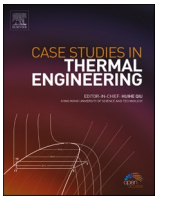
Case Studies in Thermal Engineering 52 (2023) 103653

Contents lists available at ScienceDirect

Case Studies in Thermal Engineering

journal homepage: www.elsevier.com/locate/csite



Investigating the effect of external heat flux on the thermal behaviour of hybrid paraffin-air heat sink: A molecular dynamics approach

Ke Wang [a], Dheyaa J. Jasim [b], As'ad Alizadeh [c], Ameer H. Al-Rubaye [d], Navid Nasajpour-Esfahani [e], Soheil Salahshour [f,g,h], Shadi Esmaeili [i], M. Hekmatifar [j,*]

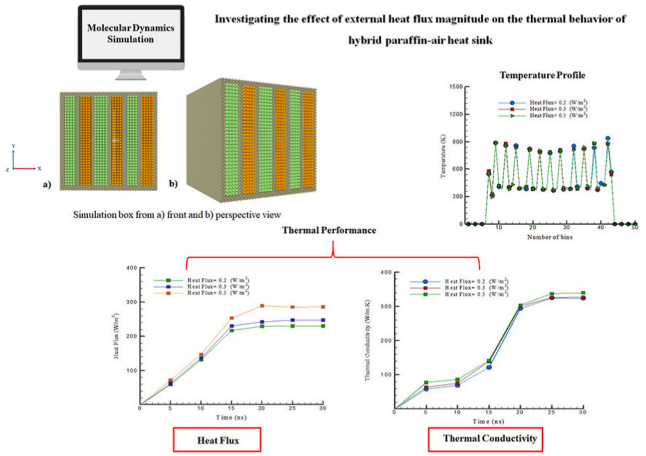
[a] Guangling College, Yangzhou University, Yangzhou 225000, Jiangsu, China
[b] Department of Petroleum Engineering, Al-Amarah University College, Maysan, Iraq
[c] Department of Civil Engineering, College of Engineering, Cihan University-Erbil, Erbil, Iraq
[d] Department of Petroleum Engineering, Al-Kitab University, Altun Kupri, Iraq
[e] Department of Material Science and Engineering, Georgia Institute of Technology, Atlanta 30332, USA
[f] Faculty of Engineering and Natural Sciences, Istanbul Okan University, Istanbul, Turkey
[g] Faculty of Engineering and Natural Sciences, Bahcesehir University, Istanbul, Turkey
[h] Department of Computer Science and Mathematics, Lebanese American University, Beirut, Lebanon
[i] Faculty of Physics, Semnan University, P.O. Box: 35195-363, Semnan, Iran
[j] Department of Mechanical Engineering, Islamic Azad University, Iran

* Corresponding author. Guangling college, Yangzhou University, Yangzhou 225000, Jiangsu, China.
E-mail addresses: 18168283886@163.com (K. Wang), maboud.hekmatifar@iaukhsh.ac.ir (M. Hekmatifar).

https://doi.org/10.1016/j.csite.2023.103653

Available online 2 November 2023

G R A P H I C A L A B S T R A C T



A R T I C L E I N F O

Handling Editor: Dr Y Su

Keywords:
Phase change material
Heat flux
Thermal performance
Heat sink
Molecular dynamics simulation

A B S T R A C T

One of today's concerns regarding energy storage units is the low rate of storage and release of thermal energy and, as a result, the efficiency loss in these units. Subsequently, different strategies are utilized to solve this concern, such as using phase change materials (PCMs) and nanostructures. The background is the low storage and release rate of thermal energy in energy storage units, which leads to efficiency loss. This issue concerns many applications, including energy storage in buildings, vehicles, and electronic devices. This study aims to investigate the effect of external heat flux (EHF) on the thermal efficiency of a specific heat sink by employing molecular dynamics (MD) simulation. After ensuring the simulated atomic structures are stable, EHF is applied to see how it affects the thermal behaviour of the combination. The obtained results show that by increasing the EHF applied to the prototype, the thermal behaviour of the structure improves. So, with the increase of EHF from 0.1 W/m^2 to 0.5 W/m^2, the heat flux and thermal conductivity (TC) increase from 212.27 W/m^2 to 317.90 W/mK to 286.71 W/m^2 and 340.03 W/mK. The findings significantly affect energy storage unit efficiency and can inform future research and development efforts.

Nomenclature

PCM	Phase change material
NP	Nanoparticle
EHF	External heat flux
MD	Molecular dynamics
TC	Thermal conductivity
MWCNT	Multiwall carbon nanotube
VF	Volume fraction

1. Introduction

Recently, due to the increase in population and the need for more energy, there has been an increase in concerns about the excessive use of fossil fuels. In this regard, renewable energy sources, especially thermal energy, have received much attention [1]. The transition to renewable energy requires the active involvement and support of community members. Knowledgeable and well-informed individuals play a crucial role in developing innovative solutions to address various challenges faced by countries and the world as a whole [2]. Thermochemical energy storage is a technique employed in various thermal energy storage methods. It is particularly intriguing because it can store significant energy in a compact space while maintaining a consistent temperature. This is accomplished using phase change materials (PCMs) operating at specific temperatures [3]. One of the ways to use renewable resources is to use a

substance that can store energy, called PCM. Heat storage by PCMs happens within the move from one stage state to another stage state. In the process of solid-solid phase transition, heat is stored due to the transfer of matter between different crystal structures. Typically, this transfer involves lower heat loss and smaller changes in volume compared to solid-liquid transitions. One key advantage of solid-solid phase change materials is that they do not necessitate highly robust storage containers, and they offer greater flexibility in terms of design [4]. A latent heat storage system needs the following parts: (1) A suitable PCM can melt at the desired temperature range. A suitable surface for transferring heat. 3: A good storage box that matches the qualities of the PCM. Latent heat storage requires understanding three imperative issues: PCMs, container materials, and heat exchangers. While PCMs have the highest latent heat, they also have low charge and discharge rates. This defect has caused their low thermal conductivity (TC) [5]. Nanoparticles (NPs) are incorporated into these materials, enhancing their ability to withstand high temperatures to resolve this problem [6]. Generally, previous studies showed that NPs are used for enhancement in heat transfer [7–10]. So far, various studies have examined the thermal performance of different nanostructures using molecular dynamics study [11–13].

