Journal of Zhejiang University-SCIENCE A in press
www.jzus.zju.edu.cn; www.springer.com/journal/11582
E-mail: jzus_a@zju.edu.cn

Research Article

https://doi.org/10.1631/jzus.A2600166

Machine learning-enabled performance prediction and operation strategy of phase-change-material-based thermal batteries

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Abstract: Thermal batteries based on phase change materials (PCMs) are a key technology for energy savings and carbon reduction in building heating since latent thermal energy storage by PCMs with high energy storage density indicates great potential to utilize renewable energies. However, the complicated structure of finned-tube heat exchangers and the nonlinear melting-solidification process of PCMs require a great deal of computation and time resources, highly restricting the engineering design and application of PCM-based thermal batteries. To address these issues, this study proposed a universal machine learning-enabled performance prediction framework for finned-tube PCM-based thermal batteries designed for residential domestic hot-water supply, in which thermal energy is stored in PCM during the charging process and released to cold water during the discharging process to provide usable hot water for end users. First, a simplified simulation method coupling a 1D tube model with a 3D CFD model is established for the rapid performance computation of thermal batteries. Second, the deep operator network framework is introduced to directly map static parameters to the time-based temperature response of outlet hot water validated by the simulation and previous experimental results. Based on the machine learning-enabled performance prediction framework, the effects of critical parameters such as tube diameter and thickness combination (Or/Th), fin distance (Fd), and flow rate (Fr) on the heat storage capacity and heat release power are systematically analyzed, providing guidelines for the proposed flowrate feedback regulation strategy of thermal batteries to satisfy different usage temperatures T_{use} and time constraints. The results show that the proposed framework can accurately predict the outlet temperature and available total volume of hot water output by thermal batteries under various conditions.

Key words: Latent thermal energy storage; Finned tube thermal battery; Simplified simulation model; Machine learning; Operation strategy

1 Introduction

With the continuous advancement of dual-carbon goals, the large-scale integration of renewables such as solar and wind power is accelerating (Li et al., 2025; Tong et al., 2025). However, the temporal and spatial mismatch between energy supply and demand (Zhai et al., 2025; Ming et al., 2026) makes efficient and reliable energy storage essential for next-generation energy systems (Xie et al., 2025; Huang et al., 2026). Thermal energy, involved in nearly 90% of global energy conversion and utilization processes (Henry et al., 2020), offers advantages over electrochemical storage in cost, safety, and service life (Freeman et al., 2023; Abdellatif et al., 2025).

Latent thermal energy storage (LTES) is widely regarded as an effective approach for high-energy-density thermal storage (Li et al., 2021; Li et al., 2023a). Owing to the high latent heat associated with phase change material (PCM) (Yu et al., 2023), PCM can store substantially more thermal energy than conventional sensible heat storage (Huang et al., 2023a), exhibiting distinct advantages in applications where space is constrained or strict

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Received Mar. 21, 2026; Revision accepted Jun. 25, 2026; Crosschecked

temperature stability is required (Liu et al., 2025). Numerous studies have demonstrated that LTES holds considerable potential in renewable energy load shifting (Moreno et al., 2014), waste heat recovery (Huang et al., 2023b), and high-power thermal management systems (Christopher Selvam et al., 2025; Yan et al., 2026b).

Although LTES possesses high energy density, its engineering application is still constrained by the low intrinsic thermal conductivity of PCM. Especially in organic phase change materials, the thermal conductivity is typically only 0.2-0.7 $Wm^{-1}K^{-1}$ (Liu et al., 2023; Tripathi et al., 2023), resulting in slow heat transfer and low power density. Material-level enhancement strategies have therefore been widely explored. Liao et al. (Liao et al., 2025) developed a PAAS/ST/DHPD flexible phase-change hydrogel. With 65 wt% DHPD, it showed a phase-change temperature of 31.0 °C, latent heat of 162.3 $J{\cdot}g^{-1}$, good thermal stability after 100 heating–cooling cycles, and compression resilience at 25 °C and 40 °C. Kumar et al. (Kumar et al., 2026) prepared anisotropic shape-stable FCPCMs using paraffin wax, OBC, SEBS, and EG. The sample with 10 wt% EG reduced the peak battery temperature by 23.5 °C at 4C discharge and narrowed the temperature difference by 50%. To address PCM leakage during phase transition, encapsulation and conductive fillers have also been adopted. Ebrahimi et al. (Ebrahimi et al., 2024) proposed an in situ synthesized nanoporous nickel/graphitized-carbon foam for organic PCM encapsulation, retaining high latent heat with only an approximately 7–12% reduction, improving shape stability, and achieving a photothermal efficiency up to ~91%. These methods have to some extent increased the thermal conductivity but may also introduce new problems, such as increased viscosity and suppressed natural convection. Li et al. (Li et al., 2026) proposed a slip-enhanced close-contact melting strategy using a pulse-heating layer and liquid-like slip surface, shortening the charging time from approximately 30 min to less than 3 min and achieving power densities up to ~1100 $kW{\cdot}m^{-3}$ while largely maintaining the energy density.

Recent studies indicate that material modification alone cannot resolve the trade-off between energy density and power density in LTES. Fin structures are widely recognized as effective passive heat-transfer enhancement methods (Elsihy et al., 2025). Properly arranged longitudinal or annular fins can enlarge the heat-transfer area and accelerate charging and discharging (Jiang et al., 2024). Accordingly, in practical engineering applications, finned-tube PCM thermal batteries are widely regarded as one of the most promising LTES configurations, thanks to their intrinsic advantages of compact structure and reliable long-term operation. Jiang et al. (Jiang et al., 2021) found that lower-shell fin placement enhanced heat conduction and natural convection, reducing melting time by up to ~62% compared with the bare-tube case. Tian et al. (Tian et al., 2024) proposed a leaf-vein-inspired self-growing fin topology with outer-tube optimization, reducing melting time by 46.4% and 57.1%, increasing specific power density by 80.6% and 125.7%, and further reducing melting time by 21.57%. Wang et al. (Wang et al., 2024) optimized the air-side fins of plate-fin heat exchangers, increasing the comprehensive performance factor by 9.53%–22.82% and heat dissipation by 26.21% under the same pumping power. Li et al. (Li et al., 2023b) combined annular-fin-induced close-contact melting with nanoenhanced PCMs, reducing the melting time to approximately 52.7% of the baseline and increasing the average power density by more than 100%. Although fin structures greatly improve heat-transfer rates, the coupled effects of multiple parameters on energy and power densities still require further study.

