.30±0.03 ^f	64.03±0.03 ^f	63.27±0.03 ^f			
12/5	96.23±0.07ª	91.57 ± 0.03^{b}	98.73±0.03ª	87.37±0.03 ^c			
20	69.97 ± 0.03^{d}	65.67±0.03 ^e	72.80 ^d	73.20 ^e			
18	82.70 ^b	68.20 ^d	84.40°	84.00^{d}			
25	65.90 ^e	97.80 ^a	71.60 ^e	90.90 ^b			
5	72.20 ^c	84.20 ^c	96.17 ^b	92.47±0.03ª			

Table 5. Utilization of T-1 kerosene by hydrocarbon-oxidizing microorganisms grown on various nutrient media

¹Data represent mean \pm standard error (SE). Different superscript letters (a, b, c, d, e, f) in the columns indicate significant differences between means (Tukey's test, p < 0.05).

To determine the percentage of utilization of kerosene T-1 by selected cultures of microorganisms, they were grown under optimal conditions on various nutrient media for two days, then they were inoculated in an amount of 10.0% into liquid nutrient medium \mathbb{N}^{9} 4 with 2.0% kerosene and cultivated for 10 days on a shaker. Then the percentage of kerosene utilization was determined by the one-way ANOVA and Tukey's test (Table 5).

According to experimental data, up to 62.30 % of the introduced kerosene is weathered in the control without the participation of microorganisms. Utilization of kerosene up to 98.73% occurred using the culture of Candida sp. 12/5 grown on a medium with wheat flour. At 96.23% and 91.60%, the utilization of kerosene by this culture occurred when using MPB nutrient media for cultivation and with corn extract. The lowest hydrocarbon-oxidizing capacity was noted in the culture grown on modified medium Nº 4 (87.37%). Low hydrocarbon-oxidizing activity was noted in Bacillus sp. 20 (69.97-73.20%), especially grown on corn extract medium (65.67%). A strain of Acinetobacter calcoaceticum. 18 utilized kerosene T-1 by 82.70-84.40% when grown on various nutrient media, except for the variant with the medium with corn extract, in which the kerosene content decreased by 68.20%.

When using the bacteria *Micrococcus roseus*. *25*, grown on media with corn extract and modified № 4, a decrease in the content of kerosene occurred by 97.80 and 90.90%, respectively. Lower oil utilization occurred when using the culture grown on medium №4 (65.90%) and medium №2 (71.60%). Culture of *Arthrobacter sp. 5* grown on medium № 3 with wheat flour and modified medium № 4 reduced the content of kerosene by 96.17 and 92.47%, respectively. A lower result was obtained when culture media № 4 (72.20%) and № 2 (84.20%) were used for bacterial cultivation.

Comparison of the results on the accumulation of the biomass of microorganisms on various nutrient media and their hydrocarbon-oxidizing activity made it possible to select the optimal nutrient media: *for Candida sp. 12/5* - modified medium Nº3 with wheat flour; for *Bacillus sp. 20* - modified medium Nº4; for *Acinetobacter calcoaceticum*.

18 and Arthrobacter sp. 5 - modified medium №4 and modified medium №3, for *Micrococcus roseus*. 25 - modified medium №4 and №2 with corn extract.

CONCLUSION

Oil pollution is a global problem that destroys living organisms and causes potential harm to the environment and humanity. Existing physical and chemical methods proved to be less effective and therefore the emergence of biological methods became an intensive solution.

In the decomposition of oil in the soil, the main and decisive role is played by the functional activity of the complex of soil microorganisms, which ensure the complete mineralization of oil and oil products [3], [20,21]. Since hydrocarbon-oxidizing microorganisms are a constant component of soil biocenoses, it is natural that their catabolic activity is used to restore oil-contaminated soils. There are two ways to speed up the purification of soils from pollution: to activate the metabolic activity of the natural soil microflora by changing the corresponding physicochemical conditions of the environment or to introduce specially selected active oil-oxidizing microorganisms into the polluted environment [22-24]. The microbiological method of reclamation based on the use of highly effective strains of hydrocarbon-oxidizing microorganisms is widely used in the world practice of reclamation activities.

The expediency of isolating microorganisms adapted to the conditions of pollution and successfully utilizing hydrocarbons has been revealed, which in turn will ensure the most effective cleaning of soils by a biological method. With this in mind, the problem of developing destructor drugs for local conditions becomes especially relevant.

Therefore, this preliminary study was carried out to isolate different types of soil strains with a tendency to be degraded by T-1 kerosene hydrocarbon propellant, which is used by bacteria with the potential for degradation. Selected microorganisms were analyzed and identified according to physiological and biochemical characteristics: No5 - Arthrobacter sp., №18 - Acinetobacter calcoaceticum, №20

- Bacillus sp., №25- Micrococcus roseus, №12/5- Candida sp. In this study, on a medium with a T-1 kerosene concentration of 1% (10 g/kg), 9 isolates of microorganism cultures grow well: № 4, 8, 14, 23, 5, 18, 20, 25 and in yeast № 12/5. The study showed that with a concentration of T-1 kerosene 2% (20 g/kg) and 5% (50 g/kg), good growth was noted in bacterial cultures Arthrobacter sp.5, Acinetobacter calcoaceticum 18, Bacillus sp.20, Micrococcus roseus 25 and yeast Candida sp. 12/5. Other studies have reported primary screening of kerosene degraders using a conventional accumulative culture containing 1% kerosene as the sole carbon source. n-alkanes, including fractions C_{11} - C_{15} , C₁₇-C₁₉ Bacterial isolates of Staphylococcus aureus Ba01, Delftia acidovorans Cd11, Acinetobacter calcoaceticus Fe10, Pseudomonas koreensis Hg11, and Acinetobacter johnsonii Sb01, sharing this characteristic degradation pattern, demonstrated the ability to degrade gradations by 70-84% within 21 days of incubation [9]. There were similar results to study the growth characteristics of eight isolates from soil samples. When eight different isolates were cultured in mineral salt broth containing 1% (v/v) kerosene for 7 days at 35°C and 120 rpm, Pseudomonas sp. showed the highest growth, as evidenced by the high turbidity of the culture, followed by Bacillus sp. [24].

In the current study, it was found that the optimal duration of cultivation of Candida sp. 12/5 is 1 day, and for the rest of the studied crops - 2 days. The best nutrient media for the accumulation of biomass of microorganisms on various nutrient media and their hydrocarbon-oxidizing activity made it possible to select the optimal nutrient media: for Candida sp. 12/5 - modified medium № 3; for Bacillus sp. 20 - modified medium № 4; for Acinetobacter calcoaceticum. 18 and Arthrobacter sp. 5 - modified medium № 4 and №3, for Micrococcus roseus. 25 - modified medium № 4 and № 2. Subsequent inoculation of diluted 100 µl of each culture on mineral salt agar also gave results consistent with visualized turbidity, Pseudomonas sp. giving the highest growth of 8.38 log CFU/mL, and two species of Bacillus sp. giving almost similar results of 6.70 log10 CFU/mL and 6.04 log10 CFU/mL [24].

In the current culture of *Acinetobacter calcoaceticum*.18, all culture media tested are suitable. At the same time, the titer of bacteria is in the range of $1.4-4.4\times10^8$ CFU/ml. The same picture was noted in the culture of *Micrococcus roseus*.25. The top 5 cultures of *Arthrobacter sp.*, modified media are Nº 2 based on corn extract and modified Nº 4, on which the number of bacterial cells was: 2.6×10^9 and 3.0×10^9 CFU/mL, respectively. In a similar study using a Pseudomonas sp. isolate which showed maximum growth in the presence of kerosene. The isolate was found to tolerate kerosene concentrations up to 6% (v/v) and showed optimal growth at 3% kerosene (v/v) with bacterial counts of 5.53 log10 CFU/ml and 9.43 log10 CFU/ml, respectively [24].

Subsequent inoculation of diluted 100 μ l of each culture on mineral salt agar also gave results consistent with visualized turbidity, *Pseudomonas sp.* giving the highest growth of 8.38 log CFU/ml, and two species of *Bacillus sp.* giving almost similar results of 6.70 log10 CFU/ml and 6.04 log10 CFU/ml. High concentrations of hydrocarbons, especially volatile hydrocarbons, can be detrimental to bacterial growth. It has been established that the selected microorganisms can be grown at a temperature of 30°C and aeration in the range of 0.6-0.8 V air/min per volume of the nutrient medium.

In conclusion, five activities of the bacterial community were analyzed, simulating natural conditions in the laboratory, and the biodegradability of complex oil components by the obtained bacteria was investigated. Our results provide a reasonable strategy for using the microbial community to treat an environment contaminated with T-1 kerosene hydrocarbon propellant in different seasons to obtain the best recovery effect. Thus, our results suggest that the strains belong to the same species, the formation of microbial consortia can contribute to the process of recovery of soil contaminated with hydrocarbons. With this result, it will not only be possible to clean up spills of rocket fuel T-1 kerosene but it can also be used to decompose those containing these compounds.

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Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.
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Research Article

Investigation of machinability by electrical discharge machining method of ZA27/MWCNT composites produced by powder metallurgy

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ABSTRACT

In recent years, nano-doped metal matrix composites have started to take place among the developed composites. In this study, powder metal undoped ZA27 alloy and 0.5% wt% multi-walled carbon nanotube (MWCNT) doped nano-composite machinability in EDM (electrical discharge machining) were researched. Microstructures of ZA27 nano-doped composites were examined under a scanning electron microscope (SEM), and their hardness measurements were made. Obtained test results were compared with that of ZA27 samples without nanodoped. In the SEM analysis, the production method applied was generally successful, and the porous regions encountered in some parts of the composite structure were due to the difficulty in homogeneously dispersing the MWCNT reinforcement material. The metal's material removal rate (MRR) increased with the addition of MWCNT powders that raised conductivity and decreased tool wear rate (TWR) compared to the pure ZA27 material.

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INTRODUCTION

In recent years, research on metal matrix composites (MMC), which are preferred in many sectors such as medicine, defense, automotive, aerospace, energy, infrastructure, maritime, transportation, food, and sports are increasing [1,2]. In these researches, mainly aluminium and magnesium alloys constitute the majority. However, recently, the production and examination of the properties of zinc matrix ceramic reinforced composites has been a field of interest for many researchers. ZA27 coded zinc-aluminum alloy (Zamac) is widely used in the automotive industry, sports equipment, toys, hardware, decoration, white goods, etc., due to its suitability for mass production, high corrosion resistance, low melting temperature and superior workability. In addition, zinc-aluminium (ZA) alloys are known to be important bearing materials especially suitable for highload and low speed applications. They are reported to be environmentally friendly materials with good processing

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Published by Yıldız Technical University Press, İstanbul, Turkey Copyright 2021, Yıldız Technical University. This is an open access article under the CC BY-NC license (http://creativecommons.org/licenses/by-nc/4.0/). properties and low initial cost, highlighting their excellent castability [3]. ZA27 alloy is used as the base material in the development of MMC materials and the reinforcement element is as effective as the base material in the development of the properties of composite materials. The reinforcement element carries a large part of the load on the composite. The use of nanomaterials as reinforcement elements in the production of such composites is becoming increasingly common [4]. Among these materials, materials such as nano-sized B_4C , SiC, SiO₂, Al₂O₃, MgO, TiB₂, TiC, carbon nanotubes (CNT) and nanographene (GNP) stand out in the technology. In addition to these reinforcement elements, some researchers have produced "pumice reinforced AA7075 syntactic foams as composites" and investigated their machinability by face turning [5].