A heat sink helps electronic and mechanical devices stay cool by removing the extra heat they produce. It does this by spreading out the heat. In this temperature change, heat sinks use materials that can transfer heat, like air or water coolers, to cool down a specific area and adjust its temperature. Heat sinks are commonly used to produce electronic devices with parts that are sensitive to getting hot. A hybrid paraffin air heat sink is a thermal energy storage system that combines PCMs and air to store and release thermal energy. The PCMs absorb and release large amounts of heat during melting and solidifying, while the air helps enhance heat transfer and improve overall efficiency. Using PCMs and air in these systems has several advantages, including high energy storage density, low thermal resistance, and improved heat transfer performance. These systems have a wide range of applications, including in buildings, vehicles, and electronic devices. They can be used to store thermal energy during periods of low demand and release it during periods of high demand, helping to reduce energy waste and improve overall energy efficiency. Additionally, using PCMs in the systems can improve the performance of energy storage units, leading to increased efficiency and reduced costs [14].

Sun et al. [15] heat transfer of waxy crude oil tank during storage heating process under dynamic thermal conditions. The results show the the study has significant applications in different fields.

So far, various studies have examined the thermal performance of different nanostructures in heat sinks. For instance, Lin and Al-Kayiem [16] said that adding copper NPs to paraffin can make it conduct heat better and stay stable at high temperatures. It can also reduce the problem of supercooling during discharge. An investigation was carried out by Gharebaghi and Sezai using a finned heat sink that had RT27 as its PCM [17]. They analyzed the heat sink in both horizontal and vertical orientations. The findings showed that by adding more fins and reducing the gap between them, the rate at which heat is transferred can be increased by up to 80 times. This also helps in accelerating the process of melting. Jailo et al. [18] used paraffin as a PCM to investigate the heat sink's cooling performance in the presence of NPs. According to the findings, PCM can lower the heat sink temperature by 18° C.

Furthermore, the heat sink's effectiveness has been enhanced by incorporating tiny particles called NPs into PCM. By adding PCM to hybrid heat sinks, Kang et al. [19] found that using PCM can lower the highest temperature and improve the thermal performance. Arshad et al. [20] concluded that when the copper NPs are added to a heat sink, the rate of heat transfer increases, and the time of melting decreases. They also concluded that using metal foam alongside NPs in electronic cooling had a similar effect. The cooling efficiency of a system utilizing PCM in reducing temperatures was examined in the research conducted by Al Shimahi et al. [21]. Findings demonstrate that increasing the amount of PCM material in the system has a greater effect on cooling efficiency than altering the voltage of the fan. Zhao et al. [22] investigated the phase change in the paraffin sample as a phase change structure utilizing the molecular dynamics (MD) method. The simulations showed that the initial structure became better when NPs were added. By adding about 10 % of NPs to the initial structure, the sample's ability to retain heat improved the most.

MD studies how atoms move and change their positions in different situations. It uses classical mechanics and calculates how molecules move. One of the unique features of this method that has led to its increasing use is that it significantly reduces laboratory costs [23]. In this paper, the original objective was to observe the effect of external heat flux (EHF) on the thermal efficiency of a specific heat sink using MD simulations. The new findings of this study include the demonstration that increasing EHF improves the thermal behavior of the structure, leading to increased heat flux and thermal conductivity. These findings contribute to understanding how EHF can enhance the thermal efficiency of energy storage units. The models developed in this study can have practical applications in designing and optimizing energy storage units, such as batteries and thermal energy storage systems. Using PCMs and nanoparticles to improve thermal behaviour makes energy storage units more efficient, reducing energy waste and increasing performance. The use of MD simulations to observe the effect of external heat flux on thermal behaviour can inform the design of energy storage systems that are better able to withstand and respond to external heat fluctuations. Overall, the models developed in this study can contribute to developing more efficient and effective energy storage systems that can help meet the growing demand for sustainable energy solutions.

2. Present simulation

By employing a computer program, computer simulation is utilized to generate a desired model of something and forecast its evolution. Using computer simulations to predict events is faster and can handle more data than traditional methods done manually on paper [24,25–27]. Because of many new developments in programming and computer simulations, scientists began using MD to study physics and chemistry. The MD tools are a way to figure out the properties of nanostructures in terms of chemical composition and force field of atoms [28]. In the MD method, molecules can be simulated using potential functions. Using statistical mechanics helps to find the atomic structure and achieve physical or mechanical equilibrium. So, we use a method to simulate molecules and find a balance in their structure using certain mathematical tools [29]. The MD simulation is a tool often used in various areas of science. The

process involves using basic equations to ascertain the motion of particles in a system over defined periods [30]. This research uses three different types of energy potentials to describe how particles interact. These potentials are called Lennard-Jones, EAM, and Coulomb potential functions.

$$U_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] r < r_c \tag{1}$$

In this equation, ε represents how much the particles attract each other. σ is the distance with no potential between the particles, and r is the distance between the particles.

