



Artificial Intelligence–Driven Control of PCM Charging and Discharging for Thermal Energy Storage in Sustainable Solar Energy

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ABSTRACT

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Artificial Intelligence, phase change material, thermal energy storage, Computational Fluid Dynamics simulation, nanoparticles, solar energy optimization

This article investigates the combination of Artificial Intelligence (AI) and Computational Fluid Dynamics (CFD) to improve the thermal performance of a phase change material (PCM)-based thermal energy storage (TES) system for solar energy applications. The geometrical model of the storage system was developed using SolidWorks and numerically analyzed in ANSYS Fluent, while the AI model was implemented in Python to predict and optimize the thermal behavior of the system. The final result reveals that the AI model could reproduce the predictions of the CFD by a high ratio, with an accuracy of approximately 98–99%, with minor deviations of ± 0.02 – 0.03 . During training, the prediction accuracy increased from 0.61 to 0.99 over 100 epochs, while prediction error decreased from 0.23 to 0.002, reflecting strong convergence of the model. The AI-enhanced model improved the thermal storage performance by reducing PCM charging times from around 3200 s to 2300 s in the conventional case and up to around 1750 s using AI optimization, indicating 20–25% reduction. Besides, AI-integrated system improved the thermal storage efficiency from 0.72 to 0.95 when it was fine-tuned compared to 0.70 to 0.84 in the conventional system. The introduction of nanoparticles significantly improved the heat transfer; the total thermal energy stored increased from 18,800 J to almost 19,900 J, and the heat transfer rate from 200 W to about 295 W at higher flow velocities. In addition, higher solar irradiance from 600 W/m² to 1000 W/m² enhanced the storage efficiency from approximately 0.71–0.81 to 0.75–0.85 according to nanoparticle concentration. It is obtained that AI-accelerated optimization with PCM enhanced through nanoparticles can enhance the heat transfer efficiency, storage effectiveness, and charge frequency of TES systems and is well-suited to sustainable solar energy applications.

1. INTRODUCTION

Over the last few decades, the global demand for clean and sustainable energy has driven an accelerated development of efficient thermal energy storage (TES) technologies to support renewable energy systems. Solar energy is one of the most valuable and sustainable renewable energy sources, considering its abundance and environmental sustainability. Solar radiation, however, is intermittent and varies throughout the day, leading to limited direct utilization of solar thermal energy. To address this shortcoming, TES has been extensively studied because these systems store extra thermal energy at times of increased solar irradiation and release thermal energy when solar input decreases or energy demand increases. Among the proposed types of thermal storage, phase

change materials (PCMs) have been under intense investigation due to their capacity to retain a great quantity of thermal energy with latent heat during phase change. It is the case that the PCM absorbs heat and melts during the process of charging, and releases the stored energy during discharge. This latent heat-storage mechanism enables PCM-type systems to retain relatively constant temperatures throughout energy storage and release, making these vehicles ideal for thermal applications in the solar sector, building energy systems, and renewable energy storage technologies. Despite these drawbacks, PCM materials often show a low thermal conductivity, thus reducing the heat transfer rate and delaying charging and discharging. In order to mitigate these obstacles, multiple improvement techniques have been developed recently in relation to the conventional PCM systems. One of

the most efficient methods is to use nanoparticles to form nano-enhanced phase change materials (NEPCM). Nanoparticle incorporation in the PCM increases thermal conductivity and improves its heat transfer properties inside the storage system. The increase in melting and solidification rate resulting from this enhancement leads to faster melting and solidification processes, as well as an increase in the TES system efficiency. At the same time as the development of thermal storage technologies, with the recent progress of technology in thermal storage technologies, Artificial Intelligence (AI) methodologies have become increasingly advanced tools for modeling, prediction, and optimization of complex energy systems. AI and machine learning methods may be used to detect nonlinear relationships in large-scale data sets as well as improve the design and working conditions of the energy system. Recent works reported are among this type of technology to predict thermal behaviors in an energy-efficient way as well as adjust operating parameters and energy efficiency to improve the energy performance in thermal storage and renewable energy systems, by utilizing AI in the most recent research. Computational Fluid Dynamics (CFD) simulations and AI tools integration can be instrumental in improving the design of thermal systems and performance assessment. The CFD simulations can provide information on temperature distribution, fluid movement, and phase transition features of PCM systems, and the AI model is able to retrieve the simulation results and predict the system response and to optimize parameters (e.g., the nanoparticle concentration, flow velocity, or operating conditions).

Aich et al. [1] studied the performance of a packed-bed TES system comprising PCM, porous media, and magnetic fields combined with a GMDH-neural network to improve performance in a packed-bed TES system using a GMDH-neural network approach. Their findings showed that, based on predictive models developed using AI, the thermal behavior can be predicted accurately and system-wide system efficiency may be greatly raised. Albarahati et al. [2] presented integration of AI for intelligent thermal management in PVT systems for better integration in photovoltaic/thermal (PVT) platforms. They demonstrated that they could improve heat recovery efficiency and energy conversion in hybrid solar energy systems by an AI algorithm. Alsehli [3] investigated solar desalination system optimization using predictive modeling as well as TES for optimization by synergizing predictive modeling with TES and predictive modeling. It was reported that the combination of AI models and TES for the improvement of water recovery for freshwater generation was a high performer to increase the efficiency and sustainability of freshwater production. Bharaneedharan et al. [4] considered the use of machine learning and AI methods in energy storage-based power systems. Intelligent forecasting and control algorithms improve system stability, efficiency, and control, the authors reported. Borhani et al. [5] proposed an AI model predicting performance for a hybrid solar cycle with trough collectors coupled with PCM storage methods. The results demonstrated that AI-enabled tools can also predict system efficiency accurately and support design parameters of the best type. Cooney and Carey [6] put forward adaptive machine learning in a controlled strategy for multi-temperature latent thermal storage. Their methodology enhanced operation control and enabled energy management of the varied storage modules on a dynamic basis. Emami et al. [7] developed deep reinforcement learning as a means to smart control of the solar-driven power cycle with TES for a smart-controlled solar

power cycle. In their Los Angeles example, they showed that the successful use of intelligent control measures can dramatically enhance energy utilization and operational efficiency. Ferrara et al. [8] developed advanced storage control approaches for energy systems of buildings and districts. Data were analyzed for AI-based optimization techniques to make the system more flexible and adaptive for energy consumption. Habib et al. [9] used a data-driven model to predict control for hybrid TES in a building management system. Their results showed that predictive control algorithms can effectively reduce energy demand and comfort with respect to temperature with regards to their energy consumption by using predictive control algorithms. Hajlaoui et al. [10] evaluated the discharge performance of hexagonal PCM storage with longitudinal smooth and Y-shaped fins in a hexagonal system on the basis of AI simulation. The experimental results of this study showed improvements in heat transfer rates and a faster thermal discharge mechanism. Huang and Hewitt [11] investigated PLC-based control over an air-source heat pump-driven PCM radiant floor heating system to control a PCM radiant floor heating system powered by air-source heat pump for the first time. They showed that automation of heating and automatic control systems for automatic heating systems could enhance both the energy efficiency and reliability of the systems of energy transfer. Isania and Galgaro [12] evaluated machine learning and AI-for-PCM-based storage design optimization in plate heat exchangers. AI was further employed as a tool for designs for energy efficient design processes and enhanced thermal storage results, as a result, which was concluded by the authors. Lv et al. [13] have advanced digital twin technologies towards secure TES systems in buildings. Their work demonstrated that real-time digital models enhance monitoring, fault detection, and operations optimization. Mamodiya et al. [14] analyzed AI hybrid solar energy systems via smart materials and adaptive photovoltaics hybrid solar systems based on AI. The study emphasized that the integration of AI enhances power production effectiveness and sustainability. Mehraj et al. [15] performed a bibliometric analysis on the use of AI in the construction of TES tanks. Their empirical study highlighted a rapid expansion of AI-based optimization approaches for TES system design. Mehta et al. [16] evaluated the performance of TES systems for solar thermal applications. The study confirmed that TES systems greatly improved solar energy use and stable energy supply system performance, significantly increasing solar capacity. Nagappan et al. [17] studied hybrid solar-PCM energy storage systems for low-carbon infrastructure. Their study offered design considerations and sustainable aspects for enhancing renewable energy storage concepts. Odoi-Yorke [18] reviewed global development of AI for solar water heating systems. AI might help in prediction and operational control and can also boost the energy consumption process of the system. Rojas Cala et al. [19] performed a bibliometric study on the feasibility of using AI in the domain of CFD modeling of TES systems. Their study showed the increasing relevance of AI-supported simulations to enhance TES design and performance prediction. Sayed et al. [20] explored AI usage for the thermal and exergy performance improvements of nanofluid-based PV/T with nano-enhanced PCM. The performance showed significant gains in thermal efficiency using AI-optimized settings. Sharma et al. [21] studied machine learning and deep learning prediction of the behavior of biodegradable PCM materials in the TES systems. Dynamic

Thermal Performance is predicted well by data-driven models. Tavakoli et al. [22] employed a physics-based approach to combine models and data-driven optimization for a latent heat thermos TES system with corrugated fins. As a result, the findings showed that the hybrid model approach is preferable for system performance and thermal responses forecasting. Yenare et al. [23] proposed a novel data-driven machine learning model for PCM charging and discharging predictions in portable cold storage and were able to successfully extract latent power from data. Their experiments validated the accuracy of the ML models in the prediction of thermal storage performance. Yilmaz et al. [24] surveyed technological progress in photovoltaic-based storage. The authors stressed the necessity of integrating renewable energy systems with advanced storage technologies for sustainable power generation. Complementing these AI-oriented studies, Agarwal [25] employed CFD to compare the thermal performance of conventional paraffin wax and an iron oxide/paraffin wax composite in a TES unit. The results showed that the incorporation of iron oxide nanoparticles improved heat absorption and modified the temperature distribution within the storage medium. Khazaa et al. [26] further investigated the time-dependent thermal behavior of NEPCMs and demonstrated that nanoparticle type and concentration significantly influenced flow development, temperature distribution, and heat-transfer performance within the enclosure. Together, these physics-based studies provide mechanistic information and simulation data that can support the development and validation of AI-assisted models for TES prediction and optimization. Comparing the AI-based performance gains reported across these studies, GMDH-neural network approaches such as Aich et al. [1] reported prediction improvements of approximately 10–15%, AI-optimized nanofluid PCM systems such as Sayed et al. [20] reported thermal efficiency gains of around 15–18%, and AI-driven solar cycle models such as Borhani et al. [5] achieved prediction accuracies of approximately 90–95%. This range of reported improvements illustrates that, while AI consistently enhances TES performance, the magnitude of improvement is highly dependent on the specific AI architecture, the quality and size of the training dataset, and the degree of coupling with high-fidelity CFD data, motivating the more tightly integrated CFD-AI framework adopted in the present study.

