

INVESTIGATION OF THE USE OF CALCIUM CARBONATE AS NANOPARTICLES IN NUCLEAR REACTORS

¹Sinem UZUN , ²Yasin GENÇ , ³Adem ACIR 

¹Erzincan Binali Yıldırım University, Engineering and Architecture Faculty, Mechanical Engineering Department, Erzincan, TÜRKİYE

²Ministry of Interior, Disaster and Emergency Management Presidency, Ankara, TÜRKİYE

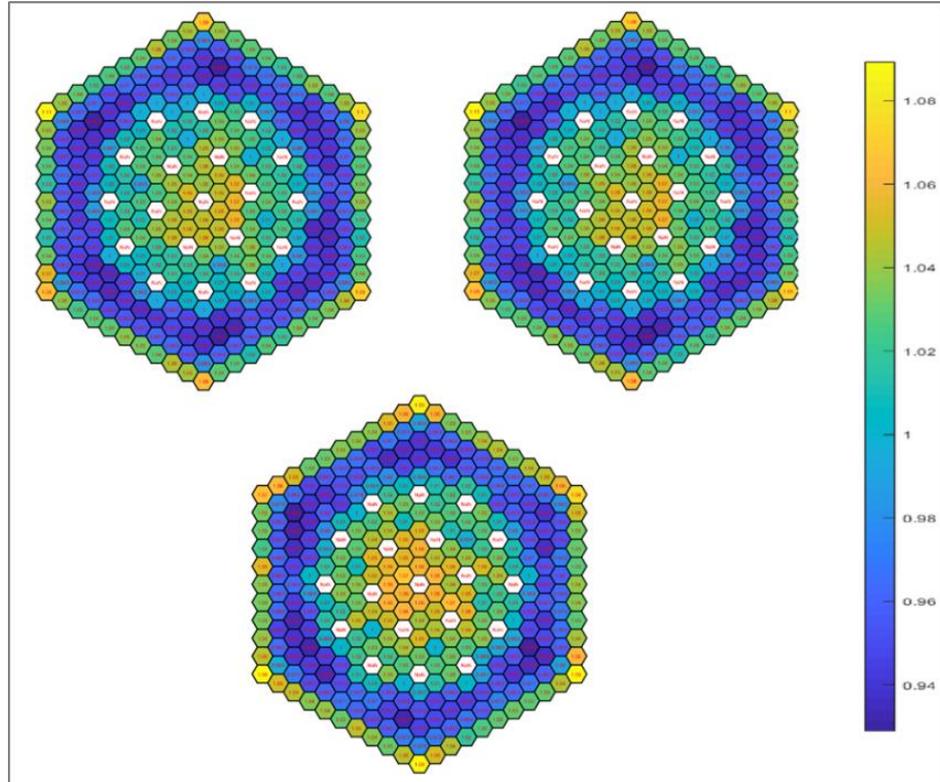
³Gazi University, Technology Faculty, Energy Systems Engineering Department, Ankara, TÜRKİYE

¹sinemuzun@erzincan.edu.tr, ²ysngnc@gmail.com, ³adema@gazi.edu.tr

Highlights

- Radiation shielding properties for CaCO₃ were investigated.
- Thermal analyzes were made with COBRA code.
- Coolant temperature increased with the nanoparticle ratio.

Graphical Abstract



Relative power distribution for CaCO₃ nanoparticle (a) 0.01%, (b) 0.02%, (c) 0.03%



INVESTIGATION OF THE USE OF CALCIUM CARBONATE AS NANOPARTICLES IN NUCLEAR REACTORS

¹Sinem UZUN , ²Yasin GENÇ , ³Adem ACIR 

¹Erzincan Binali Yıldırım University, Engineering and Architecture Faculty, Mechanical Engineering Department, Erzincan, TÜRKİYE

²Ministry of Interior, Disaster and Emergency Management Presidency, Ankara, TÜRKİYE

³Gazi University, Technology Faculty, Energy Systems Engineering Department, Ankara, TÜRKİYE

¹sinemuzun@erzincan.edu.tr, ²ysngnc@gmail.com, ³adema@gazi.edu.tr

(Received: 01.07.2022; Accepted in Revised Form: 31.10.2022)

ABSTRACT: In this study, calcium carbonate (CaCO_3) was considered as nanoparticle. In the first part of the study, half-value layer (HVL) and mean free path (MFP) values, which are radiation shielding parameters, were investigated in determined energy ranges by Phy-X open access software. At increasing energy levels, the HVL value reached approximately 10 cm, while the MFP value reached approximately 17 cm. In the second part of the study, the reactor core geometry was modeled with the MCNP code and then the relative power distribution values were determined. COBRA code input was prepared with the determined relative power distribution values and thermal analyzes were made. These analyzes were performed for three different nanoparticle ratios. As a result of the analysis, the temperature value at the end of the channel was 613 K when only water was used as a coolant, while the temperature value at the end of the channel was 611.19 K when 0.03% nanoparticles were used. Although the coolant temperature increased with the nanoparticle ratio, it was observed that the temperature decreased when only water was used.