The values of σ and ε for the interactions between the particles are calculated using the data from Table 1 and Eqs. (2) and (3) [31]:

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j} \tag{2}$$

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \tag{3}$$

The EAM non-bonding potential function is a way to show how the metal particles in the heat sink walls interact with each other. Eq. (4) is used to calculate this interaction [33].

$$U_i = F_\alpha\left(\sum_{i\neq j}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{i\neq j}\varphi_\beta(r_{ij}) \tag{4}$$

The constant F_α can have a value between 0 and 1 in this relationship. The factor ρ_β is caused by atoms' charge density, and the factor φ_β is caused by the particles present in the simulation box. In simple terms, electric potential energy or electrostatic potential energy comes from the forces created by Coulomb's constant. The force intensity between charges is determined by their arrangement, which is closely linked to energy [34]. Electric potential energy is defined from Eq. (5):

$$U_{ij}(r) = \frac{-1}{4\pi\varepsilon_0}\frac{q_i q_j}{{r_{ij}}^2} \tag{5}$$

In Eq. (5), q_j and q_i are electric charges i and j, r_{ij} is the distance between the charges and ε_0 indicates the electrical penetrance of free space and is numerically equal to 8.85×10^{-12} F m^{-1}. Simulation in experimental conditions is one of the most important objectives in MD simulations. Hangerd is considered an imperative concept in this regard, so applying this concept in the simulated system will enable the comparison of simulated results with experimental perceptions [35]. Models maintaining a constant temperature are required to simulate a system at a stable temperature. The benefit of using these models is that we can simulate the system without losing its dynamic characteristics. When MD simulation refers to a constant temperature, it signifies maintaining a steady amount of energy attributed to molecule movement. Temperature control and its time derivative help research how fluids behave. There are many ways to create the desired curves. For example, there are different ways to use the microcanonical curve to keep the temperature the same. A convenient method for ensuring a constant temperature involves adjusting the speed of an object and establishing a connection with a heat supply.

The ensembles are generally divided into three categories: (1) microcanonical ensemble, (2) canonical ensemble, and (3) grand canonical ensemble. In the microcanonical ensemble, the total energy of the system and the total number of particles of the system are constant. This ensemble is represented by (N, V, E). The canonical ensemble is a way to describe a closed system that doesn't exchange heat well with its surroundings. This group is represented by (N, V, T). This model is the most common and crucial model used in computer simulations. After ensuring the simulated structures are stable at the atomic level, the NVT ensemble changes to NVE. Then, apply heat to the heat sink using an EHF and analyze how different NPs affect the thermal behaviour of the atomic structures. How the atoms are arranged for each of the applied external fluxes can be seen in Fig. 1. Based on this figure, the integrated atomic structure of paraffin can be recognized.

This research concerns how the EHF affects a hybrid heat sink system using PCMs, and how air can disperse heat. The researchers used a MD simulation to analyze this. This study uses paraffin as a substance that can change from one phase to another. The heat sink and the structure of paraffin and air molecules are simulated using LAMMPS and Avogadro software and then analyzed further using Packmol software.

2.1. Limitation

The present exploration has several limitations that should be acknowledged. Firstly, the study used MD simulations to observe the

Table 1
Lennard-Jones potential function parameters [32].

Particle type	σ (Å)	ε (kcal/mol)
C	3.851	0.105
H	2.886	0.044
Al	4.499	0.505
O	3.50	0.06
Fe	4.540	0.055

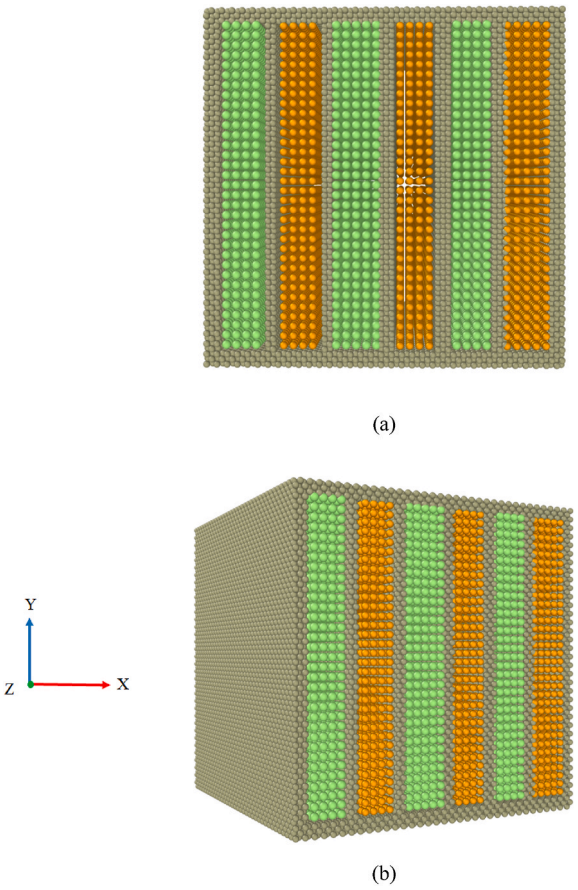


Fig. 1. Schematic of paraffin structure in the last simulation stage in the presence of EHF of 0.1 W/m^2. (a) front view, (b) perspective view.

effect of external heat flux on the thermal efficiency of a specific heat sink. While MD simulations are a powerful tool for modelling molecular behaviour, they have limitations regarding scalability and the ability to capture certain phenomena at larger scales. Secondly, the study focused on a combination of aluminium-paraffin-oxygen, which may not represent all energy storage unit configurations. Finally, the study did not consider the cost or feasibility of implementing the proposed solutions in practical applications. These limitations suggest that further research is needed to understand the proposed solutions' potential and practical applications

