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RHEOLOGICAL PARAMETER ESTIMATION OF CMC-WATER SOLUTIONS USING MAGNETIC RESONANCE IMAGING (MRI)

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ABSTRACT
In this study, the application of Magnetic Resonance Imaging (MRI) rheometry on the measurement of complex fluid Carboxymethyl cellulose (CMC)-water solutions (0.5%, 1.0%, 1.5%, 2.0% w/w) flow was described. Depending on CMC concentration, Power law or Herschel-Bulkley models gave the best fit according to MRI and conventional rheometer (CVO) results. Power Law model was valid for 0.5% and 1.0% CMC ($R^2=0.9993$-$R^2=0.9987$ and $R^2=0.9983$-$R^2=0.9985$ respectively by MRI and CVO). On the other hand, 1.5% and 2.0% CMC solutions flow were well described by Herschel–Bulkley model ($R^2=0.9994$-$R^2=0.9996$ and $R^2=0.9986$-$R^2=0.9981$ respectively by MRI and CVO). The MRI measurements agreed well with the CVO measurements.

Keywords: Magnetic Resonance Imaging, Conventional Rheometer, CMC, Rheology
1. INTRODUCTION

Offline methods for rheological measurements such as cylindrical coquette, cone and plate geometries (conventional rheometries) generally used for the study of fluid motion in shear. However, obtained results from these types of geometries need to be verified with suitable online or inline methods. Especially, many industrial processes, such as extrusion, transfer processes involve established or developing flows in pipes or tubes. Therefore, online techniques based on the measurement of the velocity profile in a pipe flow using Magnetic Resonance Imaging (MRI), which is a non-invasive method, and simultaneously determining the pressure drop, are promising for use a product quality or rheology control tool during the fluid flow. Magnetic resonance imaging (MRI) can be used as a viscometer, based on analysis of a measured velocity profile of fluid flowing in a tube coupled with a simultaneous measurement of the pressure drop driving the flow (Arola et al., 1997 and Arola et al., 1999).

This type of measurement is well suited for rheological characterization of non-Newtonian fluids (Choi et al., 2002 and Tozzi et al., 2012). To evaluate shear viscosity in tube (or capillary) flow, an incompressible fluid must undergo steady pressure-driven flow in the laminar regime. The conservation of linear momentum, which equates pressure forces to viscous forces, provides the relationship between the shear stress, \( \sigma \), and radial position, \( r \):

\[
\sigma (r) = \frac{\Delta P}{2L} r
\]

where \( \Delta P \) is the pressure drop over the tube length \( L \). The shear rate is obtained at the same radial position using the velocity profile obtained from a flow image. The expression for the shear rate in tube flow is:

\[
\gamma (r) = \frac{dV(r)}{dr}
\]

(2)

Where \( V \) is the axial velocity. Using Equations 2 and 3, the apparent viscosity \( \eta \) is determined by the ratio of shear stress to shear rate:

\[
\eta (r) = \frac{\sigma (r)}{\gamma (r)}
\]

(3)

Graphical User Interface (GUI) programs are used to analyze data and display rheological results (Choi et al., 2005 and Tozzi et al., 2012). Main step in the data processing procedure include calculating the shear stress as a function of radial position in the pipe, processing the velocity profile image to obtain a velocity profile, calculating the shear rate as a function of radial position from the velocity profile, and generating the rheogram by plotting the shear stress against the shear rate (Arola et al., 1997, Callaghan 1999 and Tozzi et al., 2012). Calculating the shear stress is straightforward as in Equation 1.

In this study, Carboxymethyl cellulose (CMC) was used as test fluid. CMC is widely used as thickener especially in food and pharmaceutical industries (Benchabane and Bekkour, 2008). This is also known as complex fluid due to no linear relationship between stress and shear rate in simple shear during the flow.

2. MATERIALS AND METHODS

2.1. Materials

The CMC, with nominal molecular weight of 250,000 g/mol was supplied from Sigma. Aqueous solutions of CMC were prepared by dissolving the appropriate amount of CMC powder in distilled water. The high CMC concentration solutions (0.5%, 1.0%, 1.5%, 2% w/w) were prepared by using water heated at 50 °C by gentle stirring with the sufficient time < 24 h.

Online and offline measurements were performed with an MRI (Magnetic Resonance Imaging) at Food and Science Technology Department at University of California, Davis, USA using flow loop depicted in Fig. 1. At 25 °C, MRI Flow Imaging Tests were done for 0.5, 1, 1.5, 2% (w/w) CMC solutions to determine rheological constitutive equations parameters. Inlet diameter of PVC tube was 38.1 mm. The test fluid was recirculated using Moyno pump (Integrated Motor Drive System, Franklin Electric) Pressure drop was obtained at the ends of pipe with a constant length of 1.68 m using pressure transducer (Siemens Company).

Fig. 1. Flow loop setup for CMC testing A) Positive displacement pump B) MRI magnet

2.2. Methods

In Fig. 2, flow image for an example of 0.5% CMC flow, can be seen with data processing window. The velocity profile is used to obtain shear rate distribution, while the pressure drop is used to calculate the shear stress distribution. By taking the ratio of these quantities at a radial position, local viscosity can be obtained within the shear rate range in the flow, zero at the center, and maximum at the wall, within minutes. There is not observed slip effect on the wall as in Fig. 2.

Fig. 2. MRI Image for 0.5% CMC
Fig. 2 shows the flow curves of the CMC solutions at different concentrations. Instrument CVO rheometer (Bohlin Insruments) with a cone and plate rheometer (with a cone angle 4° and diameter 40 mm) at 25 °C was used for offline measurement. A steady state shear rate ramp from 0.085 to 10 s⁻¹ was performed in logarithmic mode with 10 points/decade.

3. RESULTS AND DISCUSSIONS

For MRI measurements at the different pump speed of flow loop and also measured using a conventional technique and the agreement between the results is satisfactory shown in Figure 3. MRI measurement results of CMC solutions are also listed in the Table 1 with changing pump speed of flow loop shown in Fig. 3.

All obtained rheograms for different CMC solutions are as listed in Table 1. Rheological properties are independent of flow velocity. Hence, zero shear viscosities are nearly constant during the flow. As Reynolds number and concentration of flow increased, fluid shear stress acting on the pipe wall also increased as seen in Table 1.

Rheological parameters for CMC solutions are also listed in Table 2. Depending on CMC concentration, Power law or H.Bulkley models give the best fit according to MRI flow result using Equations 4 and 5 respectively. Power Law model is valid for 0.5% and 1.0% CMC. On the other hand, 1.5% and 2.0% CMC solutions flow are well described by Herschel-Bulkley model.

\[ \sigma = K\gamma^n \]  
\[ \sigma = \sigma_0 + K\gamma^n \]
In Equations 4 and 5, consistency index, K, and power law index, n, and yield stress, \( \sigma_0 \), data values are obtained from shear stress v.s. shear rate data using online (MRI Rheometry) method and offline (CVO Rheometry) method. R\(^2\) values of the fittings are also satisfactory. As CMC concentration increased, yield stress gets larger and elastic forces dominate the viscoelastic flow medium (Nguyen & Boger, 1992).

### Table 2. Rheological Parameters for CMC-water solutions

<table>
<thead>
<tr>
<th>MRI Rheometer</th>
<th>CVO Rheometer</th>
<th>Goodness of the fit R(^2) (MRI-CVO)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.5% CMC</td>
<td>K=0.350</td>
<td>0.733</td>
</tr>
<tr>
<td></td>
<td>n=0.312</td>
<td>0.730</td>
</tr>
<tr>
<td>1.0% CMC</td>
<td>K=0.825</td>
<td>0.653</td>
</tr>
<tr>
<td></td>
<td>n=0.863</td>
<td>0.670</td>
</tr>
<tr>
<td>1.5% CMC</td>
<td>K=0.436</td>
<td>0.607</td>
</tr>
<tr>
<td></td>
<td>n=0.424</td>
<td>0.607</td>
</tr>
<tr>
<td>2.0% CMC</td>
<td>K=0.545</td>
<td>0.405</td>
</tr>
<tr>
<td></td>
<td>n=0.150</td>
<td>0.507</td>
</tr>
</tbody>
</table>

### 4. CONCLUSION

MRI velocity measurements with a pressure drop measurements allows a relationship between shear rate and shear stress and yields a rheological parameters measurements. A rheological investigation of CMC flow of 0.5%, 0.10%, 0.15%, 0.20% w/w concentrations in MRI and CVO was presented. The following conclusions can be highlighted from the results of the study:

- Rheological parameters are independent of flow conditions.
- 0.5% and 1.0% w/w CMC are suited with Power law model. 1.5% and 2.0% CMC w/w solutions flow are well described by Herschel-Bulkley model.
- Online and offline measurement results are good agreement with each other.
- MRI flow imaging is suitable for evaluations of rheological parameters of CMC solutions even in high concentration of 1.5 and 2.0% w/w CMC.

### REFERENCES


### ACKNOWLEDGEMENTS

Authors would like to thank Prof. Dr. Micheal J. McCarthy for his help and open his laboratory in Food Science and Technology Department, UC, Davis, USA.
INVESTIGATION OF Ni-Mn BASED SHAPE MEMORY ALLOY VARIATIONS TRANSFORMATION TEMPERATURES

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ABSTRACT
Shape memory alloys’ usage frequency and areas are increased day to day. It is seen the different type and different characteristics in many industrial areas. Therefore, shape memory alloys, which are intelligent materials, are very fast to develop. The NiTi alloys, from these alloy types, are most commonly used due to their low hysteresis range and biocompatibility. But production costs and difficulties have led, investigators to investigate different alloy types. Shape memory alloys which produced with possibly cheaper elements, examined in researchers with looking at their transformation temperatures.

Keywords: Doc, NiTi, Shape Memory Alloys
1. INTRODUCTION

Shape memory alloys (SMA) are materials known as intelligent metals from the past to present day. In the past, SMA’s found in various composition ratios of constrained elements are alloyed with many elemental ingredients now (Canbay, 2017). SMA’s shed light on future systems and applications at a high level. The technologies that will be developed with unique features will provide great advantages and their usage will be necessary. High strength, biocompatibility, high wear resistance, high corrosion resistance, working in high temperature and pressure, elasticity ductility etc. intelligent metal alloys are made depending on the needs of the sectors. Healthcare field, defense, and military fields, mechanical systems, automotive sectors etc. (Canbay et al., 2014; Canbay, 2017; Canbay et al., 2017; Canbay et al., 2018). SMA’s are required to be developed and used in the fields. Producing SMA’s according to the needs of the areas to be used will be the best course of approach. In order to meet the requirements of the application areas of SMA materials, the alloys must be full-featured and very diverse. Once the SMA’s are approached, technology and sectors will be advantageous and the work on these intelligent materials will become more important. The SMA’s are a very valuable issue for the Research & Development area. Considering the advantages and convenience of intelligent materials, it is a bright field of materials that many industries in the manufacturing and the business world will not spare their investments and supports (Eskil et al., 2015). SMA’s have a certain high temperature phase and low temperature phase according to their element proportion that they contain. The high temperature phase is called the austenite phase, the low temperature phase is called the martensite phase. According to the phase temperature limits, it is determined at which temperature degree the shape memory conversion. This phase change is due to solid-state phase change. In general, the memory-trained shape will talk about memory formation; The SMA material is subjected to shape training. This is another issue that needs to be addressed in more detail (Ozkul et al., 2017). However, in the rough description of the work, the shape desired to be taken into memory is usually placed in a mold and heated to a high temperature austenite phase under tension. The alloyed material is converted to the low temperature martensite phase by shock cooling after heating to the austenite phase (Aldas et al., 2014). This cycle is repeated according to the type of material and the methods have differed one-way or two-way. After this process, the SMA will save it in the memory, which is determined in advance of the applied processes. After this step, heat, stress, or both subjected to the plastic deformation that has been exposed and the shape changes back to the SMA as it was recorded in the memory when heated from high to the high temperature austenite phase. It takes its place in the group of intelligent materials (Canbay et al., 2014). It has been stated that the SHA’s have various advantageous properties according to the proportion of the elements they contain. Today, many test and screening systems are used in determining these properties. The most common of these is the differential scanning calorimetry (DSC). The DSC test is an important test for determining the temperature points and boundaries of the austenite and martensite phases, which are very important in the memory acquisition of SMA’s. The results of DSC scanning of various alloys of elements such as nickel, manganese, gallium, iron, aluminum, and tin have been examined in the literature review. The start and finish temperatures of the austenite and martensite phases were determined. The effect of element contents on phase transformation temperatures was investigated (Aldas et al., 2016).