Keywords: Calcium carbonate, COBRA, MCNP, Nanoparticle, Phx-X software

1. INTRODUCTION

Calcium carbonate is a compound present in almost all food products. Although it is known as limestone among the people, it is found in the form of rock in nature. Travertines, chalks and marbles come to mind when calcium carbonate (CaCO_3) is mentioned. Although it is frequently used in the fields of construction and industry, academic research on CaCO_3 is also quite abundant [1-4]. In the literature, especially in recent years, the effect of nanoparticles in academic studies has begun to be examined. Many systems using CaCO_3 as nanoparticles are being investigated by researchers.

Some of the studies examining the mechanical properties of materials and making mechanical improvements are as follows. In one of these studies; by preparing nanocomposites containing calcium carbonate, the thermal, mechanical and morphological properties of these composites were investigated [5]. As a result of the examination, the researchers concluded that the CaCO_3 ratio was 3.75%, where the nanocomposite used showed the highest impact and tensile strength. There are researchers who examine the modification of adhesive bonds with nano- CaCO_3 to increase the shear strength of epoxy adhesives and also investigate the adhesive properties with the tensile overlap shear test [6]. In a study examining the effect of nano- CaCO_3 particles on the interlayer shear strength (ILSS) and fracture toughness properties of carbon fiber reinforced epoxy composites [7], composite materials were prepared by vacuum assisted resin method. As a result of the tests applied to the material afterwards, it was concluded that adding 2% by weight of nano- CaCO_3 to the epoxy increased the interlayer shear strength (ILSS) up to 24%. To increase the wear performance of epoxy/carbon fiber (CF) composites, CaCO_3 was added as nano

*Corresponding Author: Sinem UZUN, sinemuzun@erzincan.edu.tr

reinforcement and a 65% reduction in friction coefficient and 75% reduction in specific wear rate was observed [8]. Cementitious matrices in which nano-CaCO₃ is also used were investigated in a study that carried out studies to increase concrete strength. In particular, their mechanical and durability properties were investigated and they concluded that the use of nanomaterials in cement concrete with the necessary properties of building materials confirmed the feasibility [9]. Investigating the mechanical, thermal, morphological effect of two types of fillers, micro CaCO₃ and nano-CaCO₃, on Polypropylene (PP) composite material [10], they concluded that the inclusion of nanofillers revealed better thermomechanical properties. In the study conducted with nanocomposites containing calcium carbonate, the change of mechanical properties such as flexural strength, flexural modulus, impact strength was investigated. The sample containing 4% by weight nano CaCO₃ provided positive results in terms of flexural strength, flexural modulus, impact strength compared to pure epoxy matrix [11]. Researchers [12], who examined the effect of nano calcium carbonate particles on stone mastic asphalt (SMA), concluded, as a result of a series of mechanical tests, that the fatigue life of SMA mixtures increased and the final stresses decreased with the addition of nano CaCO₃ particles.

In the study where the effect of clinker mineral component and nanomaterials (nano-SiO₂, nano-CaCO₃ and nano-TiO₂) on cement composites was investigated [13], HCSC's (high content calcium silicate phase cement) curing time is shortened and its strength is significantly increased. There are some studies [14-16] investigating the nano-calcium carbonate effect like these, and the general conclusion from these studies is that the use of calcium carbonate as nanoparticles improves the mechanical and strength properties of the systems in which it is used.

The use of nanoparticles in nuclear systems has recently started to increase. Because of the thermal conductivity properties of the nanoparticles used, the efficiency of the system can be increased [17-18]. The nanoparticles used so far have had a positive effect on the system efficiency by increasing the coolant temperature. Some of these nanoparticles are; Al₂O₃, CuO, TiO₂, Al, Cu, Si, Ag.

In this study, firstly, open access software Phy-X [19] was used to examine the radiation shielding properties. Since radiation shielding is very important in nuclear reactors, it is important to know the radiation properties of the materials used.

In the second part of the study, it was investigated how the coolant properties of nuclear reactors containing calcium carbonate nanoparticle coolant water changed. To do this, first of all, relative power distributions were determined with the Monte Carlo N-Particle Transport (MCNP) [20] code used for neutronic analysis.

