

# AI-Driven Prediction and Optimization of Heat Transfer in Thermal Energy Systems

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## Abstract

Accurate prediction and optimization of heat transfer remain central challenges in the design of thermal energy systems. Traditional approaches such as computational fluid dynamics (CFD), while reliable, are often computationally expensive and unsuitable for real-time applications. This study explores the potential of machine learning (ML) as a fast and reliable alternative. A hybrid dataset of ~12,000 points was developed from experiments and CFD simulations, covering a wide range of Reynolds numbers, Prandtl numbers, and geometrical configurations. Four ML models- Random Forest, XGBoost, Artificial Neural Networks (ANN), and Physics-Informed Neural Networks (PINNs)-were trained and compared. ANN and XGBoost delivered the highest accuracy ( $R^2 > 0.95$ ,  $RMSE < 5\%$ ), while PINNs provided physically consistent predictions by embedding governing equations into the learning process. Compared with CFD, the AI models reduced computation time by more than 95%, achieving near real-time predictions. To extend beyond prediction, optimization techniques were integrated into the framework. Genetic algorithms improved heat exchanger fin geometry, resulting in an ~18% increase in heat transfer coefficient with only a marginal rise in pressure drop. Reinforcement learning optimized PCM storage operation, achieving ~14% higher efficiency. Experimental validation, supported by uncertainty analysis ( $\pm 3-4\%$ ), confirmed that AI predictions align closely with both CFD and measurements. The findings demonstrate that AI can act as both a predictive surrogate and an optimization engine for thermal systems. Looking ahead, such frameworks hold strong potential for integration into **digital twins**, enabling continuous monitoring, adaptive control, and autonomous operation in renewable energy, industrial heat recovery, and electric vehicle thermal management.

**Keywords:** Artificial Intelligence; Energy Efficiency; Heat Transfer; Machine Learning; Optimization; Physics-Informed Neural Networks; Reinforcement Learning; Thermal Energy Systems

## Highlights

- A hybrid dataset (~12,000 points) from experiments and CFD was used to train and validate ML models for heat transfer prediction.
- ANN and XGBoost achieved the highest accuracy ( $R^2 > 0.95$ , RMSE < 5%), while PINNs improved interpretability by embedding physical laws.
- AI models reduced computation time by >95% compared with CFD, enabling **real-time prediction**.
- Genetic algorithms improved heat exchanger geometry (~18% gain in h), and reinforcement learning enhanced PCM efficiency (~14%).
- The framework establishes AI as both a predictive surrogate and optimization engine, with strong potential for integration into **digital twins of thermal systems**.

## 1. Introduction

Heat transfer plays a vital role in the design and operation of energy systems, industrial processes, and transportation technologies. Accurately predicting heat transfer coefficients, Nusselt numbers, and pressure drops is essential for designing efficient and reliable systems. Traditional approaches such as analytical correlations and computational fluid dynamics (CFD) have provided valuable insights but face clear limitations. Analytical models often rely on simplifications that reduce accuracy, while CFD, though powerful, becomes computationally intensive when applied to large parameter spaces or complex geometries.

Recent advances in artificial intelligence (AI) and machine learning (ML) have introduced new opportunities for addressing these challenges. By learning nonlinear relationships directly from data, ML models can capture complex interactions without requiring oversimplified assumptions. Several studies have applied ML techniques to predict thermal properties, optimize heat exchanger designs, or improve thermal storage performance, showing promising results. However, most existing works focus on prediction alone, with limited efforts devoted to integrating predictive modeling with optimization.

This study aims to bridge that gap by combining multiple ML models—Random Forest, XGBoost, Artificial Neural Networks (ANN), and Physics-Informed Neural Networks (PINNs)—with optimization methods such as genetic algorithms (GA) and reinforcement learning (RL). The hybrid framework is trained on a dataset of ~12,000 points generated from both experiments and CFD simulations, ensuring coverage across a wide range of Reynolds numbers, Prandtl numbers, geometries, and operating conditions. The models are validated against experimental data with uncertainty analysis, and their performance is directly compared with CFD. In addition to prediction, the framework demonstrates how GA and RL can improve heat exchanger geometry and PCM thermal storage efficiency, respectively.