Although some research has been carried out with PCM-based TES systems and heat transfer enhancement by nanoparticles, relatively less research has integrated CFD simulation techniques with AI for the prediction of thermal performance and optimization of PCM systems. Although the work reported so far largely relies on quantitative/virtual methods, there are few intelligent models available that predict thermal behaviour, improve specific parameters (nanoparticle concentration, flow velocity, charging time), and investigate practical implementation studies to improve these technologies. AI was selected as the predictive and optimization tool in this study, rather than conventional optimization techniques such as genetic algorithms or response surface methodology, because AI-based neural networks can learn complex nonlinear relationships directly from CFD data without requiring an explicit mathematical formulation of the system physics, can evaluate new operating conditions almost instantaneously once trained, and can simultaneously optimize multiple interacting parameters (e.g., nanoparticle concentration and flow velocity) with substantially lower computational cost than repeated CFD

simulations. Therefore, a unified AI-CFD approach is justified to improve the prediction accuracy and optimization of the systems. The novelty of this study is to combine an AI model with a CFD simulation method to be able to improve the charging and discharging behaviour of a PCM TES system. The AI model trained in Python learns from CFD data to predict a system's thermal behavior and optimizes the operating conditions such as nanoparticle concentration and flow velocity that are essential for better heat transfer and enhanced energy storage efficiency. Accordingly, the purpose of this work is to optimize the thermal performance of a PCM-based energy storage system using its own computer-aided design, in which a CFD algorithm coupled with AI algorithms is developed. Notably, it involved determining the contribution of nanoparticle content, flow velocity, and operating conditions to optimizing the model charging and discharging system to improve thermal storage performance and heat transfer in solar energy applications. Unlike previous studies that apply AI or CFD in isolation (e.g., Aich et al. [1] used only a GMDH-neural network without CFD coupling; Borhani et al. [5] applied AI to a hybrid solar cycle without nanoparticle-enhanced PCM), the present work uniquely couples a CFD-trained neural network with nanoparticle-enhanced PCM to jointly optimize charging/discharging dynamics, representing a more integrated and practically actionable framework for solar TES design.

2. METHODOLOGY

This section presents the technique for studying the thermal performance of the PCM-based TES system combined with AI-based optimization. The research integrates CFD simulations and AI-based modeling to study and characterize the charging and discharging processes of the PCM system. The storage device geometrical model was built in SolidWorks, and the computational domain was imported into ANSYS Fluent for simulating heat transfer and phase change dynamics. It was concluded that an appropriate mesh representation for the thermal and flow fields in the system was developed. The thermophysical properties of the PCM material and the boundary conditions corresponding to charging and discharging were subsequently determined. The equations of mass, momentum, and energy were solved using the enthalpy-porosity method to simulate the PCM phase change. Further, a Python-based AI model was trained with the numerical output from the CFD simulation to predict and optimize the thermal performance of the system. This combined CFD-AI approach enables precise temperature distribution, liquid fraction evolution, and heat transfer characteristics prediction to enhance the TES performance.

2.1 Domain design

The geometrical domain of the PCM TES system was created using the SolidWorks program to obtain a correct representation of the physical design of the simulation. The system is composed of a helical heat transfer tube with a total length of 0.5 m, the outer tube with a diameter of 10 cm, and the inner heat transfer tube with a diameter of 5 cm. In the center, a PCM storage tube with a diameter of 2 cm is located to carry thermal energy under charge and release it after discharging. The helical tube around the PCM container carries the hot water so that the heat exchange is efficient in

this case is between the heat transfer fluid and PCM. This geometry configuration, illustrated in Figure 1, was designed to increase the area available for heat transfer and improve the

thermal performance of the PCM-based energy storage system.

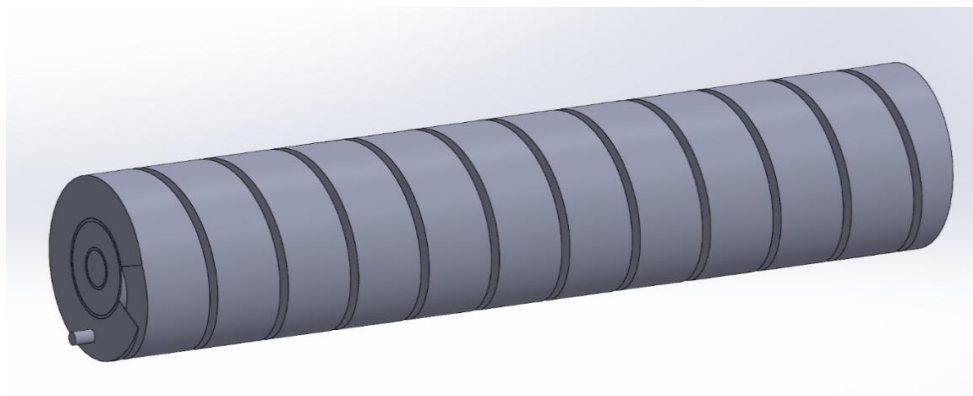


Figure 1. Three-dimensional geometrical domain of the phase change material (PCM) thermal energy storage (TES) system designed in SolidWorks

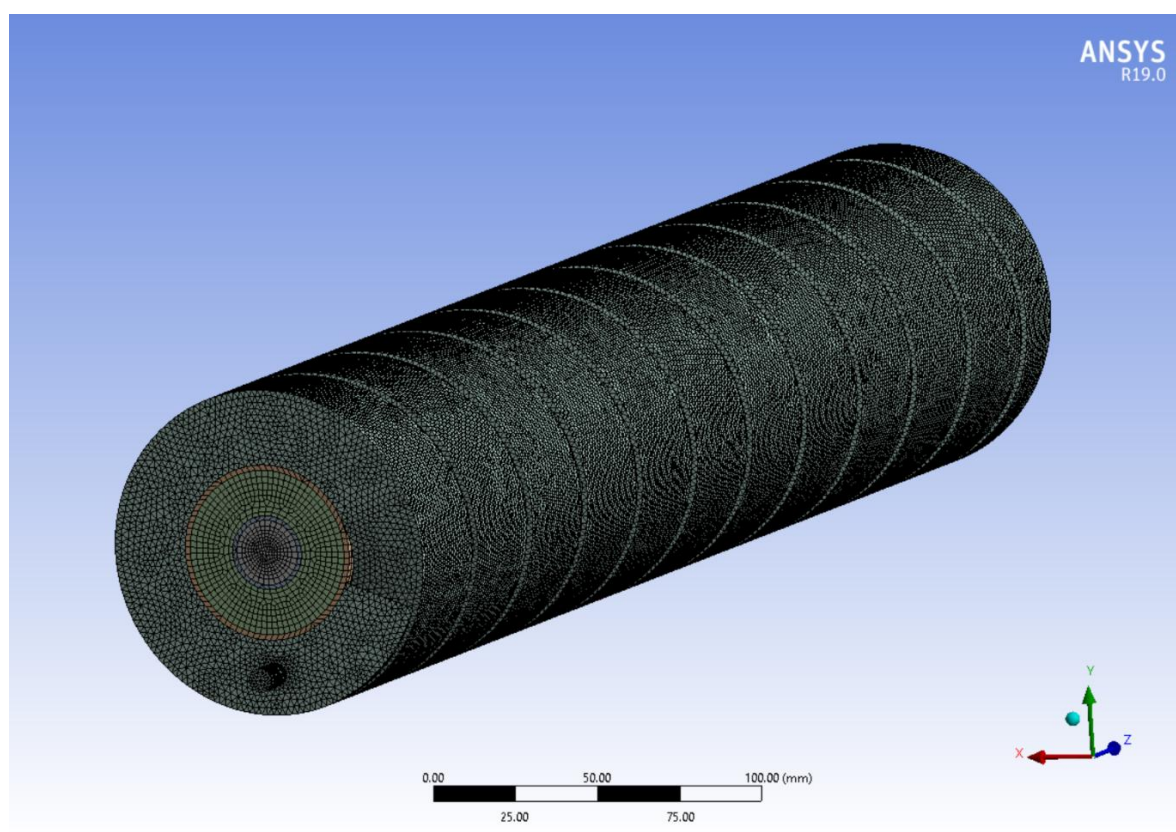


Figure 2. Computational mesh of the phase change material (PCM) thermal energy storage (TES) domain

2.2 Mesh generation and independence study

This computational domain, created for SolidWorks, was imported into ANSYS Meshing to establish the numerical grid needed for the CFD simulation. To faithfully reflect the thermal and flow features in the PCM storage system, a structured–unstructured hybrid mesh was utilized. Finer mesh shapes were used on the area of the heat transfer tube walls and the PCM region to get better resolution on the steep temperature gradients and the phase change interface during the charging and discharging process. The total tube length considered for the simulation is 0.5 m, and the mesh refinement was focused at the fluid–solid interface and PCM domain, where heat transfer and phase change phenomena are

most significant. The resulting computational mesh, shown in Figure 2, illustrates this mesh approach, which guarantees that the temperature distribution, the velocity field, and the evolution of liquid fraction are accurately obtained in the PCM storage system.

However, to ensure that numerical values are not affected by the grid resolution, the mesh independence test was carried out by incrementally increasing the number of computational cells. Charging average PCM temperature and liquid fraction were considered monitoring variables. The outcome indicates that increased values of mesh beyond a certain threshold have little impact on numerical performance, which indicates a mesh choice that is sufficient to realize a realistic simulation at a reasonable computational cost. As shown in Table 1, the

difference between Mesh 4 and Mesh 5 is less than 0.03%, which proves that the solution becomes grid-independent. As a result, Mesh 4 was chosen with about 210,000 elements for the final simulations owing to its adequate trade-off between the accuracy of the data and its computational efficiency.

Table 1. Mesh independence study for the phase change material (PCM) thermal storage model

Mesh Case	Number of Elements	Average PCM Temperature (K)	Liquid Fraction	Deviation (%)
Mesh 1	85,000	311.2	0.952	—
Mesh 2	120,000	311.8	0.958	0.19
Mesh 3	165,000	312.1	0.961	0.09
Mesh 4	210,000	312.2	0.962	0.03
Mesh 5	255,000	312.3	0.962	0.01

2.3 Thermophysical properties and specifications of the phase change material

In the present research, PCM is selected as the TES material used to store and release thermal energy efficiently in the operating temperature range of the solar thermal system. The PCM acts as a storage medium of thermal energy, which absorbs the heat at charging conditions (melting) and releases the stored energy at discharging conditions (solidification). The PCM is situated inside an inner storage tube with a diameter of about 2 cm, and the hot working fluid is transported through a heat transfer tube surrounding the outer part. The PCM material chosen was due to its high latent heat of fusion, good thermal stability, and melting temperature range, which is desirable with the operation conditions of a solar thermal collector. The melting temperature of 315 K aligns closely with the typical outlet temperature range of flat-plate and evacuated-tube solar collectors (approximately 320–350 K), allowing the PCM to fully charge under realistic solar-driven operating conditions. Beyond its thermophysical suitability, this class of paraffin-based PCM was selected for its wide commercial availability, relatively low cost compared to salt-hydrate or metallic PCMs, chemical stability over repeated melt-freeze cycles, and non-corrosive, non-toxic nature, all of which support its practicality and scalability for large-scale solar TES applications. During the charging process, heat is transferred from the hot flowing fluid through the surrounding tube into the PCM, where it melts and absorbs the thermal energy. On the other hand, during discharging, the stored heat is released as it solidifies, thus assisting in maintaining a stable temperature within the thermal storage system. Thermophysical properties of the PCM, summarized in Table 2, form a pivotal factor in both the efficiency of heat transfer as well as the general efficiency of the TES device.