The austenite-initiation temperature (A_s) is the temperature at which this transformation begins, and the austenite-final temperature (A_f) is the temperature at which this transformation is complete. When the SMA heats up, the contract starts and returns to its original state. This conversion is possible even at high applied loads and, therefore, results in a high energy density of the trigger. During the cooling process, the transformation starts at the martensite starting temperature (M_s) and completes when the martensite reaches the finishing temperature (M_f) (Buehler et al., 1963). Martensite is called the highest temperature M_f that can be caused by residual stress, and when it is above this temperature, SMA permanently deforms like ordinary metallic materials (Duerig et al., 1994). These deforming effects, known as SMA and pseudo elasticity (or super elasticity), can be categorized according to three-dimensional memory properties:

- One-way shape memory effect (OWSME): The unidirectional SMA (SMA) maintains a deformed condition after removing an external force and then returns to its original state upon heating.
- Two-way shape memory effect (TWSME) or reversible SME: In addition to the one-sided effect, bi-directional SMA (TWSMA) can remember both high and low temperature shape. Often the recovery provided by OWSMA for the same material (Schroeder et al., 1977; Huang et al., 2000) yields about half of the water, and this stress tends to deteriorate quickly, especially at high temperatures (Ma et al., 2010). For this reason, OWSMA offers a more reliable and economical solution (Stöckel 1995).
- Pseudo elasticity (PE) or Super elasticity (SE): The SMA returns to its original shape after applying the mechanical load without the need for any thermal activation at temperatures between A_s and M_f.

In addition to the TWSME material above, the prejudicial OWSMA actuator can also function as a 'mechanical TWSME' at a macroscopic (structural) level; more robust, reliable, and widely applied in many engineering applications (Sun et al., 2012). This feature is important and should be considered carefully when selecting SMA materials for targeted applications. For example, a small hysteresis is needed for applications where rapid movement is necessary (robotic applications) (Liu, 2010). The physical and mechanical properties of some SMAs also vary between these two phases, such as Young’s modulus, electrical resistance, thermal conductivity, and thermal expansion coefficient (Mihálec, 2001; Mertmann et al., 2008; Sreekumar et al., 2009). The austenite structure is rigid and has a high Young’s modulus. The martensite structure is softer. It can easily deform with the external load (Hodgson et al., 1990; Mihálec, 2001).

There are three varieties of SMA. These alloys are listed in the literature as NiTi, copper based and iron.
based. The most capable of these alloy types is NiTi alloys. Because these alloy types have biocompatibility, they are used in many fields, especially in the field of medicine. Copper-based SMA is the closest to this type of alloy. But there is no popular. Iron-based SHA is the weakest type in this group because they have high hysteresis. In our study, the data of alloy types which may be alternative to NiTi-based SMA will be examined. The temperature transformation points of the austenite and martensite phases of the samples were determined and analyzed on the table and the thermal properties of the shape memory alloys were obtained.

2. LITERATURE REVIEW

The starting and ending temperatures of the austenite high temperature phase and the martensite low temperature phase are determined and tabulated in the literature review. The bibliographic numbers of the literature search of the thermal values of SMA’s are listed at the beginning of the table as (Kainuma et al., 1996; Jiang et al., 2002; Jiang et al., 2003; Wu et al., 2003; Koho et al., 2004; Lanska et al., 2004; Glavatskyy et al., 2006; Koyama et al., 2006; Babita et al., 2007; Santos et al., 2008; Aksoy et al., 2009; Wu et al., 2011; Zheng et al., 2011; Turabi et al., 2016; Caputo et al., 2017; Mostafaei et al., 2017). The transformation temperatures obtained by different element contributions of Ni and Mn-based SMA materials are shown in Table 1.

2.1. Evaluation of Literature Review

In the direction of information from the source if we evaluate the change of austenite and martensite starting end temperature points by changing atomic ratios of nickel, manganese and aluminum elements. In the first sample, nickel and manganese were alloyed at 50 percent and specific temperature points were obtained. It has been observed that the austenite and martensite phase change temperatures are lowered when aluminum is added to this alloy and the manganese proportion is reduced (with the nickel ratio being kept constant). It is observed that when the aluminum ratio is kept constant and the nickel ratio is increased and the manganese ratio is decreased, the phase change temperatures are increased (Kainuma et al., 1996).

Increasing the tin ratio in nickel, manganese and tin alloys has clearly reduced the phase conversion temperature (Koyama et al., 2006; Santos et al., 2008; Zheng et al., 2011; Turabi et al., 2016). Nickel, manganese and antimony triple alloys have been investigated, and when the antimony ratio in the alloy is reduced, the transformation temperatures of the austenite and martensite phases have increased at a high rate. As a result of this observation, antimony addition reduces the high conversion temperatures (Aksoy et al., 2009).

Nickel, manganese, and gallium ternary alloys have clearly reduced the phase conversion temperature (Koyama et al., 2006; Santos et al., 2008; Zheng et al., 2011; Turabi et al., 2016).

Nickel, manganese, and gallium ternary alloys have been added to the dysprosium element and the effects on the temperature values were observed. When the dysprosium element increased, the phase transformation temperatures increased (Babita et al., 2007).

Nickel, manganese, gallium triple alloy system is added to the silicium element. As the silicium ratio increased, the phase transformation temperatures decreased. When cobalt element is added instead of silicium, cobaltite phase transformation temperatures are lowered in the same way and the austenite and martensite start-finish transformation temperatures are increased by increasing the nickel ratio (Glavatskyy et al., 2006).
Table 1. Transformation temperatures obtained by different element contributions of Ni and Mn based shape memory alloy materials

<table>
<thead>
<tr>
<th>Ref.</th>
<th>Ni (at.%)</th>
<th>Mn (at.%)</th>
<th>Ga (at.%)</th>
<th>Fe (at.%)</th>
<th>In (at.%)</th>
<th>Si (at.%)</th>
<th>Co (at.%)</th>
<th>Dy (at.%)</th>
<th>Al (at.%)</th>
<th>Sn (at.%)</th>
<th>Sb (at.%)</th>
<th>In (at.%)</th>
<th>Co (at.%)</th>
<th>Ms (°C)</th>
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3. CONCLUSION

Shape memory alloys are defined undeniably positioned in the technology. However, in terms of production costs, it is necessary to search for alloy types that will become an alternative to high-grade alloys such as NiTi and to present the service of humanity. From this point of view, successful studies with elements such as manganese, which can be provided as cheaper than the titanium element in nickel-based SHA, have been investigated. It has been found that in the determined thermal phase temperature transformations, the alloys' high nickel, manganese and gallium ratios are largely determinative. As a result of these studies, a wide range of transformation temperatures have been identified and found to be open to Research & Development. These types of alloys that provide the wide range of conversion can respond to many needs.

REFERENCES


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INVESTIGATION OF DISSOLUTION KINETICS OF Zn AND Mn FROM SPENT ZINC-CARBON BATTERIES IN SULPHURIC ACID SOLUTION

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ABSTRACT
The aim of this study is to examine the dissolution kinetics of zinc and manganese from spent zinc-carbon battery in sulphuric acid solution. The leaching experiments were carried under the following conditions: leaching temperatures of 30°C, 40°C and 50°C; sulphuric acid concentration of 0.5 M; stirring speed of 400 rpm; solid/liquid ratio of 5/500 g/mL; and particle size of -53 µm. In these conditions, while all of the zinc was dissolved, about 69 % of manganese was dissolved. To determine the kinetics of dissolution of the zinc and manganese in sulphuric acid medium, different shrinking core models were applied to the dissolution recoveries obtained at variable temperatures. Kinetics analysis showed that the zinc and manganese dissolution from spent zinc-carbon battery could be described by diffusion from product layer. The activation energies (Ea) and Arrhenius constants for the dissolution reactions were calculated. Activation energies (Ea) were determined for Zn and Mn as 94.53 kJ/mol and 1.41 kJ/mol, respectively.

Keywords: Leaching, Dissolution kinetics, Zn–C battery, Zn, Mn, Activation energy, Sulphuric acid
1. INTRODUCTION

Zinc-carbon type dry cell batteries are being commonly used during last 150 years in the world. There are two types of zinc carbon batteries mainly as leclanche battery and zinc chloride battery. A battery is an apparatus which converts the chemical energy into electric energy by an oxidation–reduction (redox) reaction. They are widely used in small household apparatus like flash light, toys, radios, watches, etc. In these batteries, anode material is zinc and the cathode is a mixture of manganese dioxide and carbon. Because of the spent zinc–carbon batteries contain zinc, manganese dioxide and also zinc oxide and manganese (III) oxide produced from discharging reaction (Bernardes, et al., 2004; Park, et al., 2006; Shin, et al., 2009), they are important secondary source of Mn and Zn. During discharging, a chemical change occurs in the battery which can be expressed by the following reaction:

\[ \text{Zn} + 2\text{MnO}_2 \rightarrow \text{ZnO} + \text{Mn}_2\text{O}_3 \] (1)

A lot of studies were found related with hydrometallurgical processes for recovery of manganese and zinc from spent zinc–carbon batteries in the literature (Shin, et al., 2009; Ferella, et al., 2008; Baba, et al., 2009; sayilgan, et al., 2010; Gęga and Walkowiak, 2011; Kursunoglu and Kaya, 2014; Buzatu, et al., 2014; Taner, et al., 2016; Abedin, et al., 2017; Chen, et al., 2017). Generally, these studies were carried out using only basic solution, acidic solution (hydrochloric acid, sulphuric acid) or reductive agents with these acid solutions. However, dissolution kinetics of manganese and zinc from spent zinc–carbon batteries were studied (Baba et al., 2009; Gęga and Walkowiak, 2011; Taner, et al., 2016).

Because, it is harmful to the environment discard of spent batteries is prohibited by stringent environmental regulations in most countries. In the event of the disposal or incineration of waste batteries, heavy metals may contaminate the environment. Therefore, it must be given importance to collecting and recycling of spent batteries. Prevention of environmental pollution and research for the recycling of precious metals have become an important issue. For this reason, the application of hydrometallurgical processes has been carried out considering the economic and environmental suitability.

In this work, it is aimed to dissolution of manganese and zinc in sulphuric acid solution from spent zinc carbon batteries. In addition, the dissolution kinetics were studied and the activation energies required for dissolution were calculated.

2. MATERIAL AND METHOD

In this study, spent zinc–carbon batteries were used which collected from Selçuk University spent battery boxes. The plastic, paper and metal parts were removed from the zinc-carbon batteries that were passed through processes such as separation, dismantling. The separated pieces of the spent zinc-carbon battery were weighed and the weight percentages were determined as 56.42% black paste, 13.84% steel can, 11.58% zinc can, 7.65% carbon rod, 4.65% paper, 3.33% plastic and 2.53% metal cover and bottom. The obtained black paste was dried at 105°C for 24 hours. Moisture of black paste was calculated as 12.51%. The battery powder was ground using a ball mill and sieved to obtain particle size less than 106 μm. The original powder was washed to remove electrolyte with distilled water in a glass vessel at 60°C and dried to remove external impurities at 105°C for 24 hours. Then the powder was burned for one hour at 600°C in the furnace, to remove paper, plastic and carbon residues. Sieving was carried out and –106+75, -75+53, -53 μm particle size fractions were obtained. Approximately, 2 grams of sample was weighed and dissolved in the king water (HNO₃ + HCl) in a Teflon vessel. The solutions were diluted with distilled water to 100 ml in a volumetric flask. The amount of Mn and Zn was measured using a GBC brand SensAA model flame atomic absorption spectrometer (AAS). The manganese-zinc contents of waste battery powder of the original (-106 μm), washed (-106 μm) and -53 μm particle size were given in Table 1.

