



Research Paper

Geometric–operational coupling and CatBoost-assisted rapid evaluation of charging performance in a radiator-shaped fin-enhanced latent heat thermal energy storage system

Zied Elleuch^a, Mohammad Hossein Heidarshenas^b, Hayder I. Mohammed^c, Aidar Kuttybayev^{d,*}, Maricel G. Dayaday^e, Ghada A. Alsawah^f, Mohamed Bouzidi^g, Mohammad Ghalambaz^h

^a Computer Science Department, Applied College, University of Ha'il, P.O. Box 2440, Hail City 55476, Saudi Arabia

^b Department of Mechanical and Nuclear Engineering, Kansas State University, Manhattan, KS, USA

^c Department of Physics, College of Education, University of Garmian, Kalar 46021, Iraq

^d Department of Mining, Satbayev University, Almaty 050000, Republic of Kazakhstan

^e Department of Electronics Engineering, College of Engineering and Information Technology, University of Southern Mindanao, Kabacan, Cotabato, Philippines

^f Department of Industrial and Systems Engineering, College of Engineering, Princess Nourah bint Abdulrahman University, P.O. Box 84428, Riyadh 11671, Saudi Arabia

^g Department of Physics, College of Science, University of Ha'il, Ha'il, P.O. Box 2440, Saudi Arabia

^h Department of Mathematical Sciences, Saveetha School of Engineering, SIMATS, Chennai, India

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ABSTRACT

Efficient thermal charging in latent heat thermal energy storage systems is limited by the low thermal conductivity of phase change materials and by the coupled interaction between conductive heat spreading, buoyancy-driven convection, and heat transfer fluid-side thermal resistance. In this study, a three-dimensional flat-plate fin-enhanced LHTES system was numerically investigated using the enthalpy–porosity method to clarify how geometrical and operating parameters jointly govern PCM melting dynamics. The effects of tube number, fin spacing, inlet temperature, and Reynolds number were first examined individually while preserving the total tube–fin volume, followed by a cross-parametric analysis to reveal their coupled thermo-hydrodynamic interactions. Increasing tube number accelerated melting by shortening the characteristic thermal diffusion length; however, the preferred configuration depended on the selected performance metric within the investigated range, with the four-tube case giving the shortest complete melting time and the five-tube case providing the highest average heat storage rate among the tested configurations. Reducing fin spacing from 15 mm to 5 mm decreased melting time by 50.4% and increased the average heat-storage rate by 91.2%. Meanwhile, the nominal spacing-based Rayleigh number decreased by 96.3%, indicating a reduced characteristic buoyancy scale without directly quantifying the convective heat transfer contribution. Increasing inlet temperature from 60 °C to 80 °C improved heat storage rate by 80.7%, while increasing Reynolds number from 500 to 2000 enhanced it by 106.1% through reduced HTF-side convective resistance. A relative-effect interaction analysis confirmed that the parameter effects are non-additive, with interaction magnitudes of 17.5 percentage points for fin spacing–tube number, 14.3 percentage points for inlet temperature–tube number, and 8.8 percentage points for Reynolds number–tube number based on complete melting time. A dataset comprising 38,891 transient samples from 41 CFD cases was subsequently used to train a CatBoost surrogate for simultaneous prediction of liquid fraction and stored thermal energy. Under the adopted random row-wise partition, the multi-output model reproduced the held-out CFD sample values with normalized test RMSE values of 0.0155 and 0.0169 for liquid fraction and stored energy, respectively, with corresponding R^2 values above 0.9997. Accordingly, the surrogate is presented as a bounded proof-of-concept for rapid reconstruction and comparison of transient responses within the sampled CFD design space, rather than as an extrapolative model or optimization framework. Because transient rows from the same CFD case may occur in different data subsets, these metrics represent sample-level interpolation within the simulated trajectories rather than independent validation for unseen geometrical–operational configurations.

* Corresponding author.

E-mail addresses: zi.elleuch@uoh.edu.sa (Z. Elleuch), heidarshenas@ksu.edu (M.H. Heidarshenas), hayder.i.mohammad@garmian.edu.krd (H.I. Mohammed), kuttybayev@satbayev.university (A. Kuttybayev), mdayaday@usm.edu.ph (M.G. Dayaday), gaalsawah@pnu.edu.sa (G.A. Alsawah).

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The investigation is limited to numerical charging under idealized boundary and material assumptions; discharge behavior and direct experimental validation of the proposed tube–fin geometry remain outside the present scope.

1. Introduction

Latent Heat Thermal Energy Storage (LHTES) systems are attractive for renewable-energy utilization, waste-heat recovery, and thermal management because of their high storage density and nearly isothermal operation [1]. However, the low thermal conductivity of conventional phase change materials (PCMs) leads to slow charging and discharging [2]. Proposed enhancement methods include fins, metal foams, nanoparticles, heat pipes, and hybrid techniques [3]. Metallic fins provide effective conductive pathways [4], although excessive fin density may restrict natural convection and reduce the available PCM volume [5]. Metal foams improve effective conductivity and temperature uniformity [6] but increase weight, fabrication complexity, and PCM displacement [7]. Nanoparticle-enhanced PCMs can also improve heat transfer [8], although agglomeration, viscosity increase, and long-term stability remain concerns. Therefore, fin-assisted configurations remain attractive because of their comparatively simple manufacture and integration [9], but their performance still depends on the interaction among conductive spreading, natural convection, geometric confinement, and PCM volume [10].

At the beginning of melting, heat transfer is predominantly conduction-controlled, and fins accelerate thermal penetration into the PCM [11]. As the molten region expands, buoyancy-driven convection becomes increasingly important [12], while fin geometry modifies thermal-boundary-layer development and convection-cell formation [13]. This behavior can produce stratified melting, particularly in vertically oriented rectangular PCM domains [14]. Smaller fin spacing shortens conductive pathways but may confine the molten PCM and weaken large-scale circulation [15], whereas tube arrangement controls heat-source distribution and interactions among neighboring thermal plumes [16]. This competition produces the established fin paradox, in which greater fin density improves conduction while restricting convection and reducing latent storage capacity [17]. Consequently, effective designs must balance heat transfer enhancement and PCM volume rather than simply maximize fin area [18,19]. Fin configuration also affects the solidification process [20], although the present study is restricted to charging. Similar conduction–convection and geometric-confinement effects have been reported for metal-foam and multi-shell PCM systems [21,22].

Recent investigations on LHTES have increasingly focused on the influence of geometrical and operating parameters on melting dynamics and storage efficiency. Recent studies have extended this direction through bio-inspired vascular fins combined with annular fins, topology-optimized fin–metal-foam structures, and machine-learning-assisted multi-objective optimization of geometrical and operating parameters [23–25]. These developments demonstrate the increasing integration of advanced heat transfer structures with numerical optimization and data-driven performance assessment. In flat-plate PCM heat exchangers, the arrangement of channels and heat transfer surfaces strongly affects thermal diffusion paths and the development of buoyancy-driven circulation within the molten PCM region [26]. The onset and intensity of natural convection are highly dependent on enclosure geometry and thermal stratification, since the upward motion of lighter molten PCM accelerates melting in the upper region while the lower part remains primarily conduction-dominated [27]. Consequently, several studies have attempted to optimize flow configuration and geometric design to improve thermal uniformity and reduce charging time. For example, non-uniform and S-shaped flow channels have been proposed to redistribute heat transfer more effectively throughout flat PCM domains and mitigate localized thermal resistance regions [28]. In fin-enhanced LHTES systems, parameters such as fin spacing, fin length, fin number,

and tube arrangement influence the balance between conductive heat spreading and convection-driven transport [29]. Similarly, the Heat Transfer Fluid (HTF) injection direction and flow configuration alter thermal plume evolution and phase-front morphology, indicating that operating conditions cannot be optimized independently from geometry [30]. Recent reviews further emphasized that the thermal performance of finned PCM systems depends on a delicate balance between conduction enhancement, natural convection preservation, and PCM volume fraction [31]. More advanced geometrical concepts, including triangular-shell configurations and petal-shaped tubes, have also been explored to improve melting uniformity and thermal spreading characteristics [32,33]. Among the studies on flat-plate PCM systems, Elleuch et al. [34] investigated the thermal performance of a flat-plate LHTES unit equipped with plate-mounted pin fins while preserving fin volume, and demonstrated that fin length, number, and shape strongly influence transient melting behavior and storage efficiency. However, their study was primarily focused on pin-fin geometrical variations and did not examine the influence of fin spacing or the coupled interaction between geometrical and operating parameters. In contrast to pin-fin-based configurations, the present study considers plate-like continuous fins that directly partition the PCM domain and strongly influence both conductive heat penetration and buoyancy-driven flow development. Consequently, fin spacing governs not only the thermal diffusion length, but also the formation and confinement of buoyancy-driven convection pathways within the molten PCM. Furthermore, unlike previous studies primarily focused on isolated geometric variations, the present work systematically investigates the coupled interaction between tube number, fin spacing, Reynolds number, and inlet temperature through a cross-parametric framework. Such interaction-driven analyses remain relatively limited for flat-plate fin-enhanced PCM heat exchangers, particularly when combined with machine-learning-assisted thermal performance prediction.

Recent investigations demonstrated that fin insertion and geometric modification can substantially alter thermal boundary-layer development and natural convection structures, leading to highly nonlinear melting behavior that depends simultaneously on fin arrangement, thermal driving force, and flow intensity [35]. Consequently, a configuration that performs favorably under one operating condition may not retain the same relative performance under different Reynolds numbers, inlet temperatures, or thermal loading conditions [36]. These limitations have motivated increasing interest in machine-learning-assisted frameworks for thermal energy storage analysis and optimization. Recent studies have integrated artificial intelligence techniques with numerical simulations to predict melting behavior in nano-finned PCM enclosures, petal-tube systems, and shell-and-tube latent heat storage units with promising accuracy and reduced computational cost [37–40]. In parallel, physics-informed and deep-learning-based approaches have shown strong capability in solving conduction-dominated and Stefan-type phase-change problems while preserving physical consistency [41,42]. Collectively, these studies demonstrate that coupling phase-change simulations with machine-learning prediction is already an established approach. The unresolved issue addressed here is therefore not the use of CFD or artificial intelligence itself, but the controlled characterization of coupled geometrical–operational effects in a continuous-fin flat-plate system under an approximately constant tube–fin material constraint. In particular, the combined influence of heat-source distribution, continuous-fin spacing, inlet temperature, and HTF Reynolds number on the redistribution of thermal resistance has not been systematically examined for the present configuration.

In this study, a three-dimensional flat-plate fin-enhanced LHTES system is numerically investigated to determine how tube number, fin

spacing, HTF inlet temperature, and Reynolds number jointly govern transient charging performance. The contribution is not the introduction of a new phase-change formulation, fin topology, or machine-learning algorithm. Rather, the study is differentiated from previous fin-enhanced LHTES investigations through three combined elements: a continuous-fin flat-plate configuration in which tube distribution and fin spacing jointly modify thermal pathways; controlled geometrical comparisons conducted while maintaining the total tube–fin material volume within a maximum deviation of 1.45%; and a relative-effect interaction analysis that quantitatively distinguishes geometrical–geometrical, geometrical–operational, and operational–operational coupling. The approximately constant-material constraint separates changes in heat-source distribution and conductive-pathway arrangement from improvements obtained simply by adding more conductive material. Finally, 38,891 transient samples extracted from 41 CFD cases are used to compare multi-output and independent single-output Cat-Boost models for interpolating liquid fraction and stored thermal energy within the sampled CFD trajectories. Accordingly, the work is positioned as a controlled geometrical–operational interaction analysis supported by a bounded surrogate proof-of-concept, rather than as a new CFD or machine-learning methodology, an extrapolative prediction framework, or a multi-objective optimization study. The scope is limited to numerical charging of a single PCM–HTF combination under idealized conditions, including constant thermophysical properties and adiabatic external boundaries that neglect axial and environmental heat losses. Discharge and cyclic behavior are not considered, the proposed geometry has not been validated through prototype measurements, and the random row-wise surrogate assessment represents interpolation within the sampled CFD trajectories rather than extrapolation to new geometries, materials, or working fluids.