Despite advances in material and structural optimization, the system-level coupling effects of key finned-tube parameters, including tube diameter, tube distance, and fin count, remain insufficiently understood. These parameters affect heat storage, heat release, and PCM utilization, thereby influencing both energy and power densities (Paul and Biswas, 2026). Moreover, existing studies often rely on costly full-scale CFD simulations or isolated parametric analyses, limiting rapid engineering design. Data-driven surrogate models have been increasingly used to replace high-fidelity simulations (Bai et al., 2026; Yan et al., 2026a). Intelligent and automated operation also raises new requirements for practical PCM thermal batteries (Sun et al., 2025). Therefore, this study develops an engineering-oriented simplified whole-device model to analyze the effects of key parameters on heat-storage capacity and heat-release power. Based on experimental and simulation data, a machine-learning-based rapid prediction model is then established. A flowrate feedback regulation strategy for residential hot-water supply is further proposed to match thermal-battery performance with practical operating demands. This work provides methodological guidance for the structural design and rapid performance evaluation of PCM-integrated thermal batteries.

2 Modeling methodology

This work investigates domestic hot water utilization scenarios, selecting a customized finned-tube PCM thermal battery as the research object to characterize its heat discharge performance. The equivalent volume of mixed hot water at the user target temperature is herein adopted as the practical evaluation index. Full descriptions of the prototype structure, material thermal properties, operational principle and equivalent hot water volume definition are available in Section S1 of the electronic supplementary materials (ESM).

2.1 Simplified simulation model

Due to the complex heat transfer process inside the thermal battery and the large number of grids in the computational domain, full-scale CFD simulations are computationally expensive and time-consuming. Therefore, in this study, a simplified simulation method is established. By constructing the minimum heat transfer unit, the complex heat transfer process of the cold water and the PCM is decomposed into a two-way data transfer process between the 1-dimensional tube model and the 3-dimensional CFD model. A schematic diagram of the simplified model construction is shown in Figure 1.

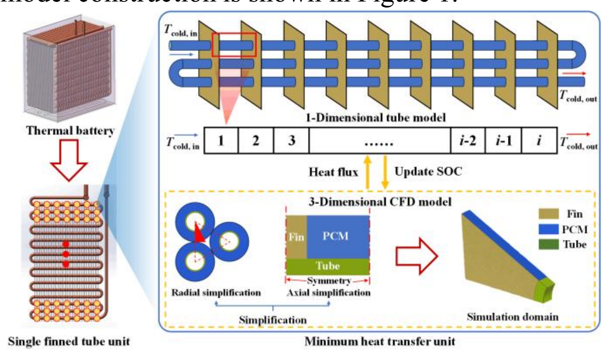

Fig. 1 Basic conception of the simplified model for thermal batteries.

Based on the periodic arrangement of the finned-tube heat exchanger, the thermal battery is decomposed into several parallel single-finned-tube units. Each unit is further divided into minimum heat-transfer units along the flow direction, representing the sequential heat exchange of cold water from inlet to outlet. Each minimum unit consists of a 1-dimensional (1D) tube model and a 3-dimensional (3D) CFD unit. The 1D tube model calculates the axial temperature evolution of flowing water, while the 3D CFD model calculates the local PCM-side phase-change heat transfer. Their coupling preserves the main heat-transfer characteristics while reducing the computational cost of full-scale CFD simulations. Through the CFD simulation model, a dataset of heat flux under different inlet temperatures of the cold water and the PCM's states of charge (SOC) is generated. The calculation for the SOC and maximum heat capacity of the 3D CFD model is as follows:

$$SOC = SOC_{\mathrm{ini}} - \frac{\int A_{\mathrm{cold}} \cdot q_{\mathrm{HF}} \mathrm{d}t}{Q_{\max}} \tag{1}$$

$$Q_{\max} = m_{\mathrm{PCM}}\left[\Delta h_{\mathrm{PCM}} + C_{\mathrm{p,PCM}}(T_{\max} - T_{\min})\right] + m_{\mathrm{tube}} C_{\mathrm{p,tube}}(T_{\max} - T_{\min}) \tag{2}$$

where SOC_{ini} represents the initial SOC; $Q_{\max}$ is the maximum heat storage capacity of the 3-dimensional CFD model; A_{cold} represents the heat transfer area between the cold water and the tube; q_{HF} represents the heat flux density between the cold water and the 1-dimensional tube model; m_{PCM} is the mass of the PCM in the model; m_{tube} is the mass of the finned tubes in the model; Δh_{PCM} is the latent heat of the PCM; C_{p} is the specific heat of the material; and $T_{\max}$ and $T_{\min}$ are the highest and lowest temperatures during operation, respectively.

During the calculation process, the corresponding heat flux is obtained based on the SOC of the current CFD unit and the inlet temperature of the cold water, which is then loaded as input into the 1D tube model. The node outlet temperature is calculated according to the energy conservation equation, while the SOC of the current CFD unit is updated. This process continues until the outlet temperature of the last node is calculated.

As shown in Figure 2, the 3D simulation domain is defined by the maximum PCM range that a single finned tube can influence and the PCM contained between two adjacent fins (Kroeger and Ostrach, 1974; Xu et al., 2024). In this study, the heat release process of the PCM within each finned tube is similar, so it is assumed that the phase change process is uniform and symmetrical between adjacent fins (Waser et al., 2020).