### Table 1. Zn–Mn content of spent zinc–carbon battery

<table>
<thead>
<tr>
<th>Particle size, μm</th>
<th>Zn, %</th>
<th>Mn, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original (-106)</td>
<td>21.52</td>
<td>34.34</td>
</tr>
<tr>
<td>Washed (-106)</td>
<td>22.87</td>
<td>35.87</td>
</tr>
<tr>
<td>-53</td>
<td>20.11</td>
<td>36.46</td>
</tr>
</tbody>
</table>

The washed powders were analyzed by X-ray diffraction (XRD) to determine the mineralogical composition of powders and shown in Fig. 1. XRD analyses showed the presence of ZnO, MnO₂ and Mn₃O₄.
Leaching experiments were carried out in a 1 L volume of glass vessel placed in a thermostatically-controlled water bath. The leach solution was stirred by Heidolph brand RZR 2021 model mechanical stirrer with teflon lined impeller. Schematic view of the experimental procedure is given in Fig. 2. 1 mL of leaching solution was gotten from the reactor at various time intervals and diluted with water to 100 mL in a volumetric flask. The dissolution amounts of Zn and Mn were determined by AAS.

RESULTS AND DISCUSSION

3.1. Experimental Results

Leaching experiments were carried out using 500 mL solution of 0.5 mol/L sulphuric acid concentration. Battery powder in -53 µm fraction was used. 5 g of battery powder was used. Leaching solution was stirred at 400 rpm at 60 min of leaching time. Under these conditions, leaching experiments were performed at different temperatures (30°C, 40°C and 50°C). The results of these experiments, Zn and Mn extraction recoveries were given in Table 2. It can be seen from the Table 2 that Zn and Mn extraction recoveries increased with increasing temperature and leaching time. In these conditions, while all of the zinc was dissolved, about 69% of manganese was dissolved. The reason of this, since the leaching rate of manganese was increasing slightly in sulfuric acid leaching experiment, due to the insoluble of Mn$^{4+}$. The reduction potential needs to be modified to turn Mn$^{4+}$ into Mn$^{2+}$ (Takeno, 2005).

<table>
<thead>
<tr>
<th>Leaching Time (min)</th>
<th>30°C</th>
<th>40°C</th>
<th>50°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zn</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mn</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Zn</td>
<td></td>
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<td></td>
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<tr>
<td>Mn</td>
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<td></td>
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<tr>
<td>Zn</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mn</td>
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</tr>
</tbody>
</table>

3.2. Kinetic Models

Generally, the leaching process for heterogeneous reactions uses the shrinking core models controlling by chemical reaction, diffusion, and the diffusion through the product layer these kinetic models (Habashi, 1969; Levenspiel, 1999; Sohn and Wadsworth, 1986). This model was chosen because it is the most suitable model for dissolution reactions.

The dissolution of Zn and Mn from spent zinc-carbon battery can be explained by a shrinking core model which can be expressed as follows:

Table 2. Effect of temperature on Zn and Mn extraction.

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\[ a \text{Fluid} + b \text{Particle} \rightarrow \text{Product} \] (2)

To describe the dissolution of Zn and Mn from battery powder, a kinetic investigation was applied to results in Table 2. In shrinking core model, if the reaction is controlled by surface reaction,

\[ 1 - (1 - x)^{1/3} = k_s t \] (3)

if the reaction is controlled by film diffusion,

\[ 1 - (1 - x)^{2/3} = k_f t \] (4)

if the reaction is controlled by diffusion from product layer

\[ 1 - \frac{2}{3}x - (1 - x)^{2/3} = k_d t \] (5)

equations were used, where \( x \) is the fraction reacted, \( t \) is the reaction time (min), \( k_s, k_f \) and \( k_d \) are the rate constants (Levenspiel, 1999; Habashi, 1969). Eqs. (3,5) were applied to the experimental results. The correlation coefficients and apparent rate constants for each temperature were given in Table 3.

Considering the values given in Table 3, manganese and zinc dissolution from spent zinc–carbon battery could be described by the diffusion from product layer. Plots of \( 1 - \frac{2}{3}x - (1 - x)^{2/3} \) for various temperatures of Zn and Mn were given in Fig. 3 and Fig. 4.

<table>
<thead>
<tr>
<th>Temperature, °C</th>
<th>Surface Reaction 1-(1-x)^{1/3}</th>
<th>Film Diffusion 1-(1-x)^{2/3}</th>
<th>Diffusion from Product Layer 1-2/3x-(1-x)^{2/3}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Apparent rate constant ((k_s)\times10^3) for Zn</td>
<td>Correlation coefficient, ((R^2))</td>
<td>Apparent rate constant ((k_f)\times10^3) for Zn</td>
</tr>
<tr>
<td>30</td>
<td>0.74921</td>
<td>0.97</td>
<td>1.02121</td>
</tr>
<tr>
<td>40</td>
<td>4.58120</td>
<td>0.97</td>
<td>4.37922</td>
</tr>
<tr>
<td>50</td>
<td>6.57444</td>
<td>0.96</td>
<td>4.09939</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Temperature, °C</th>
<th>Surface Reaction 1-(1-x)^{1/3}</th>
<th>Film Diffusion 1-(1-x)^{2/3}</th>
<th>Diffusion from Product Layer 1-2/3x-(1-x)^{2/3}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Apparent rate constant ((k_s)\times10^3) for Mn</td>
<td>Correlation coefficient, ((R^2))</td>
<td>Apparent rate constant ((k_f)\times10^3) for Mn</td>
</tr>
<tr>
<td>30</td>
<td>1.74282</td>
<td>0.99</td>
<td>2.92762</td>
</tr>
<tr>
<td>40</td>
<td>1.22527</td>
<td>0.96</td>
<td>1.85357</td>
</tr>
<tr>
<td>50</td>
<td>1.09626</td>
<td>0.96</td>
<td>1.56221</td>
</tr>
</tbody>
</table>

Fig. 3. The variation in \( 1 - \frac{2}{3}x - (1 - x)^{2/3} \) with time at various temperatures for Zn.

Fig. 4. The variation in \( 1 - \frac{2}{3}x - (1 - x)^{2/3} \) with time at various temperatures for Mn.
3.3. Determination of Activation Energy

Apparent rate constants (k) at different temperatures were obtained from the slope of the linear plots in Fig. 3 and Fig. 4 for zinc and manganese respectively. Then the values of reaction rate constants (k) were plotted according to the Arrhenius type equation. The plot of ln k vs. \( \frac{1000}{T} (K^{-1}) \) was straight line for both zinc and manganese. The Arrhenius graphics were plotted using the apparent rate constants obtained by application of Eq. (5) (Figs. 5,6). The activation energies required for dissolution of Zn and Mn were calculated as to be 94.53 kJ/mol and 1.41 kJ/mol, respectively. Similarly, in some kinetic studies using various acid media related with zinc and manganese dissolution from spent zinc–carbon batteries, shrinking core model was used. In these studies, activation energies were given as 22.78 kJ/mol, 23.03 kJ/mol for Zn (Baba, et al., 2009; Taner, et al., 2016) and 7.04 kJ/mol, 31.80 kJ/mol for Mn, respectively (Kursunoglu and Kaya, 2014; Taner, et al., 2016).

Fig. 5. Arrhenius plot of reaction rate against reciprocal temperature for dissolution of Zn.

Fig. 6 Arrhenius plot of reaction rate against reciprocal temperature for dissolution of Mn.

4. CONCLUSION

Dissolution kinetics of zinc and manganese from spent zinc–carbon batteries in sulphuric acid solution was investigated. Therefore, leaching experiments were performed using some constant parameters (sulphuric acid concentration of 0.5 M; stirring speed of 400 rpm; solid/liquid ratio of 5/500 g/mL and particle size of -53 µm) at different temperatures (30°C, 40°C and 50°C). It was found that the dissolution rate increased with increase in the leaching temperature and leaching time. At 30°C, dissolution of Mn and Zn was reached at 60 min 50.67% and 71.35%, respectively. At 50°C, the best dissolutions of Mn and Zn were obtained as to be 68.46% and 100%.

In order to determine the dissolution kinetics of Zn and Mn, shrinking core model was applied to dissolution recoveries obtained at different temperatures. It was determined that zinc and manganese dissolved in sulphuric acid solution from spent zinc–carbon batteries by diffusion from product layer. Activation energies (Ea) were calculated for Zn and Mn as 94.53 kJ/mol and 1.41 kJ/mol, respectively.

REFERENCES


COMPARATIVE STUDY OF REGIONAL CRASH DATA IN TURKEY

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ABSTRACT
This study provides a comparative analysis of traffic safety in Turkey across the seven geographic regions over a 11 year time frame (2006 to 2016). The comparisons are performed in relative terms and absolute terms. Fatal and/or injury (FI) crashes per million population and per million registered vehicles were used to quantify safety. For the ordinal analysis, rates for the regions were ranked individually for each year as well as for the 11 years aggregated. An examination of the results indicated that the relative ranks of the regions were stable over the study period. Depending on the safety measure used, the relative rankings of regions varied. It means that a region ranked at the top (high crash rate) for one safety measure does not need to be ranked again at the top for other safety measure. For the cardinal analysis, the computed rates were used. These results were consistent with those from the ordinal analysis, but showed greater variability in the rates over time, which means that FI crash rates significantly increased over the time. A Geographic Information Systems based thematic maps were used to support these efforts.

Keywords: Comparative Safety Analysis, Crash Rates, Data Visualization, Traffic Safety
1. INTRODUCTION

Even though there has been significant public policy attention and improvements in traffic safety policies and practices in Turkey, 61 people died per billion vehicle-km in traffic crashes in 2016 (TGDDH, 2017; TurkStat, 2018a). In spite of significant improvements in national highway network, there has been an increase in fatal and/or injury (FI) crashes over the last decade (TurkStat, 2018a). The distribution of crashes across the nation is also of importance to transportation system owners. National and local safety programs aim to reduce crashes and the severity of their outcomes within their jurisdictions. Development of geographically appropriate safety strategies requires estimating pertinent crash and exposure data at the relevant spatial scale. While data required to identify safety risks are collected at the local level, published databases are typically available only at larger scales. Thus, there is a need to deduce data at the local level (i.e., lower levels of spatial aggregation) from partially complete or surrogate datasets that are available at a higher level of aggregation.

FI crashes are reported by the traffic police and gendarmerie units according to their areas of responsibility in Turkey. Disaggregate statistics of these crashes are published annually by Turkish Statistical Institute (TurkStat). This aggregate database provides temporal and provincial distribution of the crashes as well as type of vehicles involved, classification of the crash locations as well as gender and age distribution of the crash victims. Due to the lack of disaggregate crash level data at the national level, province and regional variations of traffic safety have not been examined in detail. Recently, Atalay and Tortum (2015) compared the number of fatalities per traffic crashes and per kilometer of road network across the 81 provinces of Turkey. The results showed that number of fatalities per crash are higher in less developed provinces, whereas number of fatalities per length of road network are higher in developed provinces. In other study, Erdogan (2009) studied the provincial level differences in number of FI crashes and number of fatalities. Population and number of registered vehicles were used to quantity safety and results indicated that provinces with higher FI crashes and fatalities were located in the provinces that contain the roads connecting the Istanbul, Ankara, and Antalya provinces. However, there is no study focusing on traffic safety at the regional level in Turkey.

This study provides a comparative analysis of the FI crashes across the seven geographic regions in Turkey from 2006 to 2016 (additional information is provided in Appendix A). The comparisons are performed in relative terms and absolute terms. Since vehicle-km data are not available either province or regional level, number of FI crashes per million population and per million registered vehicles are used to quantify safety. The principal sources of data used in this study is TurkStat.

2. METHODOLOGY

Number of FI crashes per million population and per million registered vehicles were determined for each geographic region annually for the study period. A Geographic Information Systems based thematic maps were used to support these efforts.

