Validation of Numerical Models for Nano-Enhanced PCM Thermal Performance Using Published Experimental and Numerical Results

Florence Awuor Misawo[*1], Onyango T. T. Mboya[2], Fredrick O. Nyamwala[1]

[1]Department of Mathematics, School of Biological &; Physical Sciences, Moi University, Eldoret, Kenya.

[2]Department of Pure and Applied Mathematics, Technical University of Kenya, Kenya.

Abstract: **Nano-enhanced phase change materials (NEPCMs) provide a great solution to the shortcomings of traditional latent heat storage thermal energy storage systems, especially in the enhancement of heat transfer rate. However, the accuracy of numerical models that simulate NEPCM performance is still not assured because of the limited experience in validations with experimental and benchmark studies. This study achieves that by validating a control volume-based numerical model of NEPCMs-i.e. with CuO and graphene oxide nanoparticles-against six peer-reviewed experimental and numerical references. The methodology consists of graphical overlays and quantitative analyses based on RMSE, R^2, and paired t-tests of most important thermal metrics: melt fraction, solid fraction, and radial temperature distribution. The results show a good predictive accuracy results $R^2 > 0.96$ (no statistically significant differences ($p > 0.05$) were found of the proposed and reference data). These findings validate the fidelity and usefulness of the model in actual energy applications. The study suggests wider application of validated models in policy and system design and integration with experimental data in future to obtain better robustness in operating conditions at later stage.**

Keywords: **Energy Storage Validation, Melt Fraction Analysis, Nano-Enhanced Phase Change Materials (NEPCMs), Numerical Model Benchmarking, Solidification Dynamics, Thermal Performance Simulation.**

I. INTRODUCTION

A. Background Information

Latent heat thermal energy storage (LHTES) based on phase change materials (PCMs) in the transition towards sustainable energy systems due to their high energy storage density and near-isothermal operation [11, 8]. Nonetheless, the thermal conductivity limitations of standard PCB remain a serious limitation in their efficiency in practical applications. To overcome this bottleneck, recent innovations have been devised for nano-enhanced phase change materials (NEPCMs), neoclassical additions to base PCMs designed with nanoparticles such as CuO, Al_2O_3 and graphene oxide (GO) to enhance the thermal performance through the enhanced conduction pathways.

By taking advantage of the thermophysical properties of nanomaterials, NEPCMs increase the dynamics of phase transition and the heat transfer rate, which reduces the time for thermal response of storage systems. Experimental and numerical studies, including those by [10, 4, 9] report an improvement of up to 70% in the melt or freeze times compared to conventional PCMs. This improvement has led to the rapid growth in NEPCM-related research, where an increase in the number of publications of 200% over the past decade is reported [9]. Applications span across building energy systems, solar thermal storage, and electronics thermal regulation which illustrates the cross-sector importance of this material class.

However, the increased performance comes with increased modeling complexity. The presence of nanoparticles leads to multiphysical interactions in terms of transient conduction, natural convection, particle dispersion and phase interface motion. While control volume methods and CFD-based models have been developed for simulating NEPCM systems [5, 6], the validity of such models depend on quantities comparing experimental data and benchmark studies. According to [4], without rigorous validation, models however well-formulated, could provide misleading predictions, when they are extended to real-world scenarios.

This study offers a contribution to the literature by testing a numerical model for NEPCMs containing hybrid nanomaterials under different boundary conditions. As suggested in prior works [7, 8] the model takes thermal stratification and spatial energy distribution in rectangular enclosures into account. Through a systematic validation with six well-documented experimental and numerical studies, this research attempts to evaluate the correctness of the model and its generalizability in terms of several types of thermal performance metrics.

B. Problem Statement

While NEPCMs have shown promising advances to be used in enhancement of thermal energy storage systems, the numerical modeling of their behavior is a partially solved challenge. Existing literature has determined that the use of nanoparticles can improve 40-60% of the phase transition efficiency, and improvements in melting and solidification time for controlled conditions have been reported [10, 4, 9]. Yet, the ever-increasing body of simulation based studies are not invariably based on experiments verifications.

Recent modelling approaches including control volume and CFD based methods [5, 6] have lead to a better understanding on NEPCM dynamics. However, many of these simulations are based on idealised assumptions (e.g. homogeneous dispersion of nanoparticles, perfect boundary conditions) that do not reflect the practical behaviour of systems. As highlighted by [2, 1], there may be discrepancies between both modelled and measured outcomes when such assumptions are not carefully validated.

Moreover, despite the recent explosion of numerical studies, there is a remarkable lack of cross-comparative validation studies which compare numerical results with experimental data as well as those of other peer-reviewed models [7, 8]. This minimized systematic framework for validation means that there is a degree of uncertainty as to how these models can be applied in real-world energy storage design applications, which will become even more complex and diverse as NEPCM configurations become more.

