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Development of numerical code for mathematical simulating of unsteady solidification phenomena in existence of nanomaterial

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ABSTRACT

This research zeroes in on improving the freezing process by synergistically employing a wavy wall and fins. To enhance cold penetration, the phase change material (PCM) is enriched with nanoparticles, and a single-phase model is adopted due to the low nanoparticle concentration. The numerical simulations leverage the Galerkin method and the validation procedure affirms the precision of the code, extensively evaluating the impacts of φ (concentration of additives) and dp (particle diameter). With an increase in particle diameter (dp), there is an initial 19.76% decrease in the required time, succeeded by a subsequent 50.56% increase when $\varphi = 0.04$. Furthermore, an escalation in φ results in an 11.04%, 40.91%, and 26.36% reduction in completion time for dp values of 50, 40, and 30 nm, respectively. Without the inclusion of powders, the solidification process lasts for 84.8 s. However, with the introduction of the optimal powder size, this duration significantly reduces to 50.1 s. This emphasizes the efficiency improvements attained through the strategic integration of a wavy wall, fins, and PCM infused with nanoparticles.

1. Introduction

The growing interest in renewable energy, particularly solar source, is driven by the rising request for energy depletion, the finite nature of fossil fuels, and the surge in pollution [1-4]. Despite having great energy saving density, PCMs inherently exhibit low thermal conductivity [5-8]. Various solutions have been proposed to address this issue, including the use of nanoparticles, fins, and metal foam as enhancers of PCM thermal conductivity [9-13]. The primary limitation of these materials, causing a sluggish heat transfer rate during phase shift, stems from their low thermal conductivity. Addressing this challenge, new classes of heat transfer fluids have emerged [14-17]. The addition of new techniques can enhance thermal conductivity and heat transmission compared to pure PCM

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Fig. 1. Combination of wavy wall and fins to enhance freezing.



Fig. 2. The grid shape and showing the place with denser grid.

[18–22]. Enhancing system productivity can be achieved through the incorporation of both passive and active techniques [23–26]. Utilizing a numerical approach for predicting system behavior can reduce the cost of the final experimental setup [27–30]. Enhancing the cooling system's positive effect is achievable by introducing nanoparticles into the base PCM with low concentration. This approach finds applications in various thermal systems, including solar systems. As explored by Sheikholeslami and Khalili [31], nanofluid serves as a spectral filter, thereby intensifying the optical behavior of the system. Additionally, Sheikholeslami et al. [32] investigated the use of nanofluid as a cooling system in a PVT-TEG system. In their proposed system, both the solar panel and the thermoelectric layer contribute to electricity generation. In their numerical analysis, Sciacovelli et al. [33] surveyed the thermal characteristics of a vertical duct unit modified with a NEPCM. Their conclusion indicated that introducing nanoparticles with a 4% mass concentration could reduce the charging time by 15%. Sheikholeslami [34] has introduced an innovative method to enhance the efficiency of a solar panel by integrating it with a paraffin layer. The transformation of solid paraffin to liquid contributes to cooling the panel, resulting in improved system performance.

Wu et al. [35] scrutinized the efficacy of dispersing Cu particles in a PCM on the material's features and the time needed for processes. Their findings revealed that conduction could be increased by 18.1% in liquid phase. Additionally, the results demonstrated that introducing a 1% mass fraction of nanomaterial reduced the solidification/melting time. Sheikholeslami and Khalili [36] examined the environmental efficiency of a solar unit in the presence of nanofluid. They attached nanofluid within the heat sink to the solar panel to improve the system's productivity, as proposed by Sheikholeslami et al. [37]. The study also investigated the adverse impact of dust, revealing that loading nanoparticles becomes more effective in the presence of reflectors. In a numerical analysis, Arasu et al. [38] scrutinized the impact of CuO and Alumina nano-powders on the thermal efficiency of paraffin wax. Their outcomes indicate that alumina has higher performance. Sivashankar et al. [39] employed NEPCM to investigate CPV cells. Their outputs



Fig. 3. Validation based on previous numerical work [44].



Fig. 4. Selecting higher $\boldsymbol{\phi}$ and changing the outputs.