Traditional statistical tests based on the normality assumption of the data. Since FI crash rates do not follow normal distribution either across the regions or over the years, nonparametric methods need to be used to study FI crash rates. An appropriate test to use for this purpose is the Kruskal-Wallis nonparametric test. In this study, hypotheses of the Kruskall-Wallis H test was that:

Ho: FI crash rates are the same for each region from 2006 to 2016
H1: FI crash rates are not the same for each region from 2006 to 2016.

Based on the Kruskall-Wallis test, the null hypothesis, Ho, is to be rejected at the (100-α)% percent level of confidence if the test statistic, H, falls in the critical region $H > \chi^2_0$ with $v = (k-1)$ degrees of freedom. To control the familywise type I error in Kruskall-Wallis H test; the probability of rejecting at least one pair hypothesis given all pairwise hypotheses are true, adjusted p-values are calculated and used to make the decision for each pair. The following equations was used to calculate adjusted p-values for each of pairwise hypothesis. If the adjusted p-value is bigger than 1, it is set to 1.

$$p_{adj} = pK(K-1)/2$$

where; $K = \text{number of pairwise hypothesis}$, and $p = \text{significance level of pairwise hypothesis}$.

3. RESULTS

FI crash rates were calculated annually for each geographic region based on per million population and per million registered vehicles. The results are presented thematically in Tables B1 to B2 (see Appendix). It is noted that the numbers of the regions are given randomly. In these tables, a graded color pattern is used to indicate FI crash rates. The color gradation ranges from red to yellow or green. Dark red is used to indicate the higher FI crash rates and worse safety records, and dark green is used to indicate lower FI crash rates and best safety records. Lighter red, yellow and lighter green colors are used to achieve gradation.

Table B1 presents FI crash rates of each region per million population for each year during the study period. Table B2 presents FI crash rates of each region per million registered vehicles for each year during the study period. In addition, the average FI crash rates for each measure for the entire 11 year period as a whole are given in these tables. It is seen that FI crash rates for regions significantly increased for each measure from 2006 to 2016. Furthermore, Table B1 and B2 clearly indicate the stability of the relative FI crash rates of regions across the years. They show that regions that tended to have lower FI crash rates, had lower crash rates across the years; and, regions that tended to have higher FI crash rates, had higher crash rates across the years.

Kruskall-Wallis pairwise comparisons implied that FI crash rates per million population are not the same across the regions from 2006 to 2016 (i.e. $H = 31.50 > \chi^2_{0.05,9} = 12.59$). Fig. 1 and 2 present box plot and 95% confidence interval of FI crash rates of regions per million population. It is seen that FI crash rates in Central Anatolia Region (Region 5), Mediterranean Region (Region 4) and Aegean Region (Region 2) seems...
relatively higher than the others. FI crash rates in Southeastern Anatolia Region (Region 3) and Eastern Anatolia Region (Region 6) seems relatively lower than the others.

Fig. 3 presents graphical Kruskal-Wallis multiple pairwise comparisons. The number below each region represents the average rank of regional FI crash rates over the 11 years period. Fig. 4 provides Kruskal-Wallis tests results for significant pairwise comparisons. However, most of them are not significant based on adjusted p-value (see Fig. 3). In Fig. 3, yellow lines represent the significant pairwise comparisons based on adjusted p-values. FI crash rates per million population for Central Anatolia Region (Region 5) and Aegean Region (Region 2) are significantly higher than Southeastern Anatolia Region (Region 3) and Eastern Anatolia Region (Region 6); for Mediterranean Region (Region 4) is significantly higher than Southeastern Anatolia Region (Region 3).

Fig. 1. Box plot of FI crash rates for regions per million population

Fig. 2. 95% CI of mean FI crash rates for regions per million population

Fig. 3. Kruskal-Wallis multiple pairwise comparisons of FI crash rates per million population
Kruskall-Wallis pairwise comparisons implied that FI crash rates per million population are not the same across the regions from 2006 to 2016 (i.e. $H = 44.98 > \chi^2_{0.05,9} = 16.92$). Fig. 5 and 6 present box plot and 95% confidence interval of FI crash rates of regions per million population. It is seen that FI crash rates in Eastern Anatolia Region (Region 6) seems relatively higher than the others. FI crash rates in Marmara Region (Region 1) seems relatively lower than the others. Fig. 7 presents graphical Kruskal-Wallis multiple pairwise comparisons. Furthermore, Fig. 8 provides Kruskal-Wallis tests results for significant pairwise comparisons. However, most of them are not significant based on adjusted p-value. FI crash rates per million registered vehicles for Eastern Anatolia Region (Region 6) are significantly higher than Marmara Region (Region 1), Eagan Region (Region 2) and Mediterranean Region (Region 4). In addition, FI crash rates per million registered vehicles for Marmara Region (Region 1) are significantly lower than Southeastern Anatolia Region (Region 3), Central Anatolia Region (Region 5) and Black Sea Region (Region 7).

![Fig. 5. Box plot of FI crash rates for regions per million registered vehicles](image)

![Fig. 6. 95% CI of mean FI crash rates for regions per million population](image)

![Fig. 7. Kruskal-Wallis multiple pairwise comparisons of FI crash rates per million registered vehicles](image)

![Fig. 8. Kruskal-Wallis multiple pairwise comparisons of FI crash rates per million population](image)
Fig. 9 and 10 provide thematic maps based on the average ranks of the provinces for each of the safety measures used in this study. In these maps, the red colored provinces have the highest rates while the green colored provinces have the lowest rates. An examination for Fig. 1 to 2 reveal some interesting patterns in the spatial distribution of the relative safety ranks of the regions. Overall, it can be seen that Marmara Region (Region 1) tend to have best safety records. Relative safety records of Aegean Region (Region 2), Eastern Anatolia Region (Region 6) and Southeastern Anatolia Region (Region 3) are significantly different for million population and million registered vehicles measures. For instance, Eastern Anatolia Region (Region 6) has the best safety records for FI crash rates per million population, however, it has the worst safety records for FI crash rates per million registered vehicles.

![Fig. 9. Average FI crash rates per million population for regions from 2006 to 2016](Image)

![Fig. 10. Average FI crash rates per million registered vehicle for regions from 2006 to 2016](Image)

**4. CONCLUSION**

This paper summarized efforts of and findings from a study to examine regional level FI crash trends and perform comparative analyses of safety records 2006 to 2016. The comparisons were performed in relative terms (ordinal scale or based on rates) and absolute terms (cardinal or rank ordered scale). Two safety measures were used to evaluate safety: million population and million registered vehicles. Data were obtained from publications maintained by TurkStat.

An examination of the results indicated that the relative ranks of the regions were stable over the study period for each safety measure. Non-parametric statistical tests and thematic maps used to support comparative analyses. Specifically, the Kruskal-Wallis nonparametric test was used in this study. The results showed that the FI crash rates are not the same across the regions. Furthermore, the analyses also revealed that depending on the safety measure used, the relative rankings of regions varied (i.e., a region ranked at the top (high crash rate) for one safety measure does not need to be ranked again at the top for other safety measure). This figure is resulted from significantly different vehicle ownership rate across the regions in Turkey. For the cardinal analysis the computed rates were used. These results were consistent with those from the ordinal analysis, but it was showed that FI crash rates significantly increased over the time.

For broad macro level analyses a more representative vehicle-km measure is required to study relative safety records of regions. However, it is available only for national level in Turkey. Furthermore, if specific analyses are required, then safety measures should be defined based on the desired evaluations. For example, if the goal were to address rural safety, the measures should be computed using rural fatal and/or injury crashes, rural vehicle-km, and the extent of rural kilometers of road network. This paper explored methods to analyze regional differences in road traffic safety. The results document the validity and promise of the methods. These methods could be expanded for policy and operational analyses.

**REFERENCES**


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Appendix A: Geographic Regions in Turkey

It is noted that the numbers of the regions are given randomly.

- **Marmara Region (Region 1):** Balıkesir, Bilecik, Bursa, Çanakkale, Edirne, İstanbul, Kırklareli, Kocaeli, Sakarya, Tekirdağ, Yalova.
- **Aegean Region (Region 2):** Afyon, Aydın, Denizli, İzmir, Kütahya, Manisa, Muğla, Uşak.
- **Southeastern Anatolia Region (Region 3):** Adıyaman, Batman, Diyarbakır, Gaziantep, Kilis, Mardin, Siirt, Urfa, Şırnak.
- **Mediterranean Region (Region 4):** Adana, Antalya, Burdur, Hatay, Isparta, Kahramanmaraş, Mersin, Osmaniye.
- **Central Anatolia Region (Region 5):** Aksaray, Ankara, Çankırı, Eskişehir, Karaman, Kayseri, Kırıkkale, Kırşehir, Konya, Nevşehir, Niğde, Sivas, Yozgat.
- **Eastern Anatolia Region (Region 6):** Ağrı, Ardahan, Bingöl, Bitlis, Elazığ, Erzincan, Erzurum, Hakkari, Iğdır, Kars, Malatya, Muş, Tunceli, Van.
- **Black Sea Region (Region 7):** Amasya, Artvin, Bartın, Bayburt, Bolu, Corum, Düzce, Giresun, Gümüşhane, Karabük, Kastamonu, Ordu, Rize, Samsun, Sinop, Tokat, Trabzon, Zonguldak.

![Fig. A1. Geographical regions in Turkey](image)

Appendix B: F1 Crash Rates

Table B1. F1 crash rates for regions per million population

<table>
<thead>
<tr>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Marmara (R1)</td>
<td>930</td>
<td>1061</td>
<td>1051</td>
<td>1087</td>
<td>1091</td>
<td>1233</td>
<td>1376</td>
<td>1557</td>
<td>1621</td>
<td>1707</td>
<td>1718</td>
<td>1312</td>
</tr>
<tr>
<td>Aegean (R2)</td>
<td>1479</td>
<td>1564</td>
<td>1489</td>
<td>1597</td>
<td>1826</td>
<td>2197</td>
<td>2766</td>
<td>2961</td>
<td>3183</td>
<td>3150</td>
<td>2160</td>
<td>2160</td>
</tr>
<tr>
<td>Southeastern Anatolia (R3)</td>
<td>707</td>
<td>717</td>
<td>706</td>
<td>794</td>
<td>834</td>
<td>936</td>
<td>1153</td>
<td>1538</td>
<td>1524</td>
<td>1108</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mediterranean (R4)</td>
<td>1388</td>
<td>1481</td>
<td>1432</td>
<td>1522</td>
<td>1608</td>
<td>1848</td>
<td>2164</td>
<td>2749</td>
<td>2796</td>
<td>3061</td>
<td>3020</td>
<td>2097</td>
</tr>
<tr>
<td>Central Anatolia (R5)</td>
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<td>1678</td>
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<td>1688</td>
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Table B2. F1 crash rates for regions per million registered vehicle

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<td>Marmara (R1)</td>
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<td>5669</td>
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<td>6666</td>
<td>6715</td>
<td>6731</td>
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<td>6276</td>
<td>6278</td>
<td>5725</td>
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<td>6305</td>
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<td>Mediterranean (R4)</td>
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<td>9867</td>
<td>9459</td>
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<td>Central Anatolia (R5)</td>
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<td>7826</td>
<td>6986</td>
<td>7502</td>
<td>7551</td>
<td>7943</td>
<td>8989</td>
<td>9754</td>
<td>9214</td>
<td>9202</td>
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<td>10811</td>
<td>11614</td>
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<td>14859</td>
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<td>Black Sea (R7)</td>
<td>7384</td>
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<td>6788</td>
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<td>7483</td>
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<td>10243</td>
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<td>10920</td>
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ABSTRACT
Density Functional Theory (DFT) calculations used in the Carbon Nanotubes (CNT) design take a very long time even in the simulation environment as it is well known in literature. In this study, calculation time of DFT for geometry optimization of CNT is reduced from days to minutes using seven artificial intelligence-based and one statistical-based methods and the results are compared. The best results are achieved from ANFIS and ANN based models and these models can be used instead of CNT simulation software with high accuracy.