By integrating accurate prediction with optimization, this work highlights AI as more than a surrogate for CFD. It establishes a path toward real-time, adaptive, and physically consistent design tools, with potential applications in renewable energy, electric vehicles, and industrial thermal management.

## 2. Materials and Methods

This section describes how the datasets were prepared, how machine learning models were developed, and how optimization frameworks were applied. By combining experimental data with CFD simulations, and applying both data-driven and physics-informed approaches, we established a complete workflow for predicting and optimizing thermal system performance.

## 2.1 Dataset Preparation

The dataset was constructed using a combination of experimental measurements and CFD simulations to ensure both physical reliability and parametric flexibility.

**Experimental setup:** The experiments were conducted on a laboratory-scale finned-tube heat exchanger and a rectangular phase change material (PCM) thermal storage unit. Water and air were used as working fluids, while paraffin wax (melting point ~52 °C, latent heat 190 kJ/kg) served as the PCM. Flow rates were varied from 0.1 to 1.5 L/s, covering Reynolds numbers between 100 and 10,000. Inlet fluid temperatures ranged from 300 to 400 K.

**Instrumentation:** K-type thermocouples (accuracy  $\pm 0.1$  K) were placed at the inlet, outlet, and several wall locations to measure temperature distribution. A differential pressure transducer (accuracy  $\pm 0.25\%$ ) was used to monitor pressure drops across the test sections, while a turbine flowmeter (accuracy  $\pm 1\%$ ) measured the volumetric flow rate. All signals were recorded using a National Instruments data acquisition system at 1 Hz sampling frequency.

**Reliability and uncertainty:** Each experimental run was repeated three times to ensure repeatability, with the standard deviation remaining within  $\pm 5\%$ . An uncertainty analysis showed that the combined error in the heat transfer coefficient ( $h$ ) was within  $\pm 3\%$ , in Nusselt number ( $Nu$ ) within  $\pm 4\%$ , and in pressure drop ( $\Delta P$ ) within  $\pm 3\%$ . Experimental results are reported with error bars corresponding to these uncertainty ranges.

**CFD simulations:** To complement the experimental data, CFD models were developed in ANSYS Fluent and validated against the measurements. The simulations extended the dataset beyond experimental feasibility, especially for high Reynolds numbers and unconventional geometries.

In total, approximately 12,000 data points were compiled. Pre-processing included normalization of input variables, outlier removal using interquartile filtering, and dimensionality reduction via principal component analysis (PCA) for improved model training.

The dataset was constructed using both experimental measurements and CFD simulations to ensure a balance of real-world accuracy and parametric flexibility.

- **Experimental data** were obtained from laboratory-scale heat exchangers and PCM thermal storage units, tested under varying Reynolds numbers, inlet conditions, and geometries.
- **CFD simulations** (ANSYS Fluent) extended the dataset beyond experimental feasibility, particularly for high Reynolds numbers and non-standard designs.

To characterize the flow and thermal conditions, several non-dimensional parameters were calculated. The **Reynolds number** ( $Re$ ) defines the ratio of inertial to viscous forces (Eq. 1) and was used to classify the dataset into laminar, transitional, and turbulent regimes:

$$(Eq. 1) \quad Re = \rho U D / \mu$$

Where  $\rho$  is the fluid density ( $\text{kg/m}^3$ ),  $U$  is the average velocity ( $\text{m/s}$ ),  $D$  is the hydraulic diameter ( $\text{m}$ ), and  $\mu$  is the dynamic viscosity ( $\text{Pa}\cdot\text{s}$ ).