The power distributions values obtained from the use of the MCNP code are used in the COBRA code. The COBRA code [21] was used to obtain the thermal analysis values. The COBRA code can determine the thermal values of the reactor coolant by performing the subchannel analysis.

2. CALCIUM CARBONATE AND RADIATION SHIELDING

The issue of protection from ionizing radiation is very important in the world. Researchers working on this subject are doing improvement studies against radiation protection on some materials [4, 22-25]. For example, [22] investigated the shielding properties of some low-temperature superconducting brazing alloys. The highest mass absorption coefficient and half value layer values were determined [22]. In a study that applied solution polymerization to produce water-soluble polyurethane, CaCO₃ was used as fake gunpowder. And as a result, the tensile strength of the 40% diisocyanate-treated CaCO₃ WPU composites was increased and the elongation at break was also significantly improved [4]. Half value layer (HVL) and mean free path (MFP) values are very important in radiation protection investigations. HVL value is the thickness of the material at which the intensity of radiation entering it is reduced by one half. HVL is related to linear attenuation coefficient (μ) and it is represented by Equation 1 [26].

$$\text{HVL} = 0.693 / \mu \quad (1)$$

Another important parameter is the MFP value, which is the average path a photon can travel between two consecutive interactions with the material and it is calculated as in Equation 2 [27].

$$\text{MFP} = 1 / \mu \quad (2)$$

3. THERMAL ANALYSIS

In this part of the study, thermal properties of reactor coolant water containing calcium carbonate nanoparticles were investigated. Most nuclear reactors in the world are pressurized water reactors and generally use water as a coolant. It is expected that the coolant material used to absorb the heat generated by the chain fission reactions occurring in the nuclear reactor core will absorb the maximum heat from the system. In order to do this, there are suggestions about adding nanoparticles to the coolant water in order to improve the heat conduction properties [17-18].

The relative power distribution of the calcium carbonate nanofluid was obtained using the MCNP code which is a time-dependent Monte Carlo radiation transport code with continuous energy and generalized geometry that can track many particle types in various energy ranges. It can simulate particle interactions involving neutrons, photons and electrons, as well as for simulating the fission event. While preparing the MCNP input, data such as reactor geometry, fuel and coolant properties (such as density) are used.

With the obtained relative power values, the COBRA input that performs the subchannel analysis was prepared. COBRA code is a thermal-hydraulic code that performs subchannel analysis by dividing the examined system into channels in the number and size determined by the user. As a result of the operation of this code, thermal data of the fuel and clad regions, especially the coolant, can be obtained in the examined system. There are a total of 163 fuel bundles in the hexagonal reactor core and 312 fuel rods in each fuel bundle. The channel figure used in the COBRA code is shown in Figure 1 [28].

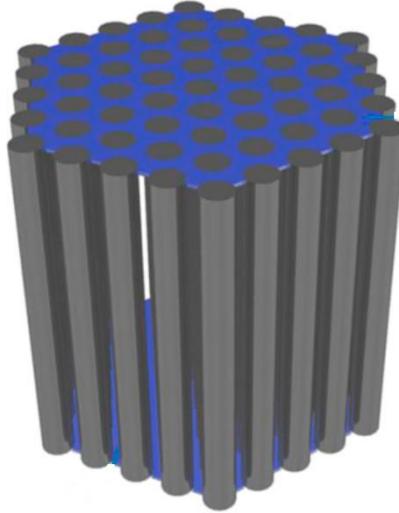


Figure 1. Schematic channel flow surface

COBRA code makes solutions by using conservation equations in its infrastructure. The mass, momentum and energy conservation equations are shown in equations 3-4 and 5, respectively [29].

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (3)$$

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla P + \nabla \cdot \bar{\tau} + \rho \vec{g} \quad (4)$$

$$\frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\rho U \vec{v}) = -\nabla \cdot \vec{q} + \dot{q}''' - P \nabla \cdot \vec{v} \quad (5)$$

4. RESULTS AND DISCUSSION

Open access software Phy-X was used to examine the radiation shielding property of the calcium carbonate compound [19]. While using this software, determined energy ranges (0.015 MeV - 15 MeV) were selected. The variation of HVL and MFP values for CaCO_3 is shown in Figure 2. According to this; While the HVL value reached approximately 10 cm at increasing energy levels, the MFP value reached approximately 17 cm. The MFP value defines the average distance between two photon interactions, while the HVL value can be defined as a measure of the thickness required to reduce radiation and represents the one-half value of the first photon that helps determine the material thickness for shielding [22]. HVL value is an indicator of radiation protection performance. In other words, the lower HVL value of any material shows better radiation shielding performance as it will need a lower thickness [30]. A low HVL value indicates that the material has good protection properties [31]. The MFP value increased with the increase in energy, which is consistent with the literature [27].