2. Numerical methodology

2.1. Computational model and geometric configuration

A three-dimensional flat-plate LHTES system was numerically investigated to analyze the influence of coupled geometrical and operating parameters on the transient melting behavior of the PCM. The computational model consists of a rectangular PCM enclosure integrated with a serpentine tube–fin structure through which the HTF flows. Copper tubes and plate-like continuous fins are embedded inside the PCM domain to enhance thermal transport from the HTF into the storage medium. The study specifically examines the effects of tube number, fin spacing, inlet temperature, and Reynolds number on melting dynamics, heat storage characteristics, and thermo-hydrodynamic interactions within the PCM region under an approximately constant tube–fin material-volume constraint during the geometrical variations. The melting process is governed by the combined effects of conductive heat diffusion through the solid structure and buoyancy-driven natural convection within the molten PCM domain.

The approximately constant tube–fin volume was selected to provide a fixed-material comparison between geometrical configurations. Because the enclosure volume is unchanged, limiting the variation in copper volume also approximately preserves copper mass, material cost, PCM displacement, and available latent-storage volume. Without this constraint, increasing tube or fin number would generally add conductive material and heat transfer surface area, making it difficult to distinguish improvements caused by material addition from those caused by spatial redistribution. For the tube-number cases, the available copper is redistributed through changes in tube diameter and flow-path arrangement. For the fin-spacing cases, fin number and thickness are adjusted together so that different conductive-path distributions can be compared under approximately the same copper-material budget.

Fig. 1 presents the geometrical configurations considered in the tube-number analysis. The four arrangements maintain approximately the

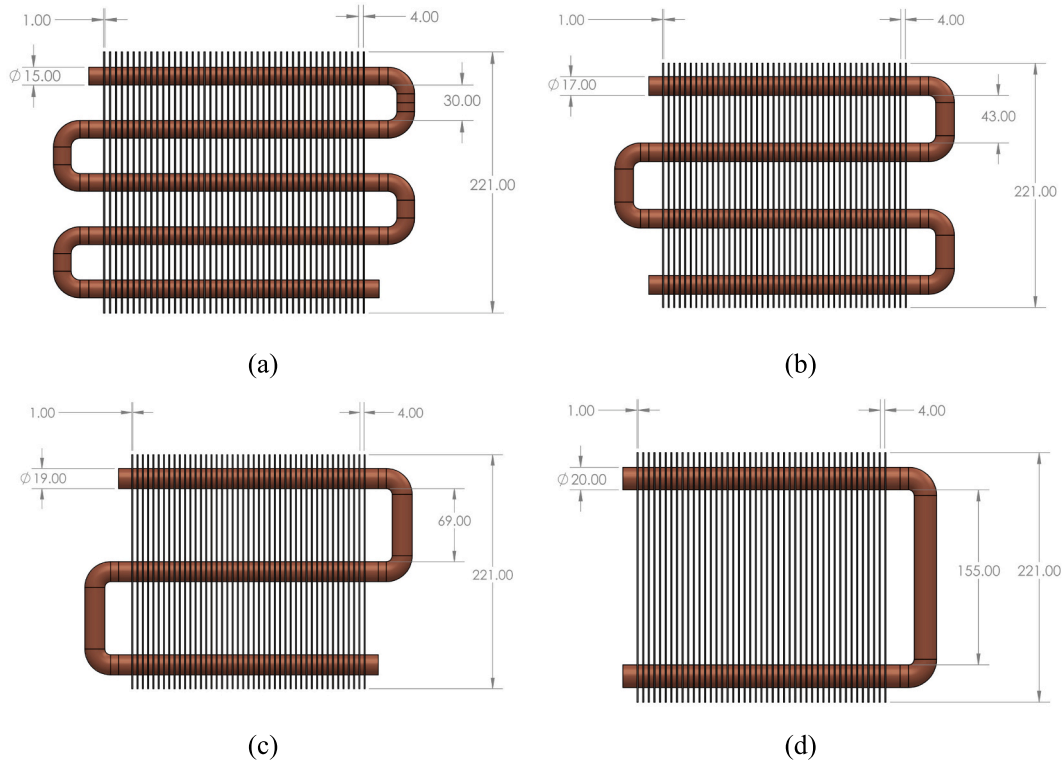


Fig. 1. Geometrical configurations of the flat-plate fin-enhanced LHTES system used in the tube-number analysis under the approximately constant tube–fin volume constraint: (a) five-tube configuration, (b) four-tube configuration, (c) three-tube configuration, and (d) two-tube configuration. The variation in tube arrangement, tube diameter, and spacing between adjacent branches modifies the heat-source distribution and the characteristic thermal diffusion length within the PCM domain.

same tube–fin volume, with a maximum deviation of 1.45%, but differ in tube diameter, hydraulic diameter, branch spacing, and HTF flow-path length. Consequently, changing the tube number simultaneously modifies the spatial distribution of the tube–fin surfaces within the PCM and the HTF-side thermo-hydraulic characteristics. The tube-number comparison is therefore interpreted as a coupled geometrical effect rather than as an isolated heat-source-distribution effect.

The total tube–fin volumes range from 174,085 to 176,650 mm³, corresponding to a maximum deviation of 1.45% from the five-tube reference configuration. This constraint limits differences in the amount of copper but does not independently isolate heat-source distribution. As summarized in Table 1, the HTF-side wetted area remains nearly constant, varying by only approximately 1.3%, whereas the hydraulic diameter decreases from 19 to 14 mm and the flow-path length increases from 4.433 to 6.009 m. The estimated mean HTF-side convection coefficient consequently increases from approximately 167 to 205 Wm⁻² K⁻¹, while L/D_h increases substantially. Thus, the tube-number effect combines PCM-side heat-source redistribution with changes in HTF-side convection and flow resistance. Accordingly, the constant-volume condition should be interpreted as a controlled material-budget constraint rather than as an assumption that tube number acts independently. It improves comparability of the PCM-side thermal response, while the accompanying changes in hydraulic diameter, flow-path length, HTF-side convection, and flow resistance remain part of the coupled geometrical effect.

A systematic parametric study was conducted to evaluate the influence of both geometrical and operating conditions on the melting performance of the flat-plate fin-enhanced LHTES system. As summarized in Table 2, the investigation was divided into two stages. In the first stage, fourteen base configurations were examined to independently assess the effects of tube number, fin spacing, inlet temperature, and Reynolds number on the transient melting behavior and thermal storage characteristics of the PCM domain. During this stage, only one parameter was varied at a time while the remaining parameters were maintained constant to isolate the contribution of each variable to the overall thermal response.

To provide a fixed-material comparison between geometrical configurations, the tube–fin volume was maintained within a maximum deviation of 1.45%. This constraint limits changes in copper usage but does not independently isolate heat-source distribution or eliminate configuration-dependent HTF-side effects. Following the single-parameter analysis, a second cross-parametric investigation was performed to examine the coupled interactions between geometrical and operating conditions. The cross-parametric matrix is summarized in Table 3 and was designed to evaluate whether the trends identified from isolated parameter sweeps remain valid when heat-source distribution, fin spacing, thermal driving force, and HTF-side convection are varied simultaneously. This additional matrix is essential because the thermal response of confined PCM systems is not governed by independent parameter effects, but by the coupled redistribution of thermal resistance between the HTF, tube–fin network, and molten PCM region. This stage was specifically intended to evaluate the robustness of the favorable configurations identified from the single-parameter analysis under different thermal and flow conditions and to reveal the nonlinear thermo-hydrodynamic interactions governing the melting process within the PCM domain.

Table 1

Geometrical and HTF-side characteristics of the tube-number configurations under the approximately constant tube–fin volume constraint. The convection coefficients are nominal values estimated using the Hausen developing-flow correlation at $Re = 2000$; bend-induced secondary-flow effects are not included.

Tubes	Total volume (mm ³)	Volume deviation (%)	D _h (mm)	Flow length (m)	A _{HTF} (m ²)	$\dot{m}$ (kg s ⁻¹)	Estimated $\bar{h}_{HTF}$ (Wm ⁻² K ⁻¹)	L/D _h
2	175,580	-0.61	19	4.433	0.2646	0.01451	167.0	233.3
3	174,085	-1.45	18	4.622	0.2614	0.01379	173.1	256.8
4	174,915	0.98	16	5.214	0.2621	0.01226	186.8	325.9
5	176,650	Ref.	14	6.009	0.2643	0.01073	205.0	429.2

The thermophysical properties employed in the numerical simulations are listed in Table 4. Water was used as the HTF, RT35 as the PCM, and copper as the tube–fin material. A reference/design temperature of 70 °C, corresponding to the midpoint of the investigated HTF inlet-temperature range, was selected for the water properties. These properties were held constant in all cases to maintain a common property basis and Reynolds-number definition and to isolate the influence of the imposed inlet-temperature difference from simultaneous changes in viscosity, density, thermal conductivity, and heat capacity. The PCM and solid components were assumed to be homogeneous and isotropic. The Boussinesq approximation was applied only to the liquid PCM, for which density variation was retained in the buoyancy term while the remaining thermophysical properties were treated as constant.

The Reynolds number of the HTF was defined as

$$Re = \frac{\rho_{HTF} u_{in} D_h}{\mu_{HTF}} \quad (1)$$

where ρ_{HTF} , u_{in} , D_h , and μ_{HTF} are the HTF density, inlet velocity, tube hydraulic diameter, and dynamic viscosity, respectively. The fixed water properties at 70 °C provide a controlled comparison in which the nominal Reynolds number remains defined on the same property basis for all inlet-temperature cases. Consequently, the reported temperature effect primarily represents the influence of the imposed thermal driving force under the adopted design assumption. This treatment does not reproduce the temperature dependence of water viscosity, density, thermal conductivity, heat capacity, or Prandtl number. Therefore, the absolute melting times, outlet-temperature histories, and HTF-side thermal resistance may differ from those of a variable-property system, particularly near the 60 and 80 °C limits. The inlet-temperature results should accordingly be interpreted as fixed-property parametric trends rather than as a complete variable-property performance assessment.

The boundary and initial conditions employed in the present simulations are summarized in Table 5. The HTF enters the tubes with a prescribed velocity corresponding to the selected Reynolds number and a constant inlet temperature determined by each operating case. A pressure outlet condition is imposed at the tube exits, while all solid–fluid interfaces satisfy the no-slip condition. Thermal coupling is applied between the HTF, tube wall, fins, and PCM domains to ensure continuity of temperature and heat flux across the interfaces. The external walls of the flat-plate enclosure are treated as adiabatic, such that heat transfer occurs exclusively through the tube–fin structure into the PCM domain. Initially, the PCM is assumed to be completely solid and maintained at a uniform temperature below its melting range. Gravity acts in the vertical direction with $g = 9.81 \text{ ms}^{-2}$, and buoyancy effects within the molten PCM are modeled using the Boussinesq approximation with a reference temperature of $T_{ref} = 35 \text{ °C}$.

2.2. Governing equations

The melting processes within the PCM domain were simulated using the enthalpy–porosity formulation, in which the solid, liquid, and mushy regions are treated simultaneously within a fixed computational domain. In this approach, the motion of the solid–liquid interface is resolved implicitly through the local liquid fraction without explicit interface tracking [45,46]. The liquid fraction, denoted by l_f , varies

Table 2

Parametric matrix used for the single-parameter analysis of the flat-plate fin-enhanced LHTES system, including tube number, fin spacing, HTF inlet temperature, and Reynolds number.