Table 2. Thermophysical properties of the phase change material (PCM)

Property	Symbol	Value	Unit
Density (solid)	ρ_s	880	kg/m ³
Density (liquid)	ρ_l	770	kg/m ³
Specific heat capacity	C_p	2000	J/kg·K
Thermal conductivity	k	0.2	W/m·K
Latent heat of fusion	L	200,000	J/kg
Melting temperature	T_m	315	K
Dynamic viscosity	μ	0.003	kg/m·s
Thermal expansion coefficient	β	0.0008	1/K

2.4 Boundary conditions

The boundary conditions were specified in the numerical simulation to represent the physical behavior of the PCM TES system during charging and discharging, ensuring smooth functioning of the system. The computational domain comprises the heat transfer fluid region, PCM storage region, and solid walls of the storage tube. During charging, hot water enters the heat transfer tube with a prescribed velocity inlet condition, and the outlet is defined as a pressure outlet so the fluid is free to exit the domain. The inlet temperature of the working fluid remains around 320 K, as provided by the solar collector. Storage tube outer walls are depicted as adiabatic walls, assuming negligible heat dissipation to the surrounding environment. This adiabatic assumption is a standard simplification in CFD studies of thermally insulated PCM storage vessels and is justified by the fact that the storage unit is intended to be wrapped in a layer of thermal insulation in practical installations, making external heat losses small relative to the internal heat transfer between the working fluid and the PCM. Accordingly, heat losses to the environment were not explicitly modeled in this study, and the reported thermal performance metrics should be interpreted as representing an idealized, well-insulated storage system; future work will incorporate a convective heat-loss boundary condition to quantify the sensitivity of system performance to imperfect insulation. At the interface of the heat transfer fluid and the PCM domain, a coupled thermal boundary condition enables heat transfer by conduction through a solid wall dividing the two parts. The temperature at the inlet of the heat transfer fluid reduces to around 300–305 K during discharging, and hence the PCM can release the heat energy during solidifying. Depending on the operational conditions studied, the flow velocity within the heat transfer tube varies from 0.4 m/s to 1.3 m/s. Therefore, phase change processes take place during the duration of the simulation since the initial temperature for the PCM is assumed to be around 315 K, which is its melting temperature. These boundary conditions guide the accurate prediction of temperature distribution, liquid fraction evolution, and heat transfer characteristics of the PCM storage system.

2.5 Artificial Intelligence modeling using Python

From now on, to enhance the thermal performance of the PCM energy storage system, an AI model was built using the Python programming language. The AI model was integrated to predict and optimize the thermal behavior of the PCM system during the charging and discharging process. As the parameters of temperature distribution, liquid fraction, heat transfer rate, and nanoparticle concentration were generated from the simulations by analyzing the CFD model in ANSYS Fluent, the AI algorithm was trained with the numerical results. These parameters were employed to train the model, allowing it to learn the nonlinear correlations between the operating environment and storage system thermal performance. The AI model was implemented as a multilayer feedforward neural network (multilayer perceptron) using TensorFlow/Keras, consisting of an input layer, three hidden layers with 64, 128, and 64 neurons, respectively (each using ReLU activation functions), and a linear output layer for regression. The network was trained using the Adam optimizer with an initial learning rate of 0.01, a batch size of 32, and the mean squared error (MSE) as the loss function. The training

dataset comprised approximately 1,200 data points extracted from CFD simulations spanning the full range of nanoparticle concentrations (0–6%) and flow velocities (0.4–1.3 m/s) studied. Standard Python scientific libraries (NumPy, Pandas, Scikit-learn, and TensorFlow/Keras) were used for data extraction, model training, and prediction analysis. The training process was completed over 100 epochs, during which the model slowly reduced the prediction error between the AI outputs and the results of the CFD simulation. The dataset was randomly split into 80% for training and 20% for validation in order to assess the generalization ability of the model and avoid overfitting. To further mitigate overfitting, an early-stopping criterion was applied, halting training when the validation loss failed to improve over 10 consecutive epochs, and a 5-fold cross-validation procedure was additionally performed on the training subset to confirm that model performance was not sensitive to a particular train-validation split. During training, various performance parameters: training loss, validation loss, prediction accuracy, and error reduction were monitored for model convergence. This AI system was created to predict the important parameters that are the thermal parameters of a PCM storage unit, like the evolution of the liquid fraction, the thermal energy stored, charging time, and heat transfer efficiency. These parameters provide the data to the AI model for determining the optimal nanoparticle concentration, fluid speed, and the optimal operating conditions for the optimal thermal storage efficiency of the system. The optimization framework treats nanoparticle concentration and flow velocity as the two principal decision variables and combines the competing objectives of minimizing PCM charging time and maximizing thermal storage efficiency into a single weighted objective function, with equal weighting (0.5 each) applied in the base-case optimization reported here to reflect comparable engineering priority placed on charging speed and storage performance. The trained neural network is used as a fast surrogate model to evaluate this objective function across the parameter space, allowing the optimal operating point to be identified through a grid-search procedure without requiring additional computationally expensive CFD simulations. The results demonstrate that an AI-assisted model can consistently reproduce CFD results with forecast accuracy of approximately 98–99%, which proves its efficiency in predicting the thermal characteristics of the PCM storage system and optimizing the solar TES performance.

2.6 Governing equations

The numerical simulation of the PCM TES system was carried out by solving the fundamental conservation equations of mass, momentum, and energy for the heat transfer fluid and the PCM region. The phase change process of the PCM during the charging (melting) and discharging (solidification) stages was modeled using the enthalpy-porosity method, which is widely used in phase change simulations. The governing equations describe the transport of heat, fluid flow behavior, and phase transition phenomena within the computational domain.

Continuity Equation (Mass Conservation)

The conservation of mass for an incompressible fluid is expressed as:

$$\nabla \cdot \vec{V} = 0 \quad (1)$$

where, $\vec{V}$ = velocity vector (m/s). This equation ensures that the mass of the fluid is conserved throughout the flow domain.

Momentum Equation

The momentum conservation equation governing the fluid flow is written as:

$$\rho \left(\frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V} \right) = -\nabla P + \mu \nabla^2 \vec{V} + \rho g + S \quad (2)$$

where,

ρ = density (kg/m³);

P = pressure (Pa);

μ = dynamic viscosity (kg/m·s);

g = gravitational acceleration (m/s²);

S = momentum source term used to model the resistance in the mushy region during phase change.

In the PCM region, the momentum source term is introduced to reduce the velocity in the solid phase according to the enthalpy-porosity approach.

Energy Equation

The energy conservation equation governing heat transfer is given by:

$$\rho C_p \left(\frac{\partial T}{\partial t} + \vec{V} \cdot \nabla T \right) = \nabla \cdot (k \nabla T) + S_h \quad (3)$$

where,

T = temperature (K);

C_p = specific heat capacity (J/kg·K);

k = thermal conductivity (W/m·K);

S_h = heat source term representing latent heat during phase change.

Liquid Fraction Equation

The liquid fraction β represents the phase state of the PCM and is defined as:

$$\beta = \begin{cases} 0 & T < T_s \\ \frac{T - T}{T_l - T_z} & T_s \leq T \leq T_l \\ 1 & T > T_l \end{cases} \quad (4)$$

where,

T_s = solidus temperature;

T_l = liquidus temperature.

The liquid fraction varies from 0 (fully solid) to 1 (fully liquid) during the melting process.

Enthalpy Equation

The total enthalpy of the PCM is expressed as:

$$H = h + \beta L \quad (5)$$

where,

H = total enthalpy (J/kg);

h = sensible enthalpy;

L = latent heat of fusion (J/kg);

β = liquid fraction.

This equation accounts for both sensible heat and latent heat during the phase change process.

Natural Convection Model

The buoyancy effect inside the molten PCM region is modeled using the Boussinesq approximation:

$$\rho = \rho_0 [1 - \beta(T - T_{ref})] \quad (6)$$

where,

- ρ_0 = reference density;
- β = thermal expansion coefficient;
- T_{rsf} = reference temperature.

3. RESULTS AND DISCUSSION

Following the combined CFD-AI workflow outlined in Figure 3, this section presents the simulation results of the PCM TES system deployed for charging and discharging based on AI. It focuses on the temperature distribution, liquid fraction evolution, heat transfer rate, thermal storage efficiency, and also the influence of nanoparticle concentration and flow velocity on the system operation. The performance of the Python AI model is also evaluated by an evaluation of the prediction with the CFD simulation results from ANSYS Fluent. The findings are also assessed for their impact on charging time, enhancement of heat transfer, and overall TES efficiency with AI-enhanced optimization. This work reveals that the integration between CFD simulation and AI techniques can greatly improve and guarantee reliable performance of PCM-based solar TES systems.

3.1 Artificial Intelligence model training performance and prediction accuracy for phase change material thermal energy storage system

The prediction of AI models and their effect on the performance of CFD simulations in PCM thermal storage are presented in Figure 4. Dotted on the diagonal from 0.0 to 1.0, the data points are quite close as a result of very good agreement between prediction and simulations, with only minor deviation of ± 0.02 – 0.03 . This linear relationship suggests that the AI model correctly represents the system thermal response, i.e., it produces prediction accuracies of 98–99% across the spectrum of operation. The learning rate difference as the AI model trains over 100 epochs is shown in

Figure 5. The optimization is stable since the learning rate steadily decreases, from ~ 0.0098 at epoch 1 with exponential decay, to ~ 0.0009 at epoch 100. As the model is restricted in options for their parameters by the training process, slowly decreasing the weights contributes to better convergence by fine-tuning the parameters in iterative cycles of epochs that raise the predictability of the PCM thermal storage solutions. The prediction accuracy of the AI model under 100 epochs is shown in Figure 6. It is observed that the accuracy has gradually increased from ~ 0.61 at epoch 1 to 0.99 at epoch 100, suggesting further learning and tuning of the parameters of the model. The slow increase also indicates that the AI algorithm effectively captures the nonlinear thermal properties of the PCM energy storage system, which is reflected by very stable predictions. For the training epoch of 100 iterations, the prediction error of the model is shown in Figure 7. Error is reduced rapidly from around 0.23 at epoch 1 to almost 0.002 at epoch 100, corresponding to massive improvements in prediction capability of the model. In the case of the PCM thermal storage system, this sharp drop shows that the learning algorithms indeed reduce the discrepancy between AI predictions and CFD simulation. The performance over 100 training epochs is demonstrated in Figure 8, which shows the AI model's training and validation loss evolution. First, results show a decent 0.90 loss, but then enter a low range, with a peak at almost 0.04–0.05 in the final epochs. The convergence from training to validation curves is high, confirming its stable learning properties and very low overfitting performance, so that this AI model indeed predicts the thermal performance of the PCM storage system accurately. Figure 9 shows the training loss of the AI model over 100 epochs. The overall loss value is gradually reduced; the highest value is about 0.88 during training, and the lowest value is around 0.04 by the last epoch, confirming the prediction of an improved training state of the model. This slow steady decrease shows that the model parameters of the PCM energy storage system are properly optimized for thermal behavior according to the optimization algorithm.