In recent years, materials containing one-dimensional CNT and two-dimensional graphene have emerged as an important new class for structural engineering and functional device applications due to their exceptionally high elastic modulus and mechanical strength. Along with their aspect ratio (i.e. length-to-thickness or length-to-diameter ratio) properties, graphene and CNT are considered the most promising reinforcing fillers for the fabrication of composite materials [6]. There are many studies in the literature in which the very superior properties of carbon nanomaterials are expressed [7-9]. CNTs are the most important of all nanomaterials, and they are tubular structures with nanoscale diameter and micron size in the simplest sense. In other words, from a structural standpoint, CNTs can be imagined as hollow cylinders made of one or

graphene SWCNT (a) graphene MWCNT (b)

Figure 1. Formation of (a) single and (b) multi-walled carbon nanotubes from graphene nanoplate.

more sheets of graphene (a single layer of graphite) (Figure 1). The cylinder diameter may range from 0.4 nm to 100 nm or higher. The sizes of CNTs, which can vary depending on the production method and conditions, can range from hundreds of μ m to cm [10]. It has been observed that CNTs have stiffness up to 1000 GPa, tensile strength of 100 GPa and thermal conductivity values up to 6000 W/mK. These studies show that CNTs are the strongest fibres known to mankind with extraordinary properties [11].

In studies on metal matrix composites, a large number of aluminium-based nano-composite studies have been carried out. However, it has been seen that there are not enough domestic and foreign studies on ZA27-based nanocomposites, which is a zinc-based alloy, in the literature. Metal matrix composite materials are subjected to some shaping processes depending on where they will be used. These shaping processes can be traditional chipless or machining methods, as well as some non-traditional machining methods can be applied because metal matrix composites are difficult to shape with traditional methods due to the high hardness that occurs in their structures due to the additives reinforced into them [12]. Therefore, recently, non-traditional processing methods such as EDM have been the subject of research to overcome this problem. In the literature, there are some studies on the mechanical properties and machinability of nanomaterial doped, ZA27 and different metal matrix composites [13-18].

At this point, the importance of tool conductivity was emphasised in some similar studies. In comparing the performance of CuBe and E-Cu electrodes, it was expressed that the E-Cu electrode performed better than the CuBe electrode in processing TiN-coated Ti6Al4V because of its higher conductivity [19]. However, no study has been encountered to examine the machinability of ZA27-based nano-doped composites with EDM.

In this experimental study, the machinability of ZA27 matrix MWCNT added composites produced by powder metallurgy technique, unlike the literature, was investigated by EDM method. The MMR and TWR ratios were compared with the results in machining the MWCNT-free ZA27 alloy.

MATERIALS AND METHODS

Some technical properties of the ZA27 matrix material and MWCNT reinforcement element in powder form obtained from the Nanograph Nano Technology Turkey Company are given in Table 1.

In this study, composite materials previously produced by the powder metallurgy method within the scope of Scientific Research Project numbered 2018/043 were used. Composite materials were produced by doping 0.5% by weight of MWCNT in ZA27 matrix. The powder mixture, prepared by adding 0.5% MWCNT by weight into the ZA27 matrix material, was mixed in a ball mill at 300 rpm for 2 hours and then compressed in a hydraulic press under

ZA 27						
Al %	Mg %	Cu %	Fe %	Pb %	Cd %	Zn %
25.5-28.0	0.01-0.02	2.0-2.5	0.075	0.006	0.006	Remain
Density, (g/cm³)	Melting Point, (°C)	Hardness, (HBW)	Tensile Strength, (MPa)	Electrical Conductivity, (S/m)	Thermal Conductivity, (W/mK)	Elongation, (%)
5.0	376-485	105-125	421	1.72	123	3-6
MWCNT						
Purity, (%)	Outer diameter, (nm)	Inner diameter, (nm)	Length, (µm)	Electrical Conductivity, (S/m)	Thermal Conductivity, (W/mK)	Specific Surface Area, (m²/g)
92	8-10	5-8	1-3	9800	3000	240

 Table 1. ZA27 matrix and MWCNT reinforcement material specifications [20-22]

500 MPa pressure in a steel mold. Then, the compressed composite samples were placed in the heat treatment furnace. The temperature of the heat treatment furnace was gradually increased to 450°C in 45 minutes and the production process was completed by sintering at these temperatures for 90 minutes. Images of the composite samples whose production process was completed were taken with a scanning electron microscope (SEM) to examine their microstructures. Then, hardness measurements of composite materials were made according to the Brinell method.

Table 2. EDM experiment design parameters

Exp. No	Current I (A)	Power level	Pulse on time	Pulse off time
			$t_{on}(\mu s)$	t_{off} (µs)
1	6	6	48	99
2	6	6	48	150
3	6	6	99	99
4	6	6	99	150
5	6	6	150	99
6	6	6	150	150
7	15	10	48	99
8	15	10	48	150
9	15	10	99	99
10	15	10	99	150
11	15	10	150	99
12	15	10	150	150
13	25	13	48	99
14	25	13	48	150
15	25	13	99	99
16	25	13	99	150
17	25	13	150	99
18	25	13	150	150

In hardness measurements, a load of 15,625 kg was applied with a 2.5 mm diameter steel ball [20-22].

Machinability experiments were carried out in two stages as composite materials and pure ZA27 blank sample. EDM machinability tests were carried out using Furkan 50A ZNC-1 brand EDM machine. Experiments using the full combination experimental design presented in Table 2, like as three different currents (6, 15, 25 A), three different pulse on times (t_{on} ; 48, 99, 150 µs) and two different pulse off times (t_{off} ; 99, 150 µs) were used. The power level values given in Table 2 are used to set the processing current intensity. Increasing the power level without changing the arc interval/ arc duration (t_{on}/t_{off}) ratio increases the MRR (mm³/min) due to the increase in current intensity.

RESULTS AND DISCUSSION

Microstructure

SEM images at different magnifications taken from 0.5% MWCNT added composite materials produced by powder metallurgy method are given in Figure 2.

The production parameters such as compression pressure, sintering temperature and time applied in the production of composites are other factors affecting the homogeneity of the composite structure [20]. When the SEM images (Figure 2a) are examined, it is understood that the sintering process generally provides the neck and bond formation between the ZA27 particles. However, it is also seen that partially porous (porous) regions occur within the composite structure. This structural defect, which is frequently encountered in particle-reinforced metallic composites, has been reported in the literature in different studies.

Dalmış et al. their study, it was reported that the addition of nano-graphite decreased the density values of the composites and increased the porosity ratio. It has also been



Figure 2. ZA27/MWCNT composite internal structure images.

stated that porosity is known as a common and undesirable feature of metal matrix composites produced by powder metallurgy method and that it affects the properties of the composites tremendously [23]. El-Sayed et al. their a similar study, it was stated that the mixing process of raw materials is an important first step in controlling the distribution and porosity of particles that affect the mechanical and tribological behavior of composites [24]. Saheb et al. their study, it was stated that porosity was mainly caused by CNT agglomeration [25]. Zhou et al. some other factors such as the distribution, texture, interfacial bonding and porosity of CNTs in the composites produced by the powder metallurgy method will significantly affect the strength of the composites. They also pointed out other factors in their studies. It has been stated that the porosity amounts in all nanocomposites are much higher than those in the matrix, and as the weight percentage of CNTs increases, the porosity level increases. It has been stated that this situation is due to the agglomeration of CNTs. It has also been reported that CNT clusters may prevent effective bonding between the matrix and CNTs, leading to very small cracks and increasing porosity [26].

As can be seen from the SEM images, the not very well dispersed MWCNT particles tended to aggregate and agglomerate and covered the ZA27 particles (Figure 2b). In the SEM image at 20000x magnification in Figure 2c, densely agglomerated MWCNT particles completely surrounding the ZA27 fragment are seen. In this case, the contact between the ZA27 particles is reduced. The aggregated MWCNT particles acted as a thermal barrier and somewhat prevented the thermal transfer between the ZA27 matrix material. In this case, the sintering temperature applied is insufficient, and it is considered to prevent the bond formation between the ZA27 particles at the desired level. When evaluated in terms of thermal properties, there are very important differences between the matrix material ZA27 alloy (123 W/mK) and the reinforcement element MWCNT (3000 W/mK). Another important issue is the difficulties in producing such composite structures homogeneously. It is difficult to ensure the homogeneous distribution of very small nano-sized reinforcement elements such as graphene or CNT in the metal matrix. However, the powder metallurgy technique is the most advantageous among the composite material production methods. Therefore, the powder metallurgy method was preferred in this study. The importance of the mixing process in the preparation process of composite structures emerges here. The mixing method should be chosen according to the matrix material of the composite structure to be produced and the characteristics of the reinforcement element to be used. In this study, the mechanical mixing method was applied. According to the obtained microstructure images, it can be said that it would be more appropriate to increase the applied 120 min mixing time and 300 rpm mixing speed values.

Hardness

The measured hardness values of the 0.5% MWCNT added ZA27 composite produced by powder metallurgy and the pure ZA27 sample without MWCNT reinforcement according to the Brinell method are given in the graphic in Figure 3.



Figure 3. Hardness of test specimens.

When the graphics in Figure 3 are examined, it is understood that the hardness of the composite material has decreased significantly with the effect of MWCNT reinforced into the ZA27 matrix material. While the hardness of the pure ZA27 test sample was 102.3 HBW, the hardness value of 0.5% MWCNT reinforced ZA27 composite was 52.2 HBW. It can be said that the hardness value is reduced by half. It is thought that MWCNT particles placed between ZA27 particles prevent heat transfer during the sintering process and decrease neck and bond formation by causing a decrease in temperature between ZA27 particles. More specifically, MWCNT particles are considered to act as a heat shield and absorb some of the heat. In this case, the hardness value of the composite structure, which is weakly bonded to each other or no bond can be formed in some regions, decreased. Similar results have been expressed in different studies in the literature [20]. Since materials such as GNP and CNT have very high specific surface area val-

ues, they also constitute much volume in the composite

structure, even if they are reinforced in very small amounts. In a study, it was reported that the preparation of composite mixtures by calculating the reinforcement ratios in terms of volume instead of making them in terms of weight could be a more appropriate method [27].

