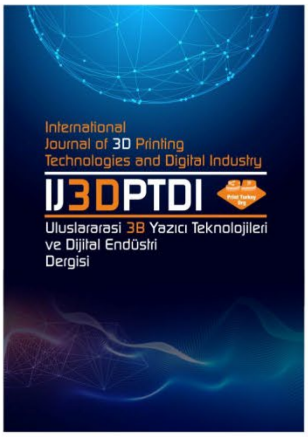

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DEVELOPMENT OF PREDICTION MODELS FOR COMPRESSIVE STRENGTH IN CEMENT MORTAR WITH BENTONITE USING MACHINE LEARNING TECHNIQUES

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ABSTRACT

In this study, the effects of bentonite-substituted cement mortar, cement compressive strength, cement quantity, spread values, water absorption percentages by weight, and porosity values on the 28-day compressive strength were investigated using Multiple Regression, Adaptive Neuro-Fuzzy Inference System and the intuitive optimization method known as Particle Swarm Optimization. Based on the results obtained from 18 data points, with 4 of them used for testing and 14 for training, effective and ineffective input parameters were identified in comparison to Multiple Regression. Subsequently, Particle Swarm Optimization and Adaptive Neuro-Fuzzy Inference System main models were designed according to the obtained results. As a result of the study, it was determined that cement compressive strength, cement quantity and water absorption parameters have a higher impact on compressive strength compared to other parameters. It was found that the best accuracy model was achieved with the Particle Swarm Optimization model, and the results of the Multiple Regression model can also be used in predicting outcomes.

Keywords: Bentonite-Substituted Cement Mortar, Cement Compressive Strength, Multiple Regression, Particle Swarm Optimization.

1. INTRODUCTION

Due to its porous structure, concrete absorbs water, leading to permeability within the concrete. Various mineral and chemical additives are used to mitigate the water permeability of concrete. One of these mineral additives is bentonite. Bentonite is a type of montmorillonite mineral formed through the weathering of volcanic ash deposits over millions of years [1]. Bentonites are classified into three groups: sodium bentonite, calcium bentonite, and active sodium-calcium Bentonite [2]. Bentonite finds applications in civil engineering, pelletizing iron ores, clarifying wine and fruit juices, animal feed, pharmaceuticals, rubber industry, paper industry, ceramic industry, petroleum refining, wastewater treatment, paint industry, fire extinguishers, fertilizer production, soil improvement, and drilling operations. One of the most significant characteristics of bentonite is its high silica content, which imparts its binding properties.

When bentonite undergoes hydration, it swells, creating a gel-like structure, and this condition imparts excellent water absorption and water retention properties to Bentonite [3]. Due to this property, bentonite can be used in the construction industry to create impermeable surfaces. Yang et al. [1], observed that by substituting natural sodium bentonite at a rate of 8% by weight in cement, after drying it in an oven at 105°C for 6 hours, it exhibited superior performance in terms of compressive strength, flexural strength, and impermeability compared to the reference sample. Wei et al. [4], have indicated that metakaolin and bentonite-substituted cements can effectively reduce concrete deterioration caused by ASR (Alkali-Silica Reaction). Memon et al. [5], found that bentonite-substituted cements perform effectively on surfaces exposed to acidity.

In addition, there is a need for the use of applications that predict concrete properties to ensure the safe utilization of materials incorporated into concrete mixtures [6]. In the literature, various studies exist where concrete's compressive strength [6–11], flexural strength [12], service life [13], workability [14] and creep behavior [15] have been predicted using different methods.

The most common methods among these include ANN (Artificial Neural Network) [16–30], SVM (Support Vector Machine) [31–37], GPR (Gaussian Process Regression) [38–44], RSM (Response Surface Methodology) [16, 18, 45], ANFIS (Adaptive Neuro-Fuzzy Inference System) [46–55] FL **(**Fuzzy Logic) [56–65] and also statistical methods such as [7, 32, 53, 66–72] and others.

In this context, the mechanical property of compressive strength of bentonite-substituted cement mortar was attempted to be determined in the study. Parameters such as cement type and substitution rate, as well as fresh property represented by the spread diameter and physical properties including hardened density, porosity, and water absorption by weight were considered. Among these properties, the significant ones were identified, and models were created using both these significant properties and all the properties combined. Models used for prediction were generated using MR (Multiple Regression), ANFIS, and the heuristic optimization method known as PSO (Particle Swarm Optimization). The prediction values obtained from these models were compared using R^2 and RMS (Root Mean Square), and the model that predicted the compressive strength of bentonite-substituted cement mortar without conducting destructive testing such as a compressive strength test was determined.