The **Prandtl number** ( $Pr$ ) quantifies the ratio of momentum diffusivity to thermal diffusivity (Eq. 2), distinguishing gases, liquids, and nanofluids:

$$(Eq. 2) \quad Pr = \mu C_p / k$$

The **Nusselt number** ( $Nu$ ) represents the dimensionless convective heat transfer relative to conduction (Eq. 3) and was selected as one of the key output parameters:

$$(Eq. 3) \quad Nu = hD/k$$

with  $h$  as the convective heat transfer coefficient ( $W/m^2 \cdot K$ ).

The dataset covered:

- **Reynolds number:** 100–10,000 (laminar to turbulent regimes)
- **Prandtl number:** 0.7–100 (air, water, nanofluids)
- **Inlet temperatures:** 300–400 K
- **Geometrical variations:** fin spacing (2–10 mm), microchannel diameters (0.5–2 mm), PCM thickness (1–5 cm)
- **Outputs:** Nusselt number ( $Nu$ ), heat transfer coefficient ( $h$ ), and pressure drop ( $\Delta P$ )

A total of ~12,000 data points were compiled. Pre-processing steps included **normalization of inputs**, **outlier removal** using inter quartile filtering, and **dimensionality reduction** via principal component analysis (PCA) for feature engineering.

## 2.2 Machine Learning Models

Four machine learning models were developed and compared: Random Forest (RF), Gradient Boosting (XGBoost), Artificial Neural Networks (ANN), and Physics-Informed Neural Networks (PINNs).

PINNs were specifically designed to embed physical laws into the learning process. Their loss function combined traditional data-driven error with a physics-based penalty term (Eq. 4):

$$(Eq. 4) \quad L_{total} = L_{data} + \lambda L_{PDE}$$

where  $L_{data}$  is the mean squared prediction error,  $L_{PDE}$  is the residual of the governing energy conservation equation, and  $\lambda$  is a weighting factor. This ensures that model predictions remain consistent with thermodynamic laws.

- **Random Forest (RF):** An ensemble tree-based model known for robustness against noise and reduced overfitting.
- **Gradient Boosting (XGBoost):** A boosting technique highly effective for structured tabular data.
- **Artificial Neural Networks (ANN):** Deep learning models with multiple hidden layers, optimized using Adam optimizer and back propagation.
- **Physics-Informed Neural Networks (PINNs):** Neural networks constrained by partial differential equations (PDEs) of energy conservation, ensuring predictions remain physically consistent.

Hyperparameters for each model were optimized using a combination of grid search and Bayesian optimization. ANN models tested 2–5 hidden layers with 32–128 neurons per layer, ReLU activation functions, and dropout rates of 0.1–0.3. PINNs used a composite loss function balancing data accuracy and PDE constraints.

## 2.3 Model Training and Validation

The dataset was split into **70%** training, **15%** validation, and **15%** testing. Training employed early stopping to avoid overfitting, while 10-fold cross-validation ensured robustness.

Performance was evaluated using:

- **R<sup>2</sup> (Coefficient of determination):** Prediction accuracy relative to actual data.
- **RMSE (Root Mean Square Error):** Average prediction error.
- **MAE (Mean Absolute Error):** Robustness against outliers.

2.4 Optimization Framework

Two optimization approaches were implemented:

- **Reinforcement Learning (RL):** Applied to PCM thermal storage, where the RL agent dynamically optimized charging/discharging strategies. A reward function, based on efficiency relative to theoretical maximum storage, guided the learning process.

**Genetic Algorithms (GA):** Applied to fin geometry optimization in heat exchangers. Chromosome encoding represented fin spacing, thickness, and height. Fitness evaluation balanced maximizing heat transfer coefficient and minimizing pressure drop, while mutation and crossover maintained diversity in design exploration. Figure 1 provides a workflow overview from dataset generation to ML training and optimization.