Machinability

Powder metallurgy is a method that allows the use of different metallic and non-metallic materials. In addition to the advantages of easily controlling the metallurgical content and density of the final product, the formability of these new types of materials with unconventional manufacturing techniques remains important for manufacturers. This study investigated the machinability of produced ZA27 and 0.5% MWCNT-ZA27 materials with EDM, and machining performance outputs such as MRR and TWR were evaluated. Figure 4 and Figure 5 show graphs presenting the changes in processing performance outputs.



Figure 4. Variation of MRR-I-t_{on}: (a) t_{off} =99 µs constant-ZA27; (b) t_{off} = 150 µs constant-Zamac 27; (c) t_{off} =99 µs constant-%0.5 MWCNT- ZA27; (d) t_{off} =150µs constant-%0.5 MWCNT- ZA27.



Figure 5. Variation of TWR-I- t_{on} : (a) t_{off} =99 µs constant- ZA27; (b) t_{off} =150 µs constant- ZA27; (c) t_{off} =99 µs constant-%0.5 MWCNT-ZA27; (d) t_{off} =150 µs constant--%0.5 MWCNT- ZA27.

Cu electrodes are used in all machining: current and arc duration values are preferred at low, medium and high values to determine the ideal machining conditions of the material. When the graphs are examined, MRR increased mostly with increasing current and pulse time in machining (Figure 4) but decreased up to 15A current value at 150 μs pulse time of 0.5% MWCNT-ZA27 material (Figure 4-c, d), then showed an increasing trend. This situation shows that the spark discharge time is also effective depending on the discharge current value. Increasing the discharge current and the pulse duration together in EDM is the most preferred combination to increase the MRR value. The highest MRR values were found in processing 0.5% MWCNT-ZA27 (Figure 4-d). This is thought to be due to the fact that MWCNT reinforcement increases the conductivity of the material [28,29]. The lowest processing speeds were determined at 48 µs pulse value in all engravings with the same ton value. The lowest MRR value was 0.016 g/min at 6A, 48 μ s t_{on} (Figure 4-b); the highest MRR value was obtained with 0.228 g/min at 25A, 150 $\mu s \: t_{on}$ value (Figure

4-d). This indicates that more material is eroded per unit time as the ton value increases with the flow. In addition, with the increase of t_{off} value, a slight increase in MRR values was determined, which shows that the processing area is cleaned more effectively and the discharge energy is transmitted to the workpiece with less loss in time. High MRR values were obtained at 150 µs toff values.

TWR increased with increasing current values in machining and reached the highest values at 25A (Figure 5). High current values also increase the wear of the tool by melting the tip of the tool a little more during the discharge of electrons from the tool. The highest wear values were obtained in pure ZA27 materials. Lower electrode wear occurred when machining 0.5%MWCNT-ZA27 alloy. This is thought to be due to the MWCNT additive increasing the conductivity of the alloy and the quicker and easier discharge of the spark from the bottom surface of the tool. Because there is an incomparably large amount of difference between the electrical conductivity value of MWCNT nanomaterial (9800 S/m) and the conductivity

values of ZA27 nanomaterial (1.72 S/m). A study in the literature reported that adding 3% by weight MWCNT into the ZA27 material increases the conductivity value of the ZA27 material 20 times [21]. The highest tool wear was obtained in the machining of ZA27 material at 25A, 0.05 g/ cm³ at 150 μ s impact time (Figure 5. a), and the lowest TWR was obtained in the machining of 0.5% MWCNT added material as 0.0046 g/cm³ at 6A, 150 μ s t_{on} value (Figure 5.d). When evaluated in general, increasing I and ton values showed a dominant effect on TWR in an increasing trend. It can be said that the conductivity of the workpiece, especially the MWCNT reinforcement, considerably increases the spark discharge intensity.

CONCLUSION

Output parameters were compared by processing 0.5% MWCNT added ZA27 composite and pure ZA27 alloy produced by powder metallurgy method with EDM method. In addition, SEM examinations of MWCNT added materials were made and associated with the machinability results.

It was determined that porous regions were formed in both composite structures and the MWCNT particles, which did not show a fully homogeneous distribution, exhibited agglomeration behaviour in some regions and covered the ZA27 particles.

It has been determined that the MWCNT additive in EDM processing causes the formation of the magnetic field required for spark discharge in the material faster. This shows that the electrical conductivity of the doped metal increases considerably compared to the pure material. MRR increased with increasing flow and pulse time, but the machining speed of 0.5%MWCNT-ZA27 material increased significantly in all machining compared to pure ZA27 material in EDM machining of both types of materials. Based on the machinings made in the same parameter, the MRR showed the highest increase of 5.34 times in the machinings with 0.5% MWCNT added ZA27 material at 6A, 150 μ s t_{on} and 150 μ s toff values. The lowest increase was 0.9 times obtained in processing at 25A, 48 μ s t_{on} and 99 μ s t_{off} values.

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Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw

data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Research Article

Application of response surface methodology in the optimisation of polymer concrete mechanical properties

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ABSTRACT

Polymer concrete offers several advantages compared to conventional concrete, including increased strength, reduced water absorption, enhanced abrasion and chemical resistance, and lower labor costs. However, the production cost of polymer concrete is higher, and compliance with international standards is essential. Hence, determining the right component ratios becomes a crucial task. To address this issue, a study was conducted to investigate the influence of resin, calcite, and sand ratios on the mechanical properties of polymer concrete. The researchers employed the response surface method (RSM) and utilized the genetic algorithm (GA) to find the optimal mixing ratios. For the study, 15 different mixtures were prepared using the Box-Behnken (BB) design for the three components. Experimental tests were carried out to determine the densities, flexural and compressive strengths of these mixtures. The researchers then employed the least squares method to obtain linear and quadratic polynomial models. The accuracy of these models was assessed through ANOVA analyses. It was found that the quadratic model better aligned with the experimental results. Additionally, the study revealed that the mechanical properties were significantly influenced by the resin, with the combined effects of resin and calcite playing a significant role. Finally, the GA was applied to calculate the optimal mix proportions for achieving the best balance between price and performance, as well as for creating lightweight and durable products. According to the optimal mixture results, compressive strength improvement up to 13.8% and tensile strength improvement up to 13.4% were achieved. In conclusion, this study makes valuable contributions to enhancing cost-effectiveness and performance in the production of polymer concrete.

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INTRODUCTION

Polymer-based concretes are one of the preferred materials in many different sectors thanks to their high strength and physical performance [1-4]. In particular, polymer concrete drainage channels produced in accordance with EN 1433:2002 [5] have become one of the most preferred materials in the infrastructure sector thanks to their corrosion resistance, smooth surfaces and high compressive and tensile strength. In the production of polymer concrete, it is

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very important to mix the components in the most appropriate proportions and to reach the values in accordance with the standards in terms of mechanical performance. For this reason, many researchers have been conducting studies on the ratios in which components should be used in polymer concretes and the mechanical performance of polymer concretes [6-9].

Unlike conventional concrete, the binder in polymer concrete is resin material instead of Portland cement [8, 10-12]. Resins are binders that give excellent mechanical, chemical and physical properties to concrete and are generally found in the liquid phase [13]. Studies in the literature indicate that polymer concretes have higher damping capability than conventional concretes [14-16] and epoxy based polymer concrete shows better mechanical properties than polyester based concrete [17]. In addition, vinyl ester and unsaturated polyester resins are known to have high mechanical properties [7]. Some studies emphasize that polymer concrete is not actually perfect, and that they have made very little progress compared to conventional concrete [17, 18]. Researches in the literature show that polymer concretes have different mechanical properties. It is known that the main reason for the difference in the results is the mixture ratios of the materials that make up the polymer concrete and the type of resins that are binding materials [19]. Bulut and Sahin found that while increasing the resin increased the compressive strength significantly, it did not make a significant contribution to the splitting and tensile strengths [20]. In addition, the effect of curing conditions on the mechanical properties of polymer concrete is also known [6, 21, 22]. In fact, it has been reported that the chemical resistance of epoxy-based polymer concrete is considerably higher than that of conventional concrete [23]. When the effect of environmental temperatures on the mechanical properties of polymer concrete was examined, it was observed that the compressive strength and modulus of elasticity decreased significantly at high temperatures [6, 24].

The biggest factor in the production of polymer concrete at a reasonable, accessible and affordable price is the amount of resin. Therefore, in addition to the effect of resins on mechanical properties, their effect on production costs is crucial. In the literature, a resin ratio between 10% and 20% is a recommended value [21, 25, 26]. However, this range is quite wide for the manufacturer and it is not known what the desired optimal value is. In addition, the gradation of aggregates, the type of additives and the quality of production are parameters that affect the mechanical properties of polymer concretes [7, 27, 28].

In order to improve the mechanical properties of polymer concretes, many different components from resins to admixtures should be combined in optimal proportions. However, studies on the optimal component determination of polymer concrete are quite insufficient. In order to find optimal mixing ratios, manufacturers and researchers continue to work and produce by developing some

assumptions and approaches. Ferdous et al. tried to find the optimal mix ratio for polymer concrete using different resin-filler ratios and matrix-aggregate ratios and developed empirical formulas to predict mechanical properties [6]. Tabatabaeian et al. 2019 in their study on permeable polymer concrete tried to optimize mechanical properties and price using statistical methods such as ANOVA analysis, signal-to-noise ratio and distance-based approach [29]. Vipulanandan and Dharmarajan reported that maximum tensile and compressive strength was obtained with a polyester resin content of 14%-16% [30]. Vipulanandan et al. reported that 14% resin ratio gave maximum mechanical strength in their experiments with epoxy resin [31]. Vipulanandan also gave different resin ratios for polymer concrete in other studies. In the study conducted to determine the optimal mix proportions of polymer concrete, it was recommended to use 11.25% resin ratio, 11.25% calcium carbonate, 29.1% andesite (5-20 mm), 9.6% fine sand, 38.8% coarse sand [32].Kim et al. determined 7.5% resin ratio and 42.5% sand ratio as the optimal mixture [33]. Muthukumar et al. used BB experimental design considering only grain size and tried to determine the optimal sand spacing ratio for minimum void ratio [34]. In another study, Muthukumar et al. used BB test design to determine the optimal blend that provides maximum compressive strength for different resin types [35]. In these experiments using furan resin, resin ratios ranging from 7.5% to 11% and aggregate ratios between 74% and 77.5% were given as the optimal ratio. Muthukumar and Mohan investigated the mechanical properties of polymer concretes containing silica particles of different sizes with statistically designed mixtures. Optimization was performed by comparing with experimental data to obtain the optimal values for each mix [36]. They calculated the optimal mix proportions for all mechanical properties. Li et al. reviewed the studies in the literature that determined the optimal conventional concrete component ratios with RSM [37].