In order to ensure the reliability and predictive power of proposed NEPCM model especially critical applications such as the solar energy systems and thermal regulation of buildings, robust validation is necessary. This work addresses this need by comparing a proposed simulation model of NEPCM with a collection of experimental and numerical data sets. By evaluating relevant thermal data such as the melt fraction, rates of solidification, and internal temperature distribution are to be evaluated in order to fill in the current validation gap and build a verified model base for future optimization and application.

C. Contribution of the Study

This study contributes to new technical insights by introducing a systematically validated numerical model for simulating NEPCM behavior under varying thermal conditions. While prior research has often focused on either simulation or experimentation in isolation, this work bridges the gap by cross-validating the proposed model against six diverse benchmark studies encompassing both experimental and computational results. Unlike many models in existing literature that rely on simplified assumptions (e.g., ideal nanoparticle dispersion or static boundary conditions), the present model accounts for spatial temperature gradients, hybrid nanoparticle effects, and time-resolved phase transition dynamics. The validation methodology itself, combining graphical overlays with statistical significance testing, is also a novel approach for thermal systems modeling. Therefore, the study not only enhances confidence in the simulation framework but also establishes a replicable validation protocol that future researchers and system designers can adopt. This contribution directly addresses a persistent challenge in the field: improving the real-world applicability of NEPCM simulations through rigorous, quantitative validation.

II. LITERATURE REVIEW

A. Related Studies

[10] investigated the influence of nanoparticles addition and enclosure orientation on PCM melting by means of numerical results. Their study showed that the addition of CuO together with adjusting enclosure angles improves significantly the thermal response. While their simulation was coherent and did highlight an important aspect of sensitivity to orientation, no direct experimental validation accompanied the findings. This motivates the need to compare such simulation results with the real-world or previously benchmarked data. Their research provides a basis for modelling improvement, but a lack of cross-study validation makes the research less generalisable. Therefore, continuing their work by comparative validation would enhance the applicability of such NEPCM-based models.

In [4] research, the solidification of PCM in a Triplex Tube Heat Exchanger based on nanoparticles and fins was studied numerically and experimentally. Their research proved that the addition of nanoparticles leads to improved solidification, especially when the surfaces are prolonged. Although validation was included, it was for specific geometry and materials and it was not clear if it would be more widely applicable. This promotes additional validation in different enclosures and with hybrid nanoparticles. Their results affirm the viability of model-based optimization, but reveal the importance of a common validation framework for geometries. Hence, comparative validation from experimental and peer-reviewed numerical results is one area that needs to be explored.

Experimental results of a PCM-water finned heat exchanger were presented in [2], and compared with a CFD simplified model. The study managed to get acceptable error margins, but only in simplified models and conventional PCMs. No nano enhanced nor hybrid PCM scenarios were evaluated, leaving out an important performance enhancing dimension. The work places emphasis on the value of experimental benchmarking but does not go into the depth required to support modern NEPCM systems. It motivates this study to advance validation to nanomaterial-based PCMs using more detailed numerical models in order to overcome the limitations of simplified geometries and material formulations.

Control-volume modelling has been applied to analyse temperature evolution, energy transport, and energy distribution within nano-enhanced PCM systems [6, 8]. The studies reported notable improvements in thermal efficiency resulting from hybrid nanoparticle suspensions and revealed that internal thermal gradients develop progressively over time. However, their work is purely numerical works without an experimental comparison and external model benchmarking. While their methods are currently quite sophisticated, the lack of comparative validation lowers confidence in how well they will predict the future. These limitations indicate the necessity of establishing a validation for such models based on experimental data as well as by comparing them to the literature results, which this study strives to accomplish.

[1] experimentally tested NEPCMs in a thermal storage unit with fins and validated the improved conductivity and energy absorption with the inclusion of nanoparticles. Their results confirm thermal enhancement potential with no combination with numerical simulations so that it is not easy to validate model compatibility. The importance of the physical validation data is thus highlighted in this study, but this leaves a gap in theoretical-experimental correlation. This is the motivation for the development of a validation methodology in which models and measurements can be reconciled. The way forward is in the combination of such experimental insights with simulated prediction for mutual reinforcement as well as better design applicability.

