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# Influence of Nanoparticle Concentrations on Heat Transfer in Nano-Enhanced Phase Change Materials

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**Abstract:** This investigation examines the effects of varied nanoparticle concentrations, such as zinc oxide (ZnO), copper oxide (CuO), and aluminum oxide ($Al_2O_3$), on the mass fraction and melting characteristics within nano-enhanced phase change materials (NEPCMs). Employing numerical simulations via ANSYS-FLUENT, the study explores these dynamics within a square enclosure subjected to distinct thermal gradients. The enclosure, measuring 10cm×10cm, incorporates a heat-supplying wall, partitioned into quarters, each exhibiting a unique temperature gradient. This setup provides a comprehensive understanding of boundary conditions relevant to NEPCM behavior. The focus lies on a comparative analysis of NEPCM's thermal properties under varying nanoparticle concentrations: 0.1, 0.3, and 0.5 weight percent. A low-temperature wall, lined with paraffin wax and integrated with these nanomaterials, facilitates the assessment of their impact on the phase change materials (PCMs). Remarkably, an inverse relationship is observed between nanoparticle concentration and mass fraction, ranging from 0.86 to 0.08. This finding underscores the significant role of nanoparticle integration in modulating NEPCM properties. Among the nanoparticles studied, CuO emerges as the most efficacious in enhancing melting due to its low density and high thermal conductivity. The temperature distribution profile within the paraffin wax shifts from a dispersed state to a more uniform and curved pattern upon nanoparticle incorporation. Such a transformation indicates an improved thermal response of the NEPCM system. The implications of this study are manifold, extending to the design and optimization of thermal energy storage systems. These insights are particularly valuable for applications in energy conservation within buildings, solar energy equipment, transportation, and storage solutions. The research elucidates the criticality of selecting appropriate nanoparticle concentrations for achieving desired phase change properties in NEPCM-based systems. Furthermore, it contributes to a deeper understanding of how nanoparticle characteristics influence the thermal behavior of PCMs, thus offering a guide for future innovations in this field.

**Keywords:** Nano-enhanced phase change materials; Nanoparticle concentration; Mass fraction; Melting behavior; Thermal energy storage; Numerical simulation; CuO; $Al_2O_3$; ZnO; Temperature gradient

## 1 Introduction

### 1.1 Background and Significance of NEPCMs

The capacity of PCMs to store and release thermal energy during phAase transitions has garnered considerable attention in diverse domains. Widely employed in thermal energy storage applications such as building heating and cooling systems, solar energy retention, and electronic cooling mechanisms, PCMs stand at the forefront of energy efficiency solutions. Nevertheless, the inherent poor thermal conductivity of standard PCMs presents a limitation, manifesting in reduced rates of charging and discharging. The advent of NEPCMs emerges as a solution to this challenge. By embedding nanoparticles within the PCM matrix, NEPCMs exhibit enhanced thermal conductivity and heat transfer performance. Research has demonstrated that the integration of nanoparticles into PCMs significantly elevates the thermal energy storage capacity and augments the efficacy of thermal energy storage systems.

## 1.2 Rationale for Investigating Nanoparticles and Melting Dynamics

The optimization of NEPCMs' thermal performance is intricately linked to the understanding of the relationship between nanoparticle concentration and the mass fraction and melting characteristics of these materials. The nanoparticle concentration within the PCM matrix is pivotal in defining key physical properties, including melting point, latent heat capacity, and thermal conductivity. By systematically exploring the influence of nanoparticle concentration on the mass fraction and melting dynamics, the design and formulation of NEPCMs can be tailored for specific applications, thereby enhancing the efficiency of thermal energy storage systems. This research aims to delve into the effects of nanoparticle concentration on the mass fraction and melting behavior of NEPCMs through comprehensive experimental and numerical analyses. Such investigations will provide valuable insights into the phase change characteristics of NEPCMs under varying nanoparticle concentrations, contributing significantly to the field of thermal energy storage system design and optimization.

## 1.3 Survey of NEPCM Research and Applications

The burgeoning field of NEPCMs has garnered substantial research interest due to its multifaceted applications across various sectors. Prior studies have predominantly focused on the augmentation of PCM matrices with nanoparticles to enhance the thermal attributes and functionality of NEPCMs. This section offers a concise synthesis of pivotal research contributions that have propelled the understanding and application of NEPCMs. It has been evidenced in earlier research [1] that the integration of nanoparticles such as ZnO, CuO, and $Al_2O_3$ into PCM matrices significantly elevates the thermal conductivity of NEPCMs. These studies underscore that nanoparticle inclusion markedly improves heat transfer rates and the thermal performance of NEPCMs, particularly noticeable as the temperature gradient between hot and cold surfaces diminishes, thereby extending container stabilization time. Ghalambaz et al. [2] embarked on an exploration focused on optimizing shell-and-tube thermal energy storage systems utilizing NEPCMs. Their investigation, which concentrated on the melting dynamics of NEPCMs, aimed at refining design parameters to bolster thermal energy storage efficiency. Notably, their optimized designs showed potential for increasing stored energy by 23.3% (Cu) and 22.5% (GO) in NEPCM compared to conventional configurations.