2. MATERIAL AND METHOD

2.1. Material

In the study, materials such as water, CEN standard sand, and cement types CEM I 42.5 R and CEM I 52.5 R, along with the cement substitute material bentonite, were used. The bentonites used in the preparation of bentonite-substituted cement mortar samples were ground and sieved. In order to determine the physical properties of the mixtures, sieve analysis, specific gravity, and specific surface area (Blaine fineness) tests were conducted according to the EN 196-6 standard. Subsequently, chemical analyses were carried out. Chemical data for the binding materials used in cement production are provided in Table 1, while physical data can be found in Table 2.

Table 1. Chemical properties of binding materials

Components	CEM I 42.5 R (%)	CEM I 52.5 R (%)	Bentonite (%)
SiO_2 (S)	21.12	20.57	63.2
Al_2O_3 (A)	6.03	4,6	14.27
Fe_2O_3 (F)	3.2	2.5	0,55
CaO	62.11	64.8	3.91
MgO	2.2	1.28	4.02
SO_3	2.69	3.25	-
Na_2O	0.35	0.21	0.17
K_2O	1.1	0.36	0,61
Cl^-	0.0068	0.01	-
TiO_2	-	-	0.03
LOI	2.79	3.18	14.46
S+A+F	30.35	27.67	78.02

Table 2. Physical properties of binding materials

Materials	Grain size (plus sieve) >40μm (%)	>90μm	Specific gravity (g/cm^3)	Specific surface (Blaine) (cm^2/g)
CEMI 42.5	15.6	7.9	3.08	3526
CEMI 52.5	1	0.1	3.11	4480
Bentonite	1.2	0.1	2.80	4700

Bentonite was substituted in bentonite-substituted cement mortar in proportions of 0%, 2.5%, 5%, 7.5%, 10%, 12.5%, 15%, 17.5%, 20%, 22.5%, 25%, 27.5%, and 30%, instead of CEM I 42.5 R and CEM I 52.5 R type cements. The codes and mixture information of bentonite-substituted cement mortar samples are provided in Table 3.

Table 3. Codes and mixture ınformation of mortar samples

Mixture code	Water (g)	CEM I 42.5 (g)	CEM I 52.5 (g)	Bentonite (g)	Standard sand (g)
A0		450.00	-	-	
A2.5		438.75	-	11.25	
A5		427.50	-	22.50	
A7.5		416.25	-	33.75	
A10		405.00	-	45.00	
A12.5		393.75	-	56.25	
A15		382.50	-	67.50	
A17.5		371.25	-	78.75	
A20	225.00	360.00	-	90.00	1350.00
B0		-	450.00	-	
B2.5		-	438.75	11.25	
B5		-	427.50	22.50	
B7.5		-	416.25	33.75	
B10		-	405.00	45.00	
B12.5		-	393.75	56.25	
B15		-	382.50	67.50	
B17.5		-	371.25	78.75	
B20		-	360.00	90.00	

The statistical analysis of the training parameters used in the model is provided in Table 4, while the statistical analysis of the test parameters used in the model is presented in Table 5.

Table 4. Statistical analysis of the training parameters used in the model

	Cement strength (MPa)	Cement amount (g)	Spread (cm)	Water absorption (%)	Porosity (%)	Density (g/cm^3)	Compressive strength (MPa)
Average	47,50	405,00	16,72	7,70	15,20	2,17	49,38
Standard error	1,39	8,75	0,19	0,16	0,31	0,00	1,53
Median	47,50	405,00	16,60	7,67	15,21	2,17	49,95
Standard deviation	5,19	32,72	0,72	0,60	1,18	0,01	5,73
Sample variance	26,92	1070,91	0,52	0,35	1,38	0,00	32,87
Kurtosis	-2,36	-1,48	0,24	-0,76	-1,62	-0,63	-0,75
Skewness	0,00	0,00	0,88	0,45	0,09	-0,08	-0,35
Range	10,00	90,00	2,41	1,87	3,37	0,04	17,95
Minimum	42,50	360,00	15,80	6,95	13,62	2,15	39,20
Maximum	52,50	450,00	18,21	8,82	16,99	2,19	57,15
Confidence level (95,0%)	3,00	18,89	0,42	0,34	0,68	0,01	3,31