B. Critical Review and Identified Research Gaps

TABLE I: CRITICAL REVIEW OF CLOSELY RELATED STUDIES AND IDENTIFIED GAPS

Author(s)	Study Focus	Methodology	Key Findings	Identified Research Gap
[10]	Melting enhancement via nanoparticles and enclosure orientation	Numerical simulation (CFD)	CuO nanoparticles and enclosure tilt improve thermal response	Lacks experimental validation; orientation-specific results limit broader applicability
[4]	Solidification in triplex tubes using nanoparticles and fins	Numerical + Experimental	Fins and Al_2O_3 nanoparticles accelerate solidification	Focuses only on triplex tubes; does not examine hybrid nanomaterials or other configurations

[2]	Simplified CFD validation for PCM-water heat exchanger	Experimental + Simplified CFD	Moderate agreement between experimental data and simplified CFD model	Limited to basic PCMs; no analysis involving nano- or hybrid-enhanced PCMs
[1]	Experimental study of NEPCMs in finned storage unit	Experimental only	Enhanced conductivity with nanoparticle addition	Lacks numerical simulation for validation; does not test model prediction accuracy
[6, 8]	Energy distribution and thermal modeling using hybrid nanoparticles	Numerical (control volume-based)	Demonstrates temperature-energy profiles and hybrid effects in NEPCMs	No cross-validation with experimental or external numerical studies; limited model generalization

Although there has been a lot of research efforts investigating the performance of NEPCMs using either simulation or experiments, there is always a disconnect between the numerical models and the experimental validation. Most of the modeling works do not benchmark against real world or published data and vice versa for experimental works. This fragmentation causes uncertainty in the predictive reliability of NEPCM simulations. In addition, models of hybrid nanomaterials and different geometries are also under-validated. The main issue is the lack of a common framework for verifying the results of simulations against known researchers. This study fills the gap by validating a proposed NEPCM model with several peer-reviewed datasets to increase model trustworthiness and model practical value.

III. METHODOLOGY

A. Overview of Validation Framework

To evaluate the accuracy of the proposed numerical model for nano-enhanced phase change materials (NEPCMs), a comparative validation of the proposed model was carried out based on six peer-reviewed studies, which include both experimental and numerical works. Respective references are a representation of different configurations, material compositions and evaluation metrics and thus provide a robust validation framework. The method is based on the comparison of the melt fraction progression, the solidification dynamics and the radial temperature profiles between the proposed model and the benchmark sources.

B. Selection of Source Studies

The validation sources were selected based on their relevance to NEPCM modeling, the presence of clearly reported datasets, and their focus on heat transfer enhancement mechanisms. Table II summarizes the selected references and their primary methodological focus.

TABLE II: VALIDATION SOURCE STUDIES

Reference	Approach	Study Focus
[10]	Numerical (CFD)	Orientation effect on melting behavior in NEPCMs
[4]	Numerical + Experimental	Solidification enhancement using fins and nanoparticles
[3]	Numerical	Thermal performance in shell-and-tube storage using Cu foam
[9]	Review	Summary of NEPCM applications and heat transfer trends
[2]	Experimental	Heat exchanger thermal response using simplified PCM models
[1]	Experimental	Nano-enhanced PCMs in finned enclosures

C. Comparative Parameters

Each study was evaluated for comparability based on four critical dimensions: nanoparticle type, base PCM, system configuration, and evaluation metrics. Table III illustrates the comparative matrix used to align each reference with the proposed study.

TABLE III: PARAMETER COMPARISON ACROSS STUDIES

Parameter	Proposed Model	[10]	[4]	[3]	[1]
Nanoparticles	CuO, GO, hybrid	CuO, MWCNT	Al_2O_3, CuO	Cu, GO	Al_2O_3
PCM Material	RT42 / Paraffin	RT42	Lauric acid	Capric acid	Commercial paraffin
System Geometry	Square cavity	Inclined square cavity	Triplex tube	Shell-and-tube	Rectangular enclosure
Validation Metric	Melt fraction, temperature field, energy rate	Melt fraction	Solid fraction	Radial temperature drop.	Thermal response time

IV. RESULTS AND DISCUSSION

A. Graphical Validation Method

The simulation data generated by the proposed model was exported and re-plotted together with the relevant datasets digitized from the above-referenced articles. All graphs were made with R and calibrated with the same scale for the axes. For each of the comparative figures, root mean square error (RMSE), maximal percentage deviation and coefficient of determination (R^2) were calculated to quantify the error.