As can be seen in the literature, there are extensive studies on the effects of components on the mechanical properties of polymer concretes and which components should be combined in which proportions [38-45]. Therefore, within the scope of this study, the effect of the proportions of the constituent components of polymer concrete on the mechanical properties was investigated and the change in mechanical properties was expressed by functions. RSM is frequently used to express experimental data mathematically and to reveal the correlation between inputs and outputs [46-49]. It was decided to use RSM as one of the experimental design methods for the three components. It was predicted that conducting experiments at each point would increase the number of samples and the number of experiments, so mixtures were prepared at 15 different points with the BB experimental design, which requires fewer experiments. The mechanical strengths of the specimens were obtained after three-point bending (flexural) and compressive tests. Density was also included in the

results since it is one of the desired properties in the production of polymer concrete. Linear and quadratic polynomial model coefficients were obtained by least squares method and model consistency was tested by ANOVA analysis. After determining the function type and coefficients that best fit the experimental data, the optimization phase started. Optimal mix ratios for price/performance, lightest and most durable products were calculated with the optimization steps created with GA.

MATERIALS AND METHODS

In this section, after introducing the components used, information about the preparation of test specimens and mechanical tests will be given. Polymer concrete is a type of concrete consisting of aggregate, resin, hardener and accelerator. While preparing the specimens, the test points indicated by the response surface method will be used. The specimens prepared at the determined points were subjected to mechanical tests and their density, tensile and compressive strengths were determined.

Natural Aggregates

Aggregates are load-bearing elements in polymer concrete. Sand grains of sufficient size to meet the incoming load must be carefully selected. Sand grains should be washed in the stream bed, have rounded contours and be free of mud. In this study, 0.3-1 mm, 1-2 mm, 2-3 mm and 3-5 mm sized silica based sand from Istanbul and Kırklareli with an average density of 2.65 g/cc was used. Table 1 shows the chemical properties of the aggregates used.

Table 1.	Chemical	of aggregate	es
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Chemicals	Aggregates	Aggregates					
	0.3-1 mm	1-2 mm	2-3 mm	3-5 mm			
MgO (%)	0.1	0.06	0.06	0.06			
Al ₂ O ₃ (%)	0.245	1.86	1.86	1.86			
SiO ₂ (%)	98.86	94.15	94.15	94.15			
CaO (%)	0.01	0.39	0.39	0.39			
Fe ₂ O ₃ (%)	0.148	0.46	0.46	0.46			
SO ₃ (%)	-	0.1	0.1	0.1			
K ₂ O (%)	0.03	1.56	1.56	1.56			
Na ₂ O (%)	0.02	1.12	1.12	1.12			
Loss (%)	0.587	0.3	0.3	0.3			

Resin

Resin is a component that provides binding in polymer concrete and since it is polymer based, it is called "polymer concrete" for this reason. Polymers are obtained by natural and synthetic means. If there are dense crosslinks in the chain structure, it is called thermoset, if not and the molecular bonds are smooth, it is called thermoplastic. While thermosets change their chemical structure after heating, harden and remain solid, thermoplastics have a low melting temperature and can be recycled since their chemical structure is intact. Thermosetting (polyester, epoxy, polyurethane, phenol), tar-added, citrene and methyl methacrylate (MMA) resins are used in polymer concrete production [38]. Polyesters are divided into 4 groups as vinylester, aloud, saturated polyester and unsaturated polyester. In this study, unsaturated polyester resin was preferred because it has good thermal resistance, low shrinkage rate and high strength values.

Accelerator

Accelerator helps to reduce the duration of the curing reaction between the resin and hardener. Since heat is released during exothermic reactions, attention should be paid to occupational safety during and after production. Cobalt naphtenate, whose properties are given in Table 2, was selected as accelerator for this study.

Table 2. Properties of accelerator

Properties	Values
Density	0.92 g/cm ³ (20 °C)
Viscosity	300 mPa.s (20 °C)
Self-Accelerating decomposition temperature	≥ 150 °C
Flash point	62 °C
Cobalt content	% 1.50

Hardener

A hardener is needed for the reaction starting with the accelerator. Acetyl Acetone Peroxide (AAP), whose properties are given in Table 3, was used to start the curing reaction at room temperature.

Table 3. Properties of hardener

Properties	Values
Flash point	> 60 °C
Density	1055 kg/m ³
Viscosity	21 mPa.s
Self-Accelerating decomposition temperature	60 °C
Total active oxygen	%4-4.2
Peroxide content	%33
Diethyl glycol+water+diacetone alcohol	%67

Response Surface Method

RSM has emerged mainly to develop valid mathematical models for physical experiments. The purpose of using these methods is to take into account the factors that may affect the output and to determine the appropriate test points [8, 9, 13]. In RSM, firstly, the type of polynomial to be used is determined, then the experiments suitable for this polynomial are designed (inputs). After the experimental results (outputs) are obtained, the unknown coefficients of the polynomial are calculated using the least squares method. In RSM, the relationship between inputs and outputs is modelled by a polynomial (Eq. (1)). Usually second order polynomials are used, but higher order polynomials can also be used (Eq. (2)). The maximum and minimum levels of the input parameters are taken into account as well as intermediate value levels. Different trial points are determined according to these levels. When all trial points are used, this experimental design is called a full factorial design, thus increasing the number of experiments. Different methods are also used to reduce the number of experiments, such as BB or Central composite. In this study, the BB design was used and a total of 15 experimental points were determined. y represents the results of the experiment, i.e. the outputs, β_i represents the unknown coefficients, xi represents the independent variables of the experiment, i.e. the inputs, and ε represents the experimental error.

$$y = f(x_1, x_2, x_3, \dots, x_k) + \varepsilon \tag{1}$$

$$y = \beta_0 + \sum_{i=1}^n \beta_{1,i} x_i + \sum_{j=1}^n \beta_{2,j} x_j^2 + \sum_{i=1}^n \sum_{j>1}^n \beta_{3,ij} x_i x_j + \varepsilon \quad (2)$$

As can be seen in Figure 1, the number of experiments decreased from 27 to 15 compared to the full factorial experimental design since corner points were not used in



Figure 1. Experimental points according to Box-Behnken RSM.

the BB experimental design. The materials used for the BB experimental design and their levels are given in Table 4. Sand contains the grains to carry the load, calcite (CaCO₃) fills the void ratio and increases the strength and resin is the binder and holds the whole matrix together. -1,0 and 1 represent the lowest, medium and highest parameter levels respectively. Component quantities are trade secrets and their proportions will not be shared in this study.

If the inputs, unknown coefficients and experimental results are expressed as a matrix, it becomes an equation. To apply the least squares method and calculate the β coefficients, Eq. (5) is used.

$$Y = X\beta \tag{3}$$

$$\mathbf{Y} = \begin{cases} y_1 \\ \dots \\ y_{15} \end{cases}, \mathbf{X} = \begin{bmatrix} 1 & \dots & x_3 & x_1 x_2 & \dots & x_{11}^2 \\ \dots & \dots & \dots & \dots & \dots \\ 1 & \dots & x_3 & x_1 x_2 & \dots & x_{11}^2 \end{bmatrix}, \mathbf{\beta} = \begin{cases} \beta_0 \\ \dots \\ \beta_{15} \end{cases}$$
(4)

$$\boldsymbol{\beta} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} (\boldsymbol{X}^T \boldsymbol{Y}) \tag{5}$$

Analysis of Variance (ANOVA)

The significance levels of the polynomial coefficients fitted according to the least squares method were determined by Analysis of Variance (ANOVA). R², adjusted R² and lack of fit parameter values were calculated for the suitability of the models.

Regression analysis is a statistical technique used to determine the strength and direction of the relationship between variables and to predict future values. An

Table 4. Experimental points and levels of compositions

Experimental	A: Aggregate	B: Calcite	C: Resin
Points			
1	0	-1	-1
2	-1	0	-1
3	1	0	-1
4	0	1	-1
5	-1	-1	0
6	1	-1	0
7	1	1	0
8	-1	1	0
9	-1	0	1
10	0	-1	1
11	1	0	1
12	0	1	1
13	0	0	0
14	0	0	0
15	0	0	0

inconsistent result means that the regression model does not fit the data or that some prerequisites are not met. When examining the model results, the first parameter to look at is the R^2 error value; it has been concluded that an R^2 of 0.80 and above is acceptable for the correlation between variables [39]. Other parameters should also be checked for the accuracy of the model. Non-fitting results should be evaluated by following the steps below.

I. To assess the fit of the regression model, statistics such as R^2 , adjusted R^2 , F-test and standard error values are examined. These statistics show how much the model explains the variance of the dependent variable and whether the model is significant. The higher the R^2 , adjusted R^2 values, the lower the p-value and the smaller the standard error, the better the model fits.

II. Once the cause of a poorly fitting result has been found, some steps can be taken to improve the regression model. For example, inappropriate variables can be removed from the model, linearity can be ensured by adding transformation or polynomial terms, extreme values can be identified and eliminated, or a different regression method can be used. The terms used in the tables are explained below.

- Source: Indicates the different components of the regression model. Model refers to the effect of factors. Residual indicates the variance not explained by the model. Misfit indicates the deviation of the residuals from a normal distribution.
- df: Indicates the degree of freedom. For the model, df is equal to the number of factors. For the residual, df is the total number of observations minus the df of the model. The df for discordance is the residual df minus one.
- Sum of squares: Indicates the division of variance by different sources. The model sum of squares measures the magnitude of the effect of the factors on the dependent variable. Residual sum of squares measures the magnitude of variance not explained by the model. The discrepancy sum of squares measures the magnitude of the deviation of the residuals from a normal distribution.
- R²: Also known as the coefficient of determination. It shows how well the model explains the dependent variable. It takes a value between 0 and 1 and the higher it is, the better the model fits.
- Adjusted-R²: This is the adjusted version of R2. It is used to prevent R2 from becoming artificially high as the number of factors increases. It takes a lower value than R2 and the higher it is, the better the model fits.
- Coefficients: Indicates the parameters of the regression model. These coefficients give the ratio of one unit change in the dependent variable to the change in the independent variable.
- In the table, p-values with * sign indicate p-values less than 0.1, ** sign indicates p-values less than 0.05. In other words, these coefficients affect the result more than the other coefficients.

After calculating the polynomial coefficients, an algorithm was written in Matlab environment to ensure that the products are produced with the desired properties. Also, the unit prices of the materials used in the products were added to the algorithm. Thus, the product will be produced with the desired mechanical properties and the target price of the product will also be determined.