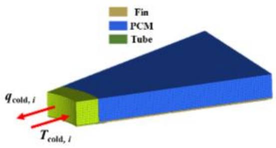

Fig. 2 Simulation domain using the finite volume method.

In this work, a numerical simulation model for the finned-tube PCM thermal battery is built via ANSYS Fluent. The corresponding governing equations and detailed model calculation principles are provided in Section S2 of the ESM.

2.1.2 1-Dimensional tube model

Modeling the heat transfer of the cold water within the heat exchanger as a 1D tube model can reduce the time required for the fluid–solid coupling calculations in the full-scale simulation. The node discretization scheme of the 1D tube model is shown in Figure 3. From the above simplification process, it can be seen that the number of nodes depends on the length of the single finned tube and the number of fins (Neumann et al., 2017). Each node adheres to the principle of energy conservation, and the outlet temperature of the cold water at node *i* can be calculated using the following formula. The outlet temperature of the cold water at node *i* can be used to calculate the outlet temperature of the cold water at node *i*+1 until the last node is reached.

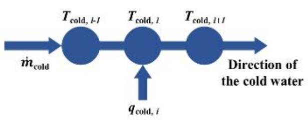

Fig. 3 Discretized node scheme of the 1-dimensional tube model.

$$T_{\text{cold},\,i} = T_{\text{cold},\,i-1} + \frac{q_{\text{cold},\,i}}{C_{\text{p,cold}}\dot{m}_{\text{cold}}} \tag{3}$$

where $T_{\text{cold},\,i}$ represents the outlet temperature of the cold water at node *i*; $T_{\text{cold},\,i-1}$ represents the outlet temperature of the cold water at node *i*-1; $q_{\text{cold},\,i}$ represents the heat flux fed back from the 3D CFD model to node i; $C_{\text{p,cold}}$ represents the specific heat capacity at constant pressure of the cold water; and $\dot{m}_{\text{cold}}$ represents the mass flow rate of the cold water.

2.1.3 Model validation

This study verifies the simplified simulation model based on the thermal battery performance test bench established by Jiang et al. (Jiang et al., 2024b) in our research group. The experimental method involved heating with 70 °C hot water for 2 hours, letting it stand for 30 minutes, and then introducing cold water at room temperature to measure the temperature curve at the outlet of the thermal battery. In addition, two situations are considered: the inlet cold water temperatures are 28 °C and 15 °C, corresponding to the summer and winter operating conditions of the thermal battery, respectively. The results showed that the simplified simulation analysis model could maintain an error of within 10% with the experimental data most of the time.

2.2 Machine learning-enabled performance prediction model

Engineering product design and optimization impose strict limits on computational cost and efficiency. Conventional experiments are time-consuming with poor repeatability, while simplified simulation models require fixed predefined parameters and involve heavy computation. With advances in artificial intelligence, machine learning surrogate models enable rapid performance prediction of thermal batteries under various key parameters, supporting product optimization and operational strategy design.

Figure 4 presents the machine learning workflow for thermal battery performance prediction. This work targets the prediction of time-varying outlet water temperature under different static critical parameters. Traditional artificial neural networks (ANNs) treat time as an extra input for pointwise regression and cannot capture temporal evolution patterns. Recurrent neural networks (RNNs), long short-term memory (LSTM) networks and transformers support autoregressive prediction but depend on historical states and fixed time steps, making them unsuitable for static parameter-driven output prediction. In contrast, Deep Operator Networks (DeepONet) (Lu et al., 2021), developed for operator learning, split the temperature prediction task into branch and trunk subnetworks (Figure 4a–c). The branch encoder receives structural parameters (outer diameter, wall thickness, fin distance) and the operational parameter (flow rate). The trunk network takes operating time to construct temporal basis functions. Their outputs are fused via the vector dot product to generate predictions. This framework efficiently learns the mapping between static parameters and time-dependent outlet temperature, with strong generalization and continuous-time adaptability.

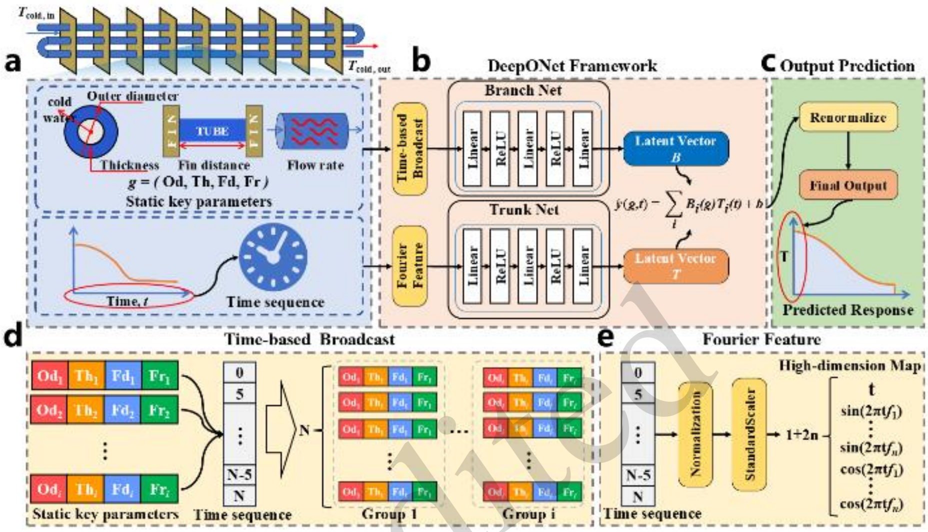

Fig. 4 The flowchart of machine learning: (a) The input parameters of the model; (b) The framework of DeepONet; (c) The prediction performance of the model; (d) The module of "Time-based Broadcast"; (e) The module of "Fourier Feature".