Table 5. Statistical analysis of the test parameters used in the model

	Cement strength (MPa)	Cement amount (g)	Spread (cm)	Water absorption (%)	Porosity (%)	Density (g/cm^3)	Compressive strength (MPa)
Average	47,50	405,00	16,58	7,61	15,33	2,17	49,81
Standard error	2,89	10,27	0,21	0,21	0,54	0,01	2,99
Median	47,50	405,00	16,55	7,57	15,41	2,17	49,91
Standard deviation	5,77	20,54	0,41	0,42	1,09	0,02	5,97
Sample variance	33,33	421,88	0,17	0,18	1,19	0,00	35,66
Kurtosis	-6,00	-3,30	1,28	0,56	-0,95	-3,90	-3,79
Skewness	0,00	0,00	0,36	0,57	-0,34	-0,37	-0,06
Range	10,00	45,00	1,00	1,01	2,53	0,03	12,84
Minimum	42,50	382,50	16,10	7,15	13,99	2,15	43,28
Maximum	52,50	427,50	17,10	8,16	16,52	2,18	56,12
Confidence level (95,0%)	9,19	32,68	0,65	0,68	1,73	0,02	9,50

2.2. Methods

2.2.1. Production Method

In the Hobart mixer's bowl, water, binding material (cement with bentonite admixture), and CEN standard sand were sequentially added, and the device was operated until the mixture became homogeneous. Then, the device was stopped, and the portion that was not well mixed under the bowl and adhered to the mixer blade was scraped into the bowl to ensure homogeneity. The mixture was then operated for a sufficient duration. After the mortar was subjected to the spread test, hardened mortar specimens were produced in 4x4x16 cm molds. The specimens were removed from the molds 24 hours after production and placed in a curing tank. After a curing period of 28 days, physical tests (water absorption, porosity, and density) and mechanical tests (compressive strength) of the specimens were completed.

2.2.2. Multiple Regression

MR is used to predict or model a dependent variable (output) using one or more independent variables (input).

MR is expressed as a linear function, as specified in Equation 1 [73]. (In the equation; Y represents the dependent variable, A represents the constant coefficient, B represents the regression coefficients, X represents the independent variables, and n represents the number of inputs.)

$$Y = A + B_1X_1 + B_2X_2 + B_3X_3 + \ldots + B_nX_n \quad (1)$$

2.2.3. Particle Swarm Optimization

PSO is a metaheuristic optimization algorithm used for the purpose of optimizing a problem, based on the movement of birds flying in flocks. In PSO, the position of each particle in the swarm (Equation 2), the velocity of each particle in the swarm (Equation 3), and the velocities of all particles are updated based on their fitness within the boundary values of particles (Equation 4) (Equation 5). The obtained velocity is then updated by adding it to the previous particle position (Equation 6), and in this way, an optimization algorithm is formed [74]. (In the equations, the symbol X_{id} represents the position, V_{id} represents the velocity, W represents the inertia weight, and C_1 and C_2 represent the scaling factors.)

$$\begin{matrix} X_{11} & X_{12} & X_{1n} \\ ' & ' & ' \\ X_{m1} & X_{m2} & X_{mn} \end{matrix} \quad (2)$$

$$\begin{matrix} V_{11} & V_{12} & V_{1n} \\ ' & ' & ' \\ V_{m1} & V_{m2} & V_{mn} \end{matrix} \quad (3)$$

$$\begin{pmatrix} f(1) = & f(X_{11}, X_{12} \ldots\ldots X_{1n}) \\ f(m) = & f(X_{m1}, X_{m2} \ldots X_{mn}) \end{pmatrix} \quad (4)$$

$$V_{id} = W * V_{id} + C_1\, x\, rand * (pbest_{id} - X_{id}) + C_2 * rand * (gbest - X_{id}) \quad (5)$$

$$X_{id} = X_{id} * V_{id} \quad (6)$$

2.2.4. Adaptive Neuro-Fuzzy Inference System

ANFIS is an artificial intelligence model designed for solving prediction problems by combining fuzzy logic and artificial neural networks, enabling data-driven and optimized inference.