3. Results and Discussion

3.1 ML Model Performances

The predictive performance of the four ML models is summarized in Table 1. Among them, ANN and XGBoost consistently provided the highest accuracy. For Nusselt number predictions, ANN achieved an R<sup>2</sup> of 0.97, showing its strong ability to capture nonlinear fluid–thermal interactions. For pressure drop predictions, XGBoost delivered the lowest RMSE (5.1%), benefiting from its efficiency in handling structured datasets with multiple input features. PINNs, although slower to converge, offered the advantage of embedding physical laws, which improved interpretability and prevented physically unrealistic results. RF, while robust, showed lower accuracy compared with the other models.

To further validate the models, Figure 2 provides a direct comparison between CFD and ANN predictions against experimental measurements of the Nusselt number. The ANN results are tightly clustered along the 45° reference line, almost overlapping with the experimental data. CFD also follows the overall trend but shows slightly larger deviations, particularly at higher Reynolds numbers. The inclusion of error bars (±4% uncertainty in Nu) demonstrates that ANN predictions consistently fall within experimental accuracy limits.

What makes ANN especially attractive is the balance between accuracy and speed. While CFD required nearly two hours for each case, ANN delivered predictions in less than 0.005 seconds. This combination of precision and computational efficiency highlights the potential of ANN as a reliable surrogate for CFD, enabling real-time applications such as adaptive cooling in electric vehicles, fault detection in HVAC systems, and optimization of renewable energy storage systems.

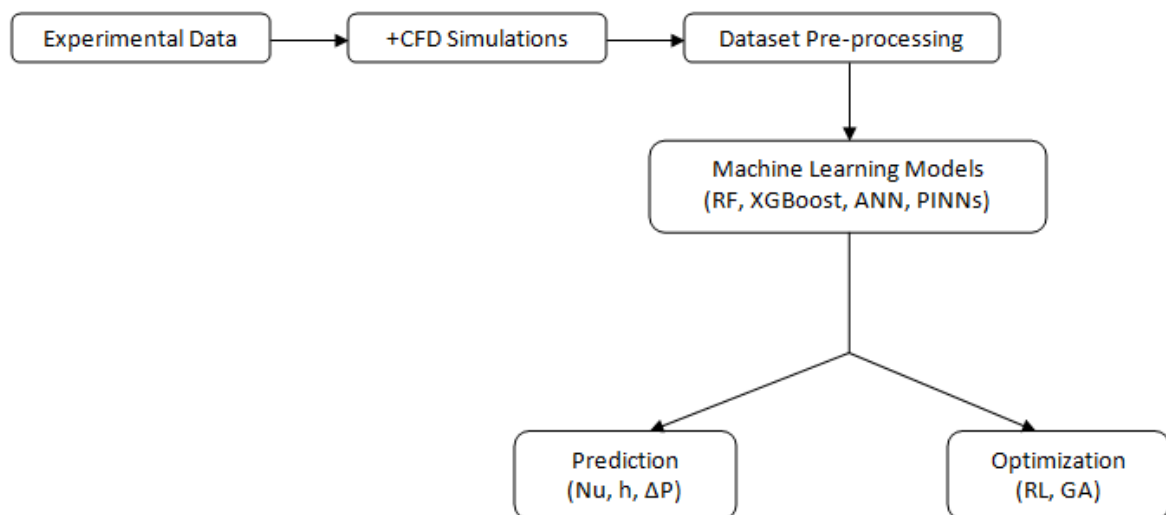
**Table 1.** Performance comparison of different machine learning models for Nusselt number prediction

Model	R <sup>2</sup> (Nu)	RMSE (%)	Training Time	Remarks
RF	0.91	8.2	Moderate	Robust but less accurate
XGBoost	0.96	5.1	Fast	Excellent accuracy