2.2.1 Data processing

In this study, the machine learning dataset is established with the thermal battery initially maintained at 70 °C (PCM fully charged), and 20 °C cold water is supplied for the heat-release process. The model output corresponds to the hourly evolution of outlet water temperature. The static input parameters adopted in this work are summarized in Table 1. Considering the comprehensive heat transfer characteristics of the thermal battery, four groups of structural parameters (tube outer diameter, wall thickness, and fin distance) and operational parameters (cold water flow rate) are selected. The diameter–thickness combinations follow commercial copper tube specifications and practical engineering standards. To guarantee engineering feasibility, the wall thickness is matched with specific outer diameters rather than varying independently.

Table 1 The input static parameters of machine learning

Parameter	Numerical range	Unit
outer diameter (Or) & thickness (Th)	6.35 & 0.8, 9.52 & 1.0, 12.7 & 1.2, 15.88 & 1.2	mm
Fin distances (Fd)	2, 4, 6, 8, 10	mm
Flow rate (Fr)	6, 8, 10	L/min

Prior to model training, the input parameters are separately processed for the two DeepONet subnetworks. The trunk network receives continuous operating time and captures temporal evolution features via Fourier transformation and MLP. As illustrated in Figure 4e, sine and cosine functions map raw time information into high-dimensional frequency features, constructing the time-dependent feature vector *T(t)*. In contrast, the branch network takes a four-dimensional static parameter vector g and compresses it into low-dimensional latent features through MLP, yielding fixed parameter embeddings *B(g)* for each parameter group. To realize operator learning, static parameter features are broadcast and aligned with all time points. As shown in Figure 4d, each static parameter group is repeatedly matched with sequential time information, constructing complete parameter–time input pairs for subsequent temperature prediction.

2.2.2 Model training

Based on the above data processing, a total of 60 unique static parameter groups are adopted for model training. Each parameter group is broadcasted and matched with 721 time points (spanning 3600 s with a 5 s interval) to construct complete training samples. Given the limited dataset size, 5-fold cross-validation is implemented to enhance model reliability and generalization. The detailed dataset settings, network hyperparameters, training configurations, and complete model validation figures are provided in Section S3 of the ESM. The results demonstrate rapid and stable model convergence, with the coefficient of determination (R^2) of both the training and test sets converging close to 1 after sufficient training, as shown in Figure S2. No obvious overfitting is observed, indicating excellent fitting and generalization capability of the network. The optimal model obtained from cross-validation is further verified under multiple typical structural and operational conditions. As shown in Figure S3, the predicted temperature evolutions show excellent consistency with the numerical simulation results, which validates that the proposed DeepONet model can accurately and reliably capture the dynamic heat-release responses of thermal batteries.

3 Results and discussion

For residential hot water applications, deliverable high-quality hot water is of primary concern. Based on the simplified simulation model, this section analyses the effects of key parameters on the available V_{40} under a fixed device volume. Two performance metrics are evaluated: the maximum V_{40} after full charging, representing the total heat storage capacity (energy density), and the cumulative V_{40} at different operating times until the outlet temperature drops to 40 °C, representing the instantaneous heat release capability (power density). The following parameter analysis is organized around these two metrics.

3.1 Effects of the outer diameter and thickness

Figure 5a–e presents the outlet water temperature profiles under different tube diameter and thickness combinations. The temperature evolution exhibits three distinct stages: an initial rapid drop driven by sensible heat release from the finned tubes and near-wall PCM; a plateau-like region corresponding to PCM latent heat release, during which the outlet temperature decreases slowly — note that the plateau temperature does not equal the phase-change temperature, as the outlet temperature is governed by coupled heat transfer among the PCM, fins, tubes and flow rate; and a final rapid decline after most latent heat is exhausted, entering the sensible cooling regime. At small fin distances, increasing the tube diameter raises the initial outlet temperature but shortens the heat release duration (with 40 °C as the threshold). For instance, the combination Or(15.88)-Th(1.2)- Fd(2) achieves an initial outlet temperature of 70.25 °C, which is 19.75% higher than Or(6.35)-Th(0.8)-Fd(2), yet its time to reach 40 °C is 1315 s, which is 30.05% shorter. First, with a fixed fin distance, a larger tube diameter reduces the PCM volume per fin-tube unit, facilitating initial heat transfer to cold water; simultaneously, the lower flow velocity at the same mass flow rate reduces the convective heat transfer coefficient but extends the water residence time, yielding more thorough heat exchange. Consequently, larger-diameter batteries deliver higher initial temperatures. Second, the increased tube diameter reduces the total PCM mass and thus the maximum storage capacity, preventing sustained heat release and causing the outlet temperature to drop below 40 °C more rapidly. This indicates that the initial-stage heat transfer resistance is dominated by the PCM itself, as heat must be gradually conducted from the interior outward.

As the fin distance increases, the heat transfer area between the PCM and tube outer wall diminishes, which disproportionately affects smaller-diameter thermal batteries. As shown in Figure 5f, the heat release duration of smaller-diameter batteries shortens more markedly than that of larger-diameter batteries. For the combination Or(6.35)-Th(0.8)-Fd(10), the time to reach 40 °C is 1315 s, 30.05% less than that of Or(6.35)-Th(0.8)-Fd(2). On the one hand, due to the reduction in fin distance, the effect of heat transfer deteriorates; on the other hand, because of the faster flow velocity, most of the PCM cannot effectively transfer the heat within itself.

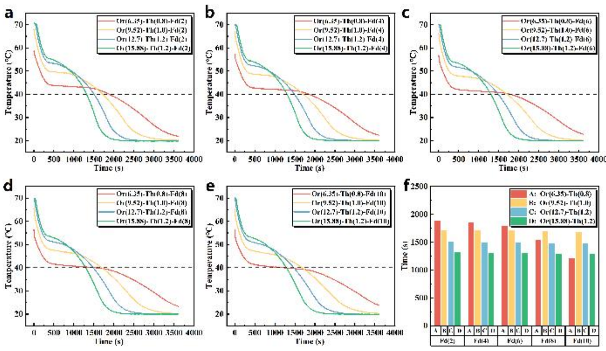

Fig. 5 The outlet water temperature of the thermal battery under different combinations of tube diameters and thickness: (a)-(e) Different fin distances; (f) The drop time of the outlet water temperature to 40 °C.