Group	Case	N	Fin spacing (mm)	HTF inlet temperature (°C)	Re	Note
Tube-number study (N)	1-4	2, 3, 4, 5	5	80	2000	Coupled tube-number effect
Fin spacing study (f_s)	5-8	5	5, 7.5, 10, 15	80	2000	Effect of fin spacing
Inlet temperature study (T_{in})	9-11	5	5	60, 70, 80	2000	Effect of thermal driving force
Reynolds-number study (Re)	12-14	5	5	80	500, 1500, 2000	Effect of HTF-side convection
Baseline		5	5	80	2000	Reference configuration

Table 3

Cross-parametric simulation matrix for assessing coupled geometrical–operational effects in the flat-plate fin-enhanced LHTES system. The matrix was constructed to examine interactions among heat-source distribution, fin spacing, thermal driving force, and HTF-side convective resistance beyond the isolated single-parameter trends.

Case group	Tube number	Fin spacing (mm)	HTF Inlet temperature (°C)	Re
Cross-set A	2	5	60/65/75/80	500/ 875/ 1625/ 2000
Cross-set B	2	15	60/65/75/80	500/ 875/ 1625/ 2000
Cross-set C	5	5	60/65/75/80	500/ 875/ 1625/ 2000
Cross-set D	5	15	60/65/75/80	500/ 875/ 1625/ 2000

Table 4

Thermophysical properties of the PCM, copper tube–fin structure, and water HTF used in the numerical simulations. Water properties were evaluated at 70 °C and treated as constant for all operating cases.

Property	Copper ^[43]	PCM (RT35) ^[33,44]	Water HTF (70 °C)	Unit
Mean density (ρ)	8978	815	977.8	kg·m ⁻³
Specific heat capacity (C_p)	381	2000	4190	J·kg ⁻¹ ·K ⁻¹
Thermal conductivity (k)	387.6	0.2	0.665	W·m ⁻¹ ·K ⁻¹
Latent heat of fusion (H_f)	-	160,000	-	J·kg ⁻¹
Thermal expansion coefficient (β)	-	0.0006	-	K ⁻¹
Dynamic viscosity (μ)	-	0.023	0.000486	Pa·s
Melting temperature range	-	32–38	-	°C

continuously between 0 and 1, corresponding to fully solid and fully liquid PCM states, respectively.

Mass conservation for the incompressible PCM is expressed as:

$$\nabla \cdot u = 0 \quad (2)$$

where u represents the velocity vector within the liquid PCM region.

The transient momentum transport is governed by the Navier–Stokes equations combined with buoyancy effects through the Boussinesq approximation [47]:

$$\rho \left(\frac{\partial u}{\partial t} + u \cdot (\nabla u) \right) = -\nabla P + \mu \nabla^2 u - \rho \beta (T - T_{ref}) g - S_m \quad (3)$$

where ρ is the density, P is the pressure, μ is the dynamic viscosity, β is the thermal expansion coefficient, and T_{ref} is the reference temperature. The buoyancy term is formulated according to the Boussinesq approximation, where the direction of g defines the sign of the buoyancy force. The term S_m represents the mushy-zone momentum resistance used to

Table 5

Boundary and initial conditions applied to the HTF, PCM, tube–fin structure, and external walls of the flat-plate LHTES model.

Region/Boundary	Applied specification	Numerical implementation
HTF inlet	Prescribed flow rate	Velocity inlet corresponding to the selected Reynolds number
HTF inlet	Temperature	60, 70, 80 °C
HTF outlet	Outflow pressure condition	Gauge pressure fixed at 0 Pa
HTF–tube interface	No-slip wall with thermal coupling	Velocity set to zero relative to the tube wall; heat transfer solved through conjugate coupling
Tube wall–PCM interface	Coupled solid–PCM heat transfer	Temperature and heat flux continuity imposed between the copper tube wall and PCM
Flat-plate inner surface	Coupled solid–PCM heat transfer	Temperature and heat flux continuity imposed between the copper fins and PCM
Flat-plate outer walls	Thermally insulated boundary	Zero normal heat flux imposed, $q'' = 0$
PCM initial condition	Uniform initial temperature	PCM initialized as solid at 30 °C
HTF–wall and PCM–solid interfaces	No-slip	Applied at all solid boundaries

suppress velocity in the solid and partially melted PCM regions [48,49].

To suppress fluid motion inside the solid and partially solidified regions, the mushy zone is modeled as a porous medium by introducing a momentum damping source term. The resistance source is defined as [50]:

$$S_m = -A_m \frac{(1 - l_f)^2}{l_f^3 + \epsilon} u \quad (4)$$

where A_m is the mushy-zone constant, l_f is liquid fraction, and $\epsilon = 10^{-5}$ is a small numerical parameter introduced to avoid singularity as $l_f \rightarrow 0$. In the present simulations, the mushy-zone coefficient was specified as $A_m = 1 \times 10^5 \text{ kg m}^{-3} \text{ s}^{-1}$, consistent with values commonly adopted in PCM phase-change simulations. This formulation progressively attenuates the velocity field as the PCM solidifies [51].

The thermal field is solved using the enthalpy-based energy Eq. [52].

$$\rho C_p \left(\frac{\partial T}{\partial t} + u \cdot \nabla T \right) = \nabla \cdot (k \nabla T) - S_L \quad (5)$$

where C_p is the specific heat capacity, k is the thermal conductivity, and S_L represents the latent heat source term associated with phase transition. The enthalpy–porosity formulation combines sensible and latent heat contributions into a unified energy framework, enabling stable simulation of melting on a stationary grid [53].

$$S_L = \rho H_f \frac{\partial l_f}{\partial t} \quad (6)$$

where H_f denotes the latent heat of fusion of the PCM. The liquid fraction

is evaluated according to the local temperature using the following piecewise relation:

$$l_f = \begin{cases} 0 & \text{if } T < T_s \\ \frac{T - T_s}{T_l - T_s} & \text{if } T_s < T < T_l \\ 1 & \text{if } T > T_l \end{cases} \quad (7)$$

where T_s and T_l are the solidus and liquidus temperatures, respectively. A linear interpolation is employed within the mushy region to ensure smooth phase transition and numerical stability [54]. To compare the thermal performance of different configurations, the total stored thermal energy Q_{st} is calculated as:

$$Q_{st} = m(E_e - E_i) \quad (8)$$

where E_i and E_e are the initial and final specific energies of the PCM, respectively, and m is the PCM mass. To compare the thermal performance of different configurations, the average heat storage rate $\dot{Q}_{avg}$ is defined as:

$$\dot{Q}_{avg} = \frac{Q_{st}}{t_m} \quad (9)$$

where t_m represents the total melting time. The average heat storage rate is therefore evaluated from the stored thermal energy and the total melting duration.

To provide a quantitative global measure of the changing thermal resistance, an apparent time-averaged charging resistance was defined as:

$$R_{ch,app} = \frac{T_{in} - T_m}{\dot{Q}_{avg}} \quad (10)$$

where $T_m = 35^\circ\text{C}$ and $\dot{Q}_{avg}$ is the average heat-storage rate over the complete melting period. The nominal HTF-side convective resistance was estimated as:

$$R_{HTF} = \frac{1}{\bar{h}_{HTF} A_{HTF}} \quad (11)$$

$R_{ch,app}$ is a global performance indicator incorporating the combined transient effects of HTF-side convection, tube-fin conduction, PCM conduction, natural convection, sensible heating, and latent heat absorption. It should not be interpreted as a steady-state resistance or used to obtain separate conductive and convective PCM resistances by direct subtraction.

Because the HTF inlet is located 0.180 m above the outlet, the raw static-pressure difference includes both gravitational head and irreversible flow loss. The mechanical pressure loss across the serpentine HTF passage was therefore calculated from the area-weighted average static pressures as

$$\Delta p_{loss} = p_{in} - p_{out} + \rho_{HTF} g(z_{in} - z_{out}) \quad (12)$$

The inlet and outlet cross-sections have the same diameter within each configuration; therefore, their area-averaged velocity-head terms cancel. The corresponding ideal hydraulic power required to overcome the component-level flow loss was evaluated as

$$P_{hyd} = \Delta p_{loss} \dot{V} \quad (13)$$

and the hydraulic work accumulated over the complete melting period was calculated as

$$W_{hyd} = P_{hyd} t_m \quad (14)$$

The thermal-storage gain per unit hydraulic work was defined as

$$\psi_{pump} = \frac{Q_{st}}{W_{hyd}} = \frac{\dot{Q}_{avg}}{P_{hyd}} \quad (15)$$

The calculated hydraulic power represents the ideal fluid power required to overcome losses within the modeled serpentine passage. Pump and motor efficiencies, external piping losses, and auxiliary-system power are not included.

The present formulation assumes that the solid PCM remains stationary and that the mushy region behaves as an isotropic porous medium with flow resistance proportional to the local liquid fraction. Although phenomena such as solid fragmentation, density-driven solid displacement, or interface instability are not captured explicitly, the enthalpy-porosity approach has been widely validated and remains one of the most reliable and computationally efficient methods for engineering-scale simulation of PCM melting processes.

To characterize the nominal buoyancy potential within the PCM domain, a height-based Rayleigh number was also evaluated as

$$Ra_H = \frac{g\beta(T_{in} - T_m)H^3}{\nu\alpha} \quad (16)$$

where $H = 0.221$ m is the enclosure height, $T_m = 35^\circ\text{C}$ is the midpoint of the PCM melting range, $\nu = \mu/\rho$ is the kinematic viscosity, and $\alpha = k/(\rho c_p)$ is the thermal diffusivity. This definition uses the inlet-to-melting temperature difference as a nominal thermal driving scale. Because the tube-fin surface temperature evolves during conjugate heat transfer, Ra_H should be interpreted as a comparative buoyancy-driving parameter rather than a local transient Rayleigh number.

To compare the HTF-side characteristics of the tube-number configurations, the total flow-path length was reconstructed from the tube material volume and annular cross-sectional area. The HTF-side wetted area was then evaluated as $A_{HTF} = \pi D_h L_{HTF}$. Because the tube-number cases were evaluated at $Re = 2000$, a nominal mean convection coefficient was estimated using the Hausen relation for thermally developing internal flow, $\bar{Nu} = 3.66 + [0.0668 Gz / (1 + 0.04 Gz^{2/3})]$ where $Gz = Re Pr D_h / L_{HTF}$, followed by $\bar{h}_{HTF} = \bar{Nu} k_{HTF} / D_h$. These estimates provide a consistent comparative scale; the absolute values do not include additional enhancement caused by the serpentine bends.

For the fin-spacing comparison, a nominal spacing-based Rayleigh number was additionally defined as:

$$Ra_s = \frac{g\beta(T_{in} - T_m)s^3}{\nu\alpha} = Ra_H \left(\frac{s}{H}\right)^3 \quad (17)$$

where s is the distance between adjacent fins. Ra_s provides a comparative measure of the buoyancy-driving scale available between neighboring fins. It does not represent a local transient Nusselt number or directly quantify convection-cell velocity or convective heat flux.

3. Computational setup and model verification

3.1. Numerical solution strategy

The numerical simulations were performed using ANSYS Fluent 2024 R1 to solve the transient conjugate heat transfer and phase-change process in the fin-enhanced LHTES system. The enthalpy-porosity formulation was adopted to capture melting of the PCM, while buoyancy-driven flow in the liquid PCM region was modeled using the Boussinesq approximation. The computational model included the PCM domain, solid fins, tube walls, and the HTF region, allowing the thermal interaction between the HTF, copper structures, and PCM to be resolved simultaneously.

The boundary and initial conditions used in the simulations are summarized in Table 5. The HTF inlet was prescribed as a velocity inlet based on the Reynolds number of each case, while a pressure outlet was imposed at the tube exits. Thermal coupling was applied at all

solid–fluid interfaces to ensure continuity of temperature and heat flux between the HTF, tube wall, fins, and PCM. The external flat-plate walls were treated as adiabatic, so that heat transfer occurred only through the tube–fin structure.