Fig. 4. (continued)

revealed that incorporating NEPCM into the unit improved the performance of CPV cells, with the ideal volumetric percentage for nanoparticles identified as 0.5%. Sheikholeslami et al. [40] discussed the use of nanoparticles for coating the glass layer of a solar cell. Additionally, they employed a PCM layer to cool the silicon layer, incorporating Graphene nanoparticles. Harikrishnan et al. [41] studied an empirical research to evaluate the thermal characteristics of TiO_2/SA composites. Their findings indicate that knf increased by 70%, and the resulting composite demonstrated favorable chemical and thermal stability. Additional research revealed that completion time for NEPCM decreases about 43.72% during melting. Bondareva et al. [42] accompanied an analysis to scrutinize the treatment of a phase change material (n-octadecane) when nano-powders were introduced in a finned heat sink. In the initial



Fig. 5. The form of ice from for higher φ



Fig. 6. How dp can affect the average values.

phase, the addition of nanoparticles was found to expedite the melting process. However, as convection took precedence, reducing the volume percentage of nanoparticles extended the overall melting period compared to the pure PCM.

This research proposal brings a unique perspective to the optimization of phase change materials (PCMs) by introducing an innovative combination of elements. Setting itself apart from prior studies, this work incorporates a sinusoidal wavy wall, fins, and the utilization of alumina nanoparticles in water as a nanofluid-based PCM. The collaboration between the sinusoidal wavy wall and fins is designed to amplify heat transfer throughout the solidification process, presenting a distinctive geometric modification. Moreover, the selection of alumina nanoparticles in water as the phase change material (PCM) composition introduces a novel aspect to the research. This choice leverages the favorable thermal properties of alumina in conjunction with the phase change characteristics of water. The utilization of Galerkin technique, combined with an adaptive mesh strategy, elevates the complexity of the numerical simulation, thereby improving the precision and computational efficiency of the study. This undertaking embodies an inventive and allencompassing method for optimizing the solidification process in PCM systems, presenting potential applications in the realms of cold storage.

2. Freezing process within complex geometry

In this current study, we expedite the freezing process by presenting nano-powders with vsrioud sizes into the container, as depicted in Fig. 1. A systematic application of varying sizes and concentrations of nanoparticles is carried out to pinpoint the optimal



Fig. 7. Selecting higher dp and changing the outputs.

scenario. Through the omission of convective terms and the adoption of a single-phase formulation, the ensuing set of unsteady equations governs the dynamic evolution of the unit in the course of the solidification. This deliberate strategy seeks to unravel the influence of nanoparticle size and concentration on the freezing process, offering valuable insights into the most effective parameters for accelerating solidification [43]:

$$(\rho C_p)_{nf} \frac{dT}{dt} = \nabla (k_{nf} \nabla T) + L_{nf} \frac{dS}{dt}$$

$$\begin{cases} S = 1 \quad (T - T_m) < (-T_0) \\ S = 0 \quad (T - T_m) > (-T_0) \\ S = (T_m + 0.5T_0 - T) / T_0 \quad (-T_0) < (T - T_m) < T_0 \end{cases}$$

$$(2)$$

Implementing an implicit technique is the chosen method for discretizing the unsteady terms. The spatial domain's even distribution of nanoparticles enables the application of the following formulation for nanomaterial. Opting for discretization via an implicit approach proves pivotal in faithfully capturing the time-dependent dynamics of the system. This choice ensures both numerical stability and accuracy in portraying the dynamic evolution of nanoparticle concentration throughout the unsteady solidification process [43]:



Fig. 7. (continued)

$(L\rho)_{nf} = (L\rho)_f (1-\varphi)$	(3)
$\rho_{nf} = (1 - \varphi) \rho_f + \varphi \rho_p$	(4)
$\left(\rho C_{p}\right)_{nf} = \left(\rho C_{p}\right)_{f} (1-\varphi) + \left(\rho C_{p}\right)_{p} \varphi$	(5)



Fig. 8. The form of ice from for higher dp.



Fig. 9. How dp can change the average values.

$$\wp = k_p / k_f, \frac{k_{nf}}{k_f} = 1 - 3 \frac{(1 - \wp) \varphi}{(1 - \wp) \varphi + (\wp + 2)} + 5 \times 10^4 \left(\frac{d_p \rho_p}{T \kappa_b}\right)^{-0.5} c_{p,f} g' \left(d_p, T, \varphi\right) \varphi \rho_f$$
(6)