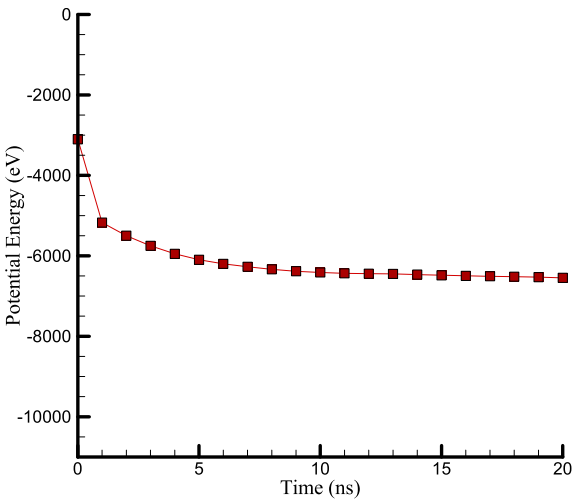


Fig. 2. Potential energy changes in the aluminum-paraffin-oxygen composite.

fully.

2.2. The equilibration process

The study of atom changes in samples can be facilitated by different forms of energy, such as potential and kinetic energy. In simple words, the combination of potential and kinetic energy in an MD simulation can be affected by many things. The potential energy of a system is a way to measure all the energy connected to how atoms interact. It can be either positive or negative, depending on the nature of the interactions. If atoms attract each other, they will have negative potential energy, while positive potential energy means they repel each other. Fig. 2 shows how the energy of the atoms in the simulated atomic composition changes over time.

The variation in the amount of kinetic energy can serve as an indication of an object's stability. This text explains the changes in the energy of a compound over time based on the information shown in Fig. 3. The kinetic energy in an MD simulation can change due to different factors, like the force field settings and the size and composition of the system. Convergence of kinetic energy indicates the suitability of settings for MD simulations, such as atomic structure modelling and the assignment of appropriate force fields.

3. Results

After ensuring the structure is appropriate for the given conditions, we study how the sample reacts to heat. For this purpose, we measure and share the amount of heat flux through the simulated samples. Heat flux is a way to measure how fast heat is being transferred in a system. It provides valuable information regarding the temperature changes in the system. In simulations of how molecules move, we can figure out how much heat flows using the Green-Kubo relation formula. The formula establishes a link between the heat transfer rate and overall heat accumulation. The Green-Kubo formula is as follows [36]:

$$K = \frac{V}{3k_B T^2}\int_0^\infty dt(J(\tau).J(0)) \tag{6}$$

In this equation, V represents the amount of space taken up by the particles in the simulation. kB stands for Boltzmann's constant, T represents the system's temperature, and J represents the amount of heat flux. Solving this equation enables us to determine the system's heat flux, and then by solving the following relation, we can find the TC.

$$K = \frac{V}{k_B T^2}\int_0^\infty (J_x(0)J_x(t))dt = \frac{V}{3k_B T^2}\int_0^\infty (J(0).J(t))dt \tag{7}$$

Heat flux measures how well a simulated sample can handle the heat and can give information about how well heat moves through the system. By studying how heat flows change over time, we can find any differences from the expected patterns and improve the simulation settings for more accurate and efficient results. Increasing the initially applied heat flux improves the thermal behaviour of the structure as much as possible. The heat flux obtained by applying an EHF of 0.1 W/m^2 is shown in Fig. 4.

To determine the cause of the improved thermal behaviour, we investigated the heat transfer efficiency in the aluminium-paraffin-oxygen combination. TC refers to the capacity of materials to transfer heat. Different levels of EHF should be applied to evaluate the effectiveness of this combination. The Green Kubo method enables us to determine the TC of a material. By examining heat conduction and system behaviour under disturbances, we can comprehend the system's heat management and modify the simulation to increase its precision and efficiency. Examining the ability of a material to conduct heat can yield significant information about the dynamic nature of atoms in response to thermal energy. This information can be combined with other measurements, like how atoms are arranged in a material, to understand the system fully. Fig. 5 shows the changes in TC resulting from applying EHF with an amount of 0.1

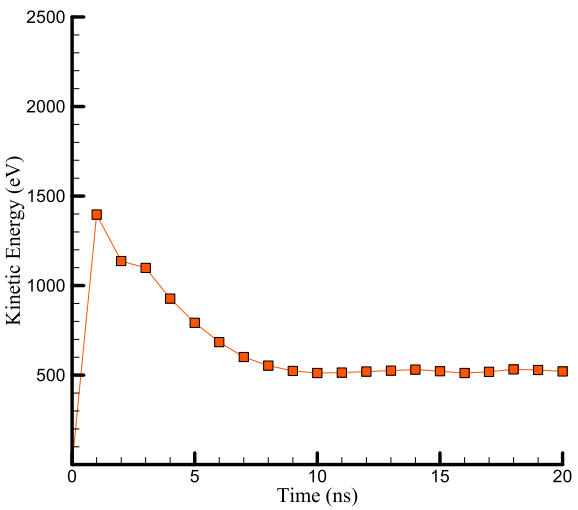


Fig. 3. Kinetic energy changes in the aluminium-paraffin-oxygen composite.