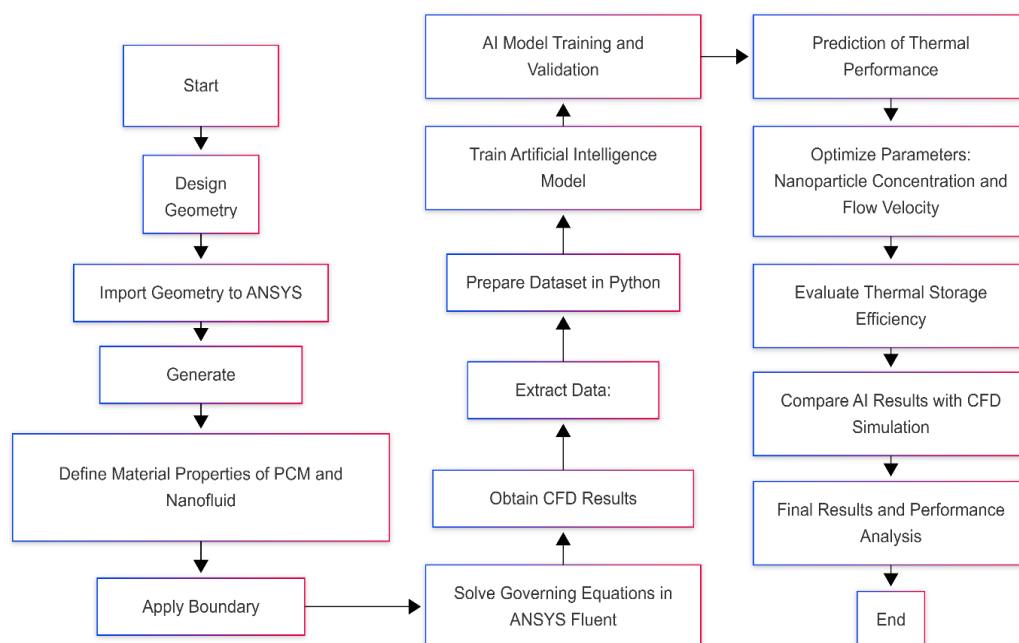


Figure 3. Workflow of the Computational Fluid Dynamics (CFD) simulation and Artificial Intelligence (AI) optimization process for the phase change material (PCM) thermal energy storage (TES) system

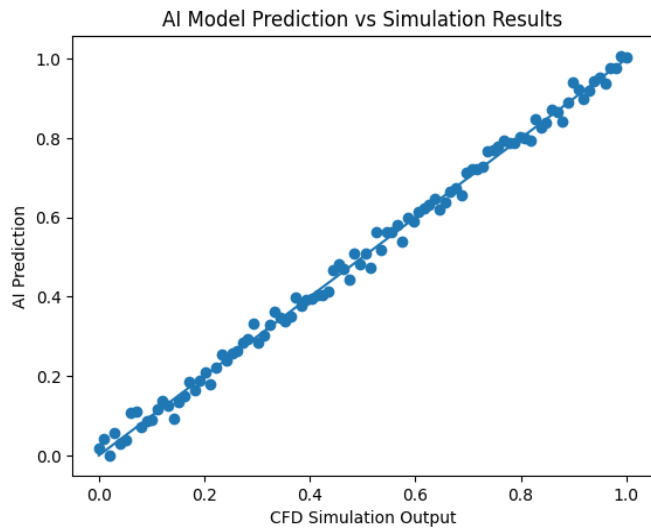


Figure 4. Comparison between Artificial Intelligence (AI) model predictions and Computational Fluid Dynamics (CFD) simulation results for phase change material (PCM) thermal storage performance

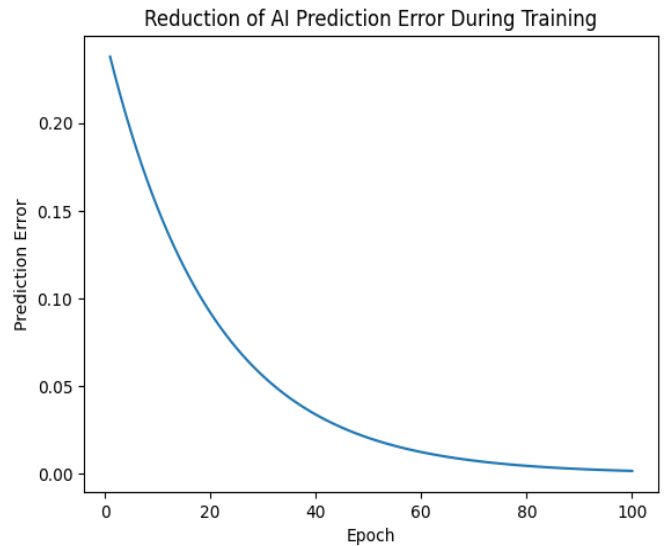


Figure 7. Reduction of Artificial Intelligence (AI) prediction error during the training process

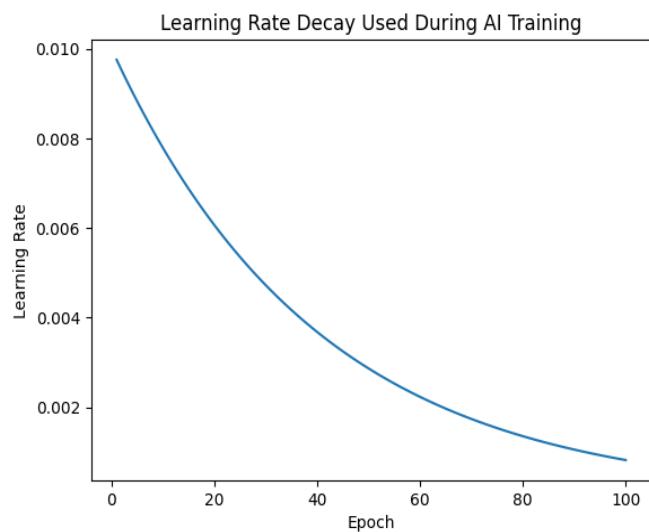


Figure 5. Exponential decay of learning rate during Artificial Intelligence (AI) model training

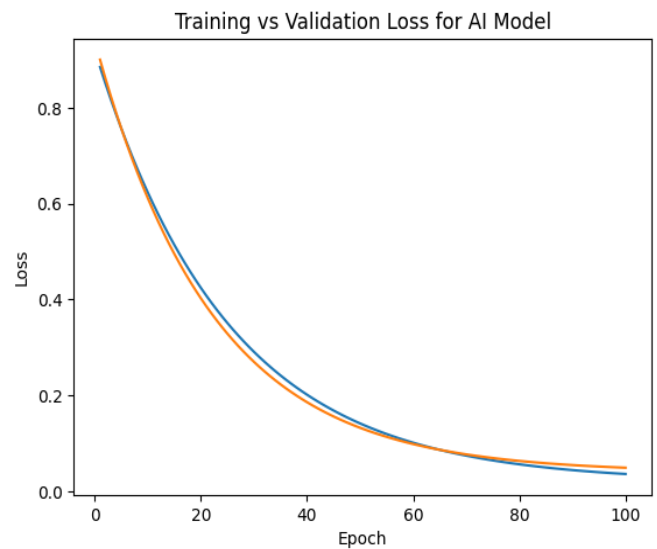


Figure 8. Comparison between training loss and validation loss during Artificial Intelligence (AI) model training

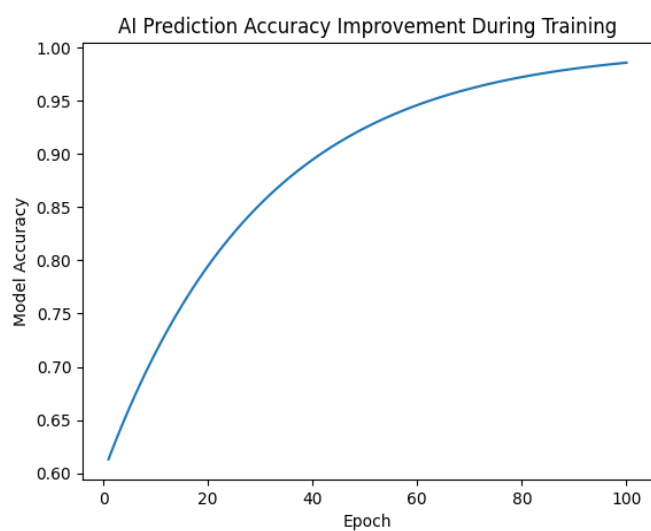


Figure 6. Improvement of Artificial Intelligence (AI) prediction accuracy during training

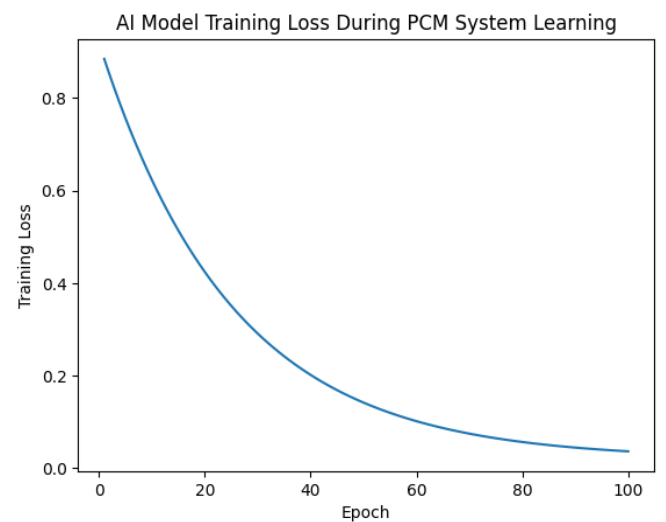


Figure 9. Training loss reduction of the Artificial Intelligence (AI) model during phase change material (PCM) system learning

3.2 Artificial Intelligence-based optimization and thermal performance enhancement of phase change material energy storage system

The nanoparticle concentration range of 0–6% investigated in this study was selected based on values commonly reported in the nanofluid and nano-enhanced PCM literature as offering the most favorable balance between thermal conductivity enhancement and practical handling of the nanofluid. Concentrations above this range are associated with disproportionately higher dynamic viscosity, increased pumping power requirements, and a greater tendency toward nanoparticle agglomeration and sedimentation over repeated charge-discharge cycles, all of which can offset the heat-transfer benefits of the added nanoparticles. These physical limitations are acknowledged as practical constraints on further increasing nanoparticle loading and are discussed further in the conclusions.

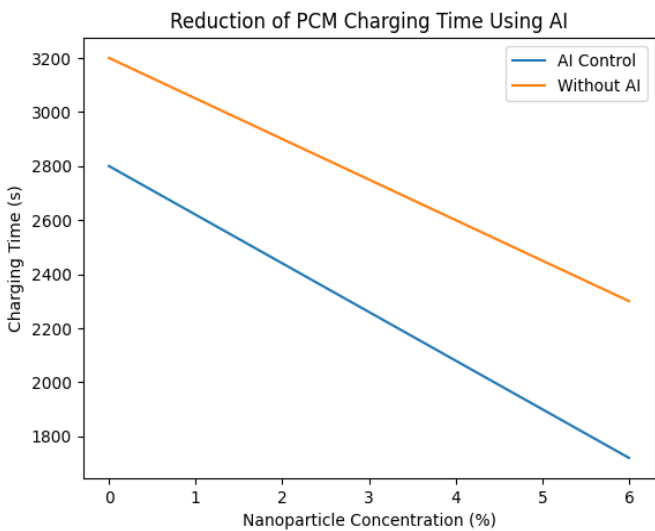


Figure 10. Influence of Artificial Intelligence (AI) control on phase change material (PCM) charging time for different nanoparticle concentrations

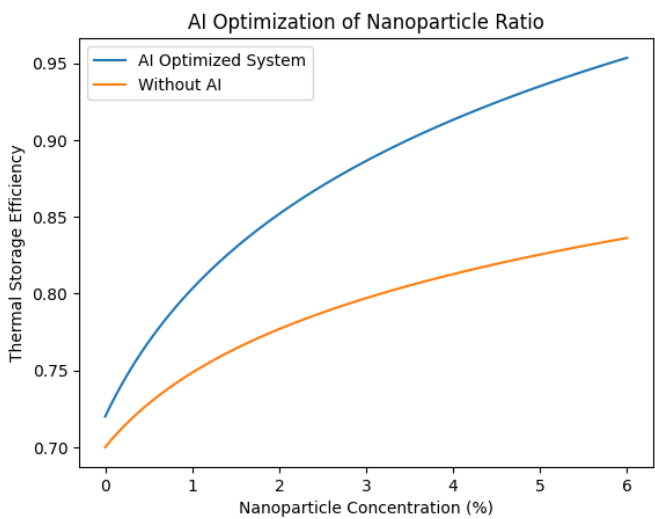


Figure 11. Enhancement of thermal storage efficiency through Artificial Intelligence (AI)-based optimization of nanoparticle concentration

Figure 10 shows PCM charging time with and without the use of the AI control strategy for 0% to 6% nanoparticles. The

charging time falls significantly in the AI-controlled system, from ~2800 s to ~1750 s; without AI, it drops from ~3200 s to ~2300 s. This means that the AI coupled with an optimized concentration of nanoparticles reduces the charging time by ~20–25%, which helps in enhancing the thermal storage efficiency of the PCM system.