The cumulative V_{40} over the full operating period is further analyzed in Figure 6a–e. Since cumulative V_{40} depends on both outlet temperature and operating time, smaller fin distances benefit smaller-diameter batteries: despite lower outlet temperatures, their longer heat release duration yields larger cumulative V_{40} that plateaus as operation proceeds. The maximum V_{40} (defined as the cumulative V_{40} from t = 0 until the outlet temperature drops to 40 °C) of the combination Or(9.52)-Th(1.0)-Fd(2) reaches 248.22 L, 12.4% higher than that of Or(15.88)-Th(1.2)-Fd(2). However, this advantage of smaller tube diameters diminishes as the fin distance increases. As shown in Figure 6f, larger-diameter batteries not only catch up and surpass smaller ones in max V_{40} but also outperform them in heat release duration. The max V_{40} of the combination Or(6.35)-Th(0.8)-Fd(10) is 136.61 L, 40.08% lower than that of Or(6.35)-Th(0.8)-Fd(2).

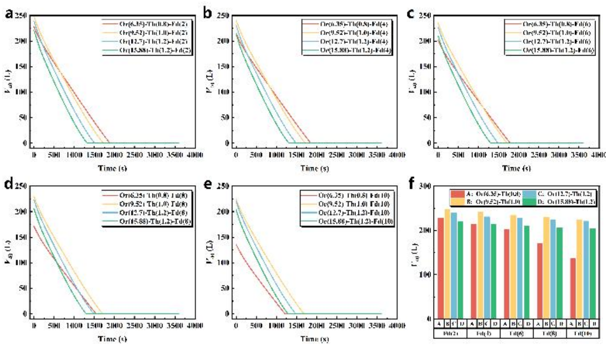

Fig. 6 Cumulative V_{40} of the thermal battery under different combinations of tube diameters and thickness: (a)-(e) Different fin distances; (f) The max V_{40}.

Therefore, thermal battery design requires careful balancing of the tube diameter and fin spacing. Smaller tube diameters extend heat release duration and can yield optimal max V_{40}, whereas larger tube diameters raise the initial outlet temperature at the cost of reduced max V_{40} and shorter heat release duration. From a thermal load management perspective, larger tube diameters enhance short-term heat release capability, making them suitable for meeting peak hot-water demand within limited time windows. Conversely, smaller tube diameters accommodate more PCM and deliver higher maximum V_{40}, making them better suited for applications requiring prolonged heat supply and greater peak-load shifting capacity.

3.2 Effects of the fin distance

For a given tube diameter and thickness combination, the fin volume has a negligible effect on the total PCM mass due to the small fin thickness (0.2 mm), especially compared with the impact of the tube diameter and thickness. As shown in Figure 7, outlet water temperatures are initially similar across different fin distances but diverge after a certain point: batteries with smaller fin distances have already released most of their latent heat, whereas those with larger fin distances retain unexploited thermal energy due to reduced heat transfer area. Notably, the influence of the fin distance weakens as the tube diameter increases. Two mechanisms contribute: first, the reduced total PCM mass and smaller per-unit PCM volume around each finned tube enable faster heat extraction; second, the lower flow velocity associated with larger diameters promotes more thorough heat exchange.

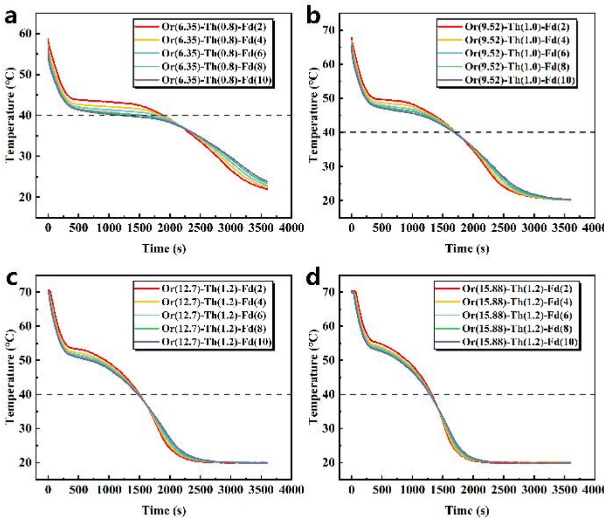

Fig. 7 The outlet water temperature of the thermal battery

under different fin distances: (a)-(d) Different combinations of tube diameters and thickness.

The cumulative V_{40} profiles over time are presented in Figure 8. Consistent with the preceding analysis, smaller fin distances yield higher cumulative V_{40}, and this effect diminishes as the tube diameter increases. Notably, for larger-diameter batteries, the enhanced heat transfer from increased tube area reduces the sensitivity of heat release duration to fin spacing. In contrast, the benefit of smaller fin distances is more pronounced for smaller-diameter batteries.

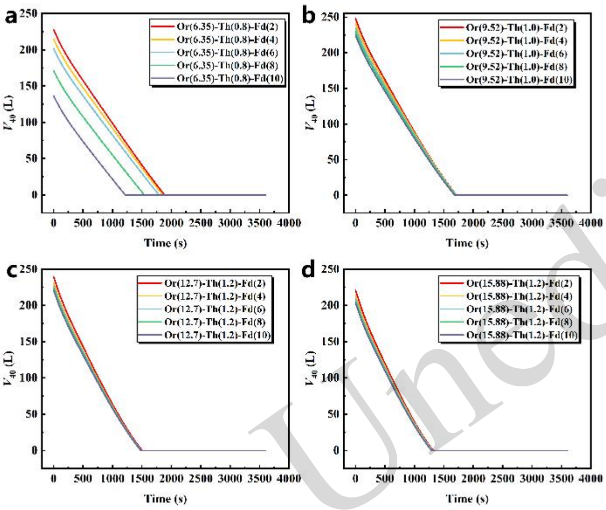

Fig. 8 Cumulative V40 of the thermal battery under different fin distances: (a)-(d) Different combinations of tube diameters and thickness.