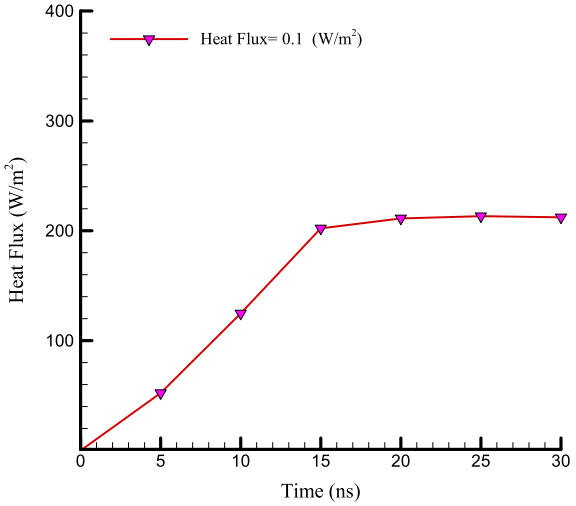


Fig. 4. The HF change in the presence of 0.1 W/m^2 EHF.

W/m^2. Previous studies show that the TC of aluminium is around 230–300 W/m.K [37,38]. The TC of paraffin ranges from 0.2 to 0.3 W/m.K [39], and the TC of air is 0.0265 W/m·K [40]. The present study's theoretical effective thermal conductivities of paraffin/aluminum/air composite are estimated at 317.90 W/m.K.

The temperature fluctuation in a blend of aluminium, paraffin, and oxygen due to applying EHF=0.1 W/m^2 can be observed in Fig. 6. The obtained results show that the EHF increases the maximum temperature.

Fig. 7 shows how we face an increase in heat flux with an increase in EHF. Numerically, with the EHF increase, the samples' heat flux increases from the numerical value of 212.27 W/m^2 to 286.71 W/m^2. As a result, it can be concluded that increasing the initially applied heat flux improves the thermal behaviour of the structure. The physical reason for increasing the initially applied HF and improving the structure's thermal behaviour is the increased heat transfer rate between the aluminium-paraffin-oxygen combination. The heat transfer rate increases as more heat is applied to the prototype, resulting in more HF and TC. This leads to better thermal behaviour of the structure and can improve the efficiency of energy storage units in real-life applications.

Fig. 8 displays how TC changes when EHF increases. The results show that this factor increases from 317.90 W/mK to 340.03 W/mK. The physical reason for the increase in thermal behaviour and TC when applying an EHF is related to the enhanced heat transfer within the aluminium-paraffin-oxygen combination. When EHF is applied, it creates a higher temperature gradient within the system. This increased temperature difference drives more efficient heat transfer, allowing heat to propagate rapidly through the material. As a result, the TC of the system increases, indicating a greater ability to conduct and transfer heat. This improvement in heat transfer efficiency contributes to the enhanced thermal behaviour observed in the study.

Fig. 9 shows the changes in TC due to the increase in EHF. According to the results, increasing the EHF from 0.1 W/m^2 to 0.5 W/m^2 increases the maximum temperature from 920.36 K to 887.64 K. The increase in the temperature gradient inside the system might

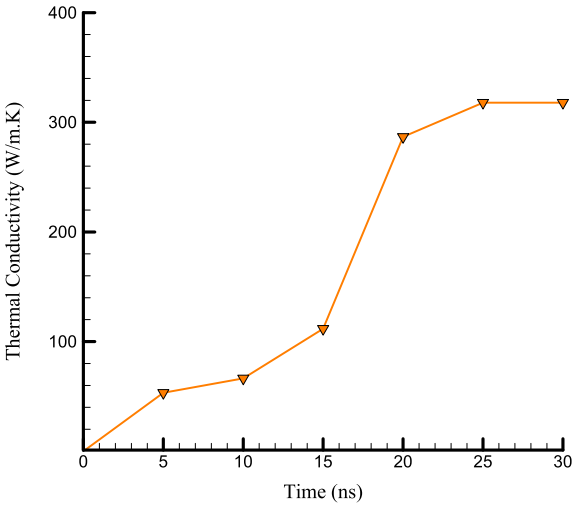


Fig. 5. The TC change in the presence of 0.1 W/m^2 EHF.

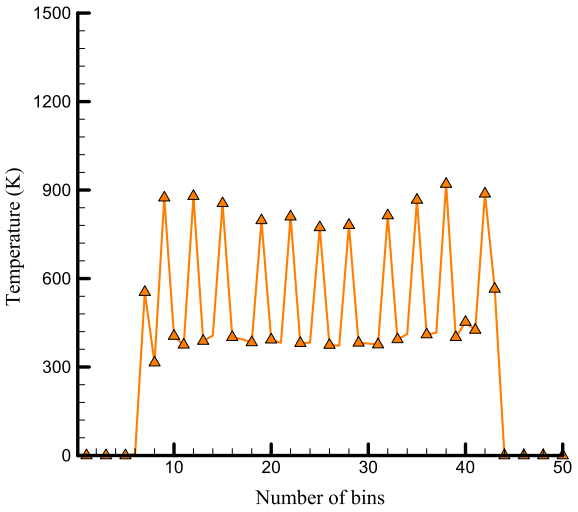


Fig. 6. The Temperature profile of the simulated sample in the presence of 0.1 W/m^2 EHF.