The governing equations were discretized using a pressure-based transient solver. Pressure–velocity coupling was handled using the SIMPLE algorithm, which provides stable convergence for incompressible flow with buoyancy effects. Spatial gradients were evaluated using the Green–Gauss cell-based method. The PRESTO! scheme was used for pressure interpolation because of its suitability for buoyancy-influenced flows, while the QUICK scheme was employed for momentum and energy discretization to reduce numerical diffusion and improve resolution of steep temperature gradients near the moving phase-change front. A first-order implicit scheme was used for temporal discretization to ensure stable advancement of the transient melting process. The influence of temporal discretization on the predicted liquid-fraction evolution was subsequently assessed through the time-step independence study, confirming that the selected time step preserved the transient phase-change response with negligible deviation.

At each time step, convergence was monitored using residual criteria and the stability of integral quantities, including liquid fraction, average PCM temperature, and stored energy. The residual tolerances were set to 10^{-4} for the continuity and momentum equations and 10^{-6} for the energy equation. These numerical settings are consistent with commonly adopted discretization strategies for transient buoyancy-driven PCM melting simulations. The mesh and time-step independence analyses were performed for the baseline case with five tubes, 5 mm fin spacing, HTF inlet temperature of 80 °C, and $Re = 2000$, unless otherwise stated.

Mesh independence and time-step sensitivity studies were performed using the temporal evolution of the liquid fraction as the main convergence criterion. For the mesh-sensitivity analysis, the solution obtained with 1.0 million cells was taken as the reference. As shown in Fig. 2(a), the coarsest mesh of 0.4 million cells underpredicts the melting rate during most of the phase-change process, indicating that the thermal boundary layer and the solid–liquid interface are not sufficiently resolved. Increasing the mesh density to 0.6 million cells substantially reduces this deviation, while the 0.8 million-cell mesh produces a liquid-fraction history very close to that of the 1.0 million-cell case. Quantitatively, the 0.8 million-cell mesh gives a mean absolute error of 9.61×10^{-4} , an RMSE of 2.53×10^{-3} , and a maximum liquid-fraction deviation of 8.43×10^{-3} relative to the 1.0 million-cell solution. The predicted time to reach liquid fraction (l_f) = 0.99 changes from 449.49 s for the 1.0 million-cell mesh to 456.44 s for the 0.8 million-cell mesh, corresponding to a deviation of approximately 1.55%. By comparison, the 0.4

and 0.6 million-cell mesh cases give deviations of approximately 4.27% and 1.73%, respectively. Therefore, the 0.8 million-cell mesh was selected as a suitable compromise between numerical accuracy and computational cost.

The time-step independence study was then conducted using the selected 0.8 million-cell mesh. As shown in Fig. 2(b), the liquid-fraction curves obtained with time steps of 0.1 s, 0.2 s, and 0.4 s almost overlap throughout the melting process, with only a small deviation visible in the magnified region. Taking the 0.1 s case as the reference, the 0.2 s time step gives a mean absolute error of 3.48×10^{-4} , an RMSE of 5.19×10^{-4} , and a maximum liquid-fraction deviation of only 1.01×10^{-3} . The corresponding time to reach $l_f = 0.99$ is 456.45 s for 0.1 s and 456.44 s for 0.2 s, giving a negligible relative difference of less than 0.01%. Although the 0.4 s time step also follows the overall trend, its maximum liquid-fraction deviation increases to 2.95×10^{-3} . Hence, a time step of 0.2 s was adopted in the final simulations because it preserves the transient melting behavior and phase-front evolution with negligible temporal discretization error, while avoiding the additional computational cost associated with the smaller 0.1 s time step.

3.2. Validation

To verify the accuracy of the present numerical framework, the predicted melting behavior was validated against the experimental measurements reported by Kamkari et al. [55] and the corresponding numerical study of Kamkari and Amlashi [56]. In these benchmark studies, the melting process of a PCM confined within a two-dimensional rectangular enclosure was investigated under natural-convection-dominated conditions. The enclosure was differentially heated from one vertical wall while the opposite wall was maintained at a lower temperature, allowing the melting front evolution to be governed by the coupled interaction between conductive heat transfer and buoyancy-driven flow inside the molten PCM region. The experimental work of Kamkari et al. [55] focused on visualizing the transient melting process and evaluating the effect of enclosure inclination angle on convection-induced melting characteristics, whereas the subsequent numerical study by Kamkari and Amlashi [56] provided detailed numerical verification of the phase-front evolution and liquid-fraction development within the same configuration.

The validation case considered in the present study reproduced the thermophysical properties, initial conditions, and thermal boundary conditions reported in Refs. [55, 56]. The PCM was initially maintained below the melting temperature and heated through a constant-temperature vertical wall, while the remaining boundaries were

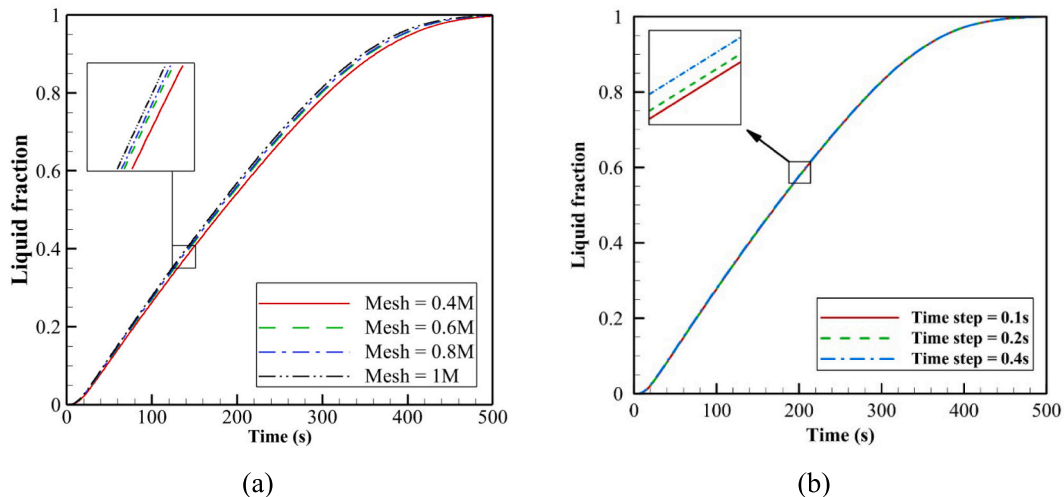


Fig. 2. Mesh independence and time-step sensitivity analyses based on liquid-fraction evolution: (a) influence of mesh resolution and (b) influence of temporal step size.

treated as adiabatic. The melting evolution was simulated using the enthalpy–porosity formulation combined with the Boussinesq approximation to account for density-driven natural convection within the liquid PCM region. The temporal evolution of the melt volume fraction (MVF) obtained in the present simulations was then compared with the corresponding experimental and numerical benchmark data.

Fig. 3 compares the variation of melt volume fraction with time between the present simulations and the reference studies. Overall, excellent agreement is observed throughout the melting process. The numerical predictions closely follow both the experimental measurements of Kamkari et al. [55] and the numerical results of Kamkari and Amlashi [56], with only minor deviations appearing during the intermediate melting stage, where natural convection becomes increasingly dominant. These small differences can be attributed to uncertainties associated with experimental measurements, mesh discretization, and the sensitivity of buoyancy-driven flow structures during transient phase change. Nevertheless, the overall agreement confirms that the adopted numerical methodology accurately captures the coupled conduction–convection melting behavior of PCM systems.

To provide a quantitative assessment of the validation, the melt volume fraction curve was compared with the present numerical prediction. The estimated mean absolute error, root-mean-square error, and maximum absolute deviation were approximately 0.012, 0.013, and 0.028 in melt volume fraction, respectively. The corresponding mean absolute percentage error was approximately 3.3%, with a coefficient of determination of about 0.998.

The largest deviation occurs during the intermediate melting stage, where the phase front is particularly sensitive to buoyancy-driven circulation. The observed agreement supports the ability of the enthalpy–porosity formulation to reproduce conduction–convection-controlled PCM melting. However, the benchmark cavity does not include forced HTF flow, conjugate heat transfer through a serpentine copper tube–fin structure, or the associated solid–fluid thermal coupling. Therefore, this comparison validates the adopted phase-change formulation and its numerical implementation but does not directly validate the absolute thermal performance or geometry-dependent trends of the proposed configuration. Direct prototype measurements of the serpentine tube–fin storage unit remain necessary for geometry-specific validation.

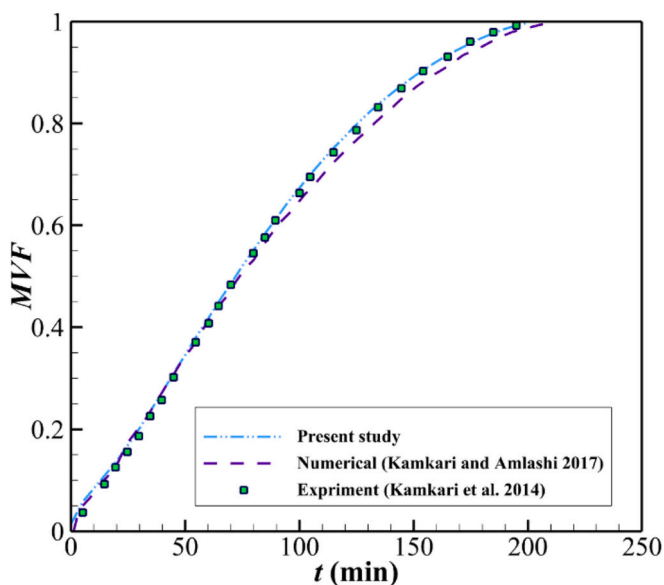


Fig. 3. Validation of the present enthalpy–porosity formulation against the experimental measurements of Kamkari et al. and the numerical results of Kamkari and Amlashi [55,56] based on melt-volume-fraction evolution.

4. Results and discussion

4.1. Influence of tube number on melting dynamics

Fig. 4 illustrates the liquid-fraction evolution for the four tube-number configurations. During the early conduction-dominated stage, increasing the tube number reduces the average PCM distance from the tube–fin surfaces and distributes heat more uniformly throughout the enclosure. However, Table 1 shows that the associated HTF-side wetted area changes by only approximately 1.3%, whereas the estimated convection coefficient increases by 22.8% because of the reduced hydraulic diameter. The observed enhancement therefore arises primarily from shorter PCM conduction paths and more distributed heat delivery, assisted by reduced HTF-side convective resistance, rather than from a substantial increase in total heat transfer area.

The resistance indicators provide a quantitative scale for this interpretation. Increasing the tube number from two to five decreases the nominal HTF-side resistance from approximately 0.0226 to 0.0185 K W^{−1}, corresponding to an 18.4% reduction. Over the same range, the apparent overall charging resistance decreases from 0.2425 to 0.1056 K W^{−1}, corresponding to a 56.5% reduction. The substantially larger change in $R_{ch,app}$ than in R_{HTF} indicates that the charging enhancement cannot be attributed solely to the estimated HTF-side convection coefficient. However, the remaining resistance cannot be uniquely divided into tube–fin conduction, PCM conduction, and natural-convection components using the retained integral data.

As melting progresses, the governing heat transfer mechanism gradually transitions from conduction-dominated transport toward convection-assisted melting. The growth and interaction of neighboring molten regions become increasingly important because they determine the formation of buoyancy-driven circulation pathways within the liquid PCM. In the higher tube-number configurations, earlier coalescence of adjacent melt zones promotes more distributed thermal stratification and enhances upward transport of thermal energy by natural convection. This behavior is particularly visible at $t = 200$ and 300 s, where the upper regions of the PCM domain melt more rapidly because of buoyancy-induced flow structures. In contrast, the $N = 2$ configuration maintains isolated melting zones for a significantly longer duration, limiting large-scale convective interaction and forcing heat transfer to remain predominantly conduction-controlled over most of the charging period. The delayed interaction between thermal plumes therefore becomes a major source of melting-rate deterioration in low tube-density configurations.