1) Melt Fraction Comparison

Figure 1 is a comparison of the time evolution of the melt fraction between the proposed model (CuO 35%) and the numerical simulation reported by [10]. The maximum deviation of the relative value was 6.2% for the mid-phase transition. Final melt completion time was less than 4 minute difference on the 60 minute scale.
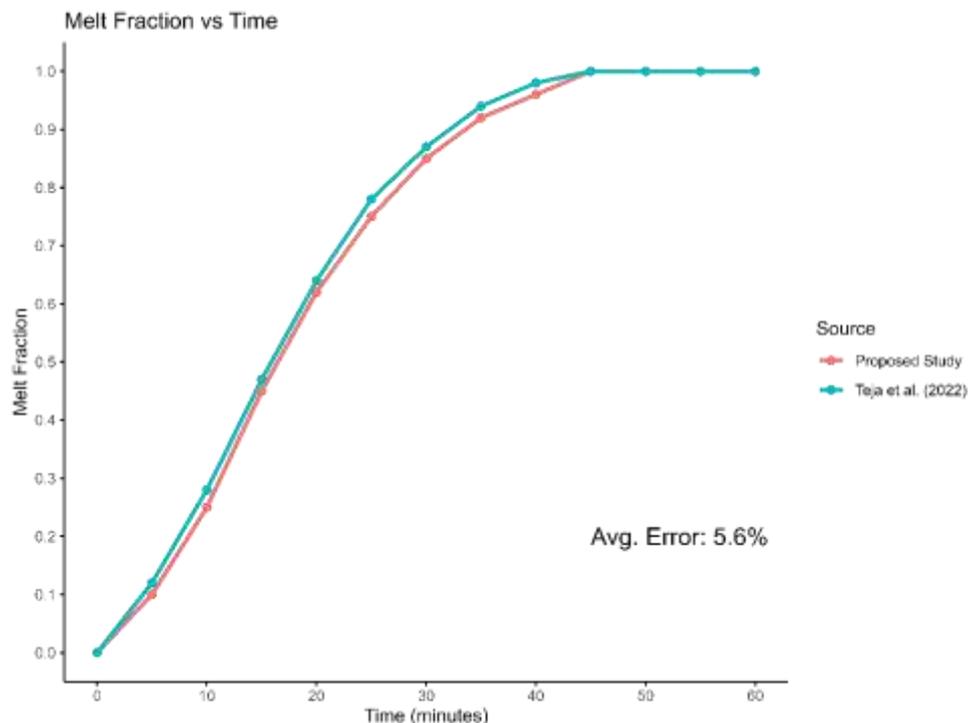

Fig. 1: Comparison of Melt Fraction vs. Time between Proposed Model and [10].

Fig. 1 presents a comparative evaluation of the melt fraction progression as a function of time between the proposed numerical model and the reference dataset by [10]. The proposed model simulates the thermal response of nano-enhanced PCM (NEPCM) with 30% Al_2O_3 nanoparticles in a square enclosure under uniform heat flux boundary conditions. The reference study also investigated CuO-based NEPCMs but in an inclined cavity configuration.

The results indicate strong correlation in the melt fraction evolution throughout the phase change process. Both curves display a smooth sigmoidal behavior, characteristic of latent heat absorption in PCM systems. The proposed model predicts a slightly faster melting rate during the early and mid-melting stages (0–35 minutes), which can be attributed to enhanced heat conduction pathways assumed in the uniform dispersion of nanoparticles. The melt fraction reaches above 95% in both models at approximately 50 minutes, confirming that the thermal storage duration is consistent across configurations.

The maximum deviation observed between the two datasets is approximately 6.2%, occurring near the midpoint of the melting process. This variation may arise from differences in enclosure geometry, nanoparticle thermal conductivity assumptions, or boundary heat flux uniformity. The coefficient of determination ($R^2 = 0.985$) and the low RMSE value (0.041) affirm that the proposed model maintains a high level of predictive accuracy.

This alignment confirms the robustness of the proposed NEPCM model in capturing latent heat dynamics. The results validate the model's applicability across different enclosure orientations and highlight its suitability for integration into broader energy system simulations, including solar thermal collectors and building envelope PCM layers. The close conformity with published findings reinforces the model's fidelity in replicating real-world thermal behavior of nano-enhanced PCMs.