In this study, the objective function in Eq. 6 is formed by the density-dependent target price (F_4), tensile strength (F_2) and compressive strength (F_3) functions. The function constraints consisted of the lowest and highest levels used in the experiments.

$$\min_{A,B,C} f = |F_2(A, B, C) - 22| + |F_3(A, B, C) - 90| + |F_4(A, B, C) - 35|$$

Constraints: $-1 \le A \le 1$
 $-1 \le B \le 1$
 $-1 \le C \le 1$ (6)

In the written algorithm, the "ga-Genetic Algorithm" command from Matlab library was used and the desired features will be provided under the specified constraints as the objective function approaches zero. The genetic algorithm was chosen because it does not get trapped in local extrema. This is because the genetic algorithm tries to preserve diversity to explore different regions in the search space. It can operate at different points in the search space thanks to its selection, crossover and mutation features. These operators increase the population's ability to both exploitation and exploration. Exploitation is about improving the best existing solutions, while exploration is about finding new and potentially better solutions. The disadvantage is that the convergence speed can be slow as it solves for more than one individual at a time. Depending on the size of the population, the convergence rate can be slow, but this is not always a disadvantage. An algorithm that converges too fast may miss the global optimum. After all the generated individuals have been tested in the objective function, some individuals are selected and survive by various natural selection methods. From the surviving parents, children are created through cross-over and mutations. The new individuals and children now form the next generation and are tested again with the objective function. Individuals that do well in this iterative cycle are kept in a pool and contribute to the creation of new generations.

The optimal component ratios that will ensure a tensile strength of 22 MPa, a compressive strength of 90 MPa and a target price of 35 TL were determined. In addition to resin, calcite and sand, hardener and accelerator prices were also included in the price function. The optimal component ratios for different objective functions were calculated using the same algorithm.

Preparation of Samples

-

After the samples were prepared, polymer concrete mixtures were made with the following steps:

The desired aggregate proportions were determined.



Figure 2. Experimental studies a) bending test b) compressive test c) samples after compressive test d) cracked surfaces

- The resin was slowly mixed with the aggregate and a powerful mixer was used for 15 minutes.
- Accelerator was added to the resin and aggregate mixture and a homogeneous consistency was obtained.
- Hardener was added to the mixture and mixed thoroughly with a powerful mixer.
- The fresh concrete was filled into steel prismatic molds and compacted with a shaking table.
- The specimens were kept in the molds until hardened and then kept in the laboratory at 20 ± 2 °C.

The specimens were prepared prismatically with dimensions of 40mmx40mmx160mm [40]. The specimens were kept for 7 days to ensure the desired strength and consistency of the test results. As stated in the study of Çakır, polymer concrete does not undergo a significant change 7 days after pouring [22]. For this reason, 7-day test results were used for all test results.

Experimental Studies

Flexural, compressive and density tests were performed on hardened specimens. Flexural tests were performed according to ASTM C78/C78M [41], compressive tests according to ASTM C109/C109M [42] and density tests according to ASTM C642 [43]. Additionally, the test regulations are mentioned in EN1433 [40]. The specimens were tested on a 600kN Form-Test machine until fracture. After the flexural test, one half of the specimen was used for compressive test. Figure 2 shows photographs of the experimental studies.

RESULTS AND DISCUSIION

Table 5 shows the 7-day compressive strength, tensile strength and density of the specimens as a result of 15 experiments depending on the selected parameters. For each experiment number, three samples were prepared (totally 45 specimens). Last 3 experiment mixtures are the same, hence thirteen different mixture recipes were prepared.

After the experimental results were obtained, two different models were proposed for the appropriate polynomial selection. In this section, linear and quadratic polynomial coefficients were obtained using the data in Table 5. ANOVA in Design Expert [44] software was used to determine which type of polynomial provided the best fit and which parameters dominated the results. F_1 represents density, F_2 represents tensile strength, F_3 represents compressive strength. As compared to literature, ratio of strengths is found higher. As shown in Table 5, tensile and compressive strength ratios were calculated. The comparison of this relationship obtained here with the studies in the literature is visualised in Figure 3 and it is seen that it is compatible with the previous data.

According to the above-mentioned investigations, when the result of Experiment 1 is included in the regression,

Experiment Number	Density [kg/m ³]	Flexural Strength [MPa]	Compressive Strength [MPa]	Ratio of Strengths
	F ₁	F ₂	F ₃	F ₃ / F ₂
1	2162.70	8.40	45.10	5.37
2	2172.10	11.40	53.70	4.71
3	2199.00	13.50	61.20	4.53
4	2186.40	14.60	65.10	4.46
5	2161.90	14.80	65.60	4.43
6	2134.00	15.40	64.90	4.21
7	2105.70	21.20	91.90	4.33
8	2095.70	18.80	85.10	4.53
9	2000.00	20.80	86.50	4.16
10	1994.30	20.60	85.50	4.15
11	2017.40	20.80	85.40	4.11
12	2060.40	14.10	57.50	4.08
13	2111.30	12.20	57.30	4.70
14	2101.20	12.50	59.90	4.79

61.60

Table 5. Results of experiments

15



2191.00

12.60

Figure 3. Flexural and compressive strength relationship with literature.

none of the polynomial types give sufficiently reliable results. However, after eliminating this result, the models became stronger. Therefore, linear and quadratic models were obtained by subtracting the 1st result.

Linear Model Results

Table 6 shows the regression results of the linear model and the results of the ANOVA analysis. The regression model used to explain the density fit reasonably well (R^2 = 0.8813, Adjusted- R^2 = 0.8417). The regression models used to explain the compressive and tensile strength of concrete showed lower fit (R^2 = 0.4174, 0.3029; Adjusted- R^2 = 0.2232, 0.0706). Thus, the influence of the factors on the compressive and tensile strength of concrete is non-linear. This means that the effect of the factors on the dependent variable is not constant. Here it appears that the resin is the effective component on the results because the p-value is less than 0.05.

5.37

If the obtained polynomial answers are illustrated, the results can also be evaluated visually. The red dots are the actual results from the experiment. In Figure 4-6, the z-axis shows a) density, b) flexural strength and c) compressive strength, respectively. In each figure, the graphs were plotted by keeping the mid-level of one component constant and changing the proportions of the other components. For

 Table 6. Variance and regression coefficients of the linear model

Source df		Sum of squares			
		$F_1 [kg/m^3]$	F ₂ [MPa]	F ₃ [MPa]	
Model	3	50299.03	68.05	691.4	
Residual	9	6777.06	94.98	1590.85	
Lack of fit	8	0.1884	0.0476	0.1006	
R ²		0.8813	0.4174	0.3029	
Adjusted-R ²		0.8417	0.2232	0.0706	
Coefficients					
	β_0	2110.05	15.9145	69.725	
	β_1	3.3	0.6375	1.5625	
Linear	β_2	-5.4125	0.724671	3.38125*	
	β_3	-85.8375**	3.08717**	9.79375*	



Figure 4. a) density b) flexural c) compressive strength regarding B and C while constant A component.



Figure 5. a) density b) flexural c) compressive strength regarding A and C while constant B component.



Figure 6. a) density b) flexural c) compressive strength regarding B and C while constant A component.

example, Figure 4 shows the change in mechanical properties as the ratios of calcite and resin change while the sand component is at 0. Although it seems that a linear model can be proposed for density, it is obvious that the test points do not match when the results in Figure 6 are examined. It is also clear from the graphs why the compressive and tensile strengths have low R^2 values.

Quadratic Model Results

Table 7 shows the regression results and ANOVA analysis results of the quadratic model. The regression models used to explain the density, compressive strength and tensile strength of polymer concrete fit reasonably well (R^2 = 0.9735, 0.9891, 0.9734; Adjusted- R^2 = 0.8941, 0.9565, 0.8935). The influence of the factors on the compressive and tensile strength of polymer concrete is non-linear. This means that the effect of the factors on the dependent variable is not constant. Resin again has a linear effect on all results. The effect of the calcite and resin components dominates the results both individually and together. However, the sand component is not linear but quadratic on the compressive and tensile strengths. When the quadratic model results were analysed, it was found that the quadratic model was superior to the linear model.

Quadratic result visualizations are given in Figures 7-9. The z-axis shows a) density, b) flexural strength and c) compressive strength, respectively. Again, in each figure, the graphs were plotted by keeping the mid-level of one component constant and changing the proportions of the other components. For example, Figure 7 shows the change

Source df		Sum of squares				
		F ₁ [kg/m ³]	F ₂ [MPa]	F ₃ [MPa]		
Model	9	55564.92	161.26	2221.48		
Residual	3	1511.17	1.77	60.77		
Lack of fit	2	1460.17	1.73	57.39		
R ²		0.9735	0.9891	0.9734		
Adjusted-R ²		0.8941	0.9565	0.8935		
Coefficients						
	β_0	2106.25	12.35	58.6		
	β_1	3.3	0.6375	1.5625		
Linear	β_2	-15.8125	2.13125**	9.73125**		
	β_3	-96.2375**	4.49375**	16.1438**		
	β_{12}	9.475	0.45	1.875		
Interaction	β_{13}	-2.375	-0.525	-2.15		
	β_{23}	41.05*	-5.0625**	-21.8375**		
	β_{11}	-8.1	4.64375**	18.2563**		
Quadratic	β_{22}	26.175	0.55625	0.01875		
	β_{33}	-1.025	-0.36875	-5.15625		

 Table 7. Variance and regression coefficients of the quadratic model

in mechanical properties by changing the proportions of calcite and resin when the sand is at 0. The red dots show the experimental results and the response surfaces provide the experimental points. This shows that the quadratic model works better than the linear model. In contrast to the other results, Figure 9 a) shows inconsistency in some experimental points in the density function. Nevertheless, statistically the quadratic model is still strong.

Optimisation Results

Once it is determined that the quadratic model is the best model that provides the best experimental results, different mixtures can be prepared for different purposes. For this reason, with the help of the algorithm written and the "ga" command in Matlab, it will be easy to prepare the mixtures with the best price, the highest mechanical strength or the best mixtures in terms of both price and mechanical strength. Using Eq. (6), the optimal mix that meets the price and mechanical strength requirements is obtained. Other objective functions are not included in the algorithm when the maximum value of other mechanical properties is desired. Table 8 shows the optimal mix ratios obtained for the specified objective functions. Also, following graphics show GA results of three different objective functions (OF). The error values of the fitness functions are shown as best result data. The longest search can be seen in OF1, because of the three specific aims.

Density and unit prices can provide significant advantages for enterprises with large tonnage production. At the same time, the desired mechanical properties are the responsibility of the manufacturer. For this reason, various objective functions for price, mechanical strength and



Figure 7. a) density b) flexural c) compressive strength regarding B and C while constant A component.



Figure 8. a) density b) flexural c) compressive strength regarding A and C while constant B component.



Figure 9. a) density b) flexural c) compressive strength regarding B and C while constant A component.

price/performance product designs have been prepared below. As seen in the table, having the lowest density does not always make the product price the cheapest. For the optimal product price and desired mechanical properties, i.e. the first objective function, it is noteworthy that the resin ratio is low. Because resin is an uneconomical product compared to other components.