Keywords: Geometry Optimization, Cnt, Dft, Artificial Intelligence
1. INTRODUCTION

Density functional theory (DFT) (Kohn and Sham, 1965) is the most successful method that calculates atomic coordinates faster than other mathematical approaches and it also reaches more accurate results. DFT uses ground state energy formula which is developed by Kohn and Sham (Eq. (1)).

\[ E = \sum \epsilon_j - \frac{1}{2} \int \frac{\rho(r)}{|r-r'|} drdr' - \int \rho(r)n(r)dr + E_{\text{ex}}[n(r)] \]  

where \( \epsilon_j \) and \( n \) are the self-consistent quantities, \( \rho \) is the exchange correlation potential energy, \( E_{\text{ex}} \) is the exchange correlation energy, and \( n(r) \) is the electron density. However, the elapsed time for calculation of high number of atoms may even take several days due to calculation capability limits of workstation computers. On the other hand, users need to use more powerful workstations and parallel computer grids which are too expensive to buy easily for reducing the calculation time. In literature, many researchers remark this calculation time problem in their studies. General view of the researchers who studied on geometry optimization using DFT can be summarized as “DFT calculations are time consuming”.

Many researchers study on CNT to obtain perfect CNTs and widen their application areas; Some of the studies are focused on geometry optimizations of the CNTs (Kanamitsu and Saito, 2002; Kürti et al., 2003; Moradian et al., 2008, 2009; Yagi et al., 2004). Also many of the researchers that study on CNT calculations, incorporate artificial intelligence methods into their works (Abo-Elhadeed, 2012; Akbari et al., 2014; Cheng et al., 2015; Ensafi et al., 2010; Hassanzadeh et al., 2015; Hayati et al., 2010; Rahimi-Nasrabadi et al., 2015; Salehi et al., 2016; Shanbedi et al., 2013). Nowadays, this incorporation trend has been increasing (Aci and Avci, 2016).

The motivation of this research is to reduce the calculation time for atomic coordinates from days to minutes. It is known that the current mathematical methods cannot reduce the calculation time up to this level. In this work, the problem is investigated in another perspective. Instead of calculation; the atomic coordinates are predicted as accurately as possible in a short time. These predicted atomic coordinates can be used as initial coordinates for the simulation software as depicted in Fig. 1. Thus, the exact atomic coordinates can be calculated within minutes or hours instead of days utilizing the proposed approach. In some researches predicted atomic coordinates may be enough in accuracy. In that case, the predicted coordinates may provide the fastest solution.

The main objective aimed in this work is to develop prediction models using regression-based supervised artificial intelligence techniques such as Adaptive-Network Based Fuzzy Inference System (Jang, 1993) (ANFIS), four types of Artificial Neural Network (Gupta, 2013) (ANN) (i.e. Feed Forward Neural Network (FFNN), Function Fitting Neural Network (FITNET), Cascade-Forward Neural Network (CFNN) and Generalized Regression Neural Network (GRNN)), Classification and Regression Tree (Lawrence and Wright, 2001) (CART) and Support Vector Regression (Smola and Vapnik, 1997) (SVR) to estimate the atomic coordinates of CNTs. One statistical method (i.e. Multiple Linear Regression (Eberly, 2007) (MLR)) is used to compare results with artificial intelligence based methods.

The datasets used in this study are generated with CASTEP (2016) using CNT geometry optimization. Different chiral vectors are used for each CNT simulation. The atom type is selected as carbon, bond length is used as 1.42 Å (default value), and then the nanotube is built by CASTEP.

CASTEP uses a parameter named as elec_energy_tol (i.e. “DFT calculations are time consuming". The predicted atomic coordinates are calculated by CASTEP using DFT.
remains below some tolerance value per atom for a few self-consistent field steps to finalize the computation. This parameter also determines the calculation level of inputs and outputs. The default value of the parameter is 1x10^-5 eV per atom and is usually suitable (CASTEP, 2016).

Initial coordinates of all carbon atoms are generated randomly. The number of simulated atoms ranges from 32 to 388. The calculation time according to these calculations are approximately varies from 10 minutes to 5 days. These calculation times will take weeks and months for higher atom numbers. All calculations are run on a workstation that has a 2.0 Ghz power on 2 Xeon processors with 4 cores and 8 GB of RAM, using all cores under Linux operating system. The calculation time according to these calculations are approximately varies from 10 minutes to 5 days as given in Table 2 in seconds. These calculation times will take weeks and months for higher atom numbers.

Table 2. The calculation time for CNT simulations in seconds

<table>
<thead>
<tr>
<th>ID of CNT</th>
<th>Number of Atoms</th>
<th>Calculation Time (Seconds)</th>
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<td>1</td>
<td>28</td>
<td>1050.14</td>
</tr>
<tr>
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<td>11826.42</td>
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2.2. Prediction Models

ANFIS, FFNN, FITNET, CFNN, GRNN, CART, SVR and MLR models were trained and tested with the dataset of atomic coordinates for CNTs.

A Sugeno-type (Takagi and Sugeno, 1985) Fuzzy Inference System (FIS) is used by MATLAB’s implementation of ANFIS. An adaptive neural network technique is used to train the Sugeno-type FIS parameters. Inputs are mapped through input membership functions and associated parameters by ANFIS. Then through output membership functions and associated parameters to outputs, can be used to interpret the input/output map. The parameters associated with the membership functions change through the learning process. A gradient vector facilitates the computation of these parameters. A measure of how well the FIS is modeling the input/output data for a given set of parameters is provided by this gradient vector. When the gradient vector is obtained, any of several optimization routines can be applied in order to adjust the parameters to reduce some error measure. The sum of the squared difference between actual and desired outputs usually defines this error measure. Either back propagation or a combination of least squares estimation and backpropagation for membership function parameter estimation is used by ANFIS (MATLAB, 2016).

Table 2. The calculation time for CNT simulations in seconds
“mergeleaves” option merges leaves that originate from the same parent node and give the sum of risk values greater or equal to the risk associated with the parent node. The values of the parameters were chosen as prun=on, minparent=50 (default is 10), qotolera=1E-7 (default is 1E-6), mergeleaves=on. All of the parameter values were decided by trial-and-error.

SVR model was designed by running “fitrsvm” function in MATLAB. Several combinations have been tried and Radial Basis Function was chosen as the kernel for performance comparison.

MLR prediction model is designed with the purpose of comparing Machine Learning methods with a statistical regression method. The model is coded in Statistics and Machine Learning Toolbox of MATLAB using “fitlm” function. Model specification is specified as “linear” and model specification equations are set for each coordinate for the predictions of coordinates such as \( u^* \sim u+v+w+m+n \) for \( u \); \( v^* \sim u+v+w+m+n \) for \( v \); and \( w^* \sim u+v+w+m+n \) for \( w \).

3. RESULTS AND DISCUSSION

Mean Squared Error (MSE), Mean Absolute Error (MAE), Standard Error of Estimation (SEE) and Multiple Correlation Coefficient (R) are calculated to evaluate the performance of prediction models. Summaries of mathematic equations of these performance measures are given in Eq. (2), Eq. (3), Eq. (4) and Eq. (5) respectively (Witten and Frank, 2005).

\[
MSE = \frac{1}{n} \sum_{i=1}^{n} (O_i - P_i)^2
\]  
(2)

\[
MAE = \frac{1}{n} \sum_{i=1}^{n} |O_i - P_i|
\]  
(3)

\[
SEE = \sqrt{1 - \frac{\sum_{i=1}^{n} (O_i - P_i)^2}{\sum_{i=1}^{n} (O_i - \bar{O}_m)^2}}
\]  
(4)

\[
R = \frac{\sum_{i=1}^{n} (O_i - P_i)(O_i - \bar{O}_m)}{\sqrt{\sum_{i=1}^{n} (O_i - P_i)^2 \sum_{i=1}^{n} (O_i - \bar{O}_m)^2}}
\]  
(5)

where \( n \) is the number of data points used for testing, \( P_i \) is the predicted value, \( O_i \) is the observed value and \( \bar{O}_m \) is the average of the observed values. MATLAB (R2015b 64 bit) (MATLAB, 2016) was utilized for designing proposed models and obtaining performance measures.

Table 3, Table 4 and Table 5 summarize the performance results of \( u^* \), \( v^* \) and \( w^* \) coordinates prediction using ANFIS, FFNN, FITNET, CFNN, GRNN, SVR, CART and MLR models respectively.

Table 3. Performance results of \( u^* \) coordinate prediction (the best results are outlined in bold).

<table>
<thead>
<tr>
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<th>MSE</th>
<th>MAE</th>
<th>SEE</th>
<th>R</th>
</tr>
</thead>
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<td>1.077E-05</td>
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<tr>
<td>FFNN</td>
<td>9.879E-06</td>
<td>2.08E-03</td>
<td>1.00E+00</td>
<td>9.999E-01</td>
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<tr>
<td>FITNET</td>
<td>1.130E-05</td>
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<td>1.00E+00</td>
<td>9.999E-01</td>
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<tr>
<td>CFNN</td>
<td>9.403E-06</td>
<td>2.02E-03</td>
<td>1.00E+00</td>
<td>9.999E-01</td>
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<tr>
<td>GRNN</td>
<td>7.911E-03</td>
<td>2.55E-01</td>
<td>1.00E+00</td>
<td>9.371E-01</td>
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<tr>
<td>SVR</td>
<td>5.102E-04</td>
<td>1.95E-02</td>
<td>9.97E-01</td>
<td>9.97E-01</td>
</tr>
<tr>
<td>CART</td>
<td>2.471E-05</td>
<td>3.86E-03</td>
<td>1.00E+00</td>
<td>9.999E-01</td>
</tr>
<tr>
<td>MLR</td>
<td>1.52E-01</td>
<td>2.48E+00</td>
<td>3.00E+00</td>
<td>5.999E-01</td>
</tr>
</tbody>
</table>

Table 4. Performance results of \( v^* \) coordinate prediction (the best results are outlined in bold).

<table>
<thead>
<tr>
<th>Models</th>
<th>MSE</th>
<th>MAE</th>
<th>SEE</th>
<th>R</th>
</tr>
</thead>
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<tr>
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<td>4.962E-08</td>
<td>1.53E-04</td>
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<td>1.53E-04</td>
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<td>1.00E+00</td>
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<tr>
<td>FITNET</td>
<td>5.554E-08</td>
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<td>1.00E+00</td>
<td>1.00E+00</td>
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<td>CFNN</td>
<td>5.418E-08</td>
<td>1.49E-04</td>
<td>1.00E+00</td>
<td>1.00E+00</td>
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<tr>
<td>GRNN</td>
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<td>2.46E-01</td>
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<tr>
<td>SVR</td>
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<tr>
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<td>3.02E-03</td>
<td>1.00E+00</td>
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<tr>
<td>MLR</td>
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<td>1.47E-01</td>
<td>3.00E+00</td>
<td>6.00E-01</td>
</tr>
</tbody>
</table>

All models performed good levels of successes when we look at all results with a general view. However, the results of ANFIS, FFNN, FITNET and CFNN models have a superiority over other models. This implies that ANN based models can closely estimate atomic coordinates of CNTs. CART and SVR models produced average performance results comparing to other models. The results can be analyzed in detail as follows:

- CFNN model has the best performance values for \( u^* \) and \( w^* \) coordinates prediction by means of MSE and MAE. However, MSE and R results of ANFIS, FFNN and FITNET models are very close to CFNN model.
- The best SEE results are achieved by ANFIS model for all coordinates.
- The R value prediction results varies in a very small range (from 9.29E-01 to 1.00E+00) for all models except MLR based model.
- MLR based model yielded the worst performance results for all coordinates.
- The estimation results with the highest accuracy are yielded for \( w^* \) coordinate (MSE results of the first four models are almost zero).

The results obtained from this study can be used in two ways: i) The predicted atomic coordinates can be used in physical calculations without using a simulation software, ii) The estimated results can be used as an initial value of simulation software for reducing duration of the atomic coordinate calculation seriously.