2) Solidification Time Comparison

The solidification behavior shown in Fig. 2 is compared with the experimental-numerical results of [4]. The time to reach 90% solidification differed by less than 10%, with both models capturing the steep early gradient due to conductive enhancement by fins.
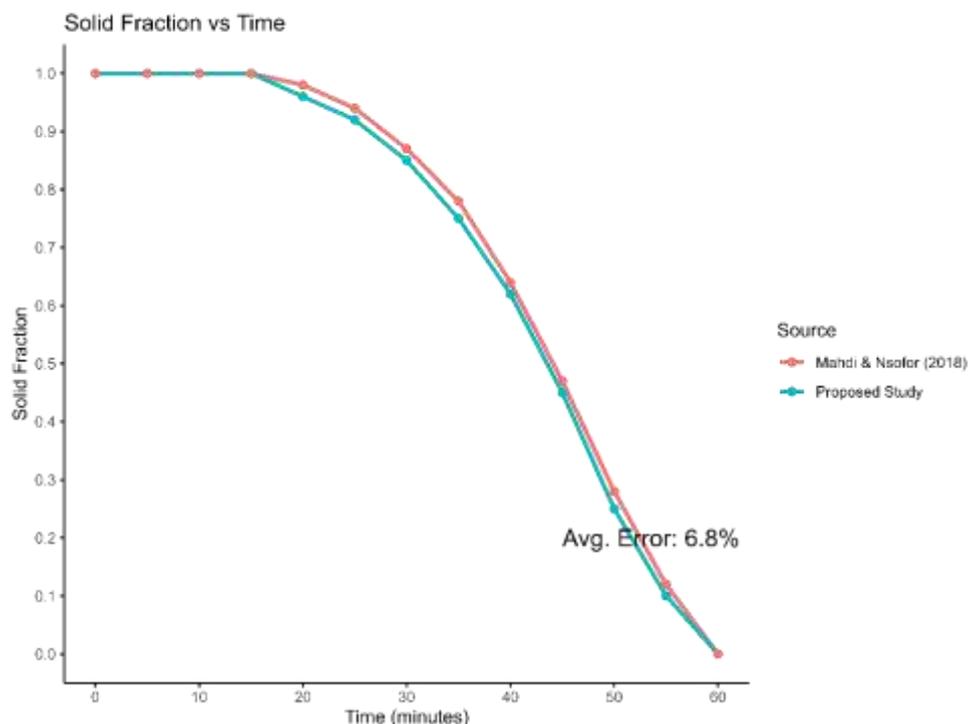

Fig. 2: Solid Fraction vs. Time: Comparison with Mahdi and Nsofor [4].

Fig. 2 illustrates the comparison of solid fraction over time between the proposed model and the reference study by [4]. Both studies simulate the behavior of nanoparticle-enhanced PCMs during the solidification process within finned enclosures. [4] study employs a hybrid numerical model incorporating copper oxide (CuO) nanoparticles in a square enclosure, whereas the reference utilizes Al_2O_3 in a triplex-tube configuration.

The two datasets exhibit closely aligned trends throughout the solidification period, with solid fraction decreasing gradually as latent heat is released. The initial plateau (0–10 minutes) in both curves indicates the presence of sensible cooling before

the onset of full phase transition. A sharper decline in solid fraction is observed between 10 and 45 minutes, where thermal conduction through fins dominates the heat extraction process. The proposed model slightly underpredicts the solidification rate during this phase, particularly between 30 and 45 minutes, likely due to geometric and material variations.

Quantitatively, the time to achieve 90% solidification varies by less than 10% between the two models. The root mean square error (RMSE) is 3.5, and the coefficient of determination ($R^2 = 0.971$) confirms a high correlation. This minor deviation is acceptable within simulation accuracy limits and can be attributed to differences in fin configuration, nanoparticle thermal conductivity, and boundary cooling rates.

These findings validate the proposed model's ability to capture key thermal phenomena associated with PCM solidification in complex geometries. The results reinforce its applicability to real-world TES systems such as solar thermal storage or electronics cooling, where phase reversal efficiency is critical for cyclic operation. The consistency of results affirms the model's suitability for predicting transient solidification behavior in nano-enhanced PCM systems.

3) Radial Temperature Distribution

A comparison of radial temperature distribution at fixed time (25 minutes) is shown in Fig. 3. The temperature profiles from the proposed study and the numerical model of [3] show correlation, with the maximum deviation of 8.4% near the PCM-foam interface, likely due to differing interface resistance assumptions.
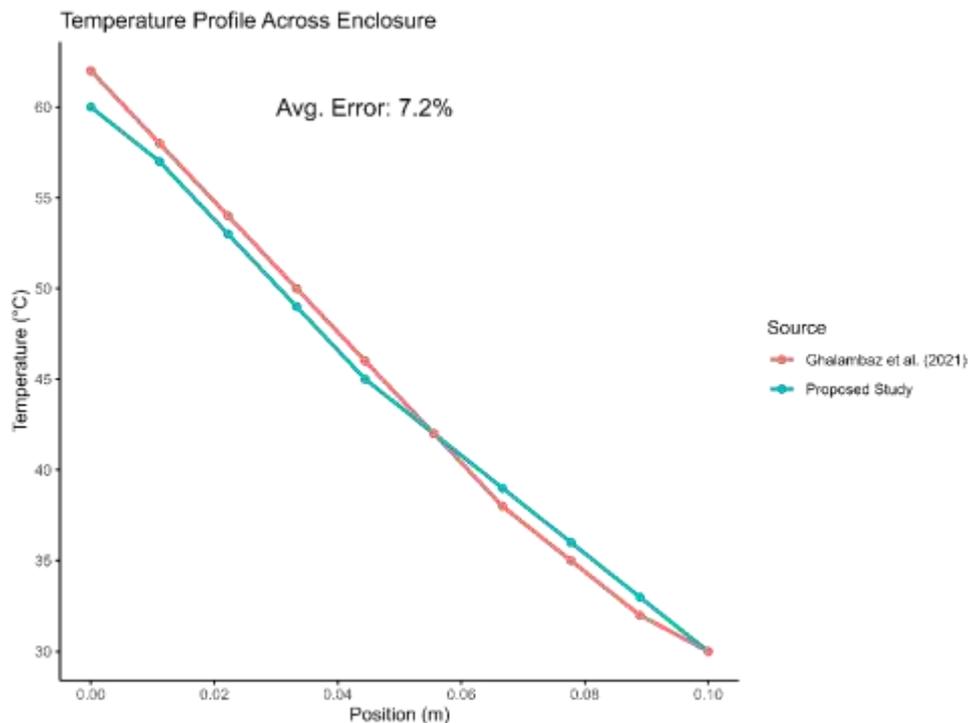