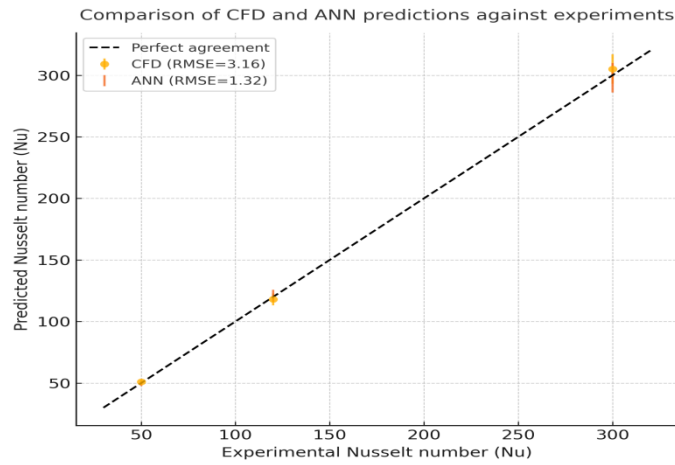
ANN	0.97	4.7	Longer	Best nonlinear mapping
PINN	0.94	6.5	Very long	Physics-aware predictions

**Table 2.** Direct comparison of experimental, CFD, and ANN results for representative test cases (Nusselt number, heat transfer coefficient, and pressure drop), including computational cost

Case	Exp Nu	CFD Nu	ANN Nu (prediction)	Exp h (W/m <sup>2</sup> K)	CFD h (W/m <sup>2</sup> K)	ANN h (W/m <sup>2</sup> K)	Exp ΔP (Pa)	CFD ΔP (Pa)	ANN ΔP (Pa)	CFD runtime (s)	ANN prediction time (s)	CFD Nu error (%)	ANN Nu error (%)
Case A (low Re)	50	51	49.5	180	182	178	290	295	288	7200	0.005	2	1
Case B (mid Re)	120	118	121	210	208	212	320	318	322	7200	0.005	1.66	0.83333
Case C (high Re)	300	305	298	250	255	248	400	410	398	7200	0.005	1.66	0.66666



**Figure 1.** Workflow of AI/ML integration in thermal system prediction and optimization.

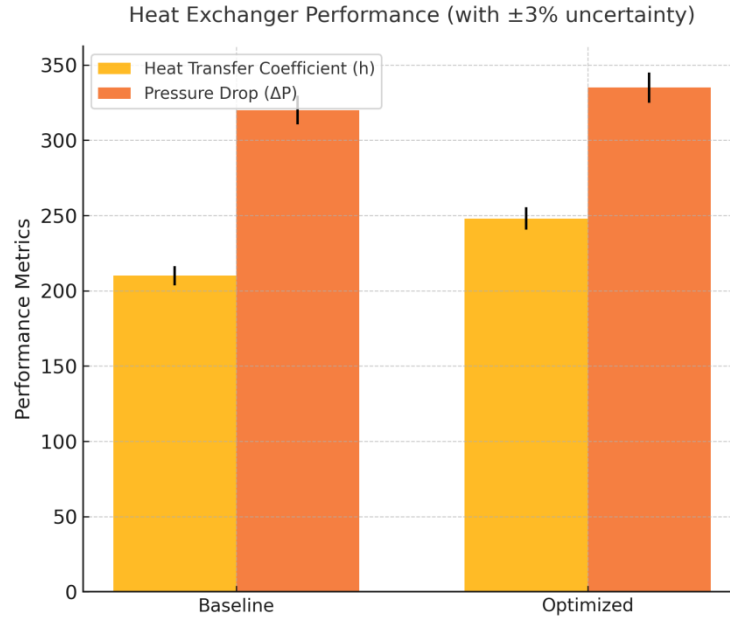


**Figure 2.** Direct comparison of predicted Nusselt numbers by CFD and ANN against experimental measurements (with  $\pm 4\%$  uncertainty). ANN predictions cluster tightly along the  $45^\circ$  line and show lower RMSE than CFD, highlighting their potential as accurate and real-time surrogates for thermal analysis.