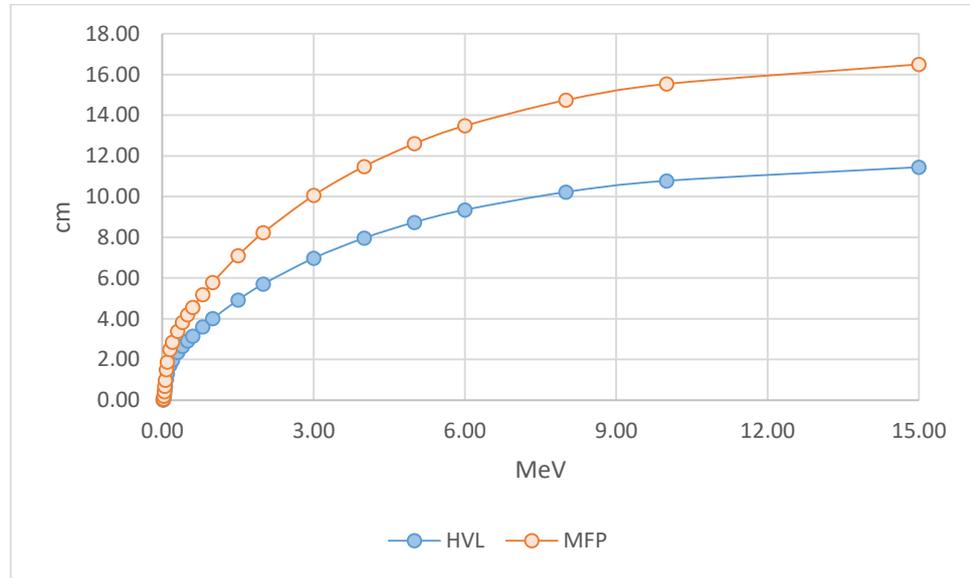


Figure 2. HVL and MFP values for CaCO_3

Low MFP and HVL values are important in radiation shielding materials. In this examination for calcium carbonate, HVL and MFP values increased in line with the literature [32].

Since the reactor type considered in this study is VVER type pressurized water reactor, the reactor geometry is hexagonal. While the image shows (a) contains 0.01% CaCO_3 , (b) 0.02% and (c) 0.03% CaCO_3 the distribution of relative power densities of the nanofluid containing in Fig.3.