An extensive review by Farid et al. [3] delved into the various facets of phase change energy storage, encompassing materials and their applications. This review accentuated the capacity of NEPCMs to enhance both the energy storage potential and efficiency of thermal energy storage systems, with encapsulation of PCMs contributing to an increased surface area for heat transfer. Investigating the melting process of NEPCMs within square cavities, Ebrahimi and Dadvand [4] scrutinized the impact of diverse parameters on the melting behavior and heat transfer properties of NEPCMs. Their findings revealed that the most substantial melting rates occurred at a volumetric nanoparticle concentration of 2%, offering crucial insights for thermal energy storage system optimization. In the realm of mathematical modeling and simulations, Dutil et al. [5] conducted a comprehensive review of PCMs. Their research highlighted the critical role of numerical modeling in understanding NEPCM behavior and enhancing performance in various applications, given the non-linear nature of the problems involved in thermal system analysis. Sharma et al. [6] presented a review focused on thermal energy storage using PCMs and their applications. This review encompassed a broad spectrum of considerations, ranging from material selection to design and performance optimization, and underscored the potential of NEPCMs in elevating the efficacy of thermal energy storage systems. The versatility of PCMs, characterized by a broad melting and solidifying temperature range, was noted as particularly advantageous for diverse applications.

Recent years have witnessed a surge in the exploration of NEPCMs, primarily due to their distinctive properties and their potential in revolutionizing thermal energy storage systems. The wealth of research conducted [1–6], and more specifically, studies [7–17], have been instrumental in advancing the understanding of NEPCMs. These studies encompass a broad spectrum of topics including radiative flow, solidification, convection effects, behavior in porous enclosures, the role of hybrid nanoparticles, and the influence of various parameters on the melting process. The synthesis of these studies offers a comprehensive perspective on the numerical simulations, experimental methodologies, and theoretical analyses pivotal in understanding the melting behavior and thermal energy storage capabilities of NEPCMs. The investigation made by Ahmed and Raizah [7] delves into the behavior of NEPCMs within inclined porous prismatic enclosures, with a particular focus on the role of radiative flow in entropy generation. This study illuminates the complexities of thermal properties in NEPCMs when subjected to intricate geometrical configurations, underscoring the enhancement in heat transmission when NEPCMs are employed.

Li et al. [8] centered on the simulation of NEPCMs within sinusoidal enclosures, and examined the impact of nanoparticle enhancement on thermal behavior. This study provides valuable insights into the heat transfer characteristics of NEPCMs in intricate geometrical settings, revealing that the most effective freezing time scenario was achieved at 198.27 seconds with specific parameters (A = 0.1 and m = 5.7). Hosseinizadeh et al. [9] made a numerical analysis of the unrestricted melting of NEPCMs inside a spherical container, enhancing the comprehension of NEPCMs' thermal performance during the melting phase. This research, conducted with an initial sub-cooling of 6°C, explored various nanoparticle Stefan numbers and volume fractions, contributing significantly to the understanding of

NEPCM behavior. Hosseini et al. [10] focused on the solidification of NEPCMs within a container, and explored the effect of nanoparticle enhancement on solidification dynamics. This investigation provides crucial data on the phase change characteristics of NEPCMs during solidification, demonstrating that the inclusion of SiC nanoparticles at 2% and 4% concentrations can increase the discharge rate by 2.8 and 4.8 times, respectively.

Lorente et al. [11] explored phase change heat storage within a pipe-centered enclosure, and examined the thermal behavior of NEPCMs in such configurations. This study offers insights into the heat transfer characteristics and performance of NEPCM-based thermal energy storage systems. Theoretical analysis first addresses the initial stages of natural convection in the liquid, followed by a detailed examination of subsequent stages. Finally, Tasnim et al. [12] investigated the influence of convection on the nano-PCM melting process within a porous enclosure. This research sheds light on the mechanisms of convective heat transfer and their impact on the thermal performance of NEPCM systems, drawing parallels with the effects observed during melting in enclosures with embedded nano-PCM in porous media. Al-Jethelah et al. [13] delved into the melting behavior of NEPCMs within porous enclosures, examining the impact of porous media on heat transfer and melting properties. The study revealed that factors such as Rayleigh number (Ra), nanoparticle volume fraction ($\phi$), and Darcy number (Da) significantly influence the enhancement of the melting process.