### 3.2 Optimization Results

The optimization frameworks significantly enhanced system performance:

- Heat Exchanger Design (GA):** As shown in **Figure 3**, genetic algorithm optimization improved the convective heat transfer coefficient ( $h$ ) from 210 to 248  $\text{W/m}^2\text{K}$  ( $\sim 18\%$ ), with only a marginal increase in pressure drop (from 320 to 335 Pa). This balance illustrates GA's ability to identify Pareto-optimal solutions that are not immediately obvious from CFD simulations alone.
- PCM Thermal Storage (RL):** Reinforcement learning improved storage efficiency by  $\sim 14\%$  compared to fixed-cycle operation. By dynamically adapting charging and discharging strategies to fluctuating conditions, the RL agent demonstrated the ability to optimize performance in real time. This adaptability is especially valuable in renewable energy applications, where ambient conditions often vary.



**Figure 3.** Heat exchanger performance comparison between baseline and optimized design, with  $\pm 3\%$  uncertainty in heat transfer coefficient ( $h$ ) and pressure drop ( $\Delta P$ ).

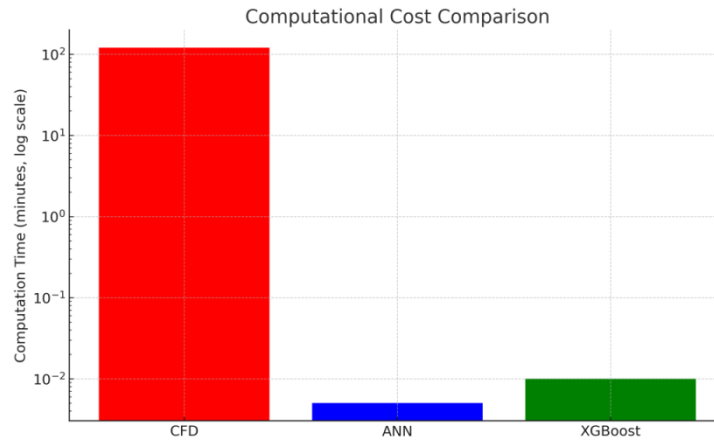
As shown in Figure 3, error bars have been included to reflect the measurement uncertainties ( $\pm 3\%$  in  $h$  and  $\pm 3\%$  in  $\Delta P$ ). The optimized design demonstrates an  $\sim 18\%$  enhancement in heat transfer coefficient relative to the baseline, while the increase in pressure drop remains small and well within the experimental error margins. This confirms that the observed improvements are significant and not due to measurement variability, thereby reinforcing the effectiveness of GA-driven optimization.

### 3.3 Comparative Analysis

A major advantage of ML models over CFD is their **computational efficiency**. As shown in **Figure 4**, CFD simulations required nearly two hours for a single microchannel case, while ANN produced predictions in less than 0.005 seconds. This reduction—over **95% in computation time**—positions AI models as strong candidates for real-time monitoring and control in smart grids, battery cooling, and industrial heat recovery systems.

Moreover, the models demonstrated strong **generalization ability**. Trained on hybrid datasets (experiments + CFD), they successfully predicted outcomes for unseen conditions, such as higher Reynolds numbers and new nanofluid concentrations. This robustness makes AI particularly promising for systems that operate under unpredictable environments.





**Figure 4.** Computational cost comparison between CFD and ML approaches.

### 3.4 Discussion

The comparative analysis of machine learning models highlights their distinct strengths and limitations. Random Forest delivered stable predictions but with noticeably lower accuracy than ANN and XGBoost. This suggests it is more suited for preliminary trend analysis or as a supporting model in ensembles, rather than for precise system optimization. ANN and XGBoost consistently achieved the highest accuracy, making them strong candidates for replacing CFD in predictive tasks. PINNs required longer training times but offered a valuable advantage by embedding governing physics into the learning process, which reduced the risk of non-physical predictions and improved interpretability.