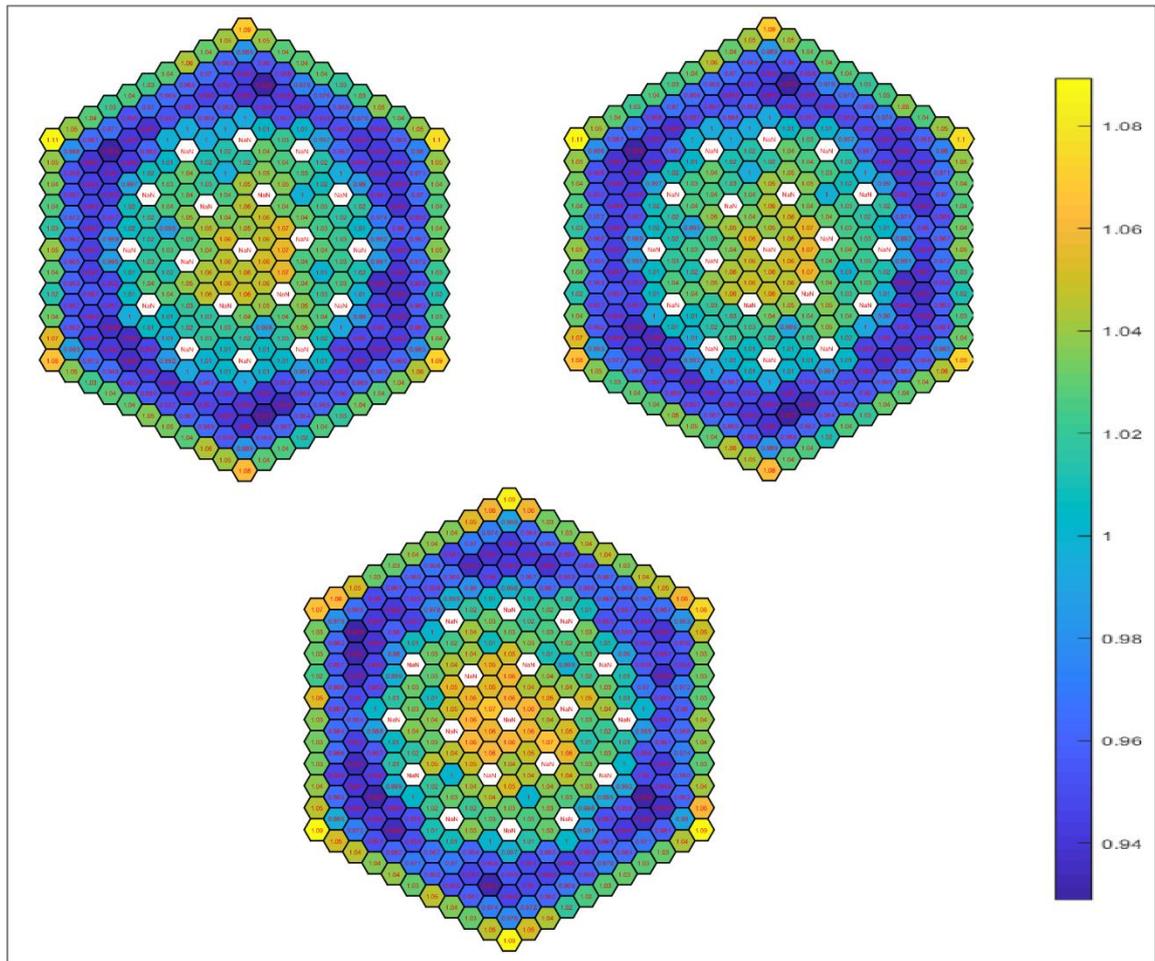


Figure 3. Relative power distribution for CaCO₃ nanoparticle (a) 0.01%, (b) 0.02%, (c) 0.03%

The changes in the thermal properties of the coolant along the channel were investigated as a result of the calculations and analysis using the varying ratios of calcium carbonate. The temperature change of the coolant containing nanoparticles along the channel was shown in Figure 4. Accordingly, although the temperature increased with the increasing ratio of CaCO₃ nanoparticles, there was a decrease in temperature when only water was used. While only water was used, the coolant temperature value at the end of the channel was approximately 613 K, while the temperature reached 610.64 K at the rate of 0.1%, 611.04 K at the rate of 0.2% and 611.19 K at the rate of 0.3% with the addition of nanoparticles. In a study using nanoparticle added coolant, the temperature increased with increasing nanoparticle ratio, similar to this study [33].

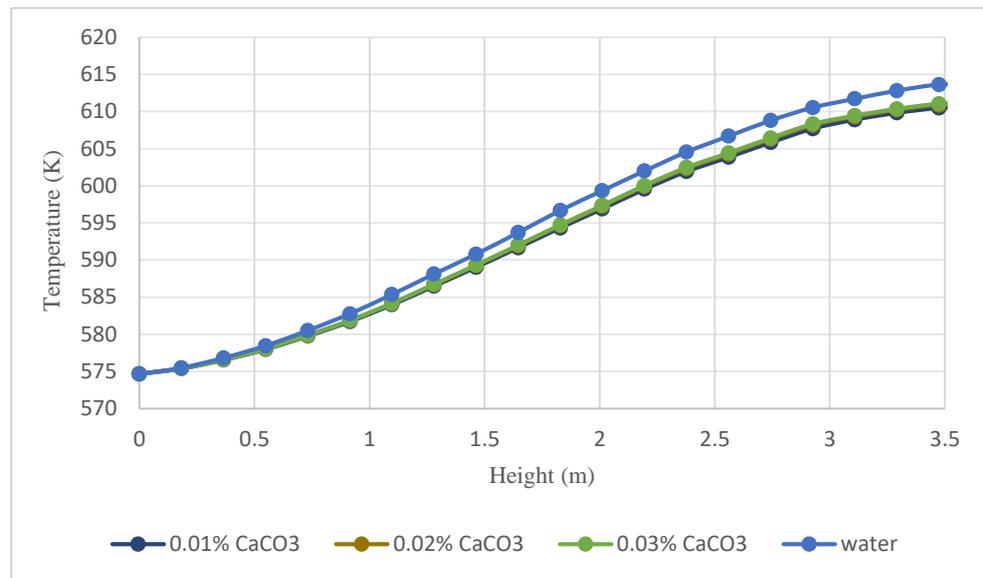


Figure 4. Temperature value

The enthalpy change of the coolant containing calcium carbonate was given in Figure 5. According to the figure, although the enthalpy increased with the increase of the nanoparticle ratio, the enthalpy value decreased compared to the case where only water was used. When only water is used at the end of the channel, the enthalpy value reaches 1598 kJ/kg, while this value reaches 1562 kJ/kg in the coolant containing 0.01% CaCO₃. The temperature and enthalpy changes are similar to other studies using nanofluid coolants [33-35].