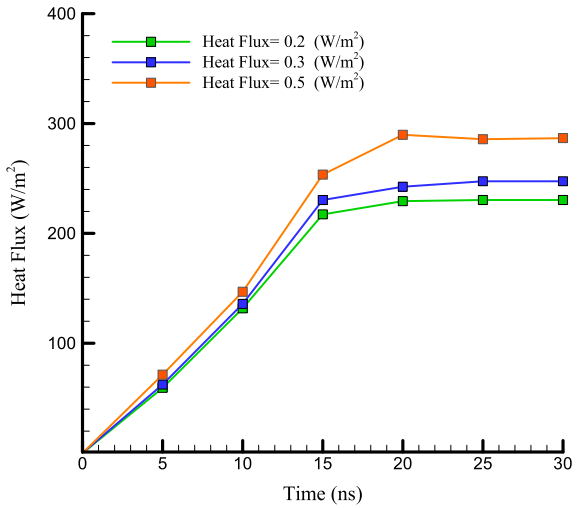


Fig. 7. The change in the HF of the sample in the presence of different EHFs.

account for the higher maximum temperature. With an increased temperature contrast, the driving force for heat transfer strengthens, subsequently facilitating a higher velocity of thermal energy transfer. The temperature in the entire system, including its maximum temperature point, has the potential to rise as a result of this. Moreover, alterations in the atom arrangement or substance composition under the influence of EHF can cause the highest temperature to rise. Numerical results are reported in Table 2.

4. Conclusion

In this study, the use of MD simulations to observe the effect of EHF on the thermal efficiency of a specific heat sink is a unique approach that has not been widely used in previous research. This research focused on investigating the behaviour of the hybrid heat sink of PCM (paraffin) and air. The experiments done in this study had two main parts. Initially, the atoms were balanced, and then the samples were subjected to heat to monitor their transformations throughout the duration. The main findings from balancing atomic samples can be divided into the following categories:

- The kinetic energy of the simulated prototype converged to 520.5522 eV after 20 ns. This convergence showed that the structure is in balance.
- The stored energy in the atom decreased to −6546.138 eV. This negative value means there is a force of attraction between the atoms in the samples, which helps keep their structure stable.
- With the increase of the EHF, the heat flux in the samples increases from the numerical value of 212.27 W/m^2 to 286.71 W/m^2

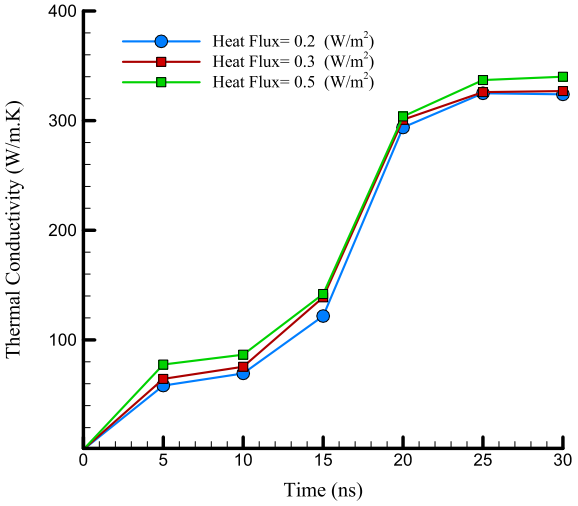


Fig. 8. The change in the TC of the sample in the presence of different EHFs.

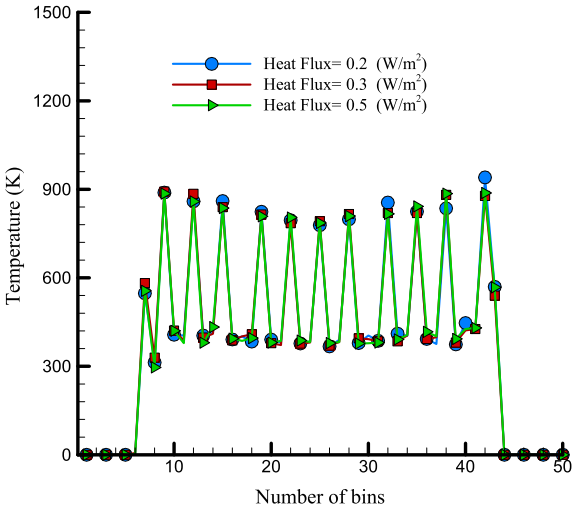


Fig. 9. The temperature profile simulated in the presence of different EHFs.

Table 2
Changes in HF, TC, and the maximum temperature in the aluminium-paraffin-oxygen atomic composition according to the magnitude of EHF.

EHF (W/m^2)	HF (W/m^2)	TC (W/m.K)	Maximum temperature (K)
0.1	212.27	317.90	920.36
0.2	230.38	323.93	940.30
0.3	247.48	326.95	892.57
0.5	286.71	340.03	887.64

- According to the results, increasing the EHF from 0.1 W/m^2 to 0.5 W/m^2 increases the maximum temperature from 920.36 K to 887.64 K. The increase in the temperature gradient inside the system might account for the higher maximum temperature.

The present exploration has limitations, including the use of MD simulations, which have scalability limitations and may not capture phenomena at larger scales. Additionally, the study focused on a specific material combination and did not consider cost or feasibility, suggesting the need for further research to understand broader applicability and practical implementation.

4.1. Future potential areas

Some potential areas for future research in this field include:

- Investigating the use of different combinations of phase change materials (PCMs) and nanoparticles to improve thermal behaviour and increase efficiency in energy storage units.
- Exploring using other simulation techniques, such as finite element analysis (FEA), to model thermal behaviour in energy storage units at larger scales.
- Investigating the use of other external factors, such as pressure on the thermal behaviour of energy storage units.

By addressing these research areas, future researchers can build upon the findings of this study and continue to advance our understanding of how to improve the efficiency and effectiveness of energy storage systems.