The influence of tube number on the global thermal response is further quantified in Figs. 6 and Table 6 through the temporal evolution of liquid fraction, average PCM temperature, and HTF outlet temperature. Increasing the tube number from 2 to 3 reduces the total melting time from 749 s to 391 s, corresponding to a reduction of approximately 47.8%, while the average heat storage rate increases by nearly 88.8%, from 185.56 W to 350.28 W. This substantial improvement confirms that the system initially operates in a strongly diffusion-limited regime, where increasing heat-source density dramatically reduces thermal resistance within the PCM domain. However, the incremental enhancement progressively decreases at higher tube numbers. Interestingly, the transition from four to five tubes does not produce a monotonic reduction in melting time: the four-tube configuration reaches complete melting in 332 s, whereas the five-tube case requires 345 s, although its average heat storage rate remains slightly higher. This indicates that, beyond a sufficiently distributed heat-source network, further subdivision of the PCM domain does not necessarily accelerate full melting. Instead, the additional tube passage modifies the local thermal-field overlap and can leave small residual unmelted regions that control the final stage of melting. Therefore, within the investigated tube-number range, the five-tube configuration provides the highest average heat storage rate, whereas the four-tube configuration gives the shortest complete-melting time. This distinction indicates that the

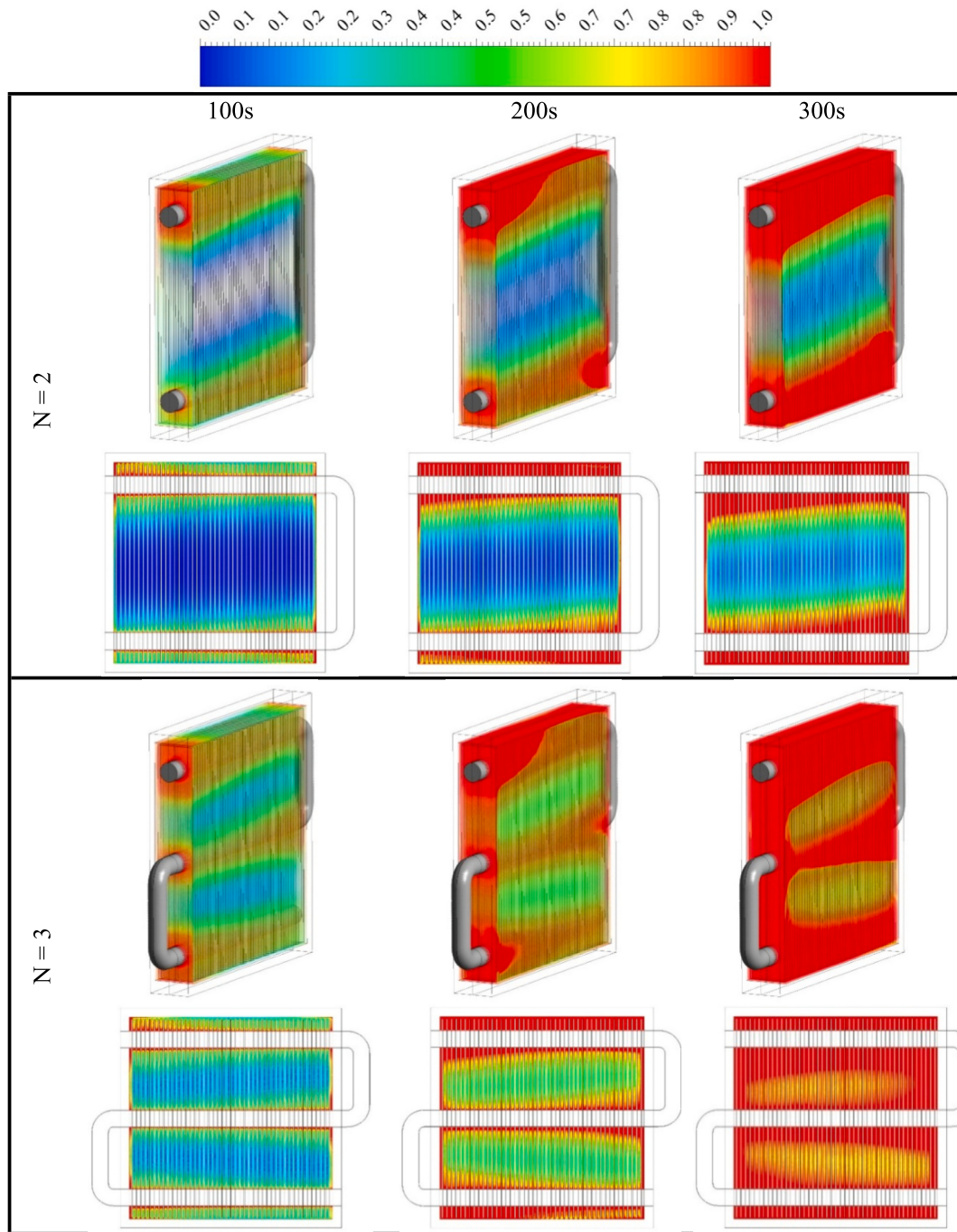


Fig. 4. Liquid-fraction and melt-front contours for different tube-number configurations ($N = 2$ – 5) at 100, 200, and 300 s, showing the effects of heat-source distribution on phase-front propagation, thermal-field overlap, and residual unmelted PCM regions.

relative preference among the tested configurations depends on whether the selected performance metric is average charging rate or complete melting time. It should be noted, however, that this comparison is based on thermal charging metrics only; pressure drop and pumping-power requirements may alter the practical thermo-hydraulic preference among the tube-number configurations.

The temperature contours shown in Fig. 5 support this interpretation. The higher tube-number configurations produce earlier overlap of thermal influence regions, resulting in a more spatially uniform temperature field and weaker thermal isolation of peripheral PCM regions. Meanwhile, the lower tube-number cases maintain steep thermal

gradients throughout most of the charging process, indicating persistent conductive resistance between the heated surfaces and the unmelted PCM. The outlet temperature behavior shown in Fig. 6(c) further reflects the same mechanism. Configurations with larger tube numbers exhibit earlier outlet-temperature recovery because the PCM approaches thermal equilibrium more rapidly and progressively loses its capacity to absorb latent heat. In contrast, the prolonged suppression of outlet temperature in the low tube-number cases indicates sustained latent heat absorption over an extended charging period.

Tube number affects charging through coupled PCM-side and HTF-side mechanisms. Increasing the number of passages shortens the

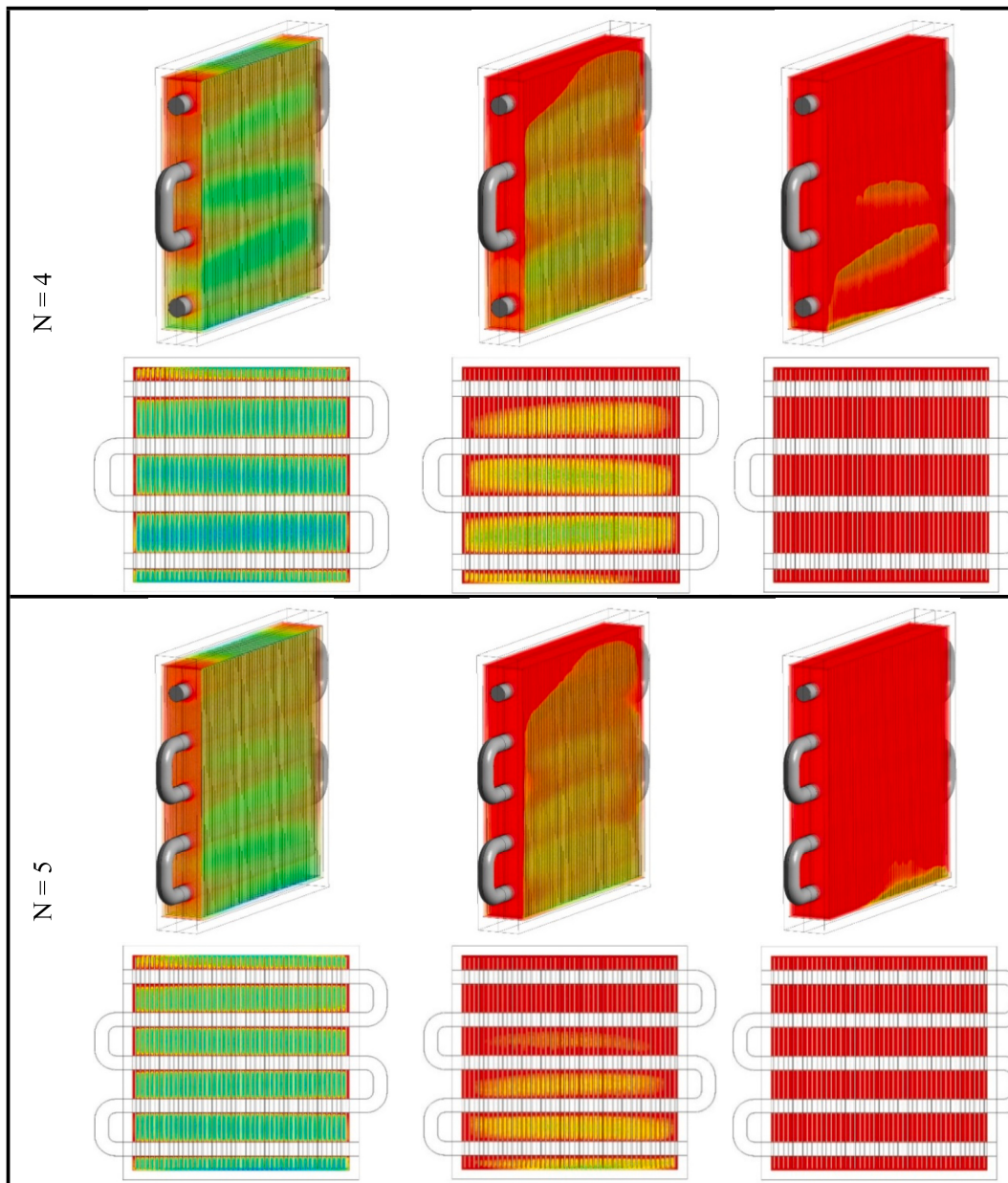


Fig. 4. (continued).

Table 6
Effect of tube number on melting time and average heat storage rate.

Configurations	Melting time (s)	Average heat storage rate (W)
$N = 2$	749	185.56
$N = 3$	391	350.28
$N = 4$	332	416.43
$N = 5$	345	425.94

characteristic conduction distance and promotes earlier interaction between neighboring melting regions. Simultaneously, the reduced hydraulic diameter increases the nominal HTF-side convection coefficient, although the longer flow path and larger L/D_h indicate increased flow resistance. Because the wetted heat transfer area remains nearly unchanged, the marked improvement from two to four tubes is attributed mainly to heat-source redistribution and reduced PCM conduction resistance, with an additional contribution from stronger HTF-side convection. The competing thermo-hydraulic effects also explain why

the five-tube configuration gives the highest average charging rate but does not produce the shortest complete-melting time.

All tube-number cases were evaluated at $T_{in} = 80^\circ\text{C}$ and therefore share the same nominal Rayleigh number, $Ra_H = 8.26 \times 10^8$. Consequently, the differences observed at equal charging times cannot be attributed to a change in the imposed buoyancy-driving scale. Instead, they arise from the redistribution of heat sources, shorter conductive pathways, and configuration-dependent development of connected liquid regions. The revised melt-front and temperature contours in Figs. 4 and 5 make this distinction visible: increasing tube number primarily improves spatial thermal penetration, while buoyancy redistributes heat after sufficiently large molten pathways have formed.