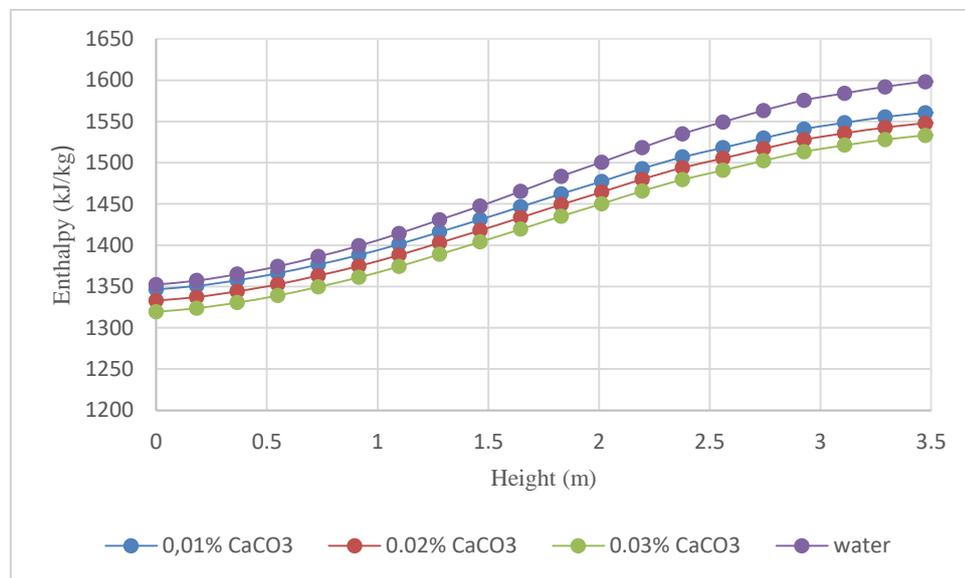


Figure 5. Enthalpy value

5. CONCLUSION

Within the scope of this study, it was carried out to examine the effect of CaCO₃ composition, which is used in many industrial and technological fields, on nuclear systems. Accordingly, firstly, the half value layer (HVL) and mean free path (MFP) values were examined using Phy-X software. According to the results obtained from the analysis for CaCO₃, the HVL value reached approximately 10 cm at increasing energy levels, while the MFP value reached approximately 17 cm.

In the thermal analysis part, although the temperature increased with the increasing ratio of CaCO₃ nanoparticles, there was a decrease in temperature compared to the case where only water was used. Similarly, the enthalpy value decreased when only water was used. While an increase in the coolant water temperature is expected in nuclear systems with the addition of nanoparticles, the use of CaCO₃ reduced the temperature a little. This shows that the heat conduction properties of the CaCO₃ compound are more ineffective than other nanoparticles (Al₂O₃, TiO₂, CuO etc.) used in nuclear systems.

Declaration of Ethical Standards

Authors declare to comply with all ethical guidelines, including authorship, citation, data reporting, and original research publication.

Credit Authorship Contribution Statement

Sinem UZUN: The author has done research and analysis.
Yasin GENÇ: The author analyzed and wrote the article.
Adem ACIR: The author has written and edited the article.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Funding / Acknowledgements

The authors declare that they have not received any funding or research grants during the review, research or assembly of the article.

Data Availability

Research data has not been made available in a repository.

REFERENCES

- [1] S. B. Baştürk, "An Investigation on the Flexural and Thermo-mechanical Properties of CaCO₃ Epoxy Composites", vol. 18, no.2, p. 161–167, 2022.
- [2] S., Leblebici, G. Işık, "The Effects of Calcium Carbonate (CaCO₃) Application At Different Concentrations on Seed Germination of Different Varieties of Carthamus Tinctorius L. (Asteraceae)", *Anadolu University Journal Of Science And Technology –C Life Sciences and Biotechnology*, vol. 7, no.1, p.1–1, 2018.
- [3] A. Şenlikci, M. Doğu, E. Eren, E. Çetinkaya, S. Karadağ, "Pressure calcimeter as a simple method for measuring the CaCO₃ content of soil and comparison with Scheibler calcimeter", *Toprak Dergisi*, vol. Special Issue, p. 24–28, 2015.
- [4] E. Wondu, Z. Lule, J. Kim, "Polyisocyanate-based water-soluble polyurethane/CaCO₃ composites for gunpowder storage", *Polymer Testing*, vol. 99, 107211, 2021.
- [5] A.E. Abd El-Hakim, A.E.M. Fettouh, A.A.A. Haroun, A.G.M. Rabie, G.A.M. Ali, M.Y.M. Abdelrahim, "Improving the mechanical and thermal properties of chlorinated poly(vinyl chloride) by incorporating modified CaCO₃ nanoparticles as a filler", *Turkish Journal of Chemistry*, vol. 43, no.3, p. 750–759, 2019.
- [6] H.B. Kaybal, H. Ulus, A. Avci, "Influence of Nano-CaCO₃ Particles on Shear Strength of Epoxy Resin Adhesives", *Uluslararası Muhendislik Arastirma ve Gelistirme Dergisi*, vol. 9, no.3, p. 29–35, 2017.