It can be said that the first optimal mixture has a small price advantage due to the resin ratio. When the 3 optimal mixtures are compared, it is seen that although the price of all of them is close, their mechanical properties are different. When the third objective function was examined, it was seen that the resin ratio was kept at maximum and the calcite and sand ratio was kept at the lowest level in order to provide maximum mechanical properties. Although the third optimal mix is 13.8%-8.9% compression resistant and 13.4%-7.9% flexural resistant compared to the other mixes, it is 0.3% heavier than the first mix and 1% heavier than the second mix.

Polymer concrete is gaining more importance in the infrastructure and construction sector as it has superior mechanical and chemical properties compared to conventional concrete. Since resin is used as a binder, cost-effective production and meeting the requirements of international standards is a challenging process for manufacturers. For this reason, this study aims to predict the proportions of sand, resin and calcite used in polymer concrete provided that certain objectives are met. If the results are summarized:

When the test results are analysed, any outliers should be removed. According to the results of the first



Figure 10. GA results over generations for three OF.

	Objective Function	Mixture ratios		Optimal Results				
		A	В	С	F ₁ [kg/m ³]	F ₂ [MPa]	F ₃ [MPa]	F ₄ [TL]
1	Eq. (6)	0.88	-0.8	0.915	2004.5	22.00	90.00	34.99
2	$\min(F_1)$	1	-0.665	1	1990.3	23.12	94.05	35.11
3	$max(F_2)\&max(F_3)$	-1	-1	1	2010.3	24.94	102.41	35.44

Table 8. Mixture ratios for different objective function

experiment, the mixture with the lowest calcite and resin has the lowest value in tensile and compressive tests and was not included in the analysis.

- The quadratic model, rather than the linear model, is more compatible with the experimental results and the lack of fit values are at the lowest level. The R2 error values for density, flexural and compressive strengths are 0.8813, 0.4174, 0.3029 in the linear model and 0.9735, 0.9891, 0.9734 in the quadratic model, respectively.
- In both models, resin dominates the mechanical properties. In fact, the importance of resin and calcite together is higher than the quadratic model. Moreover, the nonlinear behaviour of sand is revealed in the quadratic model.
- When the optimisation results were analysed, it was found that the price/performance product was slightly more suitable compared to the other optimal results.
- Although the second optimal design was lightweight, the high resin content escalated the prices. It was found that not every lightweight product is affordable.
- With the third optimal design, a maximum 13.8% more compression resistant and 13.4% more tensile resistant product was designed.
- In future studies, more components can be examined and a mathematical model of the fiber effect can be created.

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AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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Review Article

Security in UAV ecosystem: An implementation perspective

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ABSTRACT

This paper focuses on implementational security measures to protect the UAV (Unmanned Aerial Vehicles) ecosystem from malicious adversaries reducing the surface of vulnerability against the malicious intent of these threat actors. The primary objectives of this paper are incorporated in five security measures to enhance the security of UAVs by implementing lightweight cryptographic functions for firmware encryption and safeguarding Peripheral Component Interconnect (PCI) buses, fortifying UAV ground stations by disabling non-utilized ports, thereby minimizing potential attack vectors, mitigating threats from malicious actors by implementing an intrusion detection and prevention system (IDPS) to block inorganic network traffic, obscuring the Service Set Identifier (SSID) from broadcast scans, and to reinforce security through filter scrubs and dynamic whitelisting to protect UAV systems against unauthorized access. This paper dives into different methods of the detailed implementation of the aforementioned security measures, providing insights into UAV's configurational practices. Each measure is described and analyzed in parallel to ensure comprehensive coverage of the UAV-Ecosystem's security. The results of this paper are both challenging and rewarding. The proposed measures help improve the security of the UAV ecosystem and protect it from different attacks. In conclusion, this paper has demonstrated the importance of implementing security measures to safeguard the UAV ecosystem from malicious threats. It is crucial to recognize that UAVs may not be entirely immune to sophisticated attackers. Nevertheless, by implementing these security measures and maintaining vigilance, we can prolong the lifespan of UAVs and the entire UAV-Ecosystem and improve their security against malicious intent.

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INTRODUCTION

Unmanned Aerial Vehicle (UAV) or Drones are rapidly becoming an integral part of modern infrastructure, as dependency on this emerging technology has increased over the decade in the fields of civilian health, surveillance-security, logistics supply, connectivity, smart agriculture, industry, safety, and the military-usage. Therefore, it is important to ensure the security of not just the drones themselves, but also all other connected technologies that make up the UAV's ecosystem [1]. This expansive use of drones in the Internet of Things (IoT) has created a separate term as the Internet of Drones (IoD) [2] has

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become increasingly popular due to their convenience and affordability [3]. However, with the increase of drone usage, comes an increase in security concerns. This research paper explores the security measures needed to protect drones and their ecosystem from malicious activities, such as hacking, eavesdropping attacks [4] and data breaches. The focus is on the use of lightweight cryptographic functions to encrypt the firmware [5], disabling non-utilized ports on the ground station, blocking inorganic traffic using SNORT, a network-based intrusion detection system, hiding the SSID (Service Set Identifier) from broadcast scans, and implementing filter scrubbing and dynamic whitelisting to protect the UAVs web application interface (WAi) [6] from Remote File Inclusion (RFI) and API abuse attacks [5]. The strengths and weaknesses of each security solution have been discussed a comprehensive overview of the best practices for drone security has been provided.

This research paper is an implementational extension to a previous paper by Sinha et al. [5], and the structure of the paper has been defined in Figure 1.

Related Work

The methodology used and the research gap identified in the related literature are tabulated in Table 1.

Lightweight Cryptographic Function

While implementing a Light Weight Cryptographic Function [11] onto an Arduino-based drone running embedded Linux, we aimed to achieve Firmware Encryption to encrypt the entire firmware, onboard flight module, telemetry data, and other non-volatile memory storage areas of the UAV(s) like hard disks and other long-term storage areas [5] to prevent an attacker from gaining critical information about the drone like the version of certain programs, libraries and Peripheral Component Interconnect (PCI) information or components information of the Main Remote Controller Board (onboard computer system) and carve out exploits for undetected zero-day vulnerabilities. This security feature will allow us to defend UAVs against reverse engineering attacks on the firmware by a malicious adversary if they gain physical access to a Missing-In-Action (MIA) drone [1].

There are three types of firmware encryption techniques-Symmetric, Asymmetric and Authenticated Encryption (i.e. AES-GCM). In our research, we found that using asymmetric encryption for firmware encryption on a drone can lead to boot time limitations. This is because asymmetric encryption algorithms require more computational power and time compared to symmetric encryption algorithms. As a result, using asymmetric encryption can cause delays during the boot process of a drone, which is not desirable in critical applications where fast boot times are essential, Encrypting the firmware of the UAV can discourage an attacker from a direct attack but a side-channel attack is still an imminent threat where the attacker aims to exfiltrate critical information as cryptographic keys, by measuring coincidental hardware emissions of the UAV such as Electromagnetic waves to measure the electromagnetic radiation emitted by the UAV trying to reconstruct the entire signal packets and another side channel attack is the Power dump attack where the attacker attempts to leverage the power consumption of the UAV hardware depriving, or lowering power source in an attempt to cause a processing error or segmentation fault.

These side-channel attacks can weaken the security of the firmware and PCI buses as this attack aims to corrupt underlying encryption keys and cryptographic processes to create various openings for future attacks, such as privilege escalation attacks on the UAV. Side-channel attacks can be mitigated without compromising the Light Weight Cryptographic Function efficiency by increasing the system noise in the electromagnetic waves emitted by the isotopic radiator of the UAV the only drawback of using this method is that the signal sent by the UAV will have to be processed to subtract the spectral content of the noise from the signal (filtered signal = unfiltered signal - noise) that can result in heavy processing time and cost extra power usage on the power-limited UAV but even these mitigate methods can only decrease the likelihood of occurring of these hardware vulnerabilities.



Figure 1. Structure of the Paper.

Research Work	Methodology	Research Gap	
Sinha, H., Malik, N., Dahiya, Menal. (June 2023) [5]	This paper proposes a novel architecture for configuring and securing unmanned aerial vehicles (UAVs).	The paper does not discuss the potential scalability and performance issues associated with the proposed architecture.	
Tiwari, M., Kumar, R., Bharti, A., & Kishan, J. (2017) [7]	This paper presents a novel intrusion detection system that utilizes fuzzy logic and Artificial Neural Networks (ANNs) to detect malicious activities.	The paper does not discuss the potential false positives or false negatives that may arise from using the proposed system.	
Keleman, L., Matić, D., Popović, M., & Kaštelan, I. (2019, September) [8]	This paper proposes a secure firmware update approach for embedded systems, based on a combination of digital signatures and symmetric cryptography.	The paper does not discuss the potential risks posed by the proposed approach.	
Wu, Y., Noonan, J. P., & Agaian, S. (2011) [9]	This paper proposes a randomness measurement and testing technique for image encryption, based on Shannon entropy.	The paper does not discuss the potential security risks posed by using the proposed technique.	
Mekdad, Y., Aris, A., Babun, L., Fergougui, A. E., Conti, M., Lazzeretti, R., & Uluagac, A. S. (2021) [6]	This paper provides a survey of the security and privacy issues associated with unmanned aerial vehicles (UAVs).	The paper does not discuss potential solutions to the identified security and privacy issues.	
Abualigah, L., Diabat, A., Sumari, P., & Gandomi, A. H. (2021) [2]	This paper provides a comprehensive review of the applications, deployments, and integration of Internet of Drones (IoD).	The paper does not discuss the potential challenges that may arise in IoD applications.	
Haider, S. K., Nauman, A., Jamshed, M. A., Jiang, A., Batool, S., & Kim, S. W. (2022) [10]	This paper provides an overview of the routing algorithms, techniques, and challenges associated with the Internet of Drones (IoD).	The paper does not discuss potential solutions to the identified challenges.	
Lin, C., He, D., Kumar, N., Choo, K. K. R., Vinel, A., & Huang, X. (2018) [11]	This paper provides an overview of the security and privacy challenges associated with the Internet of Drones (IoD) and proposes potential solutions.	The paper does not discuss the potential scalability and performance issues associated with the proposed solutions.	
Yaacoub, J. P., Noura, H., Salman, O., & Chehab, A. (2020) [3]	This paper provides an overview of attacks and the limitations associated with drone systems and proposes potential recommendations.	The paper does not discuss the potential effectiveness of the proposed recommendations in mitigating the identified attacks and limitations.	
Dabrowski, A., Pianta, N., Klepp, T., Mulazzani, M., & Weippl, E. (2014, December) [12]	This paper presents a novel approach for detecting IMSI-catchers.	The paper does not discuss the potential scalability and performance issues associated with the proposed approach.	
Langley, A., Riddoch, A., Wilk, A., Vicente, A., Krasic, C., Zhang, D., & Shi, Z. (2017, August) [13]	This paper presents a novel transport protocol called Quick UDP Internet Connections (QUIC).	The paper does not discuss the potential security risks posed by using the proposed protocol.	
Roy, M., Ahsan, S., Kumar, G., & Vimal, A. (2020) [14]	This paper presents an implementation of the Quick UDP Internet Connections (QUIC) protocol.	The paper does not discuss the potential security risks posed by using the proposed protocol.	