Further, Elbahjaoui et al. [14] investigated the melting dynamics of NEPCMs in enclosures heated by laminar heat transfer fluids. This research illuminated the effects of fluid flow on the melting process, highlighting those adjustments in volumetric percentage, heat transfer fluid (HTF) mass flow rate, and input temperature are crucial for significant thermal performance improvements. Sushobhan and Kar [15] concentrated on the thermal modeling of nano-based PCM melting, aiming to augment thermal energy storage. The research demonstrated that an increase in the temperature differential between the melting point and the hot wall expedited the melting process of nano-based PCMs. Ghalambaz et al. [16] focused on the melting behavior of NEPCMs enhanced with hybrid nanoparticles. This study provides insights into the effects of various nanoparticle combinations on the melting and thermal performance of NEPCMs. The behavior of the liquid-solid interface was monitored across different model parameters (Nc, Nv) = (0,0), (5,18), (18,18), with the total nanoparticles volume fraction ($\upsilon$ = 0–5 percent) being a variable of interest (18,5). Dadvand et al. [17] explored the numerical modeling of NEPCM melting induced by a heated thin plate positioned at varying angles within a square enclosure. This investigation shed light on how the positioning of the heating element influences the melting behavior, revealing that an increase in nanoparticle concentration at specific points on the heated plate accelerated the melting rate of NEPCM compared to pure PCM.

This study builds upon these foundational studies to examine the interplay between nanoparticle concentration, mass fraction, and melting behavior in NEPCMs. While previous research has extensively explored the impact of nanoparticle concentration on NEPCMs, the effect of differential temperatures on the same wall remains unexplored. This study aims to fill this gap through a numerical investigation, focusing on the influence of varying temperatures, such as those induced by non-uniform solar radiation on a single wall, on the liquefaction of paraffin wax. The study is poised to contribute novel insights into the phase change characteristics of NEPCMs under varying thermal conditions, addressing the question of how different temperatures on one wall affect the melting behavior of NEPCMs.

## 2 Numerical Simulation Methodology

This section elucidates the numerical simulation methodology employed to investigate the impact of nanoparticle concentration on the mass fraction and melting behavior of NEPCMs. The simulations are designed to delineate phase change characteristics and assess thermal performance under varying nanoparticle concentrations. The methodology encompasses two principal modules:

**Preprocessing module**: This foundational module establishes the framework for calculations and matrix construction, encompassing:

a. Geometrical modeling of the calculation domain.
b. Generation of computational mesh.
c. Definition of boundary conditions.

**Solution module**: This module addresses the resolution of Navier-Stokes equations, which include continuity, momentum, and energy equations, along with the turbulent flow model.

### 2.1 Numerical Modeling of NEPCM Behavior

The computational fluid dynamics (CFD) approach is employed for solving fluid flow and heat transfer equations within the NEPCM enclosure. Utilizing the commercial CFD software package ANSYS (version 19.1), the simulation model is constructed. This model integrates the mathematics of the framework and develops a coherent state, encompassing both solidification and melting phenomena. The phase transformation model is applied to elucidate the effect of phase change, and mathematical discretization methods are employed in Cartesian coordinates (x, y, and z). The creation of two- and three-dimensional geometries is facilitated, with ANSYS supporting solid geometry mesh generation for three-dimensional models, requiring minimal user input for single-phase scenarios. In this study, a total of 51,330 cells were used, with an element size of 0.0005 m. Convergence is deemed achieved when residuals fall below a tolerance threshold of 10-6 for all fluid flow conditions as previously outlined.

### 2.2 Governing Equations and Boundary Conditions

For the simulation of fluid flow and heat transfer within the NEPCM enclosure, the model resolves a set of governing equations pertinent to incompressible flow with heat transfer, namely:

Continuity equation:

$$\nabla \cdot \vec{V} = 0 \tag{1}$$

Momentum equation:

$$\frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V} = \frac{1}{\rho} \left( -\nabla P + \mu \nabla^2 \vec{V} + \rho \vec{g} \beta \left( T - T_{ref} \right) \right) + S_m \tag{2}$$

Energy equation:

$$\frac{\partial h_{\text{sens}}}{\partial t} + \frac{\partial h_{\text{lat}}}{\partial t} + \nabla \cdot \left( \vec{V} h_{\text{sens}} \right) = \nabla \cdot \left( \frac{k}{\rho c_p} \nabla h_{\text{sens}} \right) \tag{3}$$

where, $\overrightarrow{V}$ represents the velocity vector, $P$ denotes pressure, $\rho$ is the fluid density, $\mu$ signifies the dynamic viscosity, $g$ the gravitational acceleration, $T$ temperature, $c_p$ the specific heat capacity, and $k$ the thermal conductivity.