- [7] H. B.Kaybal, "Tabakalararası kayma mukavemeti ve kırılma tokluğu üzerine deneysel bir çalışma: CaCO₃ nanoparçacıkları ile iyileştirilmiş karbon fiber takviyeli epoksi kompozitler", *Ömer Halisdemir Üniversitesi Mühendislik Bilimleri Dergisi*, vol. 10, no. 2, p. 777–783, 2021.
- [8] E. F. Şükür, "Dry Sliding Friction And Wear Properties Of Caco₃ Nanoparticle Filled Epoxy/Carbon Fiber Composites", *Ömer Halisdemir Üniversitesi Mühendislik Bilimleri Dergisi*, vol.9, no. 2, p. 1108–1117. 2020.
- [9] J.A. Abdalla, B.S. Thomas, R.A. Hawileh, J. Yang, B.B. Jindal, E. Ariyachandra, "Influence of nano-TiO₂, nano-Fe₂O₃, nanoclay and nano-CaCO₃ on the properties of cement/geopolymer concrete", *Cleaner Materials*, vol. 4(March), 100061, 2022.
- [10] M. Al-Samhan, F. Al-Attar, "Comparative analysis of the mechanical, thermal and barrier properties of polypropylene incorporated with CaCO₃ and nano CaCO₃", *Surfaces and Interfaces*, vol. 31(May), 102055, 2022.
- [11] A. Misra, M. Shukla, M.K. Shukla, D. Srivastava, A.K. Nagpal, "Nano CaCO₃ modified multifunctional epoxy nanocomposites: A study on flexural and structural properties", *Materials Today: Proceedings*, vol. 47, p. 3295–3300, 2021.
- [12] A. M. Yarahmadi, G. Shafabakhsh, A. Asakereh, "Laboratory investigation of the effect of nano Caco₃ on rutting and fatigue of stone mastic asphalt mixtures", *Construction and Building Materials*, 317, 126127, 2022.
- [13] C. Luan, Y. Zhou, Y. Liu, Z. Ren, J. Wang, L. Yuan, S. Du, Z. Zhou, Y. Huang, "Effects of nano-SiO₂, nano-CaCO₃ and nano-TiO₂ on properties and microstructure of the high content calcium silicate phase cement (HCSC)", *Construction and Building Materials*, vol. 314(PA), 125377, 2022.
- [14] T. Alomayri, "Performance evaluation of basalt fiber-reinforced geopolymer composites with various contents of nano CaCO₃", *Ceramics International*, vol. 47(21), 29949–29959, 2021.
- [15] K. Cui, D. Lau, Y. Zhang, J. Chang, "Mechanical properties and mechanism of nano-CaCO₃ enhanced sulphoaluminate cement-based reactive powder concrete", *Construction and Building Materials*, vol. 309, 125099, 2021.
- [16] M. Sun, J. Zhu, T. Sun, Y. Chen, X. Li, W. Yin, J. Han, "Multiple effects of nano-CaCO₃ and modified polyvinyl alcohol fiber on flexure–tension-resistant performance of engineered cementitious composites", *Construction and Building Materials*, vol. 303, 124426, 2021.
- [17] A. Acir, S. Uzun, Y. Genç, Ş. Asal, "Thermal Analysis Of The Vver-1000 Reactor With Thorium Fuel And Coolant Containing Al₂O₃, CuO, And TiO₂ Nanoparticles", *Heat Transfer Research*, vol. 52(4), 79-93, 2021.
- [18] Y.Genc, S. Uzun, A. Acir, "Evaluation of the al/, cu/, si/, ag/water nanofluid effects on heat transfer characteristics in vver-1200 loaded with plutonium-thorium-based fuel". *Heat Transfer Research*, vol. 52(16), 1–12, 2021.
- [19] E. Şakar, Ö. F. Özpolat, B. Alım, M.I. Sayyed, M. Kurudirek, "Phy-X / PSD: Development of a user friendly online software for calculation of parameters relevant to radiation shielding and dosimetry", *Radiation Physics and Chemistry*, vol. 166, 2020.
- [20] J.F. Briesmeister "A General Monte Carlo N-Particle Transport Code", LA-13709M, Los Alamos National Laboratory, MCNP, 2020.
- [21] B.J. Webb, "COBRA-IV PC: A Personal Computer Version of CobraIV-I For Thermal-Hydraulic Analysis of Rod Bundle Nuclear Fuel Elements and Cores". *U.S. Department of Energy under Contract DE-AC06-76RLO 1830*, 1988.
- [22] C. Aksoy, S. Dizman, B. Çakır, T. E. Koparan, E. Tıraşoğlu, "The Radiation Shielding Properties of the Low Temperature Alloys". *Afyon Kocatepe University Journal of Sciences and Engineering*, vol. 21(5), 1022–1026, 2021.
- [23] Z. Aygun, N. Yarbasi, M. Aygun, "Spectroscopic and radiation shielding features of Nemrut, Pasinler, Sarıkamis and İkizdere obsidians in Turkey: Experimental and theoretical study", *Ceramics International*, vol. 47, no. 24, p. 34207-34217, 2021.
- [24] Z. Aygun, M. Aygun, "A study on usability of Ahlat ignimbrites and pumice as radiation shielding