The influence of fin distance also reflects the trade-off between heat release rate and thermal storage capacity. A smaller fin distance enhances heat transfer and increases the available heat output within a short period, whereas a larger fin distance increases PCM loading and contributes to a greater amount of stored thermal energy. Therefore, the selection of fin distance should be based on whether the application prioritizes short-term peak demand coverage or long-term thermal load shifting.

3.3 Effects of the flow rate

For thermal batteries with identical structural parameters, V_{40} is governed by both outlet temperature and flow rate. A higher flow rate increases the convective heat transfer coefficient and instantaneous heat release power but prevents sufficient heat exchange, thereby lowering the outlet temperature. Conversely, a lower flow rate enables more thorough heat transfer and raises the outlet temperature but limits the instantaneous heat release power. These two competing effects collectively determine the net change in V_{40}.

As shown in Figure 9, as the flow rate increases, the outlet water temperature of the thermal battery shifts downward overall. This means that even at a larger flow rate, although the convective heat transfer coefficient increases, since the heat transfer resistance is mainly concentrated within the PCM, the temperature rise of the cold water within the same time period is lower compared to that at a smaller flow rate. The initial outlet water temperature of the combination *Or*(6.35)-*Th*(0.8)-*Fd*(2)-*Fr*(6) can reach 58.33 °C, which is 22.96% higher than that of the combination *Or*(6.35)-*Th*(0.8)-*Fd*(2)-*Fr*(10).

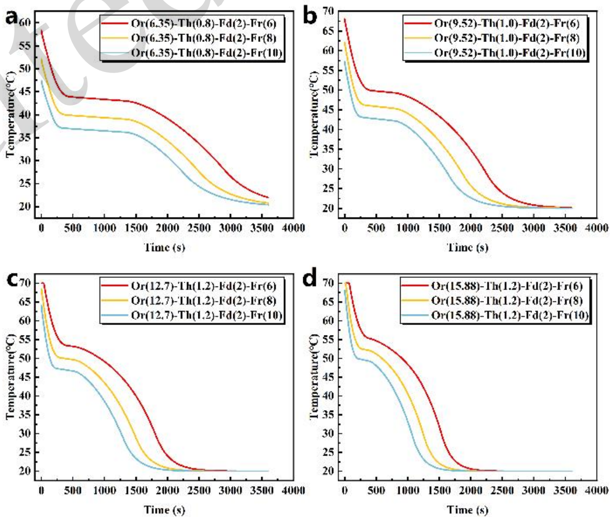

Fig. 9 The outlet water temperature of the thermal battery under different flow rates: (a)-(d) Different combinations of tube diameters and thickness.

This pattern persists throughout the entire heat release process. Notably, the influence of flow rate diminishes slightly with increasing tube diameter — consistent with the earlier observation that larger diameters reduce the per-unit PCM volume around each finned tube, enabling faster heat extraction. Nevertheless, the competing relationship between outlet temperature and flow rate remains the primary determinant of V_{40}.

Cumulative V_{40} profiles under different flow rates are shown in Figure 10. Higher flow rates do not increase the maximum V_{40}, indicating that V_{40} is ultimately limited by outlet temperature: despite higher instantaneous heat release power, the total heat extracted over the full operating period decreases, reducing max V_{40}. This effect is partially mitigated by larger tube diameters, although max V_{40} still declines slightly. For the combination *Or*(6.35)-*Th*(0.8)-*Fd*(2)-*Fr*(10), the max V_{40} is 32.38 L, 85.79% lower than that of *Or*(6.35)-*Th*(0.8)-*Fd*(2)-*Fr*(6). Further analysis of the cumulative V_{40} evolution reveals that lower flow rates extend the heat release duration, requiring more time to deliver the full max V_{40}. Conversely, while higher flow rates yield lower cumulative V_{40} at matched time points, they release heat faster and deliver more V_{40} within equal time intervals. This highlights the need to align flow rate selection with actual user usage patterns.

The effect of the flow rate is directly related to the peak-load shifting performance of the thermal battery. Increasing the flow rate enhances the heat release power and enables a larger amount of thermal energy to be delivered within a short period. However, it also reduces the maximum V_{40} due to the shortened residence time of water inside the heat exchanger. Therefore, high flow rates are advantageous when the objective is to cover short-term peak demand, whereas lower flow rates are more suitable for maximizing the utilization of stored thermal energy and extending the duration of peak-load reduction.

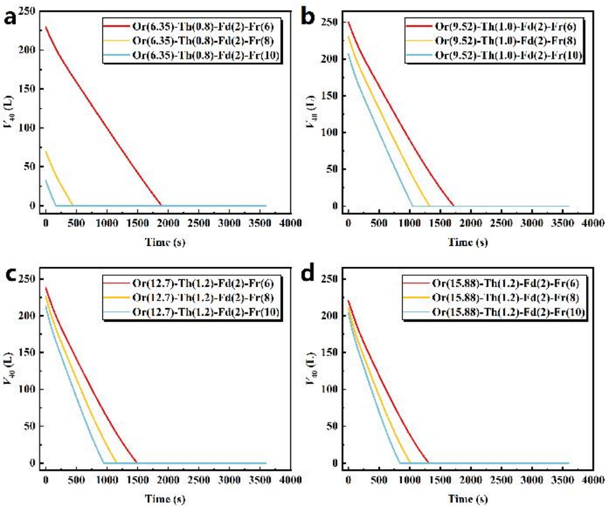

Fig. 10 Cumulative V40 of the thermal battery under different flow rates: (a)-(d) Different combinations of tube diameters and thickness.

3.4 Feedback regulation strategy for residential hot water supply

On the basis of analyzing the above parameters, different thermal battery structural selections are constructed for different heat demand scenarios. Choosing an appropriate combination of tube diameter and thickness and a smaller fin distance can achieve a larger max V_{40}. For rapid heat acquisition scenarios, choosing a larger tube diameter and an appropriate fin distance can achieve a lower heat release time, meeting the immediate heat demand.