The boundary conditions for the enclosure walls are meticulously defined to mirror realistic thermal conditions. Initial conditions of the NEPCM, including the initial temperature distribution and mass fraction distribution, are established, drawing on empirical data from prior research or specific requirements of the simulated scenario. The model employs a 10cm×10cm enclosure, featuring walls with contrasting temperatures. Two sides of the enclosure radiate high temperatures, while the remaining sides are kept at lower temperatures. This setup utilizes paraffin wax infused with three distinct nanomaterials ($Al_2O_3$, CuO, and ZnO), selected based on their prevalent usage in preceding studies, at concentrations of 0.1, 0.3, and 0.5 wt%.

A critical component of the setup is the heat-supplying wall, segmented into four distinct sections, each exhibiting a unique temperature gradient, as depicted in Figure 1. This configuration is pivotal for analyzing the melting process under varying thermal conditions. The solid phase of the material necessitates higher temperatures to initiate melting, while the opposite side undergoes a gradual temperature increase, ranging from 4 to 12°C above a specified set point (Tsp). This multi-gradient setup is instrumental in elucidating the melting behavior of materials under diverse thermal scenarios.


**Figure 1.** Division of the heat-supplying wall into four sections with varying temperature gradients

### 2.3 Simulation Assumptions and Simplifications

To facilitate the numerical simulations while ensuring computational efficiency, the following assumptions and simplifications are made:

- Incompressibility of NEPCM: The NEPCM is considered incompressible, negating any variations in density due to changes in temperature or pressure.

- Flow characterization: The fluid flow within the NEPCM is treated as laminar, and the effects of turbulence are not considered.

- Thermophysical property constancy: The thermophysical properties of NEPCM, such as density, specific heat capacity, thermal conductivity, and viscosity, are assumed to be constant and independent of temperature variations.

- Phase change modeling: The phase change process, particularly the latent heat of fusion, is modeled using an effective specific heat approach or the enthalpy-porosity method.

- Accounting for natural convection: In scenarios where natural convection is present, its impacts are incorporated by introducing appropriate buoyancy terms into the governing equations.

- Wall conditions: The enclosure walls are presumed to be adiabatic, except for the specified boundary conditions that are applied.

These assumptions are integral to the model's framework and are aligned with standard practices in the field. They strike a balance between the complexity of the physical phenomena and the need for computational tractability. The assumptions are justified based on their common application in similar studies and their acceptance in the scientific community for analyses of this nature.

## 3 Results and Discussion

This section presents the findings of the investigation into the influence of nanoparticle concentration on the mass fraction and phase change properties of NEPCMs. Utilizing numerical simulations conducted in ANSYS-FLUENT, the study delineates the impact of nanoparticle concentration on the thermal attributes of nanofluids. It is observed that the inclusion of nanoparticles significantly modifies the mass fraction, velocity stream, and temperature profile of the materials.

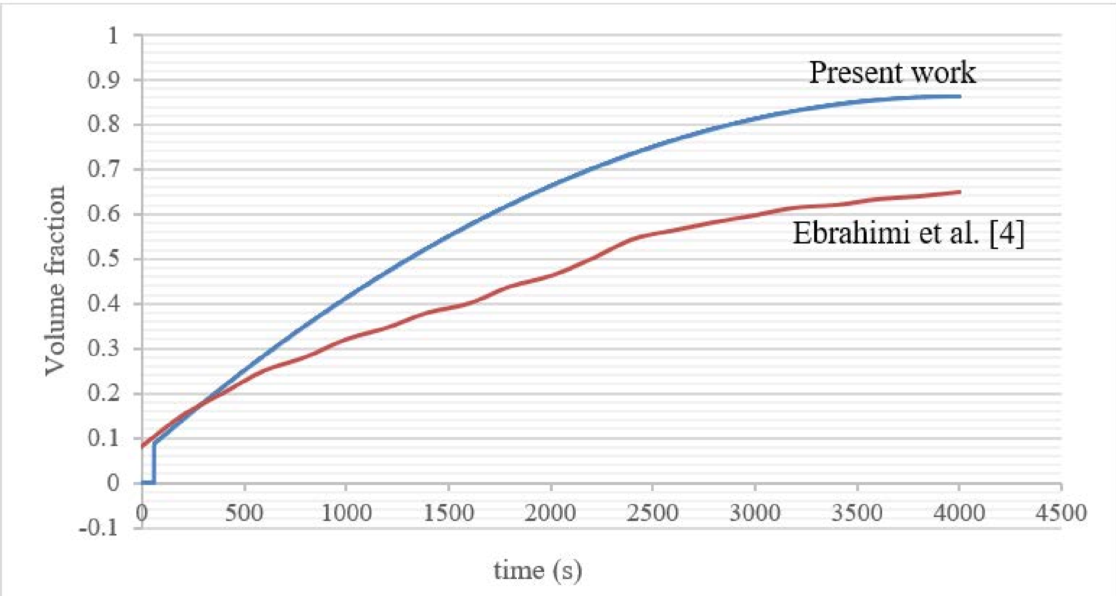



**Figure 2.** Mass fraction validation chart

A notable finding, as depicted in Figure 2, is the enhancement of volume fraction over time. The results illustrate a marked increase in the curve, with a notable point at 4,000 seconds where the fraction, previously reported as 0.65 in the study by Ebrahimi, is augmented to 0.87 in the current study.