- materials, by using EpiXS code", *International Journal of Environmental Science and Technology*, vol. 19, p. 5675–5688, 2022.
- [25] Z. Aygun, M. Aygun, "Radiation Shielding Potentials of Rene Alloys by Phy-X/PSD Code", *ACTA PHYSICA POLONICA A*, vol. 141, no. 5, p. 507-515, 2022.
- [26] H. Knipe, F. Macori, "Half-value layer". Reference article, Radiopaedia.org. (accessed on 05 Sep 2022) <https://doi.org/10.53347/rID-22271>.
- [27] M. Şekerci, H. Özdoğan, A. Kaplan, "An Investigation on Gamma-Ray Shielding Properties of Zr-Based Bulk Metallic Glasses", *HNPS Advances in Nuclear Physics*, vol. 27, p. 48–55, 2019.
- [28] M.H. Rahimi, G. Jahanfarnia, "Thermal-Hydraulic Core Analysis Of The VVER-1000 Reactor using A Porous Media Approach", *Journal Of Fluids And Structures*, vol.51, p. 85-96, 2014.
- [29] N.E. Todreas, M.S. Kazimi, "Nuclear Systems II Elements of Thermal Hydraulic Design", *Taylor & Francis*, New York, 2001.
- [30] O.E. Özkan, "Investigation of the Radiation Shielding Properties of Black Pine Wood Impregnated with Boric Acid", *Kastamonu Univ., Journal of Forestry Faculty*, 20(2), 200-207, 2020.
- [31] G. AlMisned Zakaly, SAM Issa, A. Ene, G. Kilic, O. Bawazeer, A. Almatar, D. Shamsi, E. Rabaa, Z. Sideig, HO. Tekin, "Gamma-Ray Protection Properties of Bismuth-Silicate Glasses against Some Diagnostic Nuclear Medicine Radioisotopes: A Comprehensive Study". (2021). *Materials*, 14(21), 6668.
- [32] O. Açar, "Investigation on Gamma Radiation Shielding Behaviour of CdO–WO₃–TeO₂ Glasses from 0.015 to 10 MeV", *Cumhuriyet Science Journal*, 39(4), 983-990, 2018.
- [33] V. Ghazanfari, M. Talebi, J. Khorsandi, R. Abdolahi, "Effects of water based Al₂O₃, TiO₂, and CuO nanofluids as the coolant on solid and annular fuels for a typical VVER-1000 core", *Progress in Nuclear Energy*, 91, 285–294, 2016.
- [34] E. Zarifi, G. Jahanfarnia, F. Veysi, "Thermal-hydraulic modeling of nanofluids as the coolant in VVER-1000 reactor core by the porous media approach", *Annals of Nuclear Energy*, vol. 51, p. 203-212, 2013.
- [35] H. Saadati, K. Hadad, A. Rabiee, A.H. Kamalinia, "Evaluation of nanofluid coolant effects on VVER-1000/V-446 reactor using 3-D full core coupled neutronic and thermohydraulics analysis", *Annals of Nuclear Energy*, vol. 152, 107995, 2021.