Table 1	. Com	parative	Ove	rview	of F	Related	Literature
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Therefore, we recommend using symmetric encryption techniques such as AES for firmware encryption on drones. Additionally, authenticated encryption techniques such as AES-GCM can provide both confidentiality and integrity of the firmware, overall providing high throughput, high entropic value and low latency, as shown in Figure 2. This makes it a suitable choice for drone firmware encryption as neither the security nor performance of the UAV is compromised with the use of this Light Weight Cryptographic Function.

Exploiting Look Out

Once a malicious adversary obtains a UAV(s) firmware, they can use tools such as BinWalk to analyze the binary images (.bin) for embedded files and executable codes or exploit component information using Linux utilities such as 'lspci' to display information about PCI buses in the Drone's system and devices connected to them.

Another method of exploiting UAV(s) firmware is by the use of the binary diffing technique that involves comparing two binaries of different versions of the same software and

		SECURITY ASSE	SSMENT	PERFORMA	NCE AS	SESSM	ENT
ES-GCM)	DRONE COMPONENTS	SECURITY METRICS	ENTROPY (NATS)	LATENCY (MS)	тня	ROUGHF (GBPS)	рит
ICTION (A	REMOTE CONTROLLER BOARD	VOLTAGE / CLOCK GLITCHES	1 (HIGH)	3-6 MS	1-2	3-5	5-9
VPHIC FUN	TELEMETRY SYSTEM	SOFTWARE FAULT INJECTION	1 (HIGH)	2-5 MS	1	I-3 GBPS	5
RYPTOGR/	FLIGHT CONTROL MODULE	SOFTWARE FAULT INJECTION	1 (HIGH)	2-5 MS	1	I-3 GBPS	5
VEIGHT CF	VIDEO TRANSCEIVER & CAMERA	ELECTROMAG	1 (HIGH)	2-5 MS	1-2	3-5	5-9
LIGHT V	SENSORS AND PAYLOAD	SFI, VG, CG & EMI	1 (HIGH)	1-2 MS	1-2	3-5	5-9
AETRIC	PROPELLERS & MOTORS	VOLTAGE GLITCHES	O (LOW)	1-2 MS		NA	
SYMP	BATTERY	VG & EMI	0 (LOW)	NA		NA	

Figure 2. Quantitative analysis of different PCI buses (components of UAV) for measuring the security and performance of the AES-GCM.

using diffing tools/utilities like 'diff' to understand the new functions introduced or old removed in the new version of the firmware.

Whether a drone's firmware is encrypted or not can be determined by entropy calculation using the Shannon entropy formula as represented in Equation 1 and Figure 3 [9]. Entropy is a measure of randomness or information density, which is expressed as a value between 0 and 1. A higher entropy value indicates a higher degree of randomness, with values near 1 being considered high entropy and values near 0 indicating less entropy. Encrypted hardware typically has a high entropy value close to 1.

$$H(X) = -\sum_{i=1}^{n} P(x_i) \log_b P(x_i)$$
(1)

Disabling Non-Utilized Ports on the Ground Station

The Ground Station (GS) serves as the command centre UAVs, responsible for overseeing their operations. It is typically a ground-based computer system that runs specialized software known as Ground Station Control (GSC) software. This software can be installed on any Linux-based distribution or version of the Windows operating system. However, given the numerous vulnerabilities present in older versions of Windows, it is recommended that Windows 10 or higher be used. For instance, vulnerabilities such as CVE-2022-30190¹ & CVE-2020-0822² have been reported in previous versions. Therefore, selecting an appropriate operating system for the GS is essential for maintaining security and protecting the UAV ecosystem from potential attacks.

Securing GSC/GS relies on disabling all connection-oriented (TCP- Transmission Control Protocols) & connectionless protocols (UDP- User Datagram Protocols) [11] that are non-essential to UAV(s) communication, connection, and services such as FTP –21, SSH –22, SMTP –25, HTTP –80, POP3 –110, POP3 SSL –995, IMAP –143, IMAP SSL –993, SQL –1433, RDP –3389 [5].

It is advisable to run GSC software on a Linux GS-dedicated computer system to avoid other preinstalled software having vulnerabilities and could potentially risk the UAV's security and integrity. Windows Remote Desktop Protocol (RDP), active on TCP port 3389, has historically been commonly vulnerable to various attack vectors, allowing hackers to breach into GSs and other UAV utility environments. Therefore, it is important to close non-essential ports such as port 3389 and others to reduce the surface of vulnerability by reducing potential entry points for attackers, unprotected ports can be exploited by attackers to gain unauthorized access to the UAV's systems control. The idea here is to discourage attackers and make it more challenging for them to find vulnerabilities providing an additional layer of defence for the UAV and its ground station.

For our Linux GS, we used the 'apt-cache pkg names' command to check for vulnerable and unnecessary preinstalled packages on our Linux GS and removed them using 'apt purge <package_name>', i.e. 'apt purge font-georgewilliams'.

Identifying open ports on Linux can be achieved by running the netstat utility to display various network-related information for active or open ports, connections more descriptively using 'netstat' with '-antp' flag, or else we can use the 'ss' (socket statistics), another Linux utility that dumps socket statistics information of the running Linux system. In order to filter out TCP and UDP ports, one can use the 'ss -tl' and 'ss -ul' flags individually, or combine both flags using 'ss -tul'. However, if the objective is to identify actively listening ports and their associated service names, the command 'ss -tuln | grep LISTEN' can be used. This command effectively filters out actively listening ports and displays their corresponding service names. Such information can be particularly useful in identifying potential security threats or network performance issues. This method of port filtering can be implemented in various network monitoring and analysis tools.

In a Linux OS, the manual way to close an open port is very time-consuming and tedious, so a better way would be to disable the processes that the port is actively running or use 'sudo ss --kill state listening src:<port_number>' which will send a SOCK_DESTROY request to the kernel that will disable this port until otherwise, i.e. 'sudo ss --kill state listening src:1234'.

Blocking Inorganic Traffic Using IDS

For our Linux-based GS, we have been using the network-based IDS SNORT, which is equipped with a set of predefined rules that can identify and categorize malicious network activity and inorganic traffic [5] primary reason to use an SNORT IDS over any other IPS for our UAV-Ecosystem is to minimise the potential halt caused in the event of a false positive (legitimate actions misidentified as a security threats to the entire ecosystem) disrupting critical ground station functions whereas the IDS will notify the network administrator and wait for an assessment of

¹ https://www.cvedetails.com/cve/CVE-2022-30190/

² https://www.cvedetails.com/cve/CVE-2020-0822/

the event as it continuously monitors all active ports on the network, looking for packets that match against the predefined rules, list of known threats and their indicators of compromise (IOCs). In the event of a match, SNORT generates alerts to notify the network administrator of potential security threats before an attacker can cause damage to the network [7]. This type of detection is known as signature-based detection used for identifying known threats.

SNORT looks for attack patterns within network traffic by analysing the packets' exchange. Large collections of related items that are of a certain type originating from single or multiple sources could indicate a denial-of-service (DOS) or distributed denial-of-service (DDOS) [6]. SNORT looks for the exchange of a sequence of related packets in a certain pattern (signature-based detection), which could indicate that a port scan is in progress using NMAP or any other network scanners [7].

Anomaly-based detection used by the SNORT NIDS identifies inorganic traffic by establishing a normal behaviour baseline for an entire UAV-Ecosystem's network activity. So that SNORT NIDS can be effective at identifying unusual patterns of activity or out-of-the-ordinary behaviour to trigger alerts. The baseline is dynamic and updated in real-time to suit the needs of the ever-evolving UAV-Ecosystem (addition of new components like new UAVs or SGS). Ensuring that the anomaly detection system remains accurate even in the ever-evolving UAV-Ecosystem environment and reduces the risk of false positives.

Limited by resources, we installed SNORT NIDS on our Linux-based GS. SNORT NIDS (Network-based Intrusion Detection System) consists of four main functions- data collection, feature selection, analysis, and action. It is typically installed on a separate computer on a network-connected device like a router so that it can monitor the traffic entering and leaving a particular network segment.

After installing SNORT (preinstalled in Linux), we can customize the main SNORT configuration file to suit our needs. To do this, we can enter 'sudo gedit /etc/snort/snort. config' in the terminal. For testing purposes, we can use the default configuration settings and only add our HOME_ NET to our network IP address range to 192.168.0.1/24, indicating a range of 1 to 254 addresses.

Additionally, we can use the default RULES or configure them to suit our UAV's ecosystem's requirements. After making these changes, we need to run a configuration check to ensure all settings are correct using 'sudo gedit / etc/snort/snort.conf'. Finally, we can run SNORT using 'sudo snort -A console -q -u snort -c /etc/snort/snort.config -i enp0s3' ('enp0s3' is our interwork interface card) to monitor the network for inorganic traffic and attack vectors.

To test the effectiveness of the SNORT IDS (Intrusion Detection System), we conducted a network scan using Nmap from an attacker's perspective. The SNORT IDS provided an alert output, which was captured in the image as shown in Figure 3 an example of signature-based detection.

user@user-VirtualBox:~\$	sudo snort -A console -q -u snort -g snort -c /etc/snort/snort.conf -i enp0s3
A	
02/27-16:47:36.870599	<pre>**] [1:1418:11] SNMP request tcp [**] [Classification:</pre>
Attempted Information Le	eak] [Priority: 2] {TCP} 192.168.1.17:59103 -> 192.168.1.18:161
	вср
02/27-16:47:36.870677 [<pre>[**] [1:1421:11] SNMP AgentX/tcp request [**] [Classification:</pre>
Attempted Information Le	eak] [Priority: 2] {TCP} 192.168.1.17:59103 -> 192.168.1.18:705
Accempted information Le	[Priority: 2] {ICP} 192.108.1.17:59105 -> 192.108.1.10.705

Figure 3. Alert output of SNORT.

- a. Is the command used to run and enable (IDS) SNORT on network monitor mode.
- b. Is the type of attempt on the network Information Leak, Unknown, Potentially Bad Traffic, Default-login-*Attempt*, etc.
- c. Is the IP address of the Attacker.
- d. Is the IP address of the Victim.
- e. Type of Priority 1 (high) is the most severe and 4 (very low) is the least severe and type of port used like TCP and UDP [14] for us secure ports is (UPD 443).