Further, the effects of different wall temperatures on the mass fraction of paraffin, when combined with nanoparticles, are analyzed and presented in Figure 3. The addition of three types of nanoparticles ($Al_2O_3$, CuO, and ZnO) to paraffin results in a decrease in the mass fraction of melting paraffin at consistent concentrations and test temperatures. This trend indicates that CuO is the most effective melting agent among the tested nanoparticles.

Additionally, a correlation is observed where an increase in the concentration ratio corresponds to a decrease in mass fraction for all three nanoparticle types.

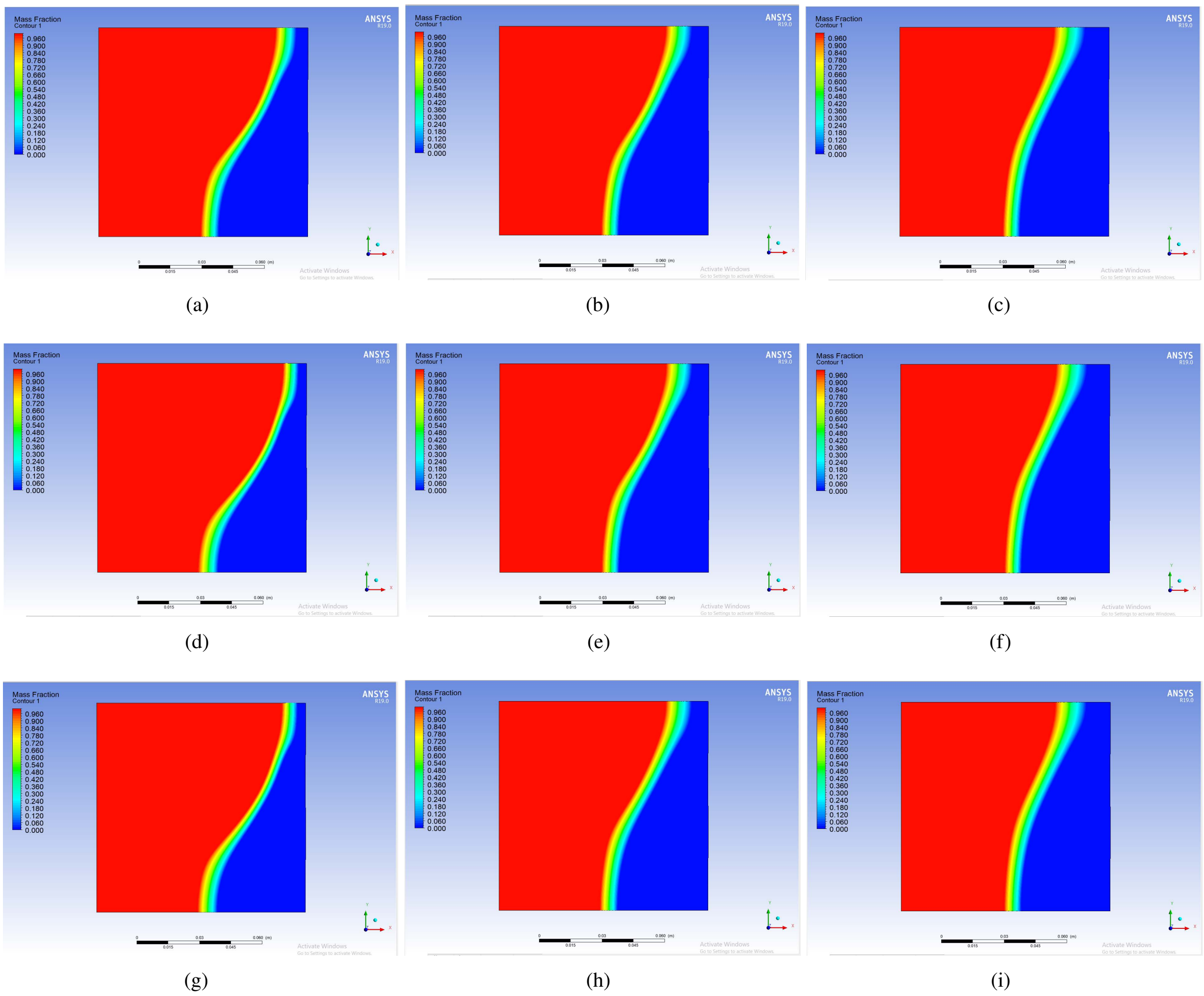
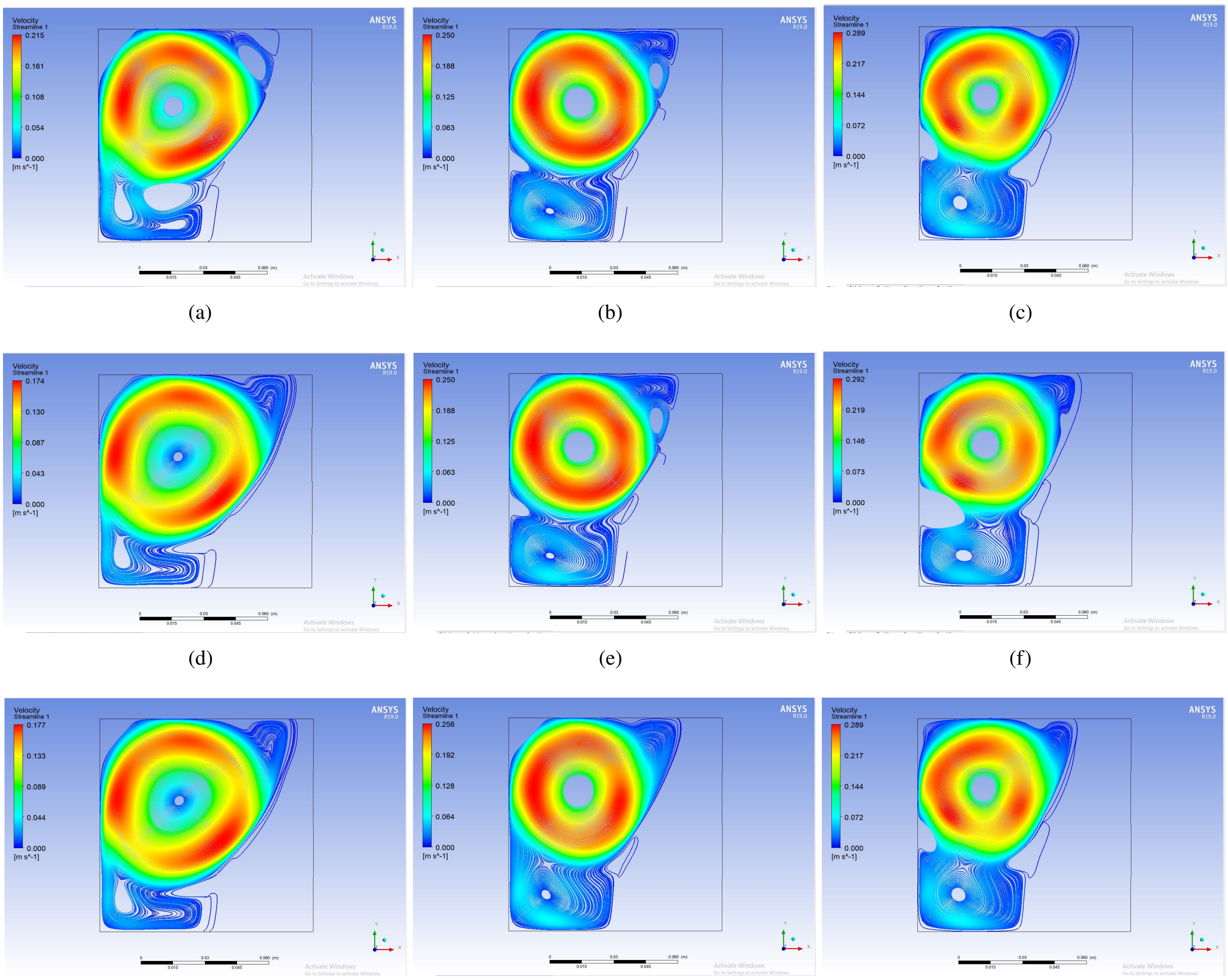