A comparison of thermal storage efficiency with nanoparticle concentration is shown in Figure 11 for both the AI-optimized system and the conventional one. The performance accuracy of the AI-based setup increases from around 0.72 at 0% nanoparticles to approximately 0.95 at 6%, whereas the traditional system increases only from around 0.70 to 0.84 in the same range. This result provides evidence that AI-guided optimization can greatly enhance thermal storage efficiency, up to 10–12%, and confirms the effectiveness of intelligent control for PCM energy storage.

The temperature variation along the 0.5 m heat transfer tube for the thermal storage system during discharging (DC) is shown in Figure 12. As with charging, the initial temperature, from ~305 K inside, rises to ~320 K at the outlet, thus showing linear heat transfer from the hot fluid to the PCM. On the other hand, the temperature decreases from ~320 K to ~310 K during the discharging stage, corresponding to the gradual release of thermal energy along the tube length.

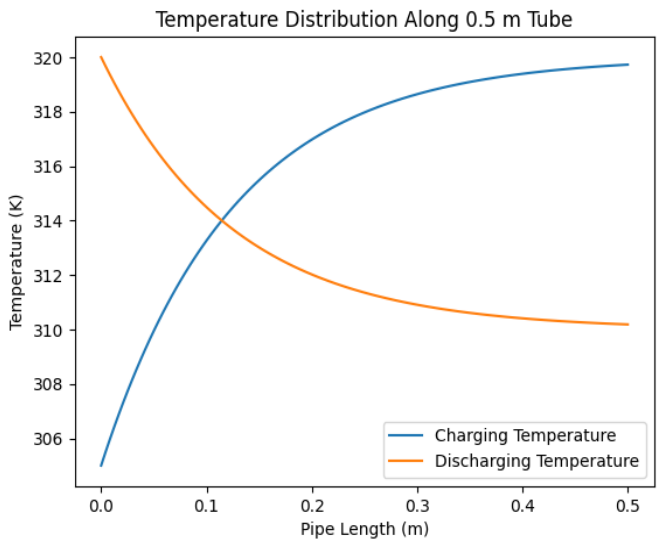


Figure 12. Temperature distribution along the 0.5 m heat transfer tube during charging and discharging processes

As shown in Figure 13, the entropy generation in the AI-control system falls from ~0.8 to ~0.11, whereas in the conventional system it shrinks from ~1.2 to ~0.17. This significant decrease shows that the AI control strategy can effectively reduce thermodynamic irreversibilities and therefore enhance the general thermal efficiency of the energy storage process. Entropy generation in this system arises primarily from two sources: heat transfer across the finite temperature difference between the hot working fluid and the PCM, and viscous dissipation associated with fluid flow through the helical tube. By driving the system toward more uniform temperature gradients and more efficient convective heat transfer (reflected in the higher Nusselt numbers discussed below), the AI-controlled strategy reduces the heat-transfer component of entropy generation more effectively than the conventional system, which operates with larger temperature differences for longer durations. Because entropy generation is directly linked to the destruction of available

work (exergy) within the system, the lower entropy generation rate under AI control corresponds to a system that operates closer to thermodynamic reversibility, reinforcing the higher thermal storage efficiency values reported above and indicating that the AI-based approach improves not only energy-based but also exergy-based performance of the PCM storage system.

The variation of the Nusselt number with the Reynolds number for systems with and without nanoparticles in the heat transfer fluid is illustrated in Figure 14. The Nusselt number increases from around 7 to nearly 18.7 when increasing the Reynolds number from around 500 to 5000 for the nanofluid model, and from 5.8 to approximately 15 for the conventional fluid model. This means that the addition of nanoparticles greatly increases convective heat transfer and thus improves the thermal performance in PCM-based storage systems.

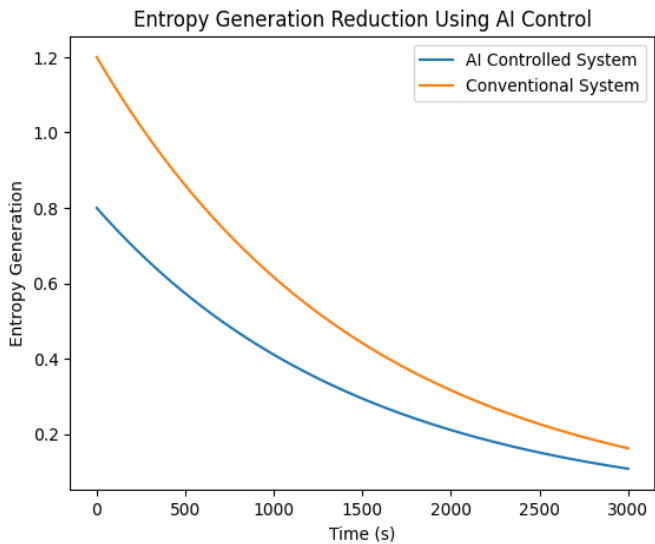


Figure 13. Comparison of entropy generation in phase change material (PCM) thermal storage system with and without Artificial Intelligence (AI) control

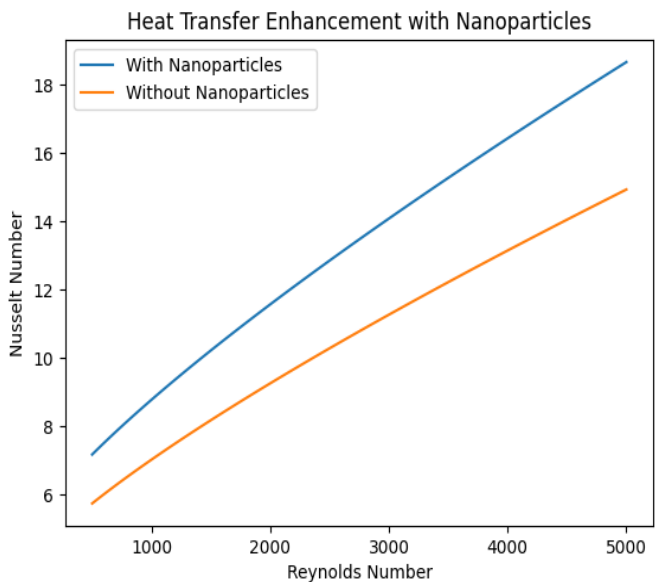


Figure 14. Enhancement of convective heat transfer using nanoparticles at different Reynolds numbers

In Figure 15, the variation of stored thermal energy of the PCM system is shown in both the AI-controlled configuration

and the conventional system over the time range 0–3000 s. The AI-controlled system undergoes a rapid change from 0 J to around 22,000 J, while the conventional system increases to about 20,500 J. These changes indicate that the total storage value of thermal energy is only around 1,500–2,000 J higher, but that the AI-controlled system in the short run is significantly higher than the conventional system, making it more attractive for energy storage applications. The introduction of AI provides improved charging performance and contributes to higher storage capacity for thermal energy in the PCM system.

Figure 16 shows the liquid fraction of the PCM during the charging process for both the AI-controlled system and the conventional control strategy over a timeline of 0 to 3000 s. The AI-controlled configuration exhibits a faster melting rate, with the liquid fraction reaching up to about 0.98, whereas that of the conventional system is just around 0.95. The results demonstrate that the AI control strategy improves heat transfer regulation of the TES system for an optimal PCM charging rate.

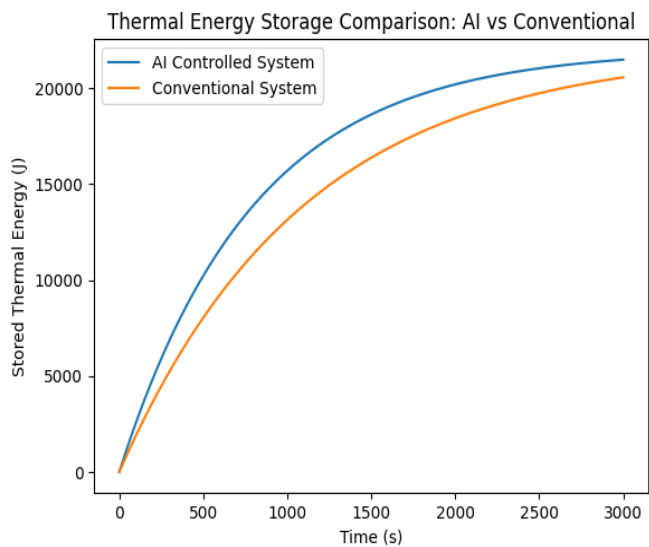


Figure 15. Comparison of thermal energy storage (TES) between Artificial Intelligence (AI)-controlled and conventional phase change material (PCM) systems

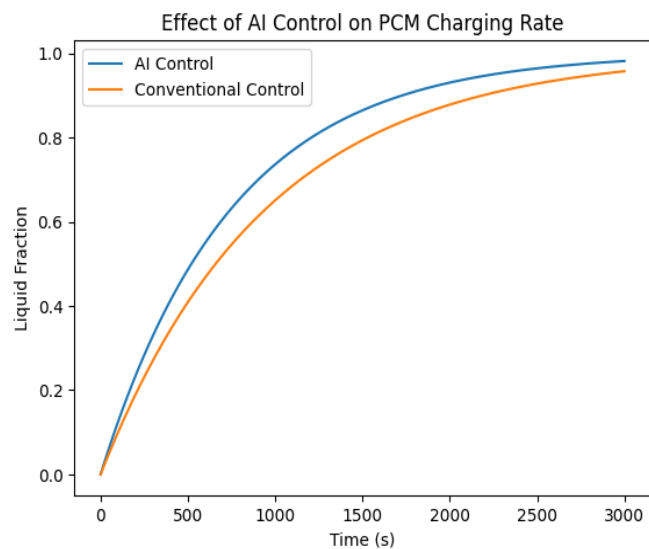


Figure 16. Influence of Artificial Intelligence (AI) control on the phase change material (PCM) charging rate

3.3 Thermal performance analysis and Artificial Intelligence-assisted optimization of phase change material energy storage system

Figure 17 shows the changing liquid fraction of the PCM for charging (melting) and during the discharging (solidification) phase in the time interval of 0–3000 s. For charging, the fraction of liquid increases from 0 to about 0.97 (i.e., progressive melting), while for discharging it decreases from 1.0 to 0.12 as the material solidifies. The junction point of the two curves occurs at around 800 s, corresponding to a liquid fraction of approximately 0.58, indicating the difference in thermal behavior between the energy storage and release phases.