This result indicates that the thermally favorable tube number depends on the selected performance objective. If minimum complete-melting time is the primary target, the four-tube configuration is preferable within the investigated range. If maximum average heat storage rate is prioritized, the five-tube configuration is slightly more favorable. Therefore, the selection of tube number within the investigated range

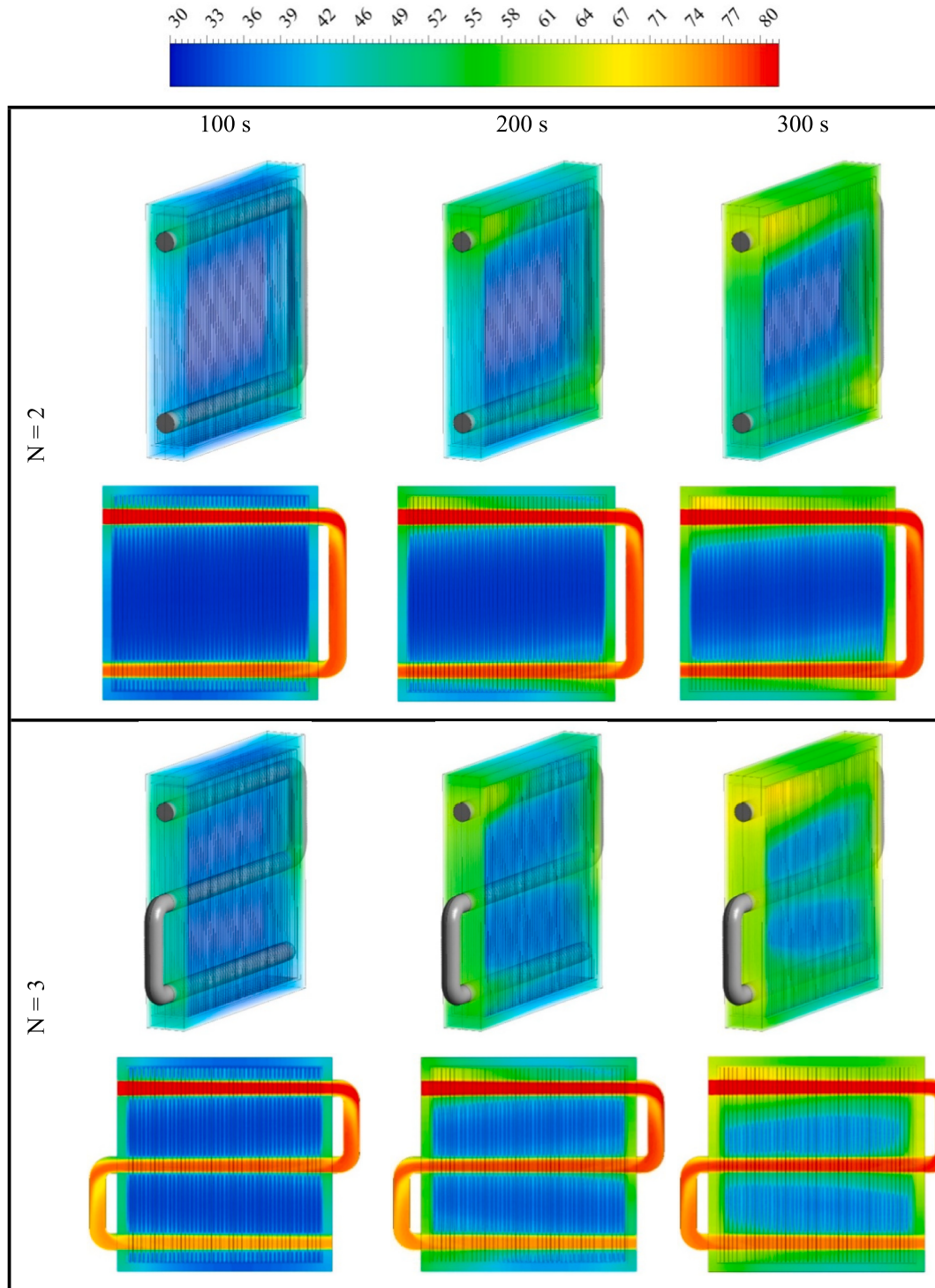


Fig. 5. Temperature contours for different tube-number configurations ($N = 2$ –5) at common charging times of 100, 200, and 300 s, illustrating the effects of tube distribution on thermal penetration, temperature uniformity, and residual low-temperature regions. All panels use an identical temperature scale and viewing orientation to enable direct comparison at common charging times.

should not be based on a single thermal metric, and the preferred configuration depends on whether the design priority is complete melting time or average charging rate.

4.2. Effect of fin spacing on net charging performance

The thermal response of the LHTEs system exhibits strong sensitivity

to fin spacing because the fins simultaneously influence conductive heat spreading and buoyancy-driven flow development within the PCM domain. Fig. 7 demonstrates that reducing the spacing between adjacent plate-like fins substantially accelerates the melting process during the early and intermediate charging stages. At small fin spacing, the conductive thermal network becomes more spatially distributed, allowing heat to penetrate the PCM domain more uniformly and

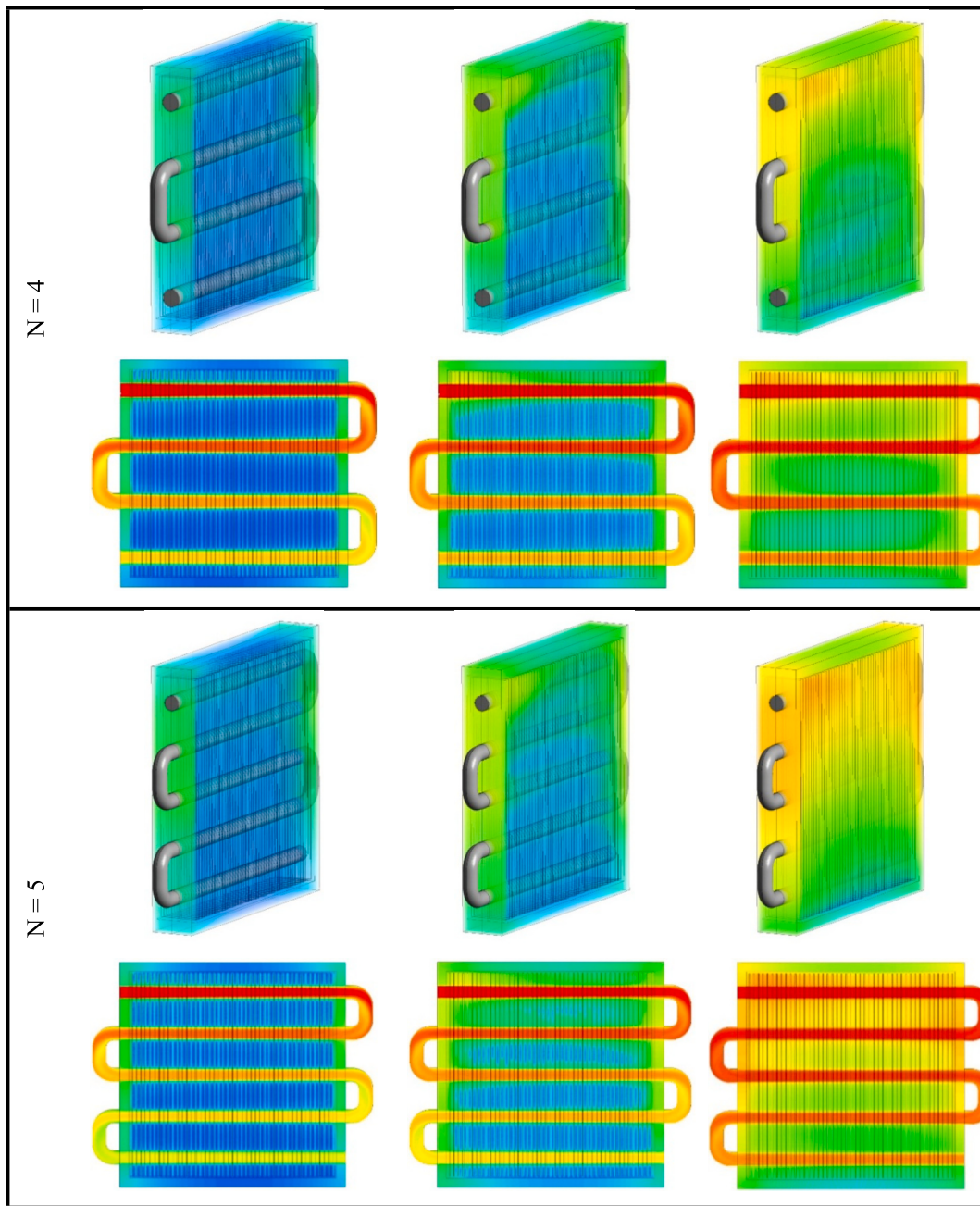


Fig. 5. (continued).

reducing the existence of thermally isolated regions. As a result, the melt front propagates more rapidly away from the tube–fin structure, particularly during the conduction-dominated stage where heat transfer is controlled primarily by local thermal diffusion through the solid PCM.

Fin spacing also changes the characteristic dimension available for buoyancy-driven motion within the molten PCM. Larger spacing provides a greater vertical and transverse length scale between neighboring fins, whereas smaller spacing partitions the liquid PCM into narrower regions. The spacing-based Rayleigh number therefore decreases substantially with decreasing fin spacing because $Ra_s \propto s^3$. This geometrical scaling indicates a lower nominal buoyancy-driving scale between closely spaced fins. However, because convection-cell velocity, circulation strength, Nusselt-number evolution, and conductive and convective heat-flux components were not separately evaluated, the degree to which natural convection is weakened cannot be quantified directly.

The liquid-fraction evolution shown in Fig. 9(a) demonstrates the net

influence of fin spacing on charging performance. Reducing the fin spacing from 15 mm to 5 mm decreases the complete melting time from 695 to 345 s, corresponding to a 50.4% reduction, while increasing the average heat-storage rate from 222.82 to 425.94 W, representing a 91.2% enhancement. Meanwhile, because the spacing-based Rayleigh number scales with the cube of the characteristic spacing, $Ra_s \propto s^3$, decreasing the spacing from 15 to 5 mm reduces Ra_s by approximately 96.3%, indicating a substantially lower propensity for buoyancy-driven circulation between adjacent fins. The simultaneous improvement in the global charging metrics demonstrates a favorable net effect of smaller fin spacing within the investigated range. However, the present results cannot determine how much of this improvement originates from conductive-path reduction or how much is offset by changes in buoyancy-driven transport, because the two heat transfer contributions were not separately decomposed. The corresponding apparent charging resistance decreases from 0.2020 K W^{-1} at 15 mm fin spacing to 0.1056