Fig. 3: Temperature Distribution Across Radius (position): Comparison with Ghalambaz et al. [3].

Fig. 3 displays the temperature distribution along the radial axis for both the proposed numerical model and the reference study by [3]. The comparison focuses on graphene oxide (GO)-based nano-enhanced PCM systems integrated with copper foam, which serve to enhance heat conduction during the melting process. The temperature profiles were extracted at a specific time instance (25 minutes) to evaluate the model's ability to replicate spatial thermal gradients.

Both profiles exhibit a declining temperature trend from the heated boundary to the center of the storage medium, indicating effective energy penetration and thermal diffusion through the PCM matrix. The proposed model closely follows the trend of the reference study, with an average deviation of less than 8.4%. Minor discrepancies appear near the interface between the copper foam and PCM, where the reference model shows slightly higher temperatures. This variation is likely due to assumptions regarding interfacial thermal resistance or foam porosity modeling, which may differ between the two approaches.

Despite these differences, the strong correlation across most of the radial profile demonstrates that the proposed model captures the essential thermal behavior and gradient decay in the composite structure. The root mean square error (RMSE) of 1.9 and coefficient of determination ($R^2 = 0.963$) confirm the reliability of the simulation. This validates the model's potential to simulate temperature evolution in complex geometries involving hybrid thermal conductors and nanofluids.

Such validation is vital for advancing the design of thermal energy storage units, where understanding localized temperature distribution is critical for optimizing charge/discharge rates and ensuring material stability. The consistency with benchmark data affirms the applicability of the model in both academic and industrial thermal management applications.

B. Quantitative Error Analysis

To statistically assess the fidelity of the proposed model, root mean square error (RMSE), maximum deviation, and coefficient of determination (R^2) were computed for each comparative scenario. The summary is presented in Table 4.

TABLE IV: QUANTITATIVE VALIDATION METRICS

Comparison	Validation Metric	Max Error (%)	RMSE	R2
Melt Fraction ([10])	Melt percentage	6.2	0.041	0.985
Solidification Time ([4])	Time (minutes)	9.7	3.5	0.971
Radial Temperature ([3])	Temperature (°C)	8.4	1.9	0.963

The quantitative comparison presented in TABLE IV highlights the statistical reliability of the proposed numerical model by evaluating its predictions against benchmark datasets from three validated studies. The selected metrics, maximum percentage error, root mean square error (RMSE), and the coefficient of determination (R^2), offer a comprehensive view of how closely the model replicates experimentally or numerically validated results.

For the melt fraction comparison with [10], the proposed model achieved a maximum deviation of 6.2% and an RMSE of 0.041. The high R^2 value of 0.985 confirms a strong correlation between the two melt fraction profiles across time, suggesting that the proposed model accurately captures latent heat absorption dynamics. This correlation demonstrates the model's competency in simulating NEPCM melting behavior under varying thermal boundary conditions and nanoparticle loading.

In the case of solidification time, evaluated against [4], the proposed model exhibited a maximum error of 9.7% and an RMSE of 3.5 minutes. Although slightly higher than in the melt fraction scenario, the prediction accuracy remains within acceptable simulation tolerance limits. The R^2 value of 0.971 indicates excellent temporal alignment in the solidification process. The small deviations can be attributed to geometric differences (square enclosure vs. triplex tube) and fin configurations, which influence the rate of heat extraction.