Author statement

Methodology, Software and Validation: Ke Wang, Dheyaa J. Jasim, As'ad Alizadeh, Ameer H. Al-Rubaye, Navid Nasajpour-Esfahani, Soheil Salahshour, M. Hekmatifar*; Writing - Original Draft: Ke Wang, Soheil Salahshour, Shadi Esmaeili, M. Hekmatifar*; Investigation: Ke Wang, Dheyaa J. Jasim, As'ad Alizadeh, Ameer H. Al-Rubaye, Navid Nasajpour-Esfahani; Revision: Ke Wang, Dheyaa J. Jasim, As'ad Alizadeh, Navid Nasajpour-Esfahani, Soheil Salahshour, Shadi Esmaeili, M. Hekmatifar*

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.

Data availability

No data was used for the research described in the article.

References

[1] J. Khodadadi, L. Fan, H. Babaei, Thermal conductivity enhancement of nanostructure-based colloidal suspensions utilized as phase change materials for thermal energy storage: a review, Renew. Sustain. Energy Rev. 24 (2013) 418–444.
[2] E. Heiskanen, K. Matschoss, Understanding the uneven diffusion of building-scale renewable energy systems: a review of household, local and country level factors in diverse European countries, Renew. Sustain. Energy Rev. 75 (2017) 580–591.
[3] N. Zhang, Y. Yuan, X. Cao, Y. Du, Z. Zhang, Y. Gui, Latent heat thermal energy storage systems with solid–liquid phase change materials: a review, Adv. Eng. Mater. 20 (6) (2018), 1700753.
[4] O. Dwekat, T. Karaki, A. Musmar, Experimental Investigation on the Performance of Phase Change Material (PCM)-Incorporated with Solar Water Heating System, 2019.
[5] A.V. Eletskii, Phase change materials with enhanced thermal conductivity and heat propagation in them, Phys. Chem. 2 (1) (2022) 18–42.
[6] S.L. Tariq, H.M. Ali, M.A. Akram, M.M. Janjua, M. Ahmadlouydarab, Nanoparticles enhanced phase change materials (NePCMs)-A recent review, Appl. Therm. Eng. 176 (2020), 115305.
[7] M. Bayat, M.R. Faridzadeh, D. Toghraie, Investigation of finned heat sink performance with nano enhanced phase change material (NePCM), Therm. Sci. Eng. Prog. 5 (2018) 50–59. https://doi.org/10.1016/j.tsep.2017.10.021.
[8] A.N. Sadr, M. Shekaramiz, M. Zarinfar, A. Esmaily, H. Khoshtarash, D. Toghraie, Simulation of mixed-convection of water and nano-encapsulated phase change material inside a square cavity with a rotating hot cylinder, J. Energy Storage 47 (103606) (2022), 103606, https://doi.org/10.1016/j.est.2021.103606.
[9] O. Younis, A. Mourad, A. Aissa, N.A.A. Qasem, A.M. Abed, O.A. Akbari, G.F. Smaisim, K. Guedri, D. Toghraie, L. Kolsi, A. Alizadeh, Numerical investigation of thermal energy storage system loaded with nano-enhanced phase change material with Koch snowflake fractal cross-section, J. Energy Storage 56 (106016) (2022), 106016, https://doi.org/10.1016/j.est.2022.106016.
[10] F. Wang, N. Nasajpour-Esfahani, A. Alizadeh, G. Fadhil Smaisim, A.M. Abed, S.K. Hadrawi, S. Aminian, R. Sabetvand, D. Toghraie, Thermal performance of a phase change material (PCM) microcapsules containing Au nanoparticles in a nanochannel: A molecular dynamics approach, J. Mol. Liq. 373 (121128) (2023), 121128, https://doi.org/10.1016/j.molliq.2022.121128.
[11] X. Liu, B. Ghafari, I. Patra, M.M. Kadhim, A. Turki Jalil, Anil Kumar, R. Sivaraman, N. Nasajpour-Esfahani, M. Taheri Andani, D. Toghraie, A molecular dynamics study of thermal behavior of ammonia/Cu nanorefrigerant flow under different initial pressures and electric fields, J. Mol. Liq. 367 (120388) (2022), 120388, https://doi.org/10.1016/j.molliq.2022.120388.
[12] X. Liu, I. Patra, O.R. Kuzichkin, M. Zaidi, S.M. Abdulnabi, Z. Mohsen Najm, U.S. Altimari, S.K. Hadrawi, M. Taheri Andani, M. Hekmatifar, Molecular dynamics study of the effect of external electric field amplitude and cavity on thermal properties of Ammonia/Copper Nano-Refrigerant, J. Mol. Liq. 365 (120125) (2022), 120125, https://doi.org/10.1016/j.molliq.2022.120125.
[13] B. Zhang, M. Hao, J. Xiong, X. Li, J. Koopman, Ab initio molecular dynamics calculations on electron ionization induced fragmentations of C4F7N and C5F10O for understanding their decompositions under discharge conditions, Phys. Chem. Chem. Phys. 25 (10) (2023) 7540–7549, https://doi.org/10.1039/D2CP03498K.
[14] H. Zhu, Y. Lu, L. Cai, Wavelength-shift-free racetrack resonator hybrided with phase change material for photonic in-memory computing, Optics Express 31 (12) (2023) 18840–18850, https://doi.org/10.1364/OE.489525.
[15] W. Sun, Y. Liu, M. Li, Q. Cheng, L. Zhao, Study on heat flow transfer characteristics and main influencing factors of waxy crude oil tank during storage heating process under dynamic thermal conditions, Energy 269 (2023) 127001.
[16] S.C. Lin, H.H. Al-Kayiem, Evaluation of copper nanoparticles–Paraffin wax compositions for solar thermal energy storage, Sol. Energy 132 (2016) 267–278.
[17] M. Gharebaghi, I. Sezai, Enhancement of heat transfer in latent heat storage modules with internal fins, Numer. Heat Tran., Part A: Applications 53 (7) (2007) 749–765.
[18] J.M. Jalil, H.S. Mahdi, A.S. Allawy, Cooling performance investigation of PCM integrated into heat sink with nano particles addition, J. Energy Storage 55 (2022), 105466.
[19] D. Kong, Y. Zhang, S. Liu, Design of additively manufactured hybrid PCM-air heat sink with a two-stage channel for enhancing thermal performance, Appl. Therm. Eng. 218 (2023), 119325.
[20] A. Arshad, M. Jabbal, H. Faraji, P. Talebizadehsardari, M.A. Bashir, Y. Yan, Thermal performance of a phase change material-based heat sink in presence of nanoparticles and metal-foam to enhance cooling performance of electronics, J. Energy Storage 48 (2022), 103882.
[21] H. Alshihmani, M.-J. Maghrebi, M. Sardarabadi, Thermal performance prediction of a phase change material based heat-sink cooling system for a printed circuit board, using response surface method, J. Energy Storage 55 (2022), 105499.