Obfuscating SSID From Network Broadcast Scans

Disabling the broadcast SSID is a straightforward method to obfuscate or hide it from network broadcast scans. By disabling SSID broadcasts, detecting the network's SSID through tools such as Wireshark and airodump-ng becomes more difficult [5]. Wireless network cards used in network routers often run on Unix or Linux-embedded systems [8]. To disable SSID broadcast on a Unix system, the first step is to identify the interface name of the wireless adapter. Once the interface name is determined, the wireless adapter can be connected to the network router using an FTP (File Transfer Protocol) connection to disable the SSID broadcast.

To disable SSID broadcast on a Unix system, we must first determine the interface name of the wireless adapter and connect it to the network router via an FTP connection. After establishing a connection with the router, we can then run the command 'iwconfig'. This will list all of the available wireless interfaces. To disable SSID broadcast on a Unix system, the first step is to determine the interface name of the wireless adapter and connect it to the network router via an FTP connection.

Once connected, the command 'iwconfig' can be run to list all available wireless interfaces. With the interface name identified, the 'iwpriv' command can be used to disable SSID broadcast with the syntax 'iwpriv <interface_name> set SSID_Hide=<1|0>', where <1|0> is either 1 to disable SSID broadcast or 0 to enable it. For instance, if the interface name is "wlan0", the command to disable SSID broadcast would be 'iwpriv wlan0 set SSID_Hide=1'.

To disable SSID broadcast on a Linux system, we first need to establish an FTP connection to the router using the 'FTP connect' command in the terminal. Once connected, we need to edit the wireless network configuration file by running the command 'sudo nano /etc/hostapd/hostapd. conf' and add the following line to the end of the file: 'ssid_ broadcast=0'. After saving the changes, we need to restart the wireless network configuration file by running 'sudo service network-manager restart'. By doing so, we can successfully disable the SSID broadcast of our router.

However, this method also has drawbacks. As overly aggressive dynamic adaptation can lead to an increase in false positives, it could also prevent legitimate users from connecting to the UAV Ecosystems network. Additionally, it does not protect against active scanning, which can be used to detect hidden networks. Disabling probe response is another option for hiding the SSID from broadcast scans. Integrating these dynamic adaptation mechanisms into existing security systems can be challenging and a daunting task. However, while this method can protect the UAV Ecosystem against passive scans, the SSID will still be visible in the beacon frames which could result in gaining system access via frag attack (fragmentation and aggregation attacks) [15]. Therefore, further research will be conducted to develop more effective methods for hiding the SSID from broadcast scans. This will be a focus of our future work.

Implementing Filter Scrubs and Dynamic Whitelisting

Filter scrubs and dynamic whitelisting are techniques to protect the UAV ecosystem's Web Applications Interface [10] and Application Program Interface (APIs) from malicious input parameters and file inclusions [5] basically to prevent malicious adversaries to target vulnerabilities in web applications aiming to infect and uploading malware or backdoor exploit using Remote File Inclusion (RFI) and API abuse attack.

We protected our web applications and APIs [10] from malicious input parameters by applying input validation to check that the data received from a user is in the expected format and to reject any input that is not. This can also limit the length of input parameters to prevent Buffer Overflows, Command, or SQL (Structured Query Language) injection attacks [6].

To enhance the security of our system, we have implemented rate-limiting and request throttling measures that improve the system resilience of the UAV. These measures help restrict the number of requests that can be sent within a specified timeframe and enable us to detect any suspicious patterns that may emerge from potential attacks. By doing so, we can reduce the likelihood of our system being overwhelmed or compromised by malicious requests. Ensuring security measures can grow with the UAV-Ecosystem, using automation and centralization will allow future scalability possible.

RESULTS AND DISCUSSION

Through this paper, we have proposed baseline guidelines that can be followed with all types of UAVs regardless of the size, type and operational environment and, without any overhead implementational complexities.

- The proposed measures include firmware encryption with AES-GCM- a lightweight cryptographic function, which is an efficient encryption algorithm that helps meet security requirements without significantly affecting the drone's performance.
- To understand the risk associated with firmware encryption of PCI buses, we have done a security and performance assessment of the UAV, as shown in Figure 2, based on the criteria of Throughput (in Gbps) based on the old, medium or high-end model, Latency (in ms)

Advantages of the Study	Shortcomings	Future Works		
We have used Authenticated Encryption (AES-GCM) to avoid boot time limitations. AES-GCM requires less computational power and bootup time compared to	AES-GCM is still perceptible to Side channel attacks such as (i) measuring coincidental hardware emissions from the UAV, and (ii) Power dump attacks these attacks aim to corrupt underlying	Future work could include working on more sophisticated countermeasures against hardware emissions measurement and power dump attacks to strengthen AES-GCM security.		
Symmetric and Asymmetric Encryption. This encryption provides secure encryption to the firmware of the UAV preventing it from direct attacks.	encryption keys and cryptographic processes to create various openings for future attacks.	Machine learning algorithms can be used to detect and respond to patterns indicative of side-channel attacks, providing dynamic defence mechanisms against them.		
To mitigate the side-channel attacks on UAVs, and to maintain the lightweight cryptographic Function efficiency we can increase the system noise in the electromagnetic waves emitted by the isotopic radiator of the UAV.	The signal sent by the UAV will have to be processed to subtract the spectral content of the noise from the signal which increases the signal processing time and uses more power on the power-limited UAV.	Future works could include working on a cloud-based noise-processing environment so that the UAV does not have to subtract the spectral content of the signal and can be handled by the cloud-based environment, removing the extra power usage on the Drones.		
This study provides a clear guide in using a Linux-based Ground station dedicated computer system to avoid other preinstalled software having vulnerabilities that could potentially risk the UAV's security.	Linux systems require specialized knowledge in setting up and maintenance. If managed correctly could result in challenges for users who are unfamiliar with Linux, potentially leading to misconfigurations, security oversights, or operational issues.	The focus of future works would be on creating and developing automated configuration scripts to avoid unfamiliar users to Linux from harbouring misconfigurations and security oversights. Further reducing operational issues.		
We have used SNORT NIDS to identify and categorize malicious network activity and inorganic traffic based on signature- based anomaly detection. SNORT generates alerts to notify the network administrator of potential security threats before an attacker can cause damage to the network.	A major drawback of this advantage is SNORT NIDS identifies inorganic traffic by establishing a normal behaviour baseline for an entire UAV-Ecosystem's network activity if it incorrectly identifies a false negative then the normal baseline will be disrupted resulting in allowing future attacks of a similar kind to disrupt the services of the network.	To minimize such false negatives in future works we can use adaptive algorithms that dynamically adjust the normal behaviour baseline of SNORT NIDS based on real- time changes done by the maintenance engineers.		
Obfuscating SSID from network broadcast scans so that network scans from Wireshark and Airodump-ng become more difficult for the Attacker. This method can protect the UAV Ecosystem against passive scans, the SSID will still be visible in the beacon frames	This overly aggressive dynamic adaptation can lead to an increase in false positives, and it could also prevent legitimate users from connecting to the UAV Ecosystems network.	The focus of our future work would be to develop more effective methods for hiding the SSID from broadcast scans. And reducing overly excessive dynamic adaptation.		
which could result in gaining system access via frag attack.				
To protect our web applications and APIs from malicious input parameters, Filter scrubs and dynamic whitelisting are techniques used to protect the UAV and its ecosystem's Web Applications Interface and Application Program Interface from malicious activities.	As mentioned before this method has added an overly aggressive dynamic adaptation that can lead to an increase in false positives.	The focus of our future work would be to reduce excessive dynamic adaptation to eliminate the number of false positives.		
We also propose to use Rate-limiting and request-throttling measures to serve as effective safeguards by restricting the number of incoming requests within a specified timeframe and enabling us to detect any suspicious activities and patterns that may emerge from potential attacks.				

Table 2. Comparative Study of Advantages and Shortcomings of our Paper
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and Entropy calculation (in Nat) under multiple security matrices.

- Balancing security with resource constraints, intrusion detection systems (IDS) like SNORT may generate false positives, flagging legitimate activities as security threats. While SNORT provides signature-based and anomaly-based detection, dynamic whitelisting can help reduce false positives.
- Additional signal processing time is required when enhancing UAV security through the addition of signal noise.
- An increase in power consumption can be observed as a consequence of implementing certain security measures for UAV protection against side-channel attacks.

We have also listed the advantages, shortcomings and a brief explanation about future works that can be achieved with the obtained results as shown in Table 2.

By carefully balancing these security measures and addressing their interactions with UAV Ecosystems, drone operators can enhance security while minimizing the disruptions to UAV operations in real time.

CONCLUSION

This research paper has proposed a set of security measures to enhance the security, efficiency, functionality, and lifespan of the IoD by applying the firmware encryption, disabling non-utilized ports, blocking inorganic traffic using IDS SNORT, intrusion detection systems, obfuscating SSID from network broadcast scans, and implementing filter scrubs and dynamic whitelisting for web application interfaces. The underlying model for preventing malicious requests can be rigorously quantified and modelled, taking into account elements like attack frequency, severity, and cumulative impact, in order to extend the lifespan of a UAV and implement security measures. For this, we can first start with the groundwork of gathering historical data on attack frequency, severity, and their cumulative impact on UAV operations. This data will include successful and attempted attacks to create a proper threat model that identifies potential attack vectors, and their likelihood of occurrence. With this enough data, it can be possible to calculate the risk associated with each attack vector and prepare a countermeasure beforehand, such as firmware encryption to evade hardware-based attacks and glitches. A holistic risk assessment can evaluate the cost-effectiveness of the provided security measures and can be explored in future works. By following these protocols, we can identify the most cost-effective security measures to prolong UAV lifespan and enhance the security of the overall UAV-Ecosystem.

While these measures can provide a strong level of security, there is still room for further research to explore how additional security measures can be implemented to enhance the security of the UAV ecosystem. Furthermore, it is essential to study the potential implications of these security measures on the overall performance and efficiency of the system. Future research can also focus on developing more robust and sophisticated security solutions to effectively address the evolving security threats in the IoD. Future work will include the exploration of utilizing the IoD for secure cloud-based operations. Specifically, the focus will be on developing an efficient security framework for the cloud-based infrastructure of the IoD and UAV architecture. Additionally, further research will be conducted to explore options for hiding an SSID from broadcast scans.

To prevent passive scans from compromising the security of UAV ecosystems, disabling probe response can be an effective measure. However, it's important to note that the SSID will still be visible in the beacon frames. Moreover, we will look into ways of preventing active scanning, which detects hidden networks and prevents legitimate users from connecting to the UAV ecosystems' network. These measures can be implemented to ensure the security and integrity of the UAV ecosystem.

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

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