**Figure 3.** Effect of different wall temperatures on mass fraction for paraffin combined with various nanoparticles with 0.1, 0.3, and 0.5 wt.%, respectively. (a)-(c) Paraffin + $Al_2O_3$; (d)-(f) Paraffin + CuO; (g)-(i) Paraffin + ZnO

These results provide insightful contributions to the understanding of NEPCM behavior under varying conditions of nanoparticle concentration and wall temperature. The findings underscore the critical role of nanoparticle type and concentration in influencing the thermal performance and phase change characteristics of NEPCMs.

The findings further reveal the impact of nanoparticle addition on the velocity or streamline of the original material. It is observed that the addition of $Al_2O_3$, CuO, and ZnO nanoparticles results in an increase in velocity across all concentration ratios. The magnitude of this increase varies with each nanoparticle type, reaching 0.177 m/s for $Al_2O_3$, 0.174 m/s for CuO, and 0.215 m/s for ZnO, compared to 0.061 m/s for pure paraffin. This enhancement is illustrated in Figure 4. With the increase in nanoparticle concentration, a corresponding increase in velocity is noted. For $Al_2O_3$, the velocities recorded are 0.215 m/s at 0.1 wt.%, 0.250 m/s at 0.3 wt.%, and 0.289 m/s at 0.5 wt.%. A similar trend is observed for CuO, with velocities of 0.174 m/s, 0.250 m/s, and 0.292 m/s at the respective concentrations. In the case of ZnO, the velocities are 0.177 m/s, 0.256 m/s, and 0.289 m/s. Among these, CuO exhibits the highest velocity of 0.292 m/s, attributable to its low density and high thermal conductivity.