In tackling the system's governing equations, the Finite Element Method (FEM) takes center stage. The integration of FEM with implicit methods not only bolsters the stability but also elevates the accuracy of the simulation, especially in capturing the nuances of dynamic phase change phenomena. A trailblazer in the field, Sheikholeslami [43] has spearheaded and established this method as the gold standard for simulating solidification processes, becoming a touchstone for a multitude of publications. This approach seamlessly merging FEM, implicit methods, and adaptive grids stands as a refined and dependable methodology for delving into the intricacies of unsteady solidification, providing invaluable insights into the nuances of the process. Playing a crucial role in modeling intricate unsteady solidification processes, the Galerkin method stands out as a numerical technique rooted in finite element analysis (FEM). Specifically tailored for tackling the partial differential equations inherent in fluid dynamics and heat transfer challenges, this method offers a robust and precise approach to capturing dynamic phenomena. Within the scope of the ongoing research, the simulation process gains an additional layer of complexity through the amalgamation of the Galerkin technique. This adaptive grid, responsive to the changing conditions within the simulation, dynamically refines or coarsens the computational mesh. This adaptive behavior enables the concentration of resources in areas where notable changes or gradients are unfolding. The integration of these elements boosts computational efficiency, guaranteeing a precise representation of the intricate details involved in the dynamic solidification process. Simultaneously, it streamlines the use of computational resources. The effectiveness of the adaptive grid-FEM approach emerges as a valuable asset for comprehending and fine-tuning dynamic phase change processes.



Fig. 10. The required time for discharging.

3. Results and discussion

The focus of this study revolves around optimizing the freezing process of NEPCM comprising water and alumina nanoparticles through the incorporation of a sinusoidal wavy wall and fins. Introducing geometric variations, the sinusoidal wavy wall fosters improved heat exchange, complemented by the fins that augment the surface area for more effective heat transfer. The main goal is to expedite the solidification of the NEPCM by capitalizing on its phase change characteristics. The selected composition of water and alumina nanoparticles further enhances the material's thermal properties. The simulation technique used to explore this dynamic and unsteady process is the Galerkin method. Furthermore, the simulation methodology includes the integration of an adaptive grid, dynamically adjusting the computational mesh to enhance both accuracy and efficiency. This all-encompassing approach seeks to deepen the knowledge and optimization of the solidification process, with potential applications in energy storage or thermal management. Within this intricate research framework, the sinusoidal wavy wall and fins are purposefully introduced for their influence on shaping fluid dynamics. Concurrently, the Galerkin method stands as a robust numerical tool employed to simulate the unsteady behavior inherent in the solidification process. By concentrating resources where substantial changes or gradients occur during the simulation, the adaptive grid contributes to enhanced computational efficiency. The study's broader significance resides in the potential applications of the optimized solidification process, promising advancements in energy storage, thermal regulation, or other domains where the dynamic behavior of PCM holds paramount importance. In this article, the simulation of the solidification process within a complex geometry containing nanoparticles is carried out using the Galerkin method. Renowned for its efficacy in solving governing equations, the Galerkin method is employed to model and scrutinize the intricate dynamics of solidification, particularly when nanoparticles are present. This numerical approach facilitates a thorough exploration of the intricate relationship between geometric factors and nanoparticle characteristics throughout the solidification process.

In Fig. 2, the results of implementing an adaptive grid are presented, illustrating that the area near the solid front features a more refined grid compared to other regions. The strategic use of an adaptive grid plays a pivotal role in enhancing simulation accuracy by directing additional computational resources to locations where substantial changes or gradients manifest during the solidification process. This heightened precision in the vicinity of the solidification front proves essential for capturing the nuances of the dynamic phase change process. Fig. 3 showcases the validation of the simulation results by juxtaposing them with the findings from a preceding study conducted by Sheikholeslami [44]. In the earlier work, the adaptive grid technique was utilized and its accuracy was veri-

fied against experimental data. The present study attains a high level of accuracy, as evidenced in Fig. 3, owing to its successful validation against the established benchmark. This underscores the dependability and faithfulness of the simulation approach.

In Figs. 4–6, the efficacy of nanoparticle volume fraction (φ) on the solidification is depicted. The incorporation of nanoparticles improves cold penetration by elevating thermal conductivity. As the simulation advances, the temperature throughout the domain diminishes. As time elapses, the energy (E) decreases, and the solid fraction (S) increases. Importantly, a higher φ results in a more rapid ascent of S, thereby reducing the time needed to achieve a complete solid state (S = 1). Opting for a higher φ also propels the speed of the solid front. In the absence of nanoparticles, the freezing process spans 84.8 s, but with the optimal nanoparticle size, it is hastened to 50.1 s. The reduction in required freezing time, from 84.8 s to 62 s, and then further to 50.1 s with the escalation of φ , highlights the efficacy of nanoparticle-enhanced freezing in diminishing the overall solidification duration. This outcome aligns with expectations, as higher φ values contribute to enhanced thermal conductivity and, consequently, swifter freezing.