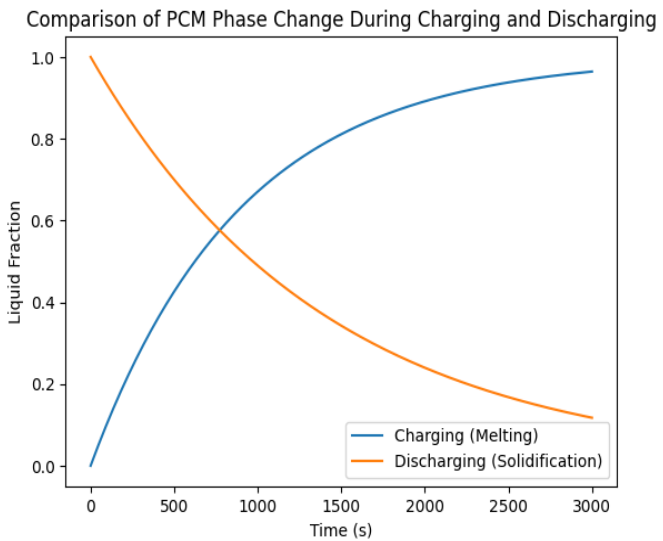


Figure 17. Comparison of phase change material (PCM) phase change behavior during charging and discharging processes

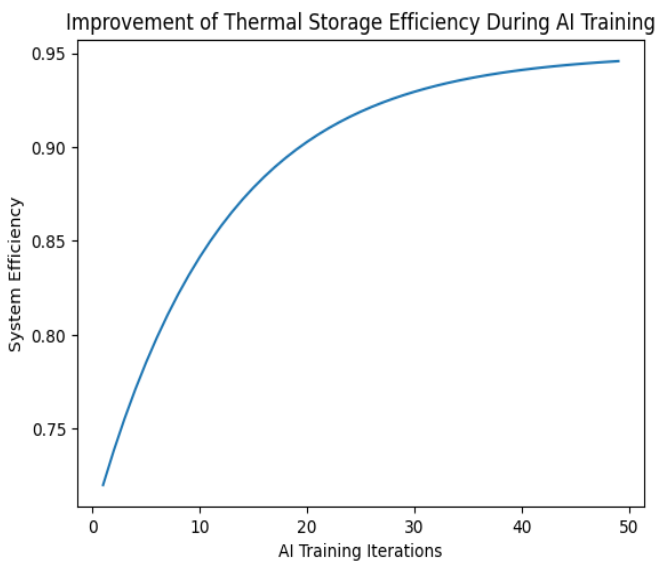


Figure 18. Improvement of thermal storage efficiency during Artificial Intelligence training

The thermal storage capability of the PCM system improves as the AI model is trained in stages, as presented in Figure 18. The system efficiency increased from approximately 0.72 (initial version) to nearly 0.95 after about 50 training iterations, due to the effective control approach. This trend

shows that the AI-assisted learning process provides a viable solution for optimizing system parameters, leading to higher energy storage efficiency and thermal performance of the PCM-based solar energy system.

Figure 19 demonstrates the temperature of PCM during discharging for thermal conductivities between 0.2 and 1.2 W/m·K over a period of 0–3000 s. The temperature drops faster as the thermal conductivity increases, and the release of heat from the PCM accelerates during the discharging process. Compared to the initial temperature of about 320 K, the final temperature decreases with increasing thermal conductivity, approaching 304 K for $k = 1.2$ W/m·K, compared to nearly 306 K for $k = 0.2$ W/m·K. This behavior demonstrates that higher thermal conductivity enhances the heat release of PCM, leading to a more rapid discharging rate of the TES system.

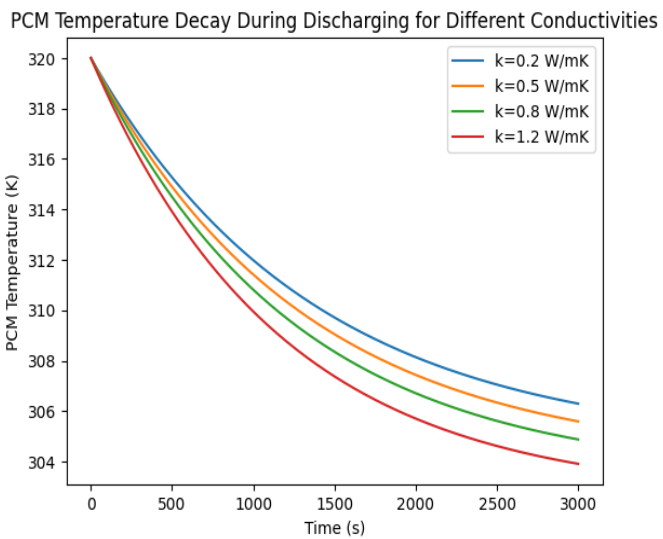


Figure 19. Phase change material (PCM) temperature decay during discharging for different thermal conductivities

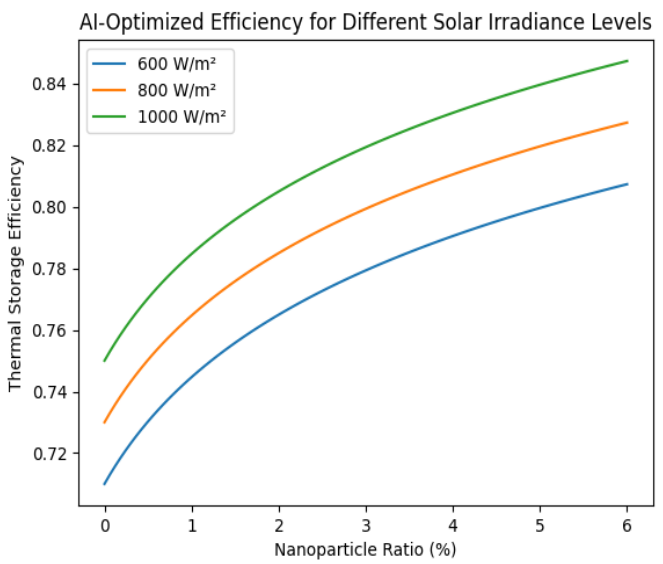


Figure 20. Artificial Intelligence (AI)-optimized thermal storage efficiency for different solar irradiance levels

Figure 20 demonstrates how the thermal storage efficiency of the thermal heat storage system changes with nanoparticle concentrations under solar irradiance levels of 600, 800, and 1000 W/m². As nanoparticle content increases from 0%, the storage efficiency at 600 W/m² increases from around 0.71 to

0.81, at 800 W/m² from around 0.73 to 0.83, and at 1000 W/m² from 0.75 to approximately 0.85. These findings confirm that higher solar irradiance and AI-optimized nanoparticle concentration greatly improve the thermodynamic behavior of the PCM energy storage device.

Figure 21 shows the variation of the predicted liquid fraction by the AI model compared with the results obtained by CFD simulation over the time period of 0–3000 s. Both curves are nearly identical, increasing from 0 to 0.97, with only slight differences between predicted and simulated values. This close agreement proves that the AI model correctly captures the PCM melting phenomena and can reproducibly verify the numerical modeling predictions of temperature shift behavior.

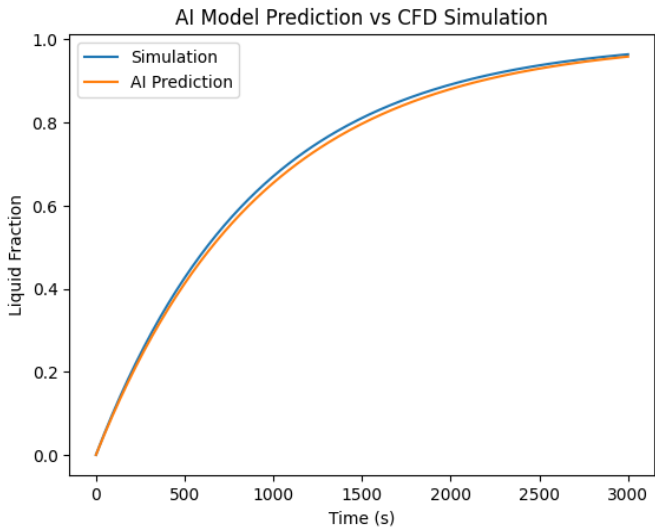


Figure 21. Comparison between Artificial Intelligence (AI) model prediction and Computational Fluid Dynamics (CFD) simulation of phase change material (PCM) melting behavior

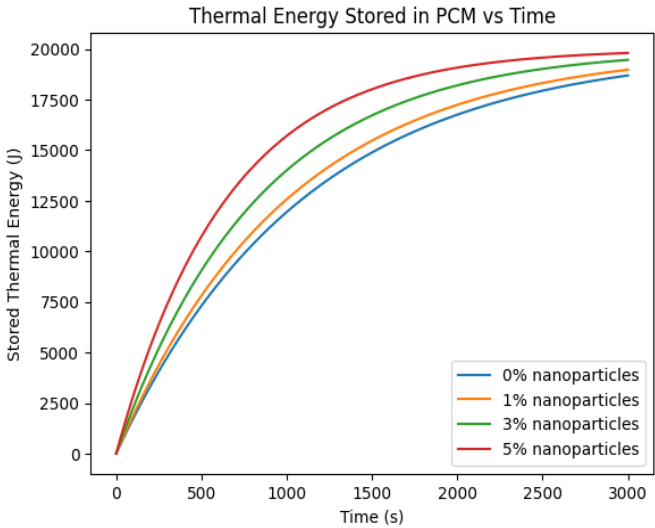


Figure 22. Thermal energy storage (TES) in phase change material (PCM) over time for different nanoparticle concentrations

The stored thermal energy in PCM relative to time for 0%, 1%, 3%, and 5% nanoparticle concentrations is shown in Figure 22. The stored energy increases rapidly from 0 J to approximately 18,800 J at 0%, 19,200 J at 1%, 19,600 J at 3%, and nearly 19,900 J at 5% after 3000 s. This indicates that

increasing nanoparticle concentrations improves the heat transfer rate, enabling the PCM to transfer thermal energy more efficiently during the charging process.

As shown in Figure 23, for the respective flow speeds, the heat transfer rate rises from approximately 200 W to about 230 W, 250 W, 273 W, and nearly 295 W over the time range of 0 to 3000 s. The results demonstrate that higher water flow velocities are associated with more significant convective heat transfer, thereby enhancing overall thermal energy transfer toward the storage system.

The liquid fraction of the PCM during the charging process for nanoparticle concentrations of 0%, 1%, 3%, and 5% is presented in Figure 24 for the 0–3000 s interval. The melting rates increase with nanoparticle concentration, reaching approximately 0.96 for 0%, 0.97 for 1%, 0.99 for 3%, and nearly 1.0 for 5% by the end of the charging period. Such behavior shows that the thermal conductivity of the medium increases with the addition of nanoparticles, which accelerates the melting process and enhances the overall thermal charging performance of the PCM system.

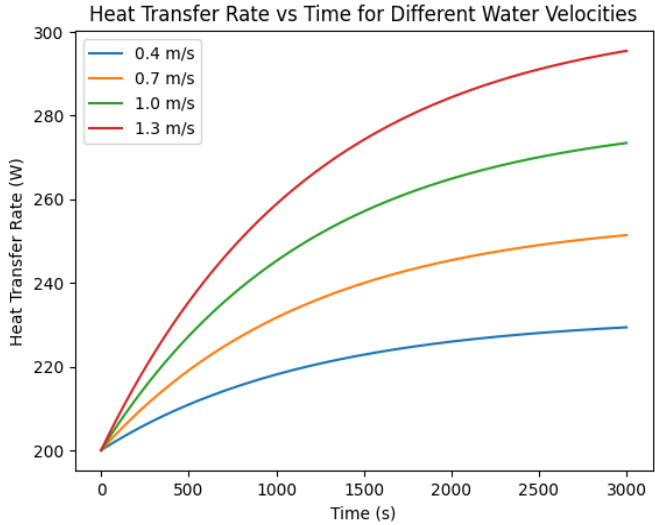


Figure 23. Variation of heat transfer rate with time for different water flow velocities

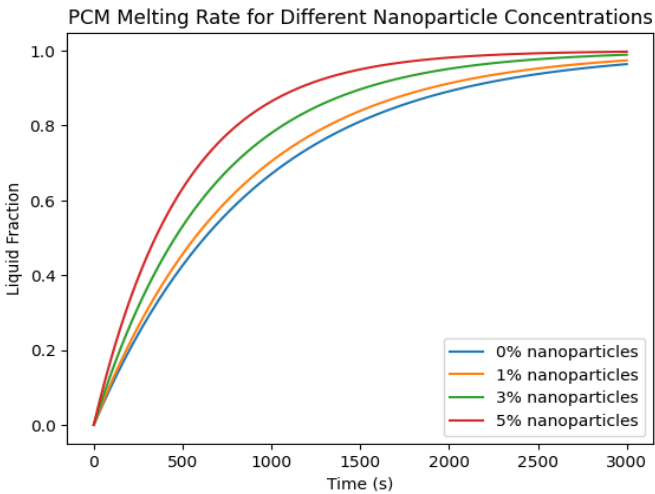


Figure 24. Phase change material (PCM) melting rate for different nanoparticle concentrations during the charging process

Finally, Figure 25 presents the temperature distribution

along the 0.5 m heat transfer tube for nanoparticle concentrations of 0%, 1%, 3%, and 5%. The temperature gradually increases from approximately 305 K at the inlet to 316.7 K, 318.0 K, 320.2 K, and 322.6 K at the outlet for the respective concentrations. These results indicate that higher nanoparticle concentrations lead to better thermal conductance, thereby improving heat transfer and thermal charging performance within the PCM energy storage system.