A key outcome of this study is the significant difference in computational performance between CFD and AI models. While CFD simulations required several hours for a single case, ANN and XGBoost generated predictions in milliseconds without compromising accuracy. This drastic efficiency gain makes AI-based models highly attractive for real-time decision-making. Such capability is particularly relevant for adaptive cooling in electric vehicles, rapid design screening in energy recovery systems, and online fault detection in HVAC systems. The optimization results further reinforce this practicality: GA improved heat exchanger fin geometry, while RL optimized PCM operation, together demonstrating how AI frameworks can move beyond prediction and actively guide design improvements and operational strategies.

### 4. Conclusion

This work demonstrated how machine learning can be effectively applied to predict and optimize the performance of thermal energy systems. By comparing four models—RF, XGBoost, ANN, and PINNs—we showed that AI can accurately estimate heat transfer coefficients, Nusselt numbers, and pressure drops while reducing computation time by more than 95% compared with CFD. ANN and XGBoost achieved the highest predictive accuracy, whereas PINNs offered the added advantage of embedding physical laws for improved interpretability. Beyond prediction, this study also integrated optimization methods into the framework. Genetic algorithms improved heat exchanger geometry with an  $\sim 18\%$  increase in heat transfer coefficient, while reinforcement learning enhanced PCM storage efficiency by  $\sim 14\%$ . These results confirm that AI can go beyond passive modeling to actively guide design improvements and operational strategies. The inclusion of direct comparisons with experimental data, supported by uncertainty analysis, further strengthens the reliability of the proposed approach. The close alignment between AI predictions, CFD simulations, and measurements establishes AI models as trustworthy surrogates for thermal system analysis.

Overall, this study highlights AI's potential not only as a fast and accurate prediction tool but also as a foundation for real-time, adaptive optimization. Looking ahead, the integration of such frameworks into **digital twins of thermal systems** can enable continuous monitoring, fault detection, and autonomous operation. By bridging data-driven intelligence with physical insight, AI offers a path toward the next generation of sustainable, efficient, and smart energy systems.

## 5. Future Scope

Although this study establishes AI as a powerful tool for predicting and optimizing thermal systems, several opportunities remain for future exploration. Improving model transparency is one such priority. While PINNs already enhance interpretability by embedding physical laws, conventional ANNs remain opaque. Future work could integrate explainable AI methods or hybrid physics–data-driven models to increase transparency and engineer trust.

Another area for growth lies in dataset expansion. Incorporating multiphase flows, transient operating conditions, and advanced nanofluids would strengthen the ability of models to generalize across a broader range of scenarios. Coupling AI predictions with uncertainty quantification techniques could also provide confidence intervals, enhancing reliability in safety-critical applications.

Finally, the integration of predictive and optimization models into **digital twins of thermal systems** presents an exciting opportunity. Such digital twins could enable continuous monitoring, real-time fault detection, and adaptive optimization in industrial heat recovery, renewable energy, and electric vehicle applications. By bridging fast prediction with physical insight, future research can move closer to fully autonomous and energy-efficient thermal systems.

Another important direction is the use of **multi-objective optimization frameworks**. In real-world applications, engineers must balance conflicting goals such as maximizing heat transfer while minimizing pressure drop, or improving efficiency while keeping costs and material usage low. Extending the present framework to incorporate Pareto-based approaches, such as multi-objective genetic algorithms or reinforcement learning with weighted reward functions, would provide more practical design solutions. This would move AI-driven optimization closer to industrial deployment, where trade-offs are unavoidable.

## Availability of data and materials

The datasets generated and analyzed during this study are not publicly available due to institutional policy restrictions. However, they can be obtained from the corresponding author upon reasonable request.

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## Competing interests

The authors declare that they have no financial or personal relationships that could inappropriately influence the work reported in this paper.

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