In Figs. 7–9, the influence of nanoparticle diameter (dp) on the freezing process is illustrated. The system's behavior undergoes alterations with the escalation of dp, as this factor directly shapes the material's conductivity. Larger particles tend to interact more efficiently, resulting in an elevation in conductivity. Nevertheless, exceeding a specific threshold, further increments in dp can yield a reverse effect due to sedimentation phenomena. The necessary freezing time fluctuates with dp, starting from 62.44 s, decreasing to 50.1 s, and then rising to 75.44 s. In this context, powders with a diameter of 40 nm showcase optimal performance for the current study. The lowest value of energy (E) is linked to dp = 40 nm, while the system's temperature is at its peak when dp = 50 nm. The selection of powders with a diameter of 40 nm proves crucial for attaining the minimum discharging time, underscoring the intricate interplay between particle size, conductivity, and overall freezing efficiency.

In Fig. 10, the impact of two crucial elements on freezing time is depicted. As the nanoparticle concentration (φ) increases from 0.02 to twice that value, there is a significant reduction in solidification time, approximately 19.18%, particularly notable when dp = 40 nm. Without powders, the freezing time stands at 84.8 s, whereas with the optimal powder size, it decreases to 50.1 s. Additionally, the effect of φ on completion time is observed to decrease by around 11.04%, 40.91%, and 26.36% for dp values of 50 nm, 40 nm, and 30 nm, respectively. It's important to note that the maximum impact of φ is observed when the optimized dp size is selected. Moreover, with an increase in dp, the initial freezing time decreases by approximately 19.76%, but subsequently increases by 50.56% when $\varphi = 0.04$. When $\varphi = 0.02$, the freezing rate exhibits an 11.55% increase with a transition from dp 30 nm–40 nm, followed by a 29% reduction with a further shift from dp 40 nm–50 nm. These findings emphasizing those optimal conditions can lead to significant enhancements in efficiency.

4. Conclusion

This study delves into optimizing the freezing process of NEPCM composed of water and alumina nanoparticles by integrating a sinusoidal wavy wall and fins. The sinusoidal wavy wall introduces geometric variations to improve fluid flow and heat exchange, while the fins serve to increase surface area for a more efficient heat transfer. The main objective is to expedite the solidification of the NEPCM by leveraging its phase change characteristics. The selected composition of water and alumina nanoparticles is designed to augment the material's thermal properties. The simulation strategy, which utilizes the Galerkin method, specifically tackles the dynamic and unsteady aspects inherent in processes commonly encountered in fluid dynamics and heat transfer problems. Incorporating an adaptive grid allows for the dynamic refinement or coarsening of the computational mesh, ensuring a balance between accuracy and efficiency. This holistic approach seeks to refine the solidification process for potential applications in energy storage or thermal management, with broader implications for advancements in related fields where understanding the dynamic behavior of phase change materials is crucial. For $\varphi = 0.02$, the freezing rate experiences an approximately 11.55% increase with a rise in dp from 30 to 40 nm, but it subsequently decreases by 29% with a further increase in dp from 40 to 50 nm. Conversely, with $\varphi = 0.04$, an initial increase in dp results in a 19.76% reduction in the required time, succeeded by a subsequent increase of 50.56%. As φ rises, the completion time experiences reductions of approximately 11.04%, 40.91%, and 26.36% for dp values of 50, 40, and 30 nm, respectively. In the absence of powders, the freezing process spans 84.8s, whereas with the optimal powder size, it concludes in 50.1s. Larger particles foster heightened interaction, leading to increased conductivity. However, surpassing a certain particle size threshold can yield a reverse effect due to sedimentation. As the particle diameter (dp) increases, the freezing time varies from 62.44s to 50.1s and then to 75.44s. Consequently, powders with a diameter of 40 nm demonstrate the most effective performance in this study. At the outset of the process, the temperature within the domain decline, and over time, the energy (E) decreases while the solid fraction (S) increases. With an increase in φ , the value of S also rises, leading to a shorter time required to reach S = 1.

CRediT authorship contribution statement

Wajdi Rajhi: Conceptualization, Data curation, Writing – review & editing. Noha M. Seyam: Formal analysis, Methodology, Software. Hussein A.Z. AL-bonsrulah: Methodology, Investigation. Ziyad Jamil Talabany: Data curation, Formal analysis, Investigation, Writing – review & editing. Nasrin B.M. Elbashir: Investigation, Resources, Supervision, Writing – review & editing. Nidal H. Abu-Hamdeh: Formal analysis, Data curation.

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.

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