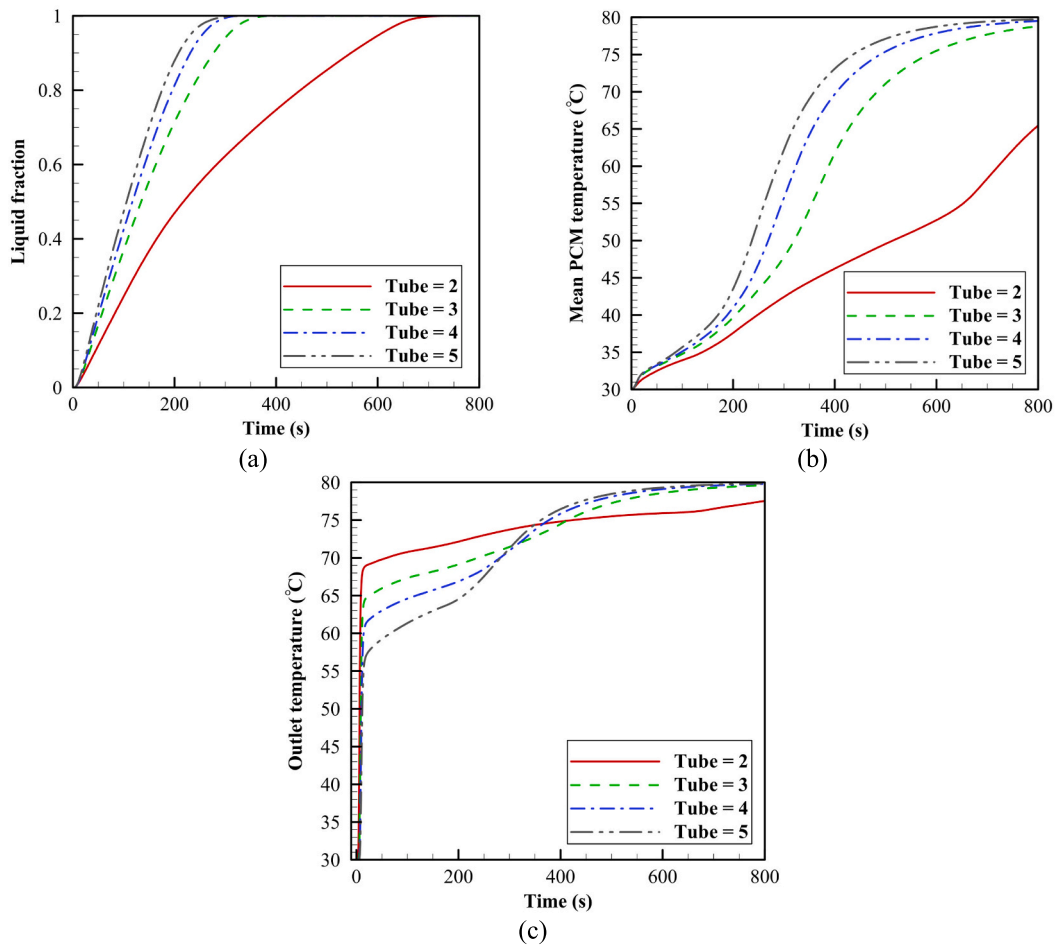


Fig. 6. Temporal response of the LHTES system for different tube-number configurations: (a) time evolution of liquid fraction, (b) variation of volume-averaged PCM temperature, and (c) temporal profile of HTF outlet temperature.

K W^{-1} at 5 mm, representing a 47.7% reduction. This value quantifies the combined system-level improvement produced by changing fin spacing, but it does not separately identify conductive and convective contributions.

The temperature contours in Fig. 8 show that larger fin spacing preserves low-temperature peripheral regions for longer periods, whereas closer fins produce earlier thermal homogenization through a more spatially distributed conduction network. The slope changes in Fig. 9 represent successive charging regimes: initial sensible heating and thin-layer melting, rapid latent heat absorption as the mean PCM temperature enters the 32–38 °C phase-change interval, and renewed sensible heating near complete melting. The corresponding rise in outlet temperature indicates progressive weakening of latent-heat demand. Smaller fin spacing shifts these transitions to earlier times, consistent with the faster propagation of the melt front.

To quantify the principal melting stage, t_{10} , t_{50} , and t_{90} are defined as the times at which the liquid fraction reaches 0.1, 0.5, and 0.9, respectively. The phase-averaged heat-storage rate is calculated as $\bar{Q}_{10-90} = [Q(t_{90}) - Q(t_{10})]/(t_{90} - t_{10})$. The corresponding apparent global thermal conductance is defined as $G_{10-90} = \bar{Q}_{10-90}/\Delta T_{10-90}$, where the denominator represents the time-averaged temperature difference over the t_{10} – t_{90} interval. This system-level metric characterizes the combined charging response and should not be interpreted as a local convection coefficient or Nusselt number. The resulting melting milestones and performance metrics for each fin spacing are summarized in Table 7.

Accordingly, fin spacing redistributes the effective thermal resistance by changing both the conductive transport distance and the

characteristic scale of buoyancy-driven circulation. Decreasing the spacing from 15 to 5 mm reduces Ra_s by approximately 96.3%, indicating stronger confinement of spacing-scale natural convection. Nevertheless, the apparent global conductance, G_{10-90} , increases from 12.01 to 19.74 W K^{-1} , corresponding to a 64.3% improvement, while the principal 10–90% melting interval decreases from 379.2 to 179.9 s. These opposite trends provide system-level evidence that the shorter and more uniformly distributed thermal pathways created by the denser fin arrangement offset the reduction in the spacing-based buoyancy scale. Therefore, within the investigated fin-spacing range, the improvement in net charging performance is consistent with a redistribution of the effective thermal resistance toward more effective fin-assisted heat spreading.

4.3. Effect of inlet temperature

The inlet temperature directly governs the thermal driving potential between the HTF and the PCM domain and therefore strongly influences the charging dynamics of the LHTES system. Fig. 10 shows that increasing the HTF inlet temperature substantially accelerates the melting process throughout the entire charging period. Unlike the geometrical parameters discussed previously, which primarily modify internal thermal transport pathways, the inlet temperature alters the magnitude of the interfacial heat flux itself. Consequently, the melting process proceeds under a stronger thermal driving force as the temperature difference between the HTF and PCM increases.

At low inlet temperatures, the thermal gradient between the heated tube–fin surfaces and the surrounding PCM remains relatively weak, as

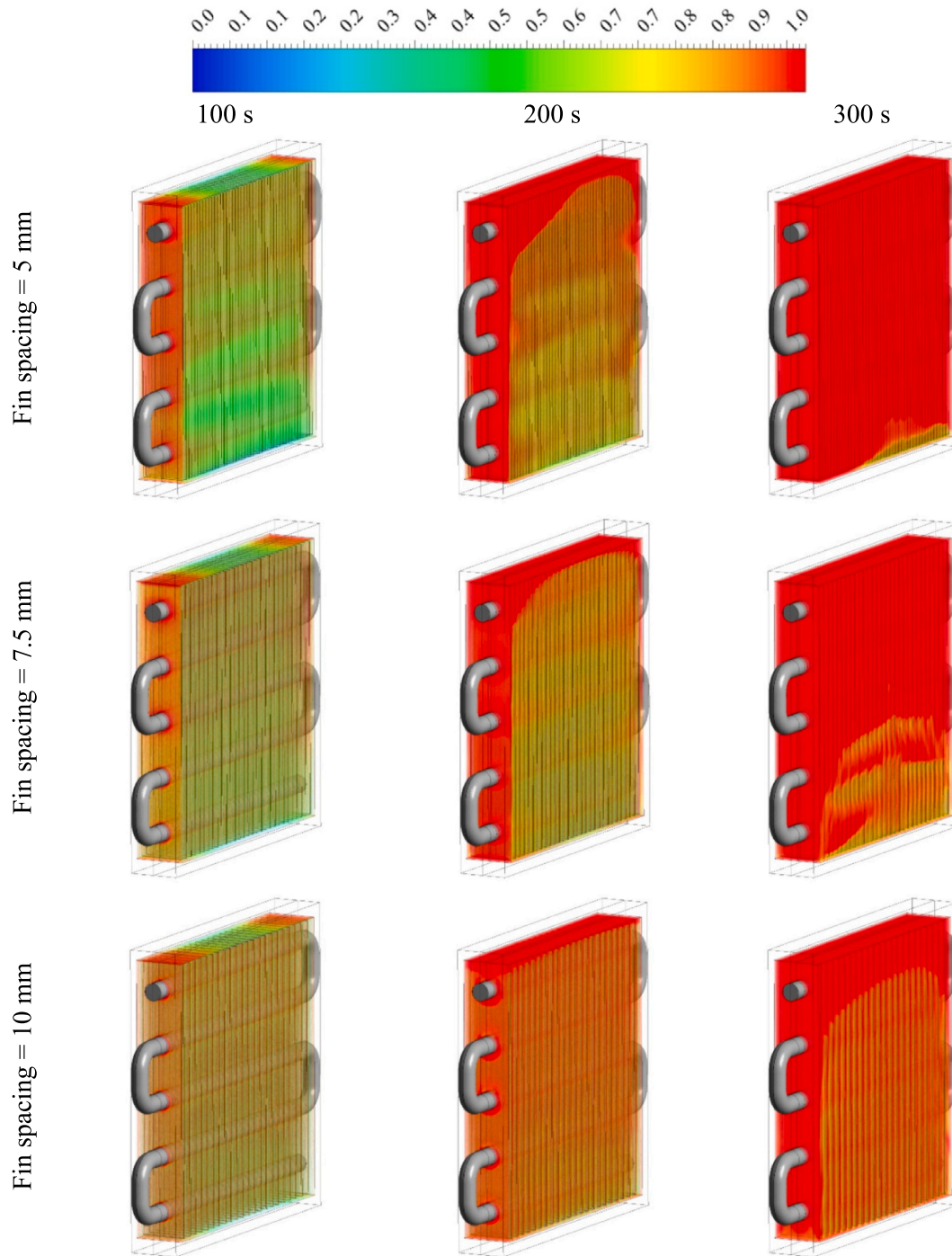


Fig. 7. Liquid-fraction contours for different fin spacings (5–15 mm) at selected charging times, showing the influence of fin density on melt-front propagation.

illustrated in Fig. 11, resulting in slower energy penetration into the solid PCM region. Under these conditions, the melting front advances gradually, and large portions of the enclosure remain below the melting temperature for extended periods. Increasing the inlet temperature strengthens the local heat flux at the tube and fin surfaces, thereby accelerating both sensible heating and latent heat absorption within the PCM. This effect becomes particularly significant during the intermediate melting stage, where stronger thermal gradients promote earlier growth of buoyancy-driven convection currents within the molten PCM region. As a result, higher inlet temperatures not only increase conductive heat transfer near the heated surfaces, but also indirectly

intensify convective transport by producing larger density gradients inside the liquid PCM.

The influence of inlet temperature on melting kinetics is quantitatively demonstrated in Fig. 12 and Table 8. Increasing the inlet temperature from 60 to 80 °C reduces the total melting time from 558 s to 345 s, corresponding to a 38.2% reduction. Over the same range, the average heat storage rate increases from 235.65 W to 425.94 W, representing an 80.7% enhancement. The nonlinear nature of this enhancement indicates that the charging process becomes increasingly sensitive to thermal driving potential as convection develops inside the molten PCM. In other words, the influence of inlet temperature extends