The study also examines the influence of temperature increases on the parameters. Once the material reaches the liquid state, the temperature on the right side is incrementally raised from 4 to 12°C + TS. Temperature is identified as a critical variable influencing the performance of PCM and nanoparticles. Upon the addition of nanoparticles, the temperature distribution profile in paraffin, initially random, transitions to a uniform and curved configuration. Interestingly, no significant difference is observed in the temperature profiles among the varying concentrations of the three nanoparticle types, as depicted in Figure 5.



(a) (b) (c)

(d) (e) (f)

(g) (h) (i)

**Figure 4.** Effect of different wall temperatures on velocity/streamline for paraffin combined with various nanoparticles with 0.1, 0.3, and 0.5 wt.%, respectively. (a)-(c) Paraffin + $Al_2O_3$; (d)-(f) Paraffin + CuO; (g)-(i) Paraffin + ZnO

This investigation delves into the effects of nanoparticle concentration on the phase change characteristics and thermal performance of NEPCMs. It is observed that an increase in nanoparticle concentration correlates with a decrease in the mass fraction, indicative of a reduction in the mixture's paraffin content. This phenomenon is attributed to the complex interaction between paraffin and nanoparticles, which governs the variations in mass fraction. Additionally, the study examines the impact of different nanoparticle concentrations on temperature, mass fraction, and velocity stream of the materials. Findings reveal that CuO emerges as the most efficient melting agent, contributing to an increase in the volume percent over time. The inclusion of nanoparticles modifies the original material's velocity, with CuO's low density and high thermal conductivity leading to higher velocity values. Furthermore, the addition of nanoparticles to paraffin results in a uniform and curved temperature distribution profile, with no significant correlation between concentration variations and their effect on temperature distribution.

The decrease in mass fraction with increasing nanoparticle concentration is influenced by factors such as packing density, agglomeration, and processing complexities. This understanding is crucial for optimizing the design and production of NEPCMs, aiming to enhance their thermal characteristics effectively. The implications for heat transfer efficiency, thermal conductivity, temperature regulation, and overall performance of NEPCMs are significant, especially considering the superior melting efficiency of CuO. This research provides insights into pivotal aspects for the development of advanced thermal management systems capable of more efficient heat storage and transfer. CuO's efficacy as a melting agent may be attributed to its inherently high thermal conductivity, which during phase transitions, could aid in maintaining a more consistent temperature distribution, thus mitigating the occurrence of isolated hotspots and temperature fluctuations.