The ANFIS model consists of five layers (fuzzification rule normalization fuzzyfication sum) and If-then rules are applied as in Equation 7 and Equation 8 [75-78]. (In the equations, the symbols x and y represent input parameters, A_1, A_2, B_1, and B_2 represent fuzzy sets, p_1, p_2, q_1, q_2, r_1, and r_2 represent output parameters, and f represents the output parameter of the ANFIS model.)

$$Rule\ 1: if\ x\ is\ A_1\ and\ y\ is\ B_1, then\ f_1 = p_{1x} + q_{1y} + r_1 \quad (7)$$

$$Rule\ 2: if\ x\ is\ A_2\ and\ y\ is\ B_2, then\ f_2 = p_{2x} + q_{2y} + r_2 \quad (8)$$

2.2.5. The Wilcoxon Test

The Wilcoxon test is a statistical method used to compare data when the normal distribution assumption is not met or when the data does not follow a normal distribution. To achieve this objective, the absolute values are computed using Equation (10), while the discrepancies between quasi-observations are determined based on Equation (9) [79]. T^+ represents the sum of rows marked with plus signs, while T^- represents the sum of rows marked with minus signs (Equation 11) [80].

$$D_i = X_i - Y_i \quad (9)$$

$$|D_i| = |X_i - Y_i| \quad (10)$$

$$T = T^{+} - T^{-} \quad (11)$$

The difference between the first half of the data, Xi, and the second half, Yi, is represented by the value Di, which serves as the test statistic for Wilcoxon, defining the trend conditions, indicated by Zw Zα/2 value in Equation (12) (for two tails) [80]. The numerical mean is denoted by μT, and the standard deviation is denoted by μT, both assumed to be zero [81]. $T^{+}= T^{-}$, indicating that the amount of difference between trial outcomes, both good and bad, is equal [80].

$$Z_W = \frac{T-\mu_T}{\sigma_T} = \frac{T}{\sigma_T} \quad (12)$$

3. RESULTS AND DISCUSSION

In the experimental results, out of the 18 values obtained from the samples, four were set aside for testing, and the remaining 14 were used for training. In the study, first, an MR model was created. Based on the results obtained from this model, PSO and ANFIS main models were designed.

Based on the available training data, an MR model was constructed, and adjusted R^2 values were examined at each stage (Table 6). Consequently, effective and ineffective input parameters were determined relative to MR. While R^2 values may increase with each new parameter, adjusted R^2 values can remain constant or decrease. Parameters associated with a constant or decreasing value can be considered as having no effect. In this study, based on this analysis, both MR, ANFIS, and PSO models including all input parameters were created, and models excluding parameters based on adjusted R^2 values were also constructed. In a single-input, single-output model, the input parameter was chosen as cement strength, and an adjusted R^2 value of 0.598 was found. Then, when the cement quantity was added, it was observed that this value increased to 0.983. However, with the addition of the third parameter, due to the decrease in the adjusted R^2 value to 0.982, it was determined that the spread table value might not be used in the model. The water absorption value was introduced in the fourth step, and because it raised the value to 0.989, it was concluded that this parameter is significant. Subsequently, the inclusion of porosity and density in the following step was found to have no effect on the results.

Table 6. The contributions of the parameters included in the model to R^2 and adjusted R^2

Model	Added	R^2	adjusted R^2
Cement strength	Cement strength	0.629	0.598
Cement strength + cement amount	Cement amount	0.986	0.983
Cement strength + cement amount + spread	Spread	0.986	0.982
Cement strength + cement amount + spread + water absorption	Water absorption	0.993	0.989
Cement strength + cement amount + spread + water absorption + porosity	Porosity	0.993	0.988
Cement strength + cement amount + spread + water absorption + porosity + density	Density	0.993	0.987

Due to the results of the adjusted R^2 values, it was determined that cement strength, cement quantity, and water absorption were more important among the 6 input parameters. Therefore, in both MR, PSO, and ANFIS, models were created with both 6-parameters and 3-parameters. The formulas for the models created with MR were determined as shown in Equation 13 and Equation 14.

$$BD = 0.714X_1 + 0.019X_2 - 0.126X_3 - 4.138X_4 - 0.273X_5 + 26.127X_6 - 17.88 \quad (13)$$

$$BD = 0.789X_1 + 0.034X_2 - 4.032X_4 + 29.004 \quad (14)$$

Table 7. The comparison of MR models

Model	Training R^2	Error (%)	Test R^2	Error (%)
3-parameter MR	0.9925	0.84	0.9987	0.88
6-parameter MR	0.9881	2.62	0.9931	2.36

When examining the R^2 values and error values in both models, it was observed that the 3-parameter regression model yielded better results (Table 7). As seen in this model as well, instead of using all available parameters in the model, conducting a preliminary evaluation to identify effective parameters is crucial.