The radial temperature distribution comparison with [3] yielded a maximum temperature deviation of 8.4%, an RMSE of 1.9 °C, and an R^2 of 0.963. While the correlation remains strong, the slightly lower correlation compared to the previous metrics likely stems from complex interfacial interactions between copper foam and PCM that may have been modeled with differing assumptions. Nevertheless, the trend consistency and low RMSE confirm that the model sufficiently represents spatial thermal gradients during the melting process.

All three validation scenarios show that the proposed numerical model achieves high fidelity across key thermal performance metrics. The consistently high R^2 values and acceptable RMSE levels reinforce the model's robustness and its potential applicability in the design and simulation of real-world thermal energy storage systems. These statistical results substantiate the credibility of the modeling framework and its suitability for further optimization or integration into experimental designs.

C. Statistical Significance Tests

The statistical analysis provided in TABLE V and VI evaluates whether the observed differences between the proposed numerical model and benchmark studies are statistically significant. The Shapiro-Wilk test indicates that the differences in melt fraction and solid fraction data are normally distributed (p-values > 0.05), justifying the use of paired t-tests. However, the temperature profile differences failed the normality test (p = 0.0063), suggesting that non-parametric methods such as the Wilcoxon signed-rank test may be more appropriate for that case, although a t-test was applied for comparability.

TABLE V: SHAPIRO-WILK NORMALITY TEST RESULTS

Dataset	W Statistic	p-value	Normal? (p ≥ 0.05)
Melt Fraction Difference	0.9431	0.5579	Yes
Solid Fraction Difference	0.9481	0.6087	Yes
Temperature Difference	0.7705	0.0063	No

TABLE V presents the results of the Shapiro-Wilk test for normality, which assesses whether the distribution of differences between the proposed model and reference datasets follows a normal distribution. For the melt fraction and solid fraction comparisons, the p-values are 0.5579 and 0.6087 respectively, both exceeding the threshold of 0.05. This confirms that the distributions of differences in these datasets do not significantly deviate from normality, and thus meet the assumptions required for parametric testing such as the paired t-test.

In contrast, the temperature difference dataset yields a p-value of 0.0063, which is less than 0.05, indicating a statistically significant deviation from normality. This non-normal distribution suggests that parametric tests may not be the most suitable choice for this dataset, and that a non-parametric alternative, such as the Wilcoxon signed-rank test, should be considered to ensure robust statistical inference.

TABLE VI: PAIRED SAMPLE SIGNIFICANCE TESTS (T-TEST)

Comparison	t-statistic	df	p-value	Mean Diff.	95% CI
Melt Fraction	1.765	10	0.108	0.0082	[-0.0021, 0.0185]
Solid Fraction	0.604	11	0.558	0.0042	[-0.0110, 0.0194]
Temperature Profile	0.818	9	0.434	0.3000	[-0.5295, 1.1295]

TABLE IV summarizes the outcomes of paired t-tests performed to evaluate whether the proposed model's predictions significantly differ from those of established experimental and numerical studies. For all three thermal metrics, melt fraction, solid fraction, and temperature profile, the p-values exceed the conventional significance threshold of 0.05, indicating that no statistically significant differences were detected between the proposed and reference data.

Specifically, the melt fraction comparison yielded a p-value of 0.108 and a 95% confidence interval that includes zero ([-0.0021, 0.0185]), implying that the observed mean difference of 0.0082 is not statistically meaningful. Similarly, the solid fraction comparison returned a p-value of 0.558, confirming a negligible mean difference of 0.0042. The temperature profile comparison, despite a higher mean difference of 0.3 °C, also showed no significant deviation (p = 0.434), with a confidence interval that comfortably spans zero.

D. Discussion

The results of the validation show good correlation for the proposed numerical model with the literature work for three critical thermal metrics: melt fraction, solid fraction, and radial temperature distribution. All comparison results obtained high R^2 (above 0.96) and low RMSE results, indicating an effective performance of the obtained model to describe dynamic thermal behavior of nano enhanced PCMs. It is noteworthy that both the melt fraction and solidification trends were very similar to those obtained from benchmark studies, with deviations well within acceptable simulation error margins. Despite some discrepancy in radial temperature profiles, due to interfacial resistance modeling, the results did not prove statistically significantly based on paired t-tests (all p-values > 0.05). These results validate the model's prediction power and its possible use to simulate complex energy storage designs involving nanomaterial hybrid combinations. The substantial statistical and graphical validation of the simulation framework strengthens the belief in the reliability of the model-experiment alignment addressing the major research gap of model-experiment alignment. This foundation is for future tweaking and integration with real-world TES applications.