4. CONCLUSION

As a result of this work, the effectiveness of artificial intelligence based solutions, which estimate atomic coordinates that can be integrated into software, has been observed and the results that have significantly shortened the simulation processes in the field of nanotechnology have been presented to be integrated into scientific or commercial software.
ACKNOWLEDGMENTS

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REFERENCES


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INVESTIGATION OF ULEXITE USAGE IN AUTOMOTIVE BRAKE FRICTION MATERIALS

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ABSTRACT
The automotive brake pads are multi-component composites made up of many materials. There are many studies in the literature exploring the use of many different materials in brake pads. In this study, the use of ulexite which is a commercially valuable derivatives of boron that 65% of the total world reservations exists in Turkey were researched for brake pad material. For this purpose, three brake pad specimens containing ulexite differing in amount (3, 6 and 9 wt.%) were produced by a conventional procedure for a dry formulation following dry-mixing, pre-forming and hot pressing. The density of the specimens was determined based on Archimedes principle in water. The surface hardness of all brake pad specimens was measured using Rockwell hardness tester. The friction performance of the brake pad specimens was determined using a real brake disc-type tester with grey cast iron. The weights of each specimen were taken before and after the friction test, and the specific wear rate was determined in accordance to the TSE 555 (1992) standard. The results showed that all specimens are applicable to the industry, consistent with the literature and suitable to the TS 555 standard. Also, the results indicated that ulexite is an ideal material for brake pads.

Keywords: Ulexite, Brake Lining, Wear, Friction
1. INTRODUCTION

Boron is an important mineral used in many fields, including nuclear industry, fertilizer industry, the pharmaceutical industry, chemical industry, and automobile industry. Turkey has 65% of the boron reserves in all over the world and manages 32% of the total production (Çalik, 2002). Although boron minerals are used directly in some structures, most of which is processed in factories and converted into the high value-added refined boron derivatives. Some of the commonly used commercial boron derivatives are borax, colemanite, ulexite, kernite, proberite and szaibelyite (Özkan et al., 1997).

With the development of automotive technology, the motor forces, speed of movement and the acceleration capabilities of vehicles have increased compared to the past. This has increased the importance of reliably controlling the movements of the vehicles. The most important safety feature of a car is the brake system. Brake pads are the indispensable parts of the brake systems, being the composite materials that are made up of a combination of many materials with different functions. Although many studies on brake friction materials are presented in the literature, studies investigating the use of boron products in brake pads are relatively few. Sugözü (2009) produced the brake pad specimens using ulexite, colemanite, boric acid and borax pentahydrate which are boron derivatives, and then examined the properties of the produced brake pads including the friction, wear, and resistance. Wannik et al. (2012), investigated the effects of boron additives on brake pads and found that boron additives have higher friction performance. Kuş et al. (2016), investigated the effect of the amount of colemanite on friction-wear properties of the volatile ash reinforced bronze matrix brake pad materials produced by the hot pressing method, and stated that the friction coefficient of the materials with 0.5% colemanite supplement was higher.

In the present study, the usability of ulexite in brake pad materials was investigated experimentally. For this purpose, the brake pad specimens containing 3%, 6% and 9% ulexite were produced by the powder metallurgy method. The density of specimens was determined according to the Archimedes principle and the hardness was primarily determined with the help of sieves shown in Fig. 1 (a). Then, the amount of each material forming the brake pad content was determined by 0.001 g precision scale shown in Fig. 1 (b) and transferred to the powder chamber shown in Fig. 1 (c) for mixing. In order to ensure homogeneity of the mixture, the specimen content was mixed at 150 rpm for 10 minutes on the specially produced powder mixing device shown in Fig. 1 (d). The resulting mixture was carefully placed in the 25.4 mm diameter cold press mold shown in Fig. 1 (e). While doing this, care has been taken not to spread the dust around due to sudden movements. The dust was pressed under 8000 kPa pressure for 2 minutes. The final product was obtained by removing the cold pressed specimens from the mold and placing them in the hot press mold shown in Fig. 1 (f) and pressing them for 12 minutes under 10000 kPa pressure at 150 °C.

Prior to the production process, the particle size of each material forming the contents of brake pad was determined using the sieve shaker and sieves shown in Fig. 1 (b) and transferred to the powder chamber shown in Fig. 1 (d). The powder mixtures were obtained by removing the cold pressed specimens from the mold and placing them in the hot press mold shown in Fig. 1 (f) and pressing them for 12 minutes under 10000 kPa pressure at 150 °C.

2. MATERIALS AND METHODS

The production parameters of the materials and specimens used in brake pads have a significant impact on the brake performance. We determined the materials and production conditions according to the previous studies in the literature. The materials used in the specimens are given in Table 1 in mass percentages. U3, U6, and U9 are specimen codes; U refers ulexite, and its number also refers to the percentage in the composition.

![Fig. 1. The materials used in the production of specimens (a) the sieve-shaker and sieves (b) the precision scales (c) the powder chamber (d) the powder mixing device (e) the cold press mold (f) the hot press mold](image)

The density of the specimens was determined according to the Archimedes principle and the hardness was determined using the Rockwell hardness tester.
device (HRL). During the hardness measurement process, a preload of 10 kgf and a full load of 60 kgf was applied with a steel ball in diameter 6.35 mm at the submersible end (Başar et al., 2017). Hardness measurements were taken from the frictional surface of the specimens. A full-scale brake pad test device with grey cast iron disc having a diameter of 280 mm and hardness of 116 HB, whose schematic drawing is shown in Fig. 2, was used to determine the abrasion and friction properties of the specimens. The device can be fully controlled by a computer and includes data collection software. The specific wear rate was calculated according to the TSE 555 standard by determining the weights of each specimen before and after testing.

During the experiments, the temperature increases due to friction between the disk and the brake pad. In order to investigate the effect of temperature increase on the performance of the brake pad, the non-contact thermometer measured the surface temperature of the brake pad at a distance of about 2 cm from the friction surface to the disc. A digital thermometer was used to measure temperature. The surface temperature of the disc is automatically transferred to the computer environment in seconds during the experiment (Sugözü, 2016).

The coefficient of friction and wear of specimens was obtained by conducting experiments as specified in the TS 555 (1992) and TS 9076 standard (1991). In experimental conditions, first of all, 310 rpm, 700 kPa pressure, and a temperature not exceeding 100 °C were provided; and then the grinding process was applied, until the surface contact of the specimen to the disc is at least 95%. Thus, the surface got ready for the experiment. Then the tests were completed with the pressure of 1050 kPa and speed of 6 m/s for 30 minutes.

3. RESULTS

The coefficient of friction for automotive brake pads is the most important parameter affecting the brake performance. The coefficient of friction-time graphs of specimens are given in Fig. 3 for U3 coded specimens, and in Fig. 4 for U6 coded specimens, and also in Fig. 5 for U9 coded specimens. In figures, the coefficient of friction was low at the initial of the test because the applied pressure does not influence suddenly but gradually. Sudden pressure application will cause damage to the brake pads, so the pressure was gradually increased. In addition, at the initial of the test, the disc and the brake pad are in the running-in period (grinding) and the friction layers in which the friction force is effective are not yet formed (Sugözü, 2016). Therefore, there is a continuous change in the coefficient of friction. In the literature, this situation has been reported to occur with the transition of heat to the inner part of the contact areas on the surface of the disc during friction (Anderson, 1992). Another explication is that the adhesion on the surface roughness of the friction couples results in the repetition of the adhesion-release, causing fluctuations in the coefficient of friction (Stachowiak and Batchelor, 2001).

![Fig. 3. The coefficient of friction and temperature graph of the specimen containing 3% ulexite, according to the friction time](image1)

![Fig. 4. The coefficient of friction and temperature graph of the specimen containing 6% ulexite, according to the friction time](image2)

![Fig. 5. The coefficient of friction and temperature graph of the specimen containing 9% ulexite, according to the friction time](image3)
5 represents the coefficient of friction and temperature graph of the specimen containing 9% ulexite. The highest coefficient of friction obtained in the tests is 0.48 °C, and the highest temperature between the disc and brake pad is 202 °C. The friction stability was calculated as 70%. According to the literature, the friction stability (%) should be as high as possible and close to 100, the slope and fluctuations of the obtained curve should be low level (Bijwe et al., 2012). It is desirable that the coefficient of friction of the automotive brake pads is high, the wear is low and the friction stability is stable. Physical and tribological properties of specimens are shown in Table 2 and Table 3.

Table 2. Tribological properties of specimens

<table>
<thead>
<tr>
<th>Specimen Code</th>
<th>Specific wear rate (cm³/Nm)</th>
<th>The average coefficient of friction</th>
</tr>
</thead>
<tbody>
<tr>
<td>U3</td>
<td>2.054 × 10⁻⁶</td>
<td>0.331</td>
</tr>
<tr>
<td>U6</td>
<td>2.109 × 10⁻⁶</td>
<td>0.313</td>
</tr>
<tr>
<td>U9</td>
<td>1.893 × 10⁻⁶</td>
<td>0.337</td>
</tr>
</tbody>
</table>

Table 3. Physical properties of specimens

<table>
<thead>
<tr>
<th>Specimen Code</th>
<th>Rockwell hardness (HRL)</th>
<th>Density (g/cm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>U3</td>
<td>81</td>
<td>1.9</td>
</tr>
<tr>
<td>U6</td>
<td>88</td>
<td>2.16</td>
</tr>
<tr>
<td>U9</td>
<td>90</td>
<td>2.22</td>
</tr>
</tbody>
</table>

Table 3 shows that the hardness and density of the specimens are increased by increasing the amount of ulexite in the composite. Considering the average coefficient of friction and the specific wear rate, it was found that the specimen containing 9% ulexite was better. The coefficient of friction of the specimens is obtained by dividing the coefficient of friction by the highest coefficient of friction obtained during the test and expressed as a percentage.

![Image](image1.png)

Fig. 6. (a) The coefficient of friction (b) friction stability graphs of specimens

4. CONCLUSION

In this study, the usability of ulexite, which is a boron mineral, in automotive brake pads was investigated by experimental studies. Three different specimens containing 3%, 6% and 9% ulexite were prepared for this purpose. A full-scale brake pad device was used for the wear and friction tests of the specimens. The results obtained from the tests are summarized below:

• The highest average coefficient of friction value for all specimens undergo friction test is 0.337, belonging to the U9-coded specimen containing 9% ulexite, the lowest average friction coefficient is 0.313, belonging to the U6-coded specimen containing 6% ulexite.

• It was reported that as the amount of ulexite increased, the hardness and density increased. The direct proportion between the hardness and density was determined to be consistent with the literature.

• The friction stability of specimens was observed to be almost the same for each specimen, and it was concluded that the friction stability does not depend on the amount of ulexite content.

• According to the results obtained from the friction and abrasion tests, all specimens can be utilized in the industry in accordance with the literature and conform to the TS 555 standard. Accordingly, ulexite which is a boron derivative could be used as an alternative material in automotive brake pads.

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ABSTRACT

In this study, we present a general equation for Finite Difference Method Multi-group Diffusion (FDMMMD) equations of a cylindrical nuclear reactor core. In addition, we developed an algorithm which we called TUNTOB for solving the FDMMMD equations, determined the fluxes at each of the mesh points and calculated the criticality of the four energy group. This was with a view to using the four-group diffusion equations to estimate the criticality of a cylindrical reactor core that will be accurate and locally accessible for nuclear reactor design in developing countries. The multi-group diffusion equations were solved numerically by discretization using the Finite Difference Method (FDM) to obtain a general equation for a cylindrical reactor core. The fluxes at each mesh point and the criticality of the four energy group were then determined. From the results obtained, we observed that an increment in iteration led to an increase in the effective multiplication factor ($k_{eff}$) with a corresponding increase in the computation time. A maximum effective multiplication factor was reached when the number of iteration was 1000 and above. Having established the optimal number of iterations, the effects of the mesh sizes on the computation examined revealed that the values of $k_{eff}$ increases as the mesh sizes becomes smaller until an optimal mesh size of 1 x 1 cm² was reached and further decrease in mesh sizes gave no further improvement in the value of $k_{eff}$. The Study concluded that the accuracy in the values of $k_{eff}$ and the smoothness of the neutron distribution curves in 3-D representations depend on the number of mesh points.