In the second part of the study, models created with PSO were developed. In these models, a six-input model was used, and a three-input model was created based on the adjusted R^2 value (Equation 15-16).

$$BD = 0.838X_1 + 0.059X_2 - 0.298X_3 - 3.11X_4 + 0.085X_5 + 3.76X_6 + 4.85 \quad (15)$$

$$BD = 0.79X_1 + 0.033X_2 - 4.189X_4 + 29.294 \quad (16)$$

Table 8. The comparison of PSO models

Model	Training R^2	Error (%)	Test R^2	Error (%)
3-parameter PSO	0.9925	0.75	0.9987	0.78
6-parameter PSO	0.9925	0.84	0.9931	0.85

When Table 8 is examined, it is observed that there is not a significant difference between both the 3-parameter and 6-parameter PSO models. Therefore, it is considered that both models can be used. The proximity of the results indicates that predictions can be made with fewer parameters, which is important both in terms of time and cost.

Finally, in the study, ANFIS models were constructed by varying the cluster numbers of input parameters, and these models are summarized in Table 9. In addition to the 6-parameter models for ANFIS, 3-parameter models were also constructed (determined based on adjusted R^2 values in MR). A common characteristic of all ANFIS models is that the training results come out close to perfection. However, in the test results, it has been revealed that most ANFIS models tend to memorize and cannot generalize. In ANFIS models, having a large number of subsets and parameters does not necessarily imply a more accurate model. In the study, it is important to identify the ideal parameters and models divided into subsets. It can be said that in the study, the model with 2-4-3 subsets, using cement strength, cement quantity, and water absorption parameters in that order, is the most suitable among ANFIS models.

Table 9. The comparison of ANFIS models

Number of clusters	Training R^2	Error (%)	Test R^2	Error (%)
2,3,3	1	0.0005	0.8213	3.7063
2,3,4	1	0.0002	0.5899	6.6289
2,3,5	1	0.0002	0.6729	14.9330
2,4,3	1	0.0002	0.9946	2.4057
2,4,4	1	0.0002	0.7800	5.0333
2,4,5	1	0.0001	0.7383	10.4069
2,5,3	1	0.0001	0.4493	9,7674
2,5,4	1	0.0001	0.1302	13,4016
2,5,5	1	0.0001	0.1847	25,0392
2,7,7	1	0.0001	0.1045	66.4502
2,3,4,3,3,3	1	0.0005	0.3019	15.3642
2,3,5,3,3,4	1	0.0005	0.3019	15.3642
2,4,3,3,3,5	1	0.0004	0.8279	15.1278
2,5,4,3,3,3	1	0.0005	0.1439	23.0605

In the study, the best results obtained in all models were compared in Table 10 and Figure 1. When examining the results, it is observed that the 3-parameter PSO model is better than all other models, but it is also possible to achieve very close results when the MR model is used. The results of the ANFIS model also approach the truth (Figure 1), but it is seen that there is a significant deviation when the correct ANFIS model cannot be established (Table 9). In addition, Wilcoxon values were also examined for the best results of each model in Table 10. According to these values, all results were found to be significant.

Table 10. The comparison of the best models

Model	Training R^2	Error (%)	Z_W	Test R^2	Error (%)	Z_W
3-parameter MR	0.9925	0.84	-1.16	0.9987	0.88	-0.73
3-parameter PSO	0.9925	0.75	-0.09	0.9987	0.78	0.01
ANFIS (2,4,3)	1	0.0002	-1.44	0.9946	2.4057	-1.83