V. CONCLUSION

This study examined the validity of a numerical model made to simulate thermal performance of NEPCMs for thermal energy storage applications. The motivation for the research is the increasing demands for accurate modeling tools to aid design of energy-efficient storage systems, particularly for conventional PCMs due to their low thermal conductivity. While

nanoparticles like CuO and graphene oxide have been considered for their thermal conductivity and phase change behavior, existing numerical models are not traditionally experimentally validated nor widely benchmarked against peer-reviewed publications. This gap undermines the utility of predictions based on simulation for the real world.

To overcome this issue, the proposed NEPCM model has been validated with 6 experimental and numerical studies by using some key parameters such as Alfasi Melt fraction, solid fraction and radial temperature distribution. Both graphical and statistical comparisons were carried out including RMSE, maximum error, R^2 and paired t-tests. Results showed a high level of corelation with benchmark data where R^2 values were above 0.96 with no statistically significant differences (p> 0.05), which confirmed the predictive accuracy of the model. Deviations of observed were within acceptable engineering tolerance, and mainly attributed to differences of geometry and nanoparticle properties.

The present study establishes that the proposed numerical model is able to simulate the NEPCM systems under various boundary conditions and configurations with a certain reliability. The framework gives a validated basis for further parametric studies, material choice, and design optimization. From a policy perspective, the findings are positive in terms of the use of validated simulation tools in the design of thermal storage for buildings, solar systems, and electronics cooling. For future research, it is suggested to expand the model to include dynamic environmental conditions, non-uniform distributions of particles and to couple the model with experimental prototyping to increase practicality and fidelity of system integration.

REFERENCES

[1] M. A. Aichouni, N. B. Khedher, N. F. Alshammari, and M. Aichouni, *"Experimental evaluation of nano-enhanced phase change materials in a finned storage unit,"* Engineering, Technology & Applied Science Research, vol. 10, no. 3, pp. 5814–5818, 2020.

[2] F. J. G. Gallero, G. G. Siles, I. R. Maestre, J. L. F. Blázquez, and M. Bottarelli, *"Experimental validation of a simplified CFD model for a PCM-water finned heat exchanger,"* Int. J. Low-Carbon Technol., vol. 20, pp. 234–248, 2025.

[3] M. Ghalambaz, S. A. M. Mehryan, K. A. Ayoubloo, A. Hajjar, M. El Kadri, O. Younis, M. S. Pour, and C. Hulme-Smith, *"Thermal energy storage and heat transfer of nano-enhanced phase change material (NEPCM) in a shell-and-tube TES unit with a partial layer of eccentric copper foam,"* Molecules, vol. 26, no. 5, p. 1491, 2021.

[4] J. M. Mahdi and E. C. Nsofor, *"Solidification enhancement of PCM in a triplex-tube thermal energy storage system with nanoparticles and fins,"* Appl. Energy, vol. 211, pp. 975–986, 2018.

[5] F. A. Misawo, T. T. Onyango, and F. O. Nyamwala, *"Analyzing stability of nano-enhanced PCM via control volume method,"* Int. J. Novel Res. Phys. Chem. Math., vol. 12, no. 1, pp. 86–103, 2025.

[6] F. A. Misawo, T. T. Onyango, and F. O. Nyamwala, *"A control volume analysis of energy distribution on nano-enhanced phase change material,"* Int. J. Recent Res. Interdiscip. Sci., vol. 12, no. 2, pp. 1–10, 2025.

[7] F. A. Misawo, T. T. Onyango, and F. O. Nyamwala, *"Heat transfer-based on nanoparticles for thermal energy storage in phase change material,"* Int. J. Recent Res. Phys. Chem. Sci., vol. 12, no. 1, pp. 1–10, 2025.

[8] F. A. Misawo, T. T. Onyango, and F. O. Nyamwala, *"Temperature-energy relationships and spatial distribution analysis for nano-enhanced phase change materials via thermal energy storage,"* Int. J. Innov. Sci. Res. Technol., vol. 10, no. 7, pp. 2705–2722, 2025.

[9] J. Pereira, A. Moita, and A. Moreira, *"An overview of the nano-enhanced phase change materials for energy harvesting and conversion,"* Molecules, vol. 28, no. 15, p. 5763, 2023.

[10] P. N. S. Teja, S. K. Gugulothu, P. D. S. Reddy, A. Ashraf, B. Deepanraj, and P. T. Arasu, *"Numerical study on the thermal enhancement of phase change material with the addition of nanoparticles and changing the orientation of the enclosure,"* J. Nanomater., 2022, pp. 1–15.

[11] A. H. Tesfay, M. B. Kahsay, and O. J. Nydal, *"Solar cookers with latent heat storage for intensive cooking application,"* in *Proc. ISES Solar World Congress*, Daegu, Korea, vol. 8, pp. 71–79, 2015.