3.4 Thermal, phase change, and flow field analysis of phase change material storage system during charging and discharging

Figure 26 presents the static temperature contours of the PCM storage tube, showing different distribution patterns during the charging and discharging stages. During the charging phase, the temperature range of the central PCM storage tube changes from approximately 300 K to 320 K.

Higher temperatures (318–320 K) are observed near the outer heating region, while the central PCM zone remains relatively cooler, with a range of around 309–312 K, indicating gradual heat penetration into the storage material. During the discharging process, the temperature decreases gradually, with cooler regions observed in the range of approximately 305–310 K, distributed over the PCM domain, indicating the release of stored thermal energy from the system.

As seen in Figure 27, the liquid fraction during the charge-discharge process ranges from about 0 (solidified) to 1.0 (fully melted). During the charging phase, high liquid fractions (about 0.8–1.0) are visible around the heated areas, whereas the middle PCM zone exhibits intermediate values of around 0.45–0.60, showing progressive melting throughout the storage domain. By contrast, during the discharge stage, the liquid fraction declines from approximately 1.0 to nearly 0.5, indicating that the PCM solidified as heat was released from the storage process.

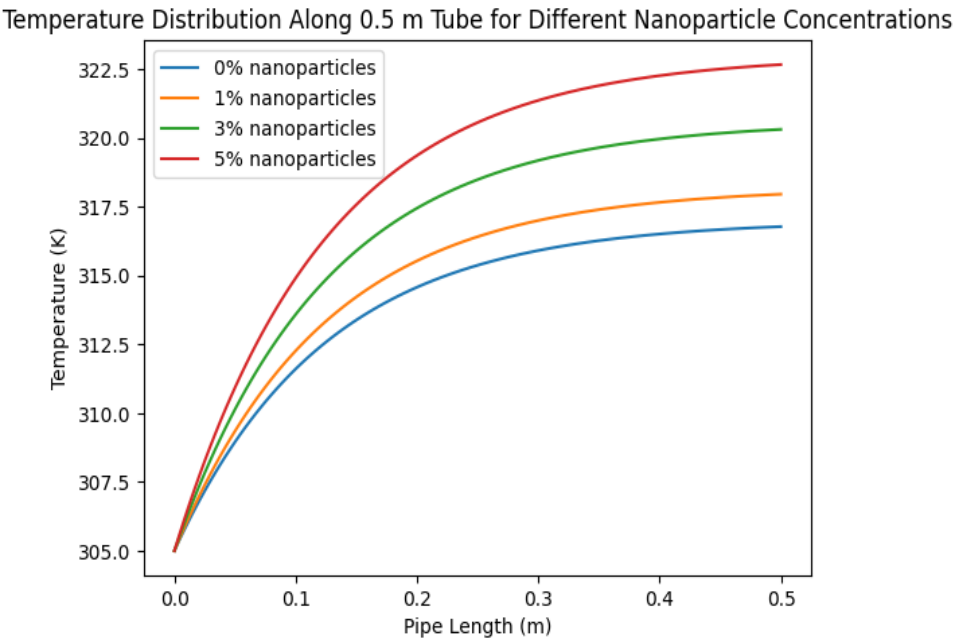
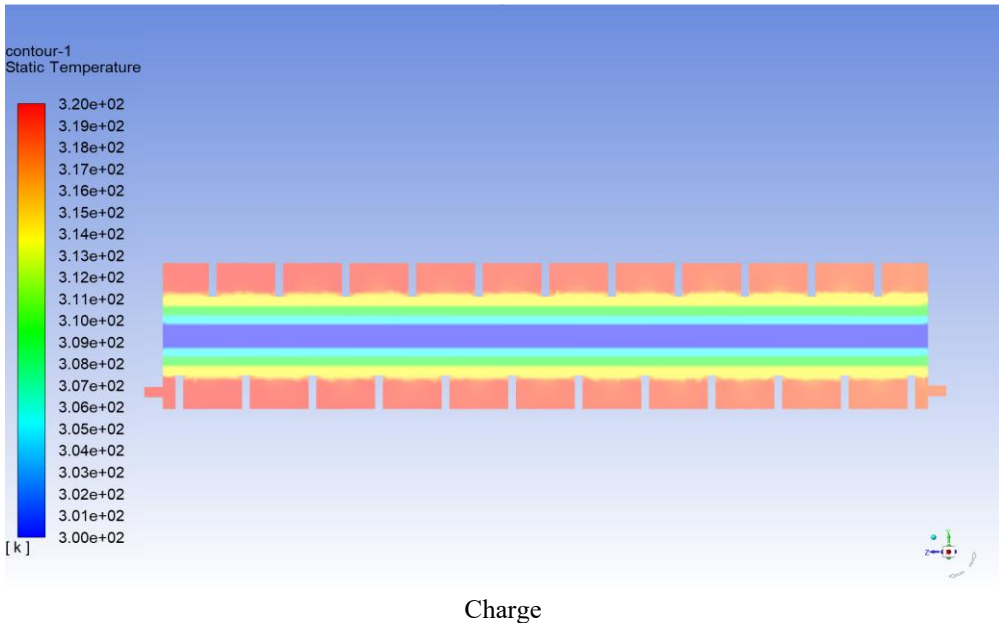
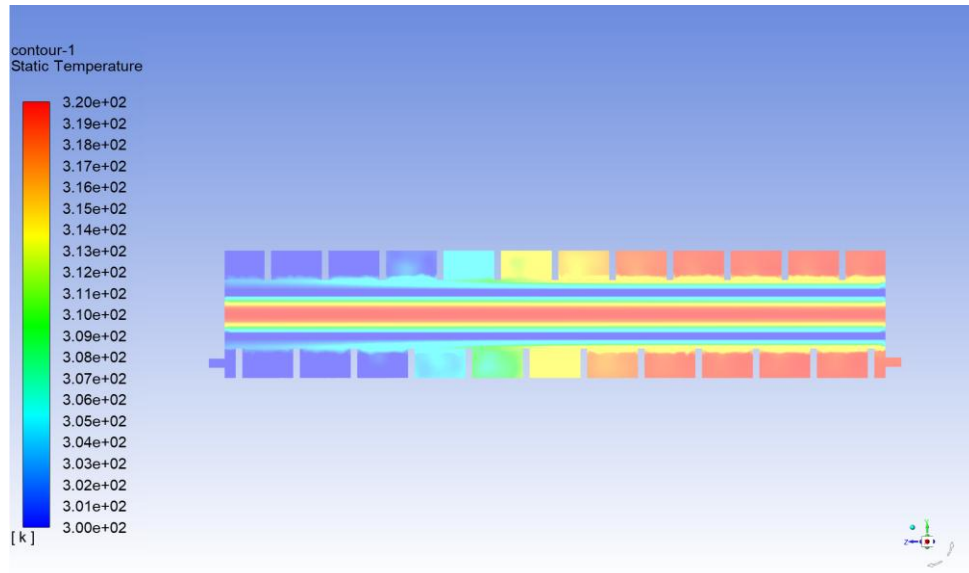


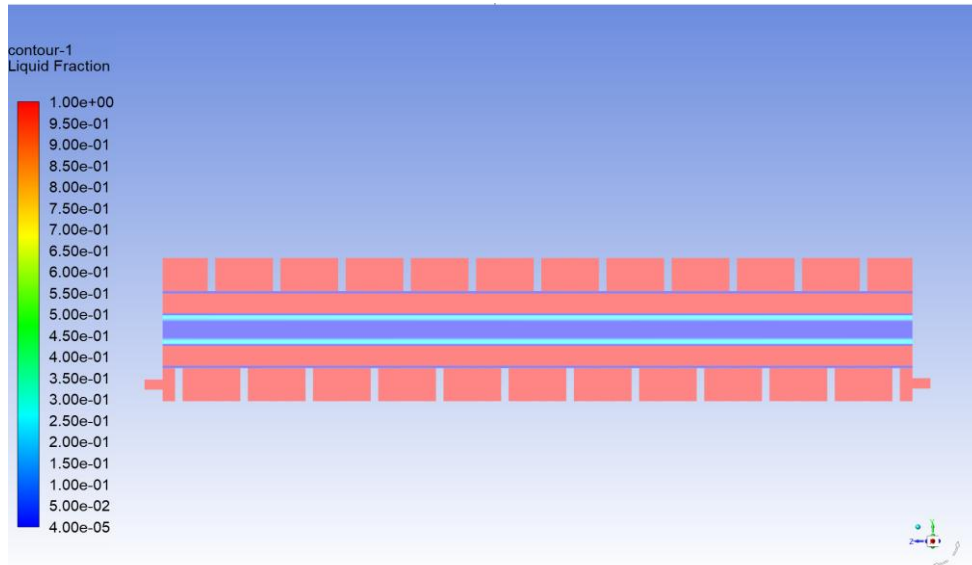
Figure 25. Temperature distribution along the 0.5 m heat transfer tube for different nanoparticle concentrations



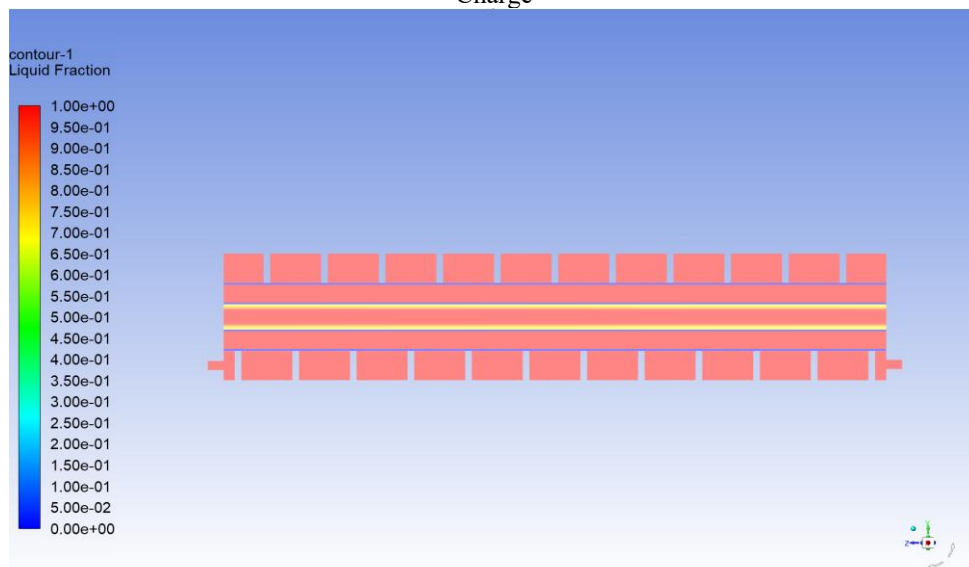


Discharge

Figure 26. Temperature contours of phase change material (PCM) tube during charging and discharging processes



Charge



Discharge

Figure 27. Liquid fraction contours of phase change material (PCM) during charging and discharging processes