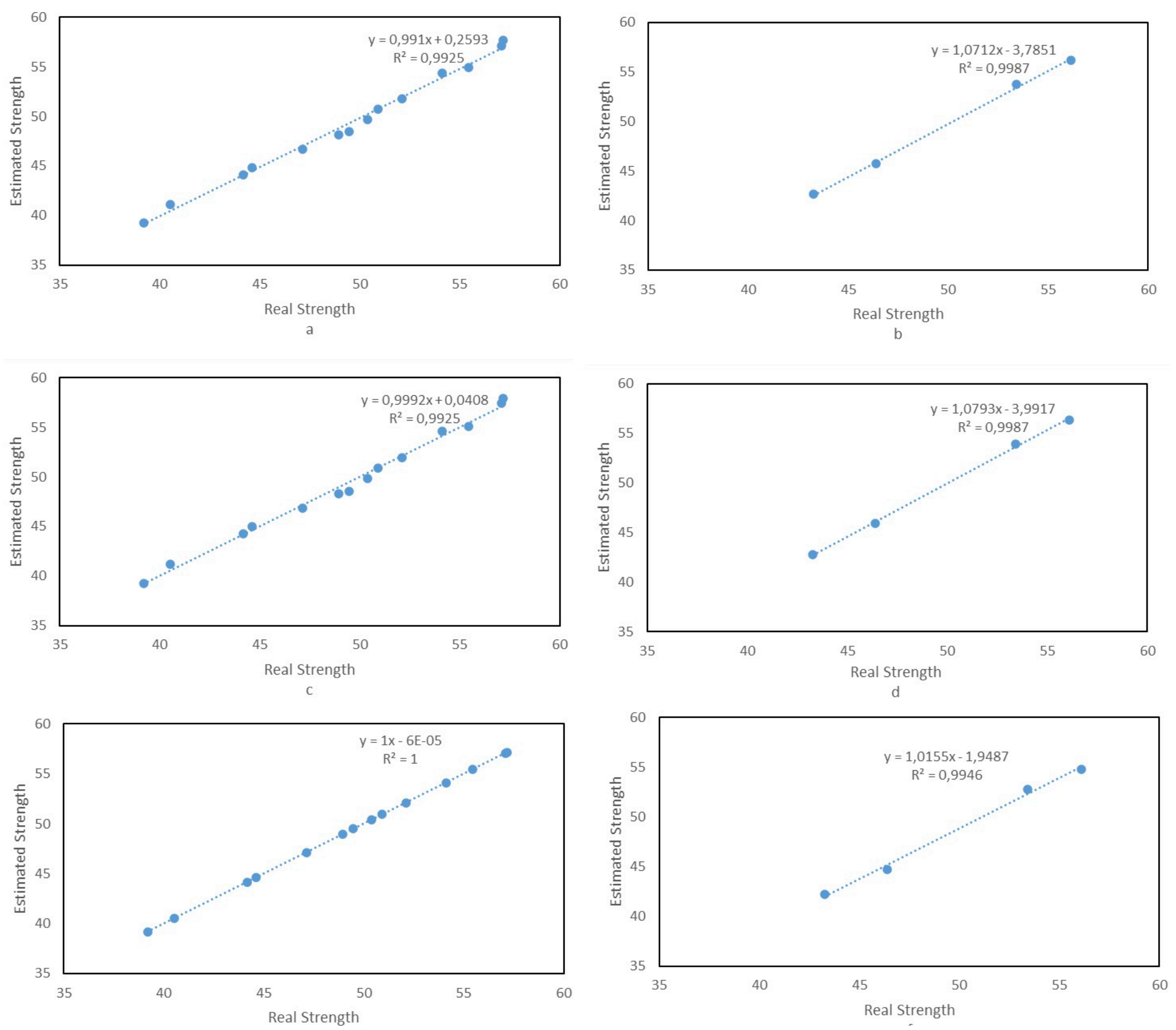

Figure 1. Comparison of scatter plots of prediction models (a-3-parameter MR training b-3-parameter MR test c-3-parameter PSO training d-3-parameter PSO test e-ANFIS (2-4-3) training f-ANFIS (2-4-3) test)

4. CONCLUSION

In this study, three models, namely MR, ANFIS, and PSO were employed to predict the compressive strength of bentonite-substituted cement mortar. The input parameters used in the models were cement strength, cement quantity, spread, water absorption, porosity, and density. The results obtained from the models indicated that both PSO and MR models could be used to predict the outcomes. However, it can be stated that cement strength, cement quantity, and water absorption parameters have a greater influence on compressive strength compared to other parameters. The results also demonstrated that PSO provided the highest accuracy in predicting the compressive strength of bentonite-substituted cement mortar. The developed PSO model can serve as a valuable database to facilitate the design of cement mortar mixtures.

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