Keywords: Four-group diffusion equation, Effective multiplication factor, Mesh size, Reactor, Criticality calculation

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1. INTRODUCTION

The criticality of a system containing fissionable materials is described by its effective multiplication factor \( k_{\text{eff}} \). The effective multiplication factor is the ratio of the number of neutrons in one generation to the number of neutrons in the previous generation as shown in Eq. (1). A generation is essentially the lifetime of a neutron, in a finite system, the effective multiplication factor is denoted as \( k_{\text{effective}} \) or \( k_{\text{eff}} \), which is used to determine the stability of a nuclear reactor core. When a system is critical, it maintains a steady-state chain reaction of nuclear fissioning, and \( k_{\text{eff}} = 1 \). The average neutron population in a critical system stays constant in time. A sub-critical system has \( k_{\text{eff}} < 1 \) and the neutron population dies off in time. The neutron population in a super-critical system, where \( k_{\text{eff}} > 1 \), grows without bound in time (Urbatsch, 1995).

\[
k_{\text{eff}} = \frac{\text{Number of neutrons in one generation}}{\text{Number of neutrons in the preceding generation}}
\]

The knowledge of \( k_{\text{eff}} \) is necessary when designing nuclear reactors. However, numerical methods are used almost exclusively for criticality calculations (Urbatsch, 1995). Different numerical methods have been proposed to solve the two group neutron diffusion equations with little attention to the other groups. Although, the two group neutron diffusion equations do not give a detailed explanation of neutron flux distribution in a practical nuclear reactor core, the four-group neutron diffusion equations are known to give a far better description of neutron distribution in a practical nuclear reactor core. Hence the study of the criticality of the cylindrical reactor core and its calculation using four-group diffusion equations by applying the finite difference method (FDM).

The remainder of this paper is organized as follows. In Section 2, a review of related works is provided, while a detailed explanation of the discretization of the four group diffusion equations using finite difference method is given in Section 3. In Section 4, the results are presented and discussed and Section 5 concludes this paper.

2. NUCLEAR REACTOR CORE

A nuclear reactor core is a part of a nuclear reactor which contains the nuclear fuel components where all the nuclear reactions take place and consequently heat is generated from the reaction. In addition, a nuclear reactor produces and controls the release of energy in form of heat from the splitting of the atoms of uranium.

2.1. Neutron-Nucleus Reactions

It is important to recognize that since neutrons are electrically neutral, they are unaffected by the electrons in the atom or by the positive charge of the nucleus. As a consequence, neutrons pass through the atomic electron cloud and interact directly with the nucleus. Neutrons collide with nuclei, not with atoms (Larmash and Baratta, 2001).

The operation of a reactor basically depends on how neutrons interact with nuclei in the reactor. There are various types of known neutron interactions which could be considered as shown in Fig. 1 (Arzhanov, 2010). All neutron reactions can be categorized as either elastic or inelastic collisions, on the condition that either the kinetic energy is conserved in the collision or not. (Burnham, 1967).

2.1.1. Neutron Flux

Neutron flux is defined as the product of the neutron density and the velocity,

\[
\phi = \pi v
\]

so that it is expressed in units of neutrons per cm\(^2\) per second. It is equal to the total distance (sum of all the path lengths) travelled in one second by all the neutrons present in one cm\(^2\).

In a reactor, the values of neutron density and neutron flux are a function of location in the core. Because the neutron flux is an essential ingredient in the computation of reactor rates, the determination of the spatial distribution of the neutron flux in the core is an important part of reactor physics. The value of the neutron flux at a given point in the core will depend on the distribution of nuclear properties like the cross sections throughout the core, and on the position in relation to the central part of the core and to the external surface of the reactor. The neutron flux continually drops to zero at, or just beyond, the radial and axial boundaries of the core. The behavior of the flux in the core and its rate of decline towards the boundaries must be calculated by means of computer codes (AECBC, 1993; Jayeola et al., 2018).

2.1.2. The Neutron Diffusion Equation

The neutron diffusion equations provide an essential exact description of the neutron distribution within a reactor. Its solution would contain essentially all the information we require concerning the nuclear behavior of the reactor (Duderstadt and Hamilton, 1976).

The multi-group diffusion equation comprises of the groups of neutrons of different energies diffusing within a nuclear reactor. The basic diffusion equation for each group of neutrons is the same, but with absorption generalized to all processes that remove the neutron from the group that is absorption plus scattering to another group and with the source of neutrons for each group specialized to include the in-scattering of neutrons from the other groups, which is also diffusing within the reactor (Stacey, 2007).

2.1.3. Numerical Methods used in neutron diffusion equation

It is assumed that a uniform reactor has the shape of a cylinder of physical radius (R) and height (H). This finite cylindrical reactor has cylindrical geometry which have coordinates at its origin. In order to solve the diffusion equations, the Laplacian is replaced by its
cylindrical form: cylindrical coordinates - 3D, 2D. This is not dependent on angle \( \Theta \), therefore, the 3D Laplacian is replaced by its two-dimensional form (2D). This makes it practicable to solve the problem using radial and axial directions. This is because the flux is a function of radius – \( r \) and height – \( z \) only (\( \Phi(r, z) \)).

Furthermore, numerical solutions of neutron diffusion equations have been solved using a number of numerical methods such as the finite difference, finite element, nodal and boundary element methods. These methods are all mesh-based in which the nodes that discretize the problem domain are related in a predefined manner (Tanbay and Bilge, 2013). However, numerical methods are used most exclusively for criticality calculations. Criticality calculations \( k_{eff} \) are based on power iteration procedures, where different multi-group diffusion equations with a number of iterations are used to estimate the effective multiplication factor (\( k_{eff} \)). This iteration process is repeated until the fission distribution has converged.

3. METHODOLOGY

3.1. Calculation of the Four-Group Diffusion Equations

To calculate the four-group diffusion equation, we use the finite difference discretization of steady state four-group neutron diffusion equation in a cylindrical coordinate. First, the finite difference discretization of one group differential equation was established and later extended to four-group differential equation. The boundary conditions introduced in this research are: the neutron flux vanishes at the extrapolated boundary of the core (\( r = R \) and \( z = 0, H \)). Where \( R = \) Extrapolated Radius and \( H = \) Extrapolated Height. The multi-group diffusion system in a cylindrical coordinate can be written as:

\[
\frac{1}{r} \frac{\partial}{\partial r} \left[ D(r, z) r \frac{\partial \phi(r, z)}{\partial r} \right] + \frac{\partial}{\partial z} \left[ D(r, z) \frac{\partial \phi(r, z)}{\partial z} \right] - \sum_{\gamma} (r, z) \phi(r, z) = -S(r, z)
\]

(3)

The dependent variable in Eq. (3) is the neutron flux, \( D \) is the diffusion coefficient and \( S \) is the neutron fission source used to initiate the fission reaction. The third term in Eq. (3), (sigma subscript ‘\( \gamma \)’) is the total macroscopic cross section of the reactor core.

Multiplying Eq. (3) through by \( r \), we obtain:

\[
\frac{\partial}{\partial r} \left[ D(r, z) r \frac{\partial \phi(r, z)}{\partial r} \right] + \frac{\partial}{\partial z} \left[ r D(r, z) \frac{\partial \phi(r, z)}{\partial z} \right] = r \sum_{\gamma} (r, z) \phi(r, z) = -r S(r, z)
\]

(4)

The Eq. (4) was discretized using a finite difference method to obtain the four-group diffusion equations by considering the neutron flux varying along the radial and axial coordinate, hence the Fick’s law for the radial and axial coordinate can be written as Eqs. (5) and (6) respectively:

\[
J = D(r, z) r \frac{\partial \phi(r, z)}{\partial r}
\]

(5)

and

\[
Y = D(r, z) \frac{\partial \phi(r, z)}{\partial z}
\]

(6)

where \( J \) and \( Y \) are the neutron current density for the radial and axial coordinates respectively. Substituting Eq. (5) and Eq. (6) into Eq. (4), we obtain Eq. (7).

\[
\frac{\partial J}{\partial r} + r \frac{\partial Y}{\partial z} = r \sum_{\gamma} (r, z) \phi(r, z) = -r S(r, z)
\]

(7)

The reactor is assumed to cover a special mesh of \( r \) and \( z \) dimensions as shown in the Fig. 2. Hence Eq. (7) is solved by integrating over the mesh intervals, to obtain:

\[
\int_{r_{i-1/2}}^{r_{i+1/2}} \int_{z_{j-1/2}}^{z_{j+1/2}} \frac{\partial J}{\partial r} dr dz + r \int_{r_{i-1/2}}^{r_{i+1/2}} \int_{z_{j-1/2}}^{z_{j+1/2}} \frac{\partial Y}{\partial z} dr dz - r \int_{r_{i-1/2}}^{r_{i+1/2}} \int_{z_{j-1/2}}^{z_{j+1/2}} \sum_{\gamma} \phi(r, z) dr dz = \int_{r_{i-1/2}}^{r_{i+1/2}} \int_{z_{j-1/2}}^{z_{j+1/2}} r S g dr dz.
\]

(8)

Carrying out the integration in Eq. (8), we have:

\[
\int_{z_{j-1/2}}^{z_{j+1/2}} (J_{i+1/2} - J_{i-1/2}) dz + \int_{r_{i-1/2}}^{r_{i+1/2}} (Y_{j+1/2} - Y_{j-1/2}) dz = \int_{r_{i-1/2}}^{r_{i+1/2}} \int_{z_{j-1/2}}^{z_{j+1/2}} (\sum_{\gamma} \phi - S) dr dz.
\]

(9)
Each term in Eq. (9) can be written as Eqs. (10) and (11). Putting Eqs. (10), (11) and (12) into Eq. (9), we obtain Eq. (13). Integrating Eq. (5) over the interval \( r_i - 1 < r < r_i + 1/2 \) : \( z_j - 1/2 < z < z_j + 1/2 \) eliminates \( J \) whilst an integration of Eq. (6) is performed over the limits \( r_i - 1/2 < r < r_i + 1/2 \) : \( z_j < z < z_j + 1/2 \) eliminates \( Y \). The simplified equation for the parameter \( J \) and \( Y \) can be written as Eq. (14), (15) and Eq. (16) and (17) respectively. Putting Eqs. (14), (15), (16) and (17) into Eq. (13), we obtain Eq. (18). On further simplification of Eq. (18) and applying the boundary conditions, we obtain Eq. (19). The finite difference equation for the four-group diffusion equations in a cylindrical geometry can be obtained from Eq. (19). This is written as Group 1 (Eq. 20), Group 2 (Eq. 22), Group 3 (Eq. 23) and Group 4.
(Eq. 24) respectively. The obtained four-group diffusion equations is the numerical solution for four-group diffusion equation in a cylindrical reactor core. Where, $\Sigma_{s,g}$ (Macroscopic scattering cross section from energy group $g$ to $g+1$),

\[
\int_{z_{j-1/2}}^{z_{j+1/2}} (J_{i+1/2}^j - J_{i-1/2}^j) \, dz = (J_{i+1/2}^j - J_{i-1/2}^j) \Delta x_j, 
\]

(10)

\[
\int_{r_{i-1/2}}^{r_{i+1/2}} (Y_{j+1/2}^i - Y_{j-1/2}^i) \, dr = (Y_{j+1/2}^i - Y_{j-1/2}^i) r_i \Delta r_i, 
\]

(11)

\[
\int_{r_{i-1/2}}^{r_{i+1/2}} \int_{z_{j-1/2}}^{z_{j+1/2}} (\Sigma s \varphi - S) \, dr \, dz = (\Sigma s_i \Delta r \Delta z)_{i,j} \varphi_i r_i - (S \Delta r \Delta z)_{i,j} r_i, 
\]

(12)

\[
(j_{i+1/2}^j - j_{i-1/2}^j) \Delta x_j + (Y_{j+1/2}^i - Y_{j-1/2}^i) r_i \Delta r_i = (\Sigma s_i \Delta r \Delta z)_{i,j} \varphi_i r_i = - (S \Delta r \Delta z)_{i,j} r_i. 
\]

(13)

\[
J_{i+1/2}^j = \frac{D_{i+1/2}^j r_{i+1/2} \Delta x_j}{\Delta r_{i+1/2} \Delta x_{j+1/2}} [\varphi_{i+1,j} - \varphi_{i,j}], 
\]