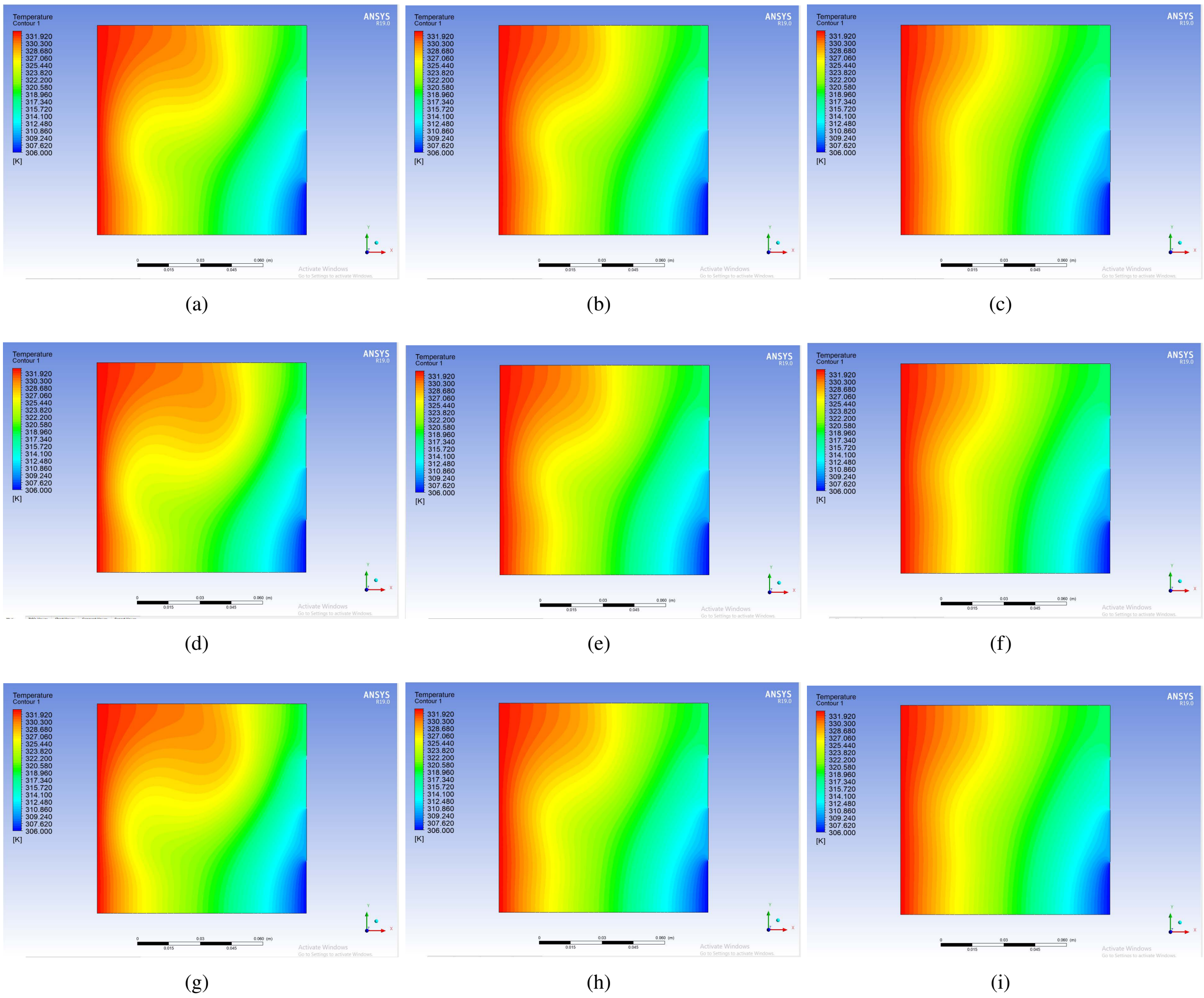



**Figure 5.** Temperature profile for the first case of all materials combined with paraffin and different nanoparticles at concentrations of 0.1, 0.3, and 0.5 wt.%, respectively. (a)-(c) Concentrations of $Al_2O_3$; (d)-(f) Concentrations of CuO; (g)-(i) Concentrations of ZnO

## 4 Conclusions

In this research, the influence of nanoparticles on the mass fraction within a PCM, specifically paraffin wax, was investigated. The study employed nanomaterials ($Al_2O_3$, CuO, and ZnO) at concentrations of 0.1, 0.3, and 0.5 wt.% and examined their effects under varying temperature conditions within a square enclosure. It was observed that the thermal characteristics of NEPCMs are notably improved with the addition of nanoparticles, particularly CuO. CuO distinguished itself as the most effective melting agent, markedly enhancing the composite material's thermal conductivity. Furthermore, the mass fraction of PCM was found to be influenced by the nanoparticle concentration, highlighting the need for careful optimization to maximize heat transfer capabilities. The outcomes of this study underline:

- It has been conclusively demonstrated that the concentration of nanoparticles exerts a significant influence on the mass fraction of NEPCMs.

- An inverse relationship is noted between the mass fraction and nanoparticle concentration; with increasing nanoparticle concentration, the mass fraction decreases. Specifically, the efficacy of CuO as a melting agent facilitates a more efficient and expedited phase transition process, a critical attribute for applications necessitating rapid heat absorption or release.

- The velocity or streamline of the base material, namely paraffin, is observed to increase with the inclusion of all three types of nanoparticles ($Al_2O_3$, CuO, ZnO), with the highest velocity recorded for ZnO at 0.215 m/s, compared to 0.061 m/s for pure paraffin.

- CuO, when added to paraffin, is identified as the most effective agent in enhancing the melting process under similar concentration and testing conditions.

- The introduction of nanoparticles into paraffin wax significantly improves the NEPCM's melting behavior, resulting in a more rapid and uniform phase transition from solid to liquid. This improvement is primarily attributed to the enhanced thermal conductivity of the nanoparticles.

- Future research should explore the impact of nanoparticle size and shape on the mass fraction and melting behavior of NEPCMs, offering the potential for further optimization.

- The findings from this study are poised to contribute significantly to the advancement of more efficient thermal energy storage systems and broaden the application scope of NEPCMs in various engineering fields.

## 5 Future Work

Future investigations should focus on the effects of nanoparticle size and shape on the mass fraction and melting behavior of NEPCMs. Detailed analysis of different nanoparticle characteristics will deepen understanding of optimization opportunities, guiding the development of tailored NEPCM solutions for diverse applications. Comprehensive exploration of these aspects will provide insights into the intricate interactions within the composite material, paving the way for advancements in this burgeoning field of research.

## Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

## Conflicts of Interest

The authors declare no conflict of interest.

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