In practical applications, in addition to the design optimization for the structural selection of thermal batteries, it is also necessary to consider the resolution of the contradiction between the time and total amount of heat acquisition during the operation of the thermal battery, that is, the heat release power of the thermal battery. Therefore, based on a typical structure of a thermal battery with parameter combination Or(12.7)-Th(1.2)-Fd(2), this study proposes a heat release power regulation strategy based on intelligent flowrate feedback control, considering the different time and heat requirements of users. As shown in Figure 11, the core of the strategy lies in the regulation of the flow rate. Specifically, the demands of users include usage temperature (T_{use}), the required time, and the equivalent water volume of the usage temperature (V_{use}). Based on the constructed thermal battery performance prediction model, the cumulative V_{use} changes can be quickly calculated. Furthermore, if the user has no limit on the usage time, then it is only necessary to compare whether the max V_{use} provided by the thermal battery under the current flow rate is larger than the required value. If it is larger, hot water is output; if it is less, the flow rate is reduced to increase the total V_{use}. If the user has a limited usage time, then the cumulative V_{use} that can be provided within the time interval is calculated and judged whether it is larger than the required V_{use}. If it is larger, hot water is output; if it is less, the flow rate is adjusted to meet the requirements.

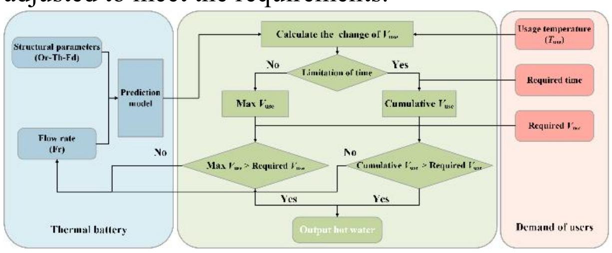

Fig. 11 Thermal battery intelligent operation strategy based on flow rate regulation.

This study demonstrates the impact of regulating the flow rate on the cumulative V_{use} under different T_{use} conditions, as shown in Figure 12. Under the same T_{use} conditions, as the flow rate (6.5 L/min, 7.5 L/min, 8.5 L/min) increases, it can be observed that the max V_{use} slightly decreases, indicating a reduction in the total heat storage capacity of the thermal battery. However, when the fully charged thermal battery operates at different time intervals (10 min, 20 min, 30 min), as the flow rate increases, the accumulative V_{use} shows an upward trend, indicating an increase in the heat release power of the thermal battery, which is consistent with the results of the above parameter analysis. As shown in Figure 12a, at a flow rate of 8.5 L/min within 10 minutes, the accumulative V_{use} obtained is 13.96% higher than that at 6.5 L/min, and it can increase by 11.02% within 20 minutes. It is worth noting that the accumulative V_{use} obtained within 30 minutes is consistent with the max V_{use}, meaning that at this time, the thermal battery has completed the heat release of the required T_{use}, and then the outlet water temperature is lower than T_{use}.

However, as T_{use} increases (30 °C to 50 °C), as shown in Figure 12c, due to the insufficient total heat storage capacity at higher flow rates, the max V_{use} decreases significantly. At a flow rate of 8.5 L/min, the maximum V_{use} decreases by up to 69.86% compared to 6.5 L/min. At this point, the heat release power at higher flow rates is limited by the max V_{use} and thus no longer has an advantage. It is worth noting that as T_{use} increases, due to the higher requirements for the outlet water temperature, the max V_{use} is reduced. At a flow rate of 6.5 L/min, the maximum V_{use} of 50 °C is 80.27% lower than that at 30 °C, and the thermal energy is released over a shorter duration. At this time, it is advisable to consider connecting multiple thermal battery modules to increase the max V_{use} output.

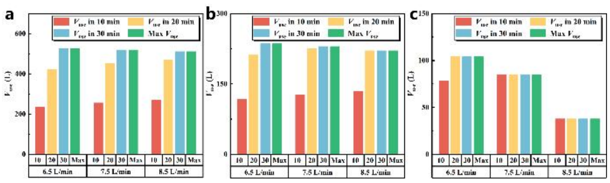

Fig. 12 Comparison of flow rate (6.5 L/min, 7.5 L/min, 8.5 L/min) regulation under different usage temperature demands: (a) T_{use} = 30 °C; (b) T_{use} = 40 °C; (c) T_{use} = 50 °C.

These results demonstrate that the proposed prediction and regulation framework can provide guidance for balancing thermal storage capacity and heat release power according to different user demands, thereby improving the operational flexibility of residential hot-water systems.

4 Conclusions

This study proposes a machine-learning-enabled design and operation strategy for thermal batteries in residential hot-water supplies. By developing a simplified simulation model and introducing the DeepONet architecture, rapid performance prediction is achieved. Based on these models, the effects of key structural and operating parameters on high-grade hot-water supply are systematically analyzed, and an intelligent flowrate feedback regulation strategy is proposed. The main conclusions are as follows:

(1) This study establishes an efficient modeling and prediction framework to reduce the high computational cost of full-scale CFD simulations and enable rapid design iteration and time-series performance evaluation. A simplified model coupling a 1D tube model with a 3D CFD unit is developed to decompose the complex multiphysics heat-transfer process. The model maintains prediction errors within 10% while greatly reducing computational time. In addition, the DeepONet framework is introduced to directly map structural and operating parameters to the time-dependent outlet water temperature response. The 5-fold cross-validation results show an R^2 approaching 1, with predictions highly consistent with simulation results, demonstrating its reliability for rapid engineering evaluation.

(2) This study reveals the coupling mechanisms among key structural and operating parameters, as well as the trade-off between energy density and power density in finned-tube thermal batteries. Tube outer diameter and thickness combinations (*Or/Th*), fin distance (*Fd*), and flow rate (*Fr*) are selected as key parameters, while the equivalent 40 °C hot-water volume (V_{40}) is used to characterize high-grade hot-water release capability. Parametric analysis results show that at small fin distances, increasing the tube diameter elevates the initial outlet water temperature but shortens the heat release duration. Increasing the flow rate improves the heat release power but significantly reduces the maximum V_{40}. At

10 L/min, the max V_{40} decreases by 85.79% compared to 6 L/min, which clearly highlights the trade-off between energy density and power density.