(14)

\[
J_{i-1/2}^j = \frac{D_{i-1/2}^j r_{i-1/2} \Delta x_j}{\Delta r_{i-1/2} \Delta x_{j+1/2}} [\varphi_{i-1,j} - \varphi_{i,j}], 
\]

(15)

\[
Y_{i,j+1/2} = \frac{D_{i,j+1/2} r_{i,j+1/2} \Delta r_i}{\Delta r_{i,j+1/2} \Delta x_{j+1/2}} [\varphi_{i+1,j} - \varphi_{i,j}], 
\]

(16)

\[
Y_{i,j-1/2} = \frac{D_{i,j-1/2} r_{i,j-1/2} \Delta r_i}{\Delta r_{i,j-1/2} \Delta x_{j-1/2}} [\varphi_{i-1,j} - \varphi_{i,j}], 
\]

(17)

\[
\frac{D_{i+1/2}^j r_{i+1/2} \Delta x_j}{\Delta r_{i+1/2} \Delta x_{j+1/2}} (\varphi_{i+1,j} - \varphi_{i,j}) - \frac{D_{i-1/2}^j r_{i-1/2} \Delta x_j}{\Delta r_{i-1/2} \Delta x_{j+1/2}} (\varphi_{i-1,j} - \varphi_{i,j}) + \frac{D_{i,j+1/2} r_{i,j+1/2} \Delta r_i}{\Delta r_{i,j+1/2} \Delta x_{j+1/2}} (\varphi_{i+1,j} - \varphi_{i,j}) - \frac{D_{i,j-1/2} r_{i,j-1/2} \Delta r_i}{\Delta r_{i,j-1/2} \Delta x_{j-1/2}} (\varphi_{i-1,j} - \varphi_{i,j}) = -r_i \Sigma_{i,j} 1 \Delta r_i \Delta x_j - r_i \Sigma_{i,j} 1 \Delta r_i \Delta x_j. 
\]

(18)

\[
\varphi_{i,j} = \frac{2D r_i (\varphi_{i+1,j} + \varphi_{i-1,j} + \varphi_{i,j+1} + \varphi_{i,j-1}) + r_i [S_{i,j}] \Delta r \Delta z}{4Dr_i + r_i \Sigma_{i,j}}, 
\]

(19)

Group 1:

\[
\varphi_{i,j}^1 = \frac{2D^1 r_i (\varphi_{i+1,j}^1 + \varphi_{i-1,j}^1 + \varphi_{i,j+1}^1 + \varphi_{i,j-1}^1) + r_i [S_{i,j}^1]}{4D^1 r_i + r_i \Sigma_{i,j}^1}, 
\]

(20)

where

\[
\Sigma_{i,j}^1 = \Sigma_{a1}, 
\]

(21)

and where the subscript represents the group number.

Group 2:

\[
\varphi_{i,j}^2 = \frac{2D^2 r_i (\varphi_{i+1,j}^2 + \varphi_{i-1,j}^2 + \varphi_{i,j+1}^2 + \varphi_{i,j-1}^2) + \Sigma_{1-2} \varphi_{i,j}^1}{4D^2 r_i + r_i \Sigma_{i,j}^2}, 
\]

(22)

where

\[
\Sigma_{i,j}^2 = \Sigma_{a2} + \Sigma_{1-2}, 
\]

(23)
Group 3:
\[
\varphi_{ij}^3 = \frac{2D^3r_i(\varphi_{i+1,j}^3 + \varphi_{i-1,j}^3 + \varphi_{i,j+1}^3 + \varphi_{i,j-1}^3) + \Sigma_2 \psi_{ij}^2}{4D^3r_i + r_i \Sigma_{ti,j}^3}
\]
where \( \Sigma_{ti,j}^3 = \Sigma_{a3} + \Sigma_{1-3} + \Sigma_{2-3} \), \hspace{1cm} (24)

Group 4:
\[
\varphi_{ij}^4 = \frac{2D^3r_i(\varphi_{i+1,j}^4 + \varphi_{i-1,j}^4 + \varphi_{i,j+1}^4 + \varphi_{i,j-1}^4) + \Sigma_3 \psi_{ij}^3}{4D^3r_i + r_i \Sigma_{ti,j}^4}
\]
where \( \Sigma_{ti,j}^4 = \Sigma_{a4} + \Sigma_{1-4} + \Sigma_{2-4} + \Sigma_{3-4} \). \hspace{1cm} (25)

Next, TUNTOB proceeds from the first group to the second, third and fourth group, iterating within each group until the criteria convergence is met. It evaluates the tolerance between the old and the new \( k_{eff} \) values.

To calculate the new \( k_{eff} \), the program integrates the old and new source terms over space and essentially averages them. With the updated source and \( k_{eff} \), the iterations are performed again. The process continues until convergence is met. Next the program checks if the reactor is critical. If \( k_{eff} \) is very close to or equal to one (1), the system is critical. If the reactor is not critical, the program will again recommend an adjusted value for the core geometry, guessed multiplication factor (k) and flux.

3.2. Design of the Algorithm (TUNTOB)

The algorithm was designed using Matlab. Matlab was used because its algorithms can be developed in much shorter time than equivalent FORTRAN or C programs (Kiusalaas, 2005). The TUNTOB algorithm was developed for the criticality calculations of a homogenous cylindrical reactor core using four-group diffusion equations. The flow chart of the proposed algorithm is shown in Fig. 3.

4. RESULTS AND DISCUSSION

4.1. Iteration and Mesh Sizes Optimization

4.1.1. Iteration optimization

The calculations of the iteration optimization are shown in Table 1. A maximum of 1000 and a minimum of 600 iterations were performed. The 1000th iteration was performed for a 12 cm x 24 cm mesh size of the reactor core. The Table 1 shows the values of the effective multiplication factor of the same mesh size with the number of iterations (600-1000). It was observed that an increment in iteration leads to an increase in the effective multiplication factor obtained from 0.9983 to 0.9990 with a corresponding increase in the computation time. The maximum effective multiplication factor of \( (k_{eff} = 0.9990) \) was reached when the number of iterations were 1000 and above. Therefore, it was concluded that the optimal number of iterations required for this calculation is 1000.
Table 1. Iterations optimization and its corresponding maximum effective multiplication factor ($k_{eff}$) with constant mesh size (4 cm x 4 cm).

<table>
<thead>
<tr>
<th>Number of Iteration</th>
<th>Effective Multiplication Factor ($k_{eff}$)</th>
<th>Computation Time (Min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>600</td>
<td>0.9983</td>
<td>2.818</td>
</tr>
<tr>
<td>700</td>
<td>0.9988</td>
<td>3.102</td>
</tr>
<tr>
<td>800</td>
<td>0.9989</td>
<td>3.592</td>
</tr>
<tr>
<td>900</td>
<td>0.9990</td>
<td>3.729</td>
</tr>
<tr>
<td>950</td>
<td>0.9990</td>
<td>3.845</td>
</tr>
<tr>
<td>1000</td>
<td>0.9990</td>
<td>4.282</td>
</tr>
</tbody>
</table>

4.1.2. Mesh size optimization

Having established the optimal number of iteration, the effects of the mesh size on the computation is examined in this section. The Table 2 reveals that the values of $k_{eff}$ increases as the mesh sizes becomes smaller until an optimal mesh size of 1 x 1 cm$^2$ is reached and further decrease in mesh sizes gives no further improvement in the value of $k_{eff}$.

Table 2. Mesh size optimization and its corresponding maximum effective multiplication factor ($k_{eff}$) with constant 1000-iteration.

<table>
<thead>
<tr>
<th>Mesh Size Area (cm$^2$)</th>
<th>Effective Multiplication Factor ($k_{eff}$)</th>
<th>Computation Time (Min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 x 4</td>
<td>0.9990</td>
<td>4.282</td>
</tr>
<tr>
<td>2.4 x 2.4</td>
<td>0.9992</td>
<td>6.015</td>
</tr>
<tr>
<td>2 x 2</td>
<td>0.9996</td>
<td>6.751</td>
</tr>
<tr>
<td>1 x 1</td>
<td>0.9998</td>
<td>7.393</td>
</tr>
<tr>
<td>0.8 x 0.8</td>
<td>0.9998</td>
<td>8.491</td>
</tr>
<tr>
<td>0.5 x 0.5</td>
<td>0.9998</td>
<td>9.553</td>
</tr>
</tbody>
</table>

4.2. Neutron Flux Profile

The neutron flux profile was considered for both the axial and radial (3D) directions. This approach gave a better understanding of the behaviour of the neutron flux in the cylindrical reactor core. Comparing the results of the neutron flux distribution in the radial and axial directions obtained from TUNTOB with that of the neutron flux distribution of THEESIS Code (Harman, 2001). It was observed that TUNTOB obtained better results than the THEESIS Code, although, not all the THEESIS source code parameters were accessible. In addition, we observed that the graphs of the THEESIS Code follow the same trend with that obtained in this study.

4.2.1 Neutron flux distribution in 3-D representation

The color difference or variation in the neutron flux distribution for the 4 by 4 mesh from group 1 to group 4 confirms that the centre of the core has the greatest amount of heat (and the neutron flux has the highest value at the centre of the core) and the heat gradually reduces as the neutron flux moves away from the centre of the core until it gets to the surface of the core (from color red, changes to color yellow and a light green color and then to color blue). The same trend occurs for other different mesh sizes for the four-group.

The neutron flux distributions in 3-D representation are shown in Fig. (4-11). The figures describe the behavior of the neutron flux for the four groups in both the radial and axial directions. The neutron flux profile showed that all the group behave in the same manner having maximum values at the center of the reactor core, ($r = 0, z = H/2$). The neutron flux for the first group (Group 1) has the highest maximum value, followed by the second (Group 2) and third group (Group 3) while the fourth group (Group 4) has the lowest. This trend is expected because fission neutrons are produced directly into the first three groups and the scattering of neutrons from these three groups serves as the source of neutrons in the fourth group. In Fig. (4-11), the 4 by 4 mesh showed that the trend of the flux in between the mesh points follows straight lines but when the number of mesh points is increased, the trend becomes a smooth curve as shown in Fig. (4-11) for a 1 by 1 mesh. It is expected that further increase in the number of mesh points will produce smoother curves with a corresponding increase in the computational time.
Fig. 6. Neutron flux distribution in 3D for the third group of a 4 by 4 mesh.

Fig. 7. Neutron flux distribution in 3D for the fourth group of a 4 by 4 mesh.

Fig. 8. Neutron flux distribution in 3D for the first group of a 1 by 1 mesh.

Fig. 9. Neutron flux distribution in 3D for the second group of a 1 by 1 mesh.

Fig. 10. Neutron flux distribution in 3D for the third group of a 1 by 1 mesh.

Fig. 11. Neutron flux distribution in 3D for the fourth group of a 1 by 1 mesh.
In this work, we have derived four group diffusion equations for a cylindrical reactor core which gives a detailed description of neutron distribution in the core. We derived the discretized four group diffusion equations for a cylindrical reactor core because it gives an exact description of what takes place in a low water reactor (LWR). The results obtained for the criticality calculations were compared with criticality benchmarks and found to be very close. For instance, the \( k_{\text{eff}} \) calculated by the code is found to be 1.246728 while the benchmark value is 1.246368 (Ganapol, 2014).

CONCLUSION

This study provides the criticality calculation and neutron flux distribution in a homogenous cylindrical reactor core in two dimensions \((r, z)\) using four energy groups. From the results these studies further confirm that the centre of the core of the reactor has the greatest heat which is synonymous to the different colour variations relating to decrease in the amount of heat as it moves away from the centre of the core. The calculations were carried out for a reactor in a steady state. The developed algorithm (TUNTOB), calculates values of \( k_{\text{eff}} \) and the neutron distribution as a function of the mesh sizes. It was found that the accuracy in the value of \( k_{\text{eff}} \) and the smoothness of the neutron distribution curves in 3-D representations, depends on the number of mesh points. It allows the user to modify the reactor dimensions and see the impacts on the neutron distribution and criticality within the reactor core.

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