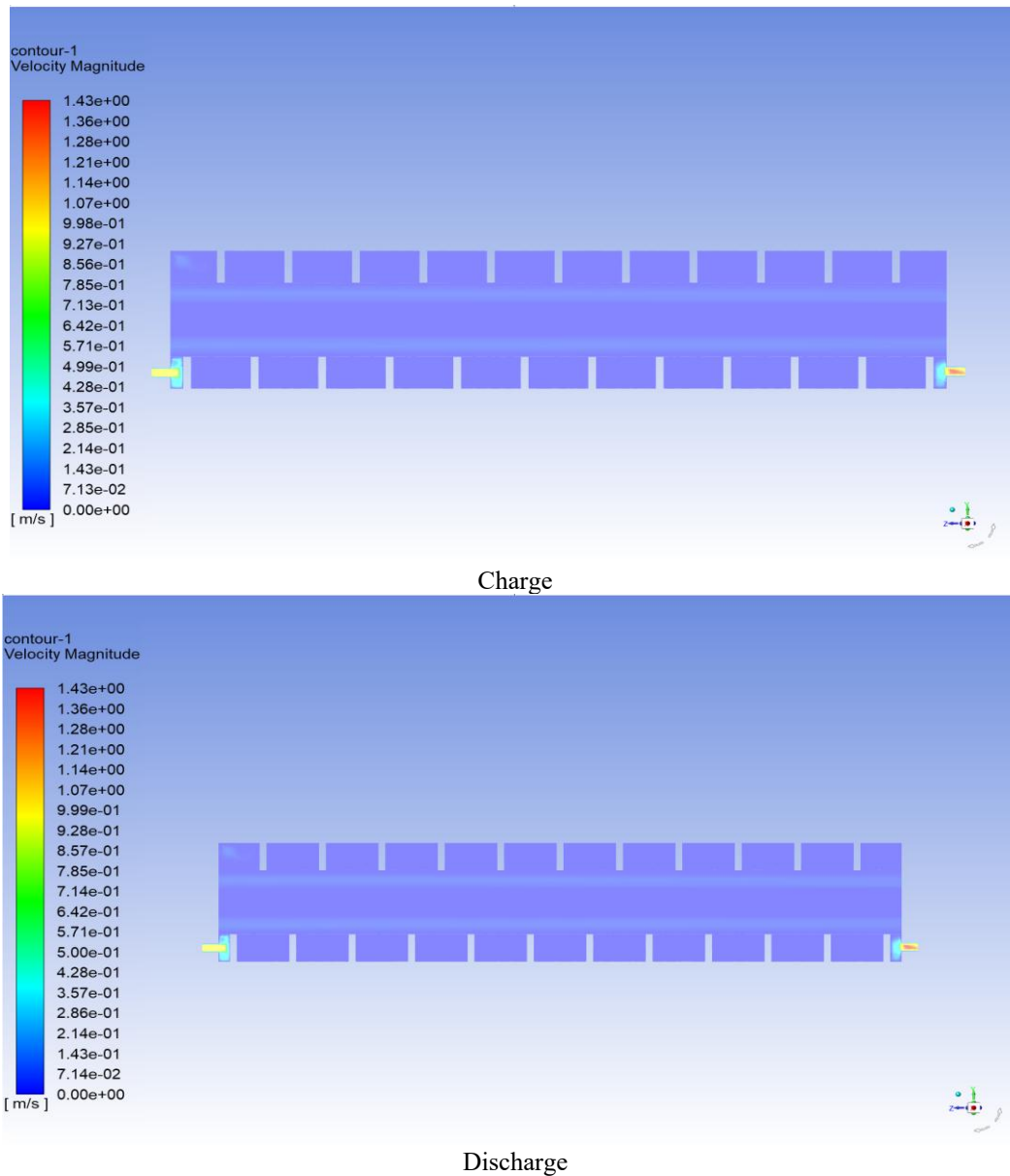


Figure 28. Velocity magnitude contours in the phase change material (PCM) heat transfer tube during charging and discharging processes

The magnitude distribution of the heat transfer fluid velocity in the tube during charging and discharging is shown in Figure 28, with a velocity range of approximately 0 m/s to 1.43 m/s, as indicated by the color scale. Maximum velocities are observed near the inlet and outlet (~ 1.2 – 1.4 m/s), while the velocity along the central tube is more uniform (~ 0.5 – 0.7 m/s), suggesting consistent convective heat transfer throughout the region. The flow field is uniformly distributed along the tube length, ensuring good convective heat transfer during both charging and discharging of the PCM storage material.

Direct experimental validation of the present CFD model was not performed; however, confidence in the numerical results is supported in several ways. First, the mesh independence study (Table 1) confirms that the reported results are numerically converged and not artifacts of grid resolution. Second, the predicted melting behavior, liquid-fraction evolution, and temperature trends are consistent with those reported in experimentally validated CFD studies of analogous helical-tube and shell-and-tube PCM storage configurations in the literature [10, 20], which employed similar enthalpy-porosity formulations and reported

comparable charging/discharging timescales and liquid-fraction profiles. This qualitative agreement with previously validated numerical and experimental studies lends confidence to the accuracy of the present CFD predictions, although direct experimental validation of this specific geometry remains an important objective for future work, as noted in the conclusions.

The thermal performance of PCM-based TES systems proved to be significantly more efficient in the current study compared to previous work. These differences are summarized in the results of the present study. For example, Aich et al. [1] used a GMDH-neural network model to predict the performance of a packed-bed PCM storage system and observed gains in prediction performance of about 10–15% (accuracy of system forecast performance estimation and thermal efficiency enhancement). By contrast, the current study achieved a higher prediction accuracy of around 98–99%, with the AI model reducing prediction error from 0.23 to 0.002, suggesting better prediction of the thermal behavior of PCM.

Similarly, Sayed et al. [20] studied AI-optimized nano-

enhanced PCM systems and found a thermal efficiency enhancement of around 15–18%, attributed to the incorporation of nanofluids. In the current study, combining nanoparticles with AI optimization enhanced the thermal storage efficiency from 0.72 to 0.95, representing an improvement of up to 30–32%, significantly more than existing results. Furthermore, Hajlaoui et al. [10] investigated AI-based PCM discharge enhancement with finned tube set-ups and reported an approximate 20% enhancement in heat transfer compared to previous studies, while the present study reported a 20–25% decrease in charging time and improved stored thermal energy from about 18,800 J to nearly 19,900 J following the addition of nanoparticles.

Additionally, Borhani et al. [5] used AI models for predicting the performance of PCM-based solar thermal systems and reported prediction accuracies of ~90–95%, while the current work achieved ~98–99% accuracy, with close agreement between AI predictions and CFD simulations. In general, the findings validate that the combination of AI-based optimization with nanoparticle-assisted PCM storage has exhibited significantly enhanced efficacy in heat transfer performance, charging rate, and thermal storage efficiency compared to many previously reported studies.

4. CONCLUSIONS

This work focused on research combining AI and CFD analysis for enhancing the thermal performance of PCM-based TES systems in solar applications. Results indicated it was able to predict the thermal behavior of PCM storage systems with an accuracy of about 98–99%, with only about ± 0.02 – 0.03 deviation of the results obtained in CFD simulations. Model performance improved in the AI training step. The prediction ability improved from around 0.61 in the very first epoch to nearly 0.99 after 100 training epochs, and the prediction error went down from 0.23 to about 0.002, which showed good convergence of the learning model. Furthermore, the training & validation losses decreased from approximately 0.90 to approximately 0.04–0.05, indicating the stability of the AI model and the absence of overfitting during training. Furthermore, the incorporation of AI optimization resulted in a substantial improvement in the thermal efficiency of the PCM storage system. In the traditional system, PCM charging time decreased from about 3200 s to 2800 s, and that of the AI-controlled system decreased further from 2300 s to almost 1750 s, which is equal to about a 20%–25% improvement. AI optimization improves the thermal storage efficiency from around 0.72 to 0.95, while the conventional system achieved only 0.70 to 0.84, indicating an overall efficiency improvement of 10–12%. Furthermore, the nanoparticles provided an extra layer in the storage system, which also enhanced the heat transfer behavior. Then, with the increase of water velocity from 0.4 m/s to 1.3 m/s, the heat transfer efficiency increased from roughly about 200 W to almost 295 W and the accumulated thermal energy increased from about 18,800 J for 0% NPs to nearly 19,900 J for 5% NPs, the PCM melting rate ranged between 0.96 for 0% and a little over 1.0 for 5% NPs as the latter improved with the thermal conductivity, leading to a faster phase transfer. Solar was, however, found to influence the system significantly. Thermal storage efficiency of the nanoparticles increased from about 0.71 to 0.81 in 600 W/m², 0.73 to 0.83 at 800 W/m², and between 0.75 and 0.85 in 1000 W/m² as they were applied and

the nanoparticles increased in concentration. Moreover, the PCM discharging process was accelerated with larger thermal conductivity, i.e., the PCM temperature decreased from 320 K to about 304 K with $k = 1.2$ W/m·K and 306 K with $k = 0.2$ W/m·K, confirming heat transfer behavior for the storage system. During charging, PCM temperature was raised from ~300 K to ~320 K, and dropped to ~305–310 K during discharging as stored heat was liberated. This heat transfer fluid has a velocity magnitude (m/s) between 0 and 1.43 m/s, providing large convective heat transfer along the heat transfer tube. Consequently, this work is shown to be more efficient for sustainable solar thermal energy and high performance in areas like charging and storage owing to combining AI technologies with PCM-based TES systems.

Practical Feasibility and Economic Considerations. Beyond the thermal performance metrics discussed above, the practical feasibility of deploying the proposed AI-enhanced, nanoparticle-augmented PCM storage system depends on several economic and operational factors. From an economic perspective, the 20–25% reduction in PCM charging time achieved through AI optimization translates into a higher number of charge-discharge cycles achievable per day, which can improve the effective utilization rate of the storage unit and the associated return on capital investment for a given installed storage capacity. The ease of fabrication of the proposed helical-tube geometry is comparable to conventional shell-and-tube PCM storage units already used commercially, suggesting that manufacturing complexity would not be a significant barrier to adoption. The principal additional costs relative to a conventional PCM system are the procurement of nanoparticles, which adds a marginal material cost that scales with concentration, and the computational cost of training the AI model, which is incurred once during system design and is negligible during operation since the trained model evaluates new operating conditions almost instantaneously. Potential limitations affecting large-scale deployment include the long-term stability of the nanofluid against sedimentation over thousands of charge-discharge cycles, the need for periodic recalibration of the AI model if operating conditions drift outside the range of the original training data, and the upfront cost of instrumentation required to supply the real-time temperature and flow data needed for AI-based control in a real installation. A detailed techno-economic analysis quantifying these costs against the efficiency gains reported here is identified as an important direction for future work.

Although the present work describes practical performance and applicability of combining AI with PCM-based TES systems, the system performance observed here with this proposed method may be judged across many methods for system improvement and operation. To improve the thermal conductivity and heat transfer properties of PCM, the current work can try either hybrid nanomaterials or other types of nanoparticles to improve the above performance. Second, the AI-CFD model proposed must be tested experimentally; a recommended validation methodology would involve fabricating a prototype of the helical-tube PCM storage unit instrumented with thermocouples at multiple radial and axial positions and flow meters at the inlet/outlet, operating it under controlled hot-water inlet temperatures and flow rates matching the simulated boundary conditions, and comparing the measured temperature evolution and charging/discharging times directly against both the CFD predictions and the AI model outputs to quantify prediction error under real operating environments. Additionally, other cutting-edge AI systems

can be adopted, such as deep learning, reinforcement learning, and digital twin solutions, which enable real-time optimization and intelligent control of TES systems. Future work as such might also test the different geometries of heat absorption tubes, fins, and porous media for the efficient charging and discharging of PCM materials. Lastly, the integration and calibration of the PCM storage system with large-scale solar thermal collectors or photovoltaic-thermal systems may provide in-depth knowledge to improve the utilization of renewable energy and planning of sustainable energy storage systems.

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