[22] C. Zhao, Y. Tao, Y. Yu, Molecular dynamics simulation of nanoparticle effect on melting enthalpy of paraffin phase change material, Int. J. Heat Mass Tran. 150 (2020), 119382.
[23] P. Xue, S. Pauly, W. Gan, S. Jiang, H. Fan, Z. Ning, Y. Huang, J. Sun, Enhanced tensile plasticity of a CuZr-based bulk metallic glass composite induced by ion irradiation, J. Mater. Sci. Technol. 35 (10) (2019) 2221–2226.
[24] H.N. Abdelhamid, M. Dowaidar, M. Hällbrink, Ü. Langel, Gene delivery using cell penetrating peptides-zeolitic imidazolate frameworks, Microporous Mesoporous Mater. 300 (2020), 110173.
[25] D. Toghraie Semironi, A.R. Azimian, Molecular dynamics simulation of liquid–vapor phase equilibrium by using the modified Lennard-Jones potential function, Heat Mass Tran. 46 (2010) 287–294.
[26] N.A. Jolfaei, N.A. Jolfaei, M. Hekmatifar, A. Piranfar, D. Toghraie, R. Sabetvand, S. Rostami, Investigation of thermal properties of DNA structure with precise atomic arrangement via equilibrium and non-equilibrium molecular dynamics approaches, Comput. Methods Progr. Biomed. 185 (105169) (2020), 105169.
[27] S.-R. Yan, N. Shirani, M. Zarringhalam, D. Toghraie, Q. Nguyen, A. Karimipour, Prediction of boiling flow characteristics in rough and smooth microchannels using molecular dynamics simulation: investigation the effects of boundary wall temperatures, J. Mol. Liq. 306 (112937) (2020), 112937.
[28] M. Moeini, R. Barbaz Isfahani, S. Saber-Samandari, M.M. Aghdam, Molecular dynamics simulations of the effect of temperature and strain rate on mechanical properties of graphene–epoxy nanocomposites, Mol. Simulat. 46 (6) (2020) 476–486.
[29] M. Monshi, S. Esmaeili, A. Kolooshani, B.K. Moghadas, S. Saber-Samandari, A. Khandan, A novel three-dimensional printing of electroconductive scaffolds for bone cancer therapy application, Nanomedicine Journal 7 (2) (2020).
[30] R. Trobec, F. Merzel, D. Janežič, Computational complexity of split symplectic MD integration method, in: Advances in Parallel Computing, Elsevier, 1998, pp. 541–548.
[31] H.J. Berendsen, J.R. Grigera, T.P. Straatsma, The missing term in effective pair potentials, J. Phys. Chem. 91 (24) (1987) 6269–6271.
[32] A.K. Rappé, C.J. Casewit, K. Colwell, W.A. Goddard III, W.M. Skiff, UFF, a full periodic table force field for molecular mechanics and molecular dynamics simulations, J. Am. Chem. Soc. 114 (25) (1992) 10024–10035.
[33] M.S. Daw, M.I. Baskes, Embedded-atom method: derivation and application to impurities, surfaces, and other defects in metals, Phys. Rev. B 29 (12) (1984) 6443.
[34] P.G. Huray, Maxwell's Equations, John Wiley & Sons, 2011.
[35] D.C. Rapaport, The Art of Molecular Dynamics Simulation, Cambridge university press, 2004.
[36] M.S. Green, Markoff random processes and the statistical mechanics of time-dependent phenomena. II. Irreversible processes in fluids, J. Chem. Phys. 22 (3) (1954) 398–413.
[37] A. Zhang, Y. Li, Thermal conductivity of aluminum alloys—a review, Materials 16 (8) (2023) 2972.
[38] E. Kaschnitz, W. Funk, T. Pabel, Electrical Resistivity Measured by Millisecond Pulse-Heating in Comparison to Thermal Conductivity of the Aluminium Alloy Al-7Si-0.3 Mg at Elevated Temperature, vol. 43, High Temp Press, 2014, pp. 175–191.
[39] Z. Wang, Z. Zhang, L. Jia, L. Yang, Paraffin and paraffin/aluminum foam composite phase change material heat storage experimental study based on thermal management of Li-ion battery, Appl. Therm. Eng. 78 (2015) 428–436.
[40] Y. Yao, H. Wu, Z. Liu, Pore scale investigation of heat conduction of high porosity open-cell metal foam/paraffin composite, J. Heat Tran. 139 (9) (2017), 091302.