(3) This study proposes an intelligent flowrate feedback operation strategy to resolve the dynamic mismatch between heat extraction time and total heat demand under different user scenarios for thermal batteries with fixed structures. Specifically, for a typical structural design, a regulation logic is constructed considering usage temperature (T_{use}), time constraints, and required hot water volume (V_{use}). The rapid prediction model is employed to evaluate cumulative V_{use} in real time and adjust the flow rate accordingly. The results demonstrate that in time-constrained scenarios, increasing the flow rate enhances short-term cumulative V_{use}. For example, increasing the flow rate from 6.5 L/min to 8.5 L/min raises the cumulative V_{use} by 13.96% within 10 minutes. However, under scenarios with high T_{use} requirements, higher flow rates significantly reduce the maximum V_{use}, indicating that modular expansion may be required to improve the total output capacity. This strategy provides methodological support for intelligent control in practical engineering applications of thermal batteries.

(4) Future work should validate the proposed prediction framework and explore its application in practical thermal energy management scenarios. The developed prediction and regulation approach is expected to support intelligent operation of PCM-based thermal batteries, improve the flexibility of residential hot-water systems, and facilitate thermal load shifting and renewable energy integration in building energy systems.

Acknowledgments

The present study is supported by the National Natural Science Foundation of China (Grant No. 524762247 and No. 5220602), Young Elite Scientists Sponsorship Program by Zhejiang Association for Science and Technology (Grant No. ZJSKXQT2025038) and Special Program of Hangzhou Chengxi Sci-tech Innovation Corridor.

Author contributions

Yanyu Shen and Zhi Li designed the research. Yanyu Shen, Linfeng Zhu, and Ruicheng Jiang developed the simplified simulation model and processed the corresponding data. Yanyu Shen and Ruicheng Jiang established and validated the machine-learning prediction model. Zhen Zhang provided engineering support for the thermal battery design and parameter settings. Yuqi Huang and Xiaoli Yu helped to organize the manuscript and prepare the figures. Yanyu Shen wrote the first draft of the manuscript. Peiwang Zhu and Zhi Li supervised the research, revised the manuscript, and edited the final version. All authors read and approved the final manuscript.

Conflict of interest

The authors declare that they have no conflict of interest.

Declaration on the use of generative AI tools

The authors declare that no generative artificial intelligence tools or AI-assisted technologies were used in the preparation of this manuscript.

Data availability

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

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Electronic supplementary materials

Section S1, Table S1, Figs. S1, Formula S1-S2; Section S2, Formula S3-S7; Section S3, Table S2, Figs. S2-S3

中文概要

题　目：基于机器学习的相变材料热电池性能预测与运行策略

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目　的：相变材料热电池具有较高的储能密度，在建筑生活热水供应和可再生能源消纳中具有良好的应用潜力。然而，翅片管换热结构复杂，相变材料熔化–凝固过程具有明显非线性，传统全尺度 CFD 仿真计算成本高、耗时长，限制了热电池的快速设计与工程应用。本文旨在建立一种面向住宅生活热水供应的相变材料热电池机器学习性能预测与运行调节方法，实现热电池出口水温和可用热水输出量的快速预测，并为不同用水需求下的运行策略提供指导。

创新点：1、建立了 1D 管模型与 3D CFD 模型耦合的简化仿真方法，将复杂的整机传热过程分解为最小传热单元的数据传递过程，在保持主要传热特征的同时降低计算成本；2、引入 DeepONet 深度算子网络，将结构参数和运行参数直接映射到出口热水温度的时间响应，实现热电池动态放热性能的快速预测；3、以 Or/Th、Fd 和 Fr 为关键参数，系统分析其对热储存能力和放热功率的影响，并提出面向不同使用温度和时间约束的流量反馈调节策略。

方　法：1、基于翅片管换热器的周期性结构特征，构建单翅片管单元和最小传热单元，将热电池内部冷水与相变材料之间的传热过程转化为 1D 管模型和 3D CFD 模型之间的耦合计算过程；2、以热电池满充状态下的放热过程为研究对象，选取管径与壁厚组合 Or/Th、翅片间距 Fd 和流量 Fr 作为输入参数，建立机器学习数据集，并通过 DeepONet 模型预测出口水温随时间的变化；3、基于简化仿真模型和机器学习预测结果，分析不同管径、壁厚、翅片间距和流量对等效 40 °C 热水体积 V40、热储存能力和放热功率的影响；4、针对住宅生活热水供应需求，构建考虑使用温度 Tuse、用水时间和所需热水体积 Vuse 的流量反馈调节策略，并通过典型工况验证其可行性和有效性。

结　论：1、所建立的 1D 管模型–3D CFD 耦合简化模型能够有效降低全尺度 CFD 仿真的计算成本，并保持较高的预测精度；结合 DeepONet 模型后，可实现热电池出口水温时间响应的快速预测；2、Or/Th、Fd 和 Fr 对热电池的储热能力和放热功率具有显著影响。较小翅片间距有利于提高短时放热能力，较小管径有利于增加相变材料装载量和延长放热时间，而较高流量可提高瞬时放热功率，但会降低最

大可用热水输出量；3、热电池运行过程中存在能量密度与功率密度之间的权衡关系。提高流量能够增强短时热水输出能力，但在高使用温度需求下可能显著降低最大 Vuse；4、所提出的流量反馈调节策略能够根据用户使用温度、时间约束和热水需求量对运行参数进行适应性调节，为相变材料热电池在住宅生活热水系统中的智能运行提供了方法支持。

关键词： 潜热储能；翅片管热电池；相变材料；简化仿真模型；机器学习；DeepONet；运行策略。