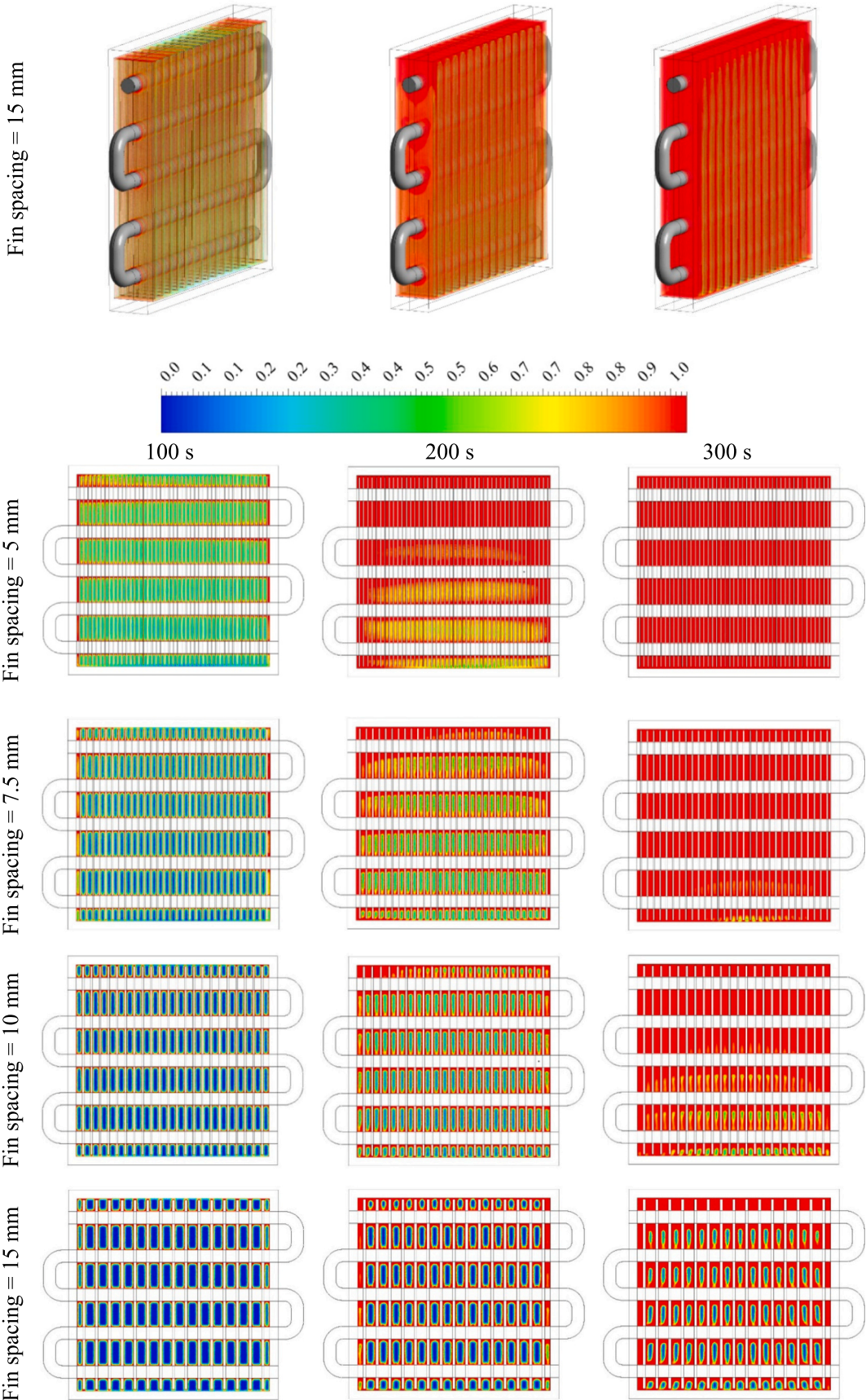


Fig. 7. (continued).

beyond simple conductive scaling because stronger buoyancy forces progressively enhance thermal transport throughout the liquid PCM

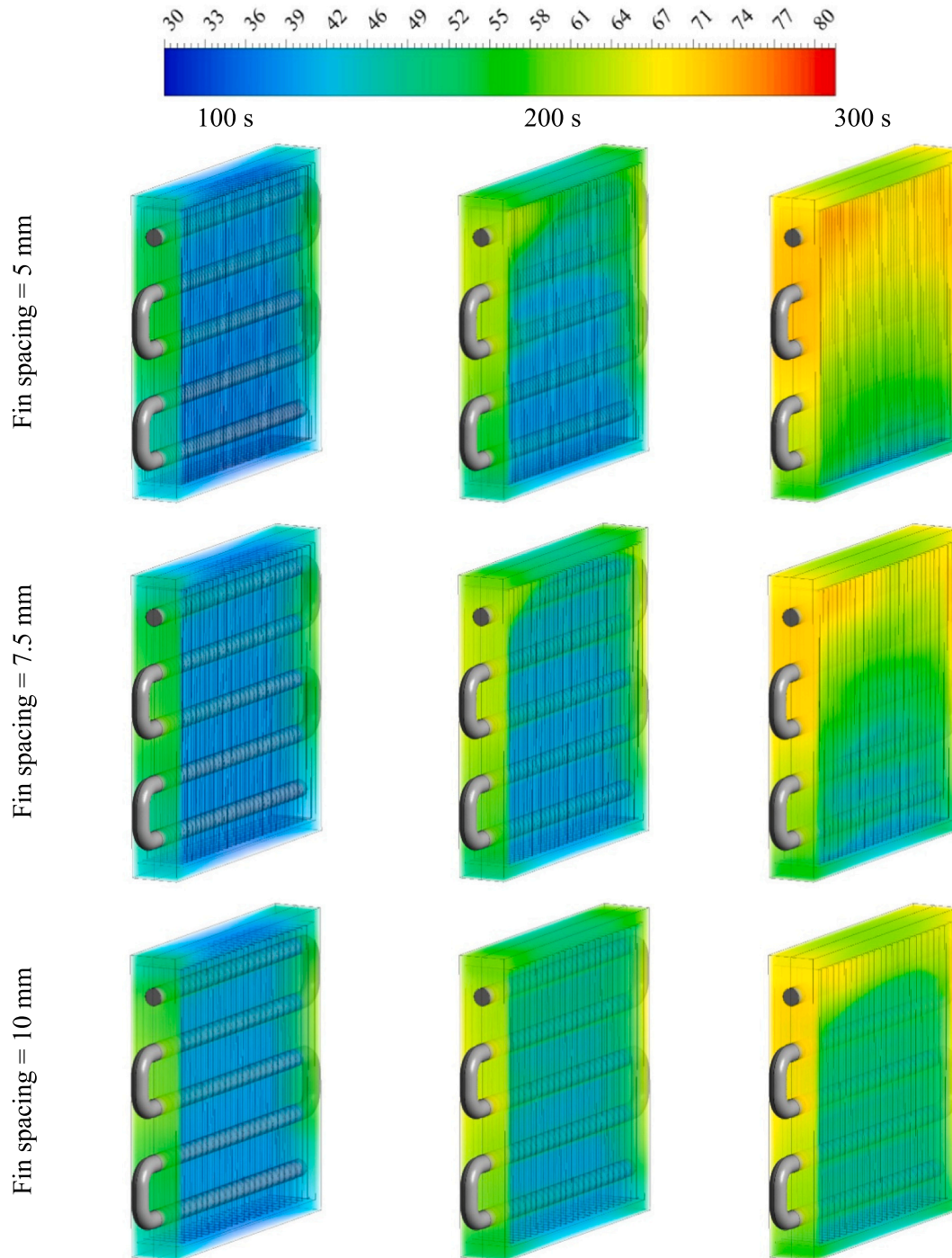


Fig. 8. Temperature contours for different fin spacings (5–15 mm) at selected charging times, illustrating the balance between conductive heat spreading and thermal nonuniformity within the PCM domain. All panels use an identical temperature scale and viewing orientation to enable direct comparison at common charging times.

region. The temperature distributions presented in Fig. 11 further illustrate this behavior. Higher inlet temperatures produce earlier thermal penetration into the lower and peripheral regions of the PCM enclosure, resulting in faster elimination of thermally stratified solid zones. In contrast, lower inlet temperatures maintain strong thermal nonuniformity for longer durations because the weaker thermal driving force limits both conductive propagation and buoyancy-induced mixing. This difference is also reflected in the outlet-temperature histories shown in Fig. 12(c). At higher inlet temperatures, the outlet temperature

rises more rapidly because the PCM approaches thermal equilibrium earlier and its latent heat absorption capacity is depleted within a shorter charging duration.

The inflection points in Fig. 12 identify changes in the dominant energy-storage regime. The initial response corresponds mainly to sensible heating and conduction-controlled melting. When the mean PCM temperature enters the 32–38 °C phase-change interval, latent heat absorption limits the temperature-rise rate while the liquid fraction increases more rapidly. As melting approaches completion, the liquid-

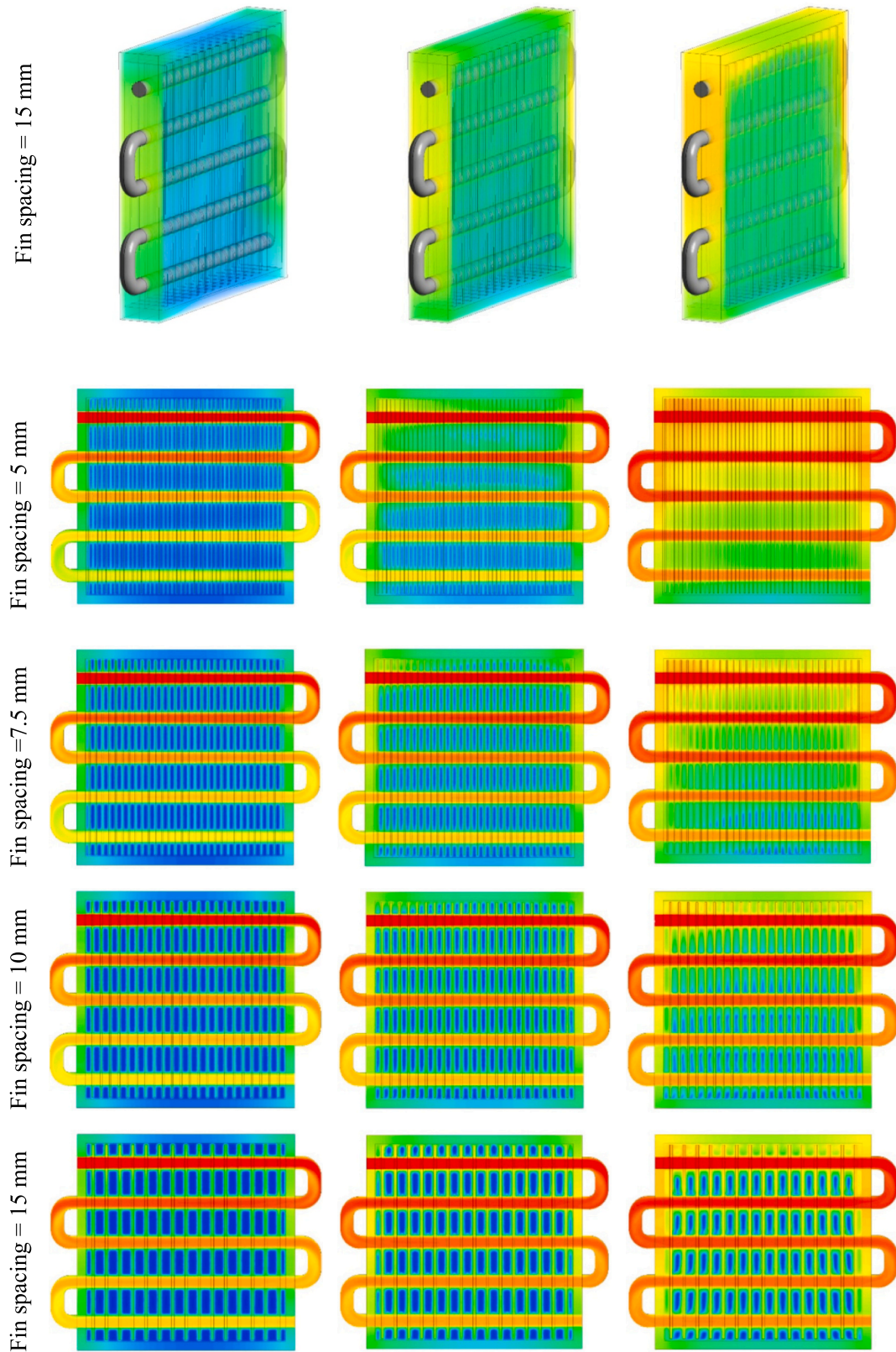


Fig. 8. (continued).

fraction slope decreases and the PCM and outlet temperatures rise toward their respective equilibrium values. Increasing the inlet temperature shifts these transitions to earlier times because it increases both the thermal driving force and the nominal Rayleigh number.

From a physical perspective, the inlet temperature primarily controls

the competition between energy absorption capacity and heat transfer intensity within the storage system. Increasing the thermal driving potential accelerates phase-front propagation and enhances convection-assisted transport, thereby reducing the duration over which conduction-limited melting persists inside the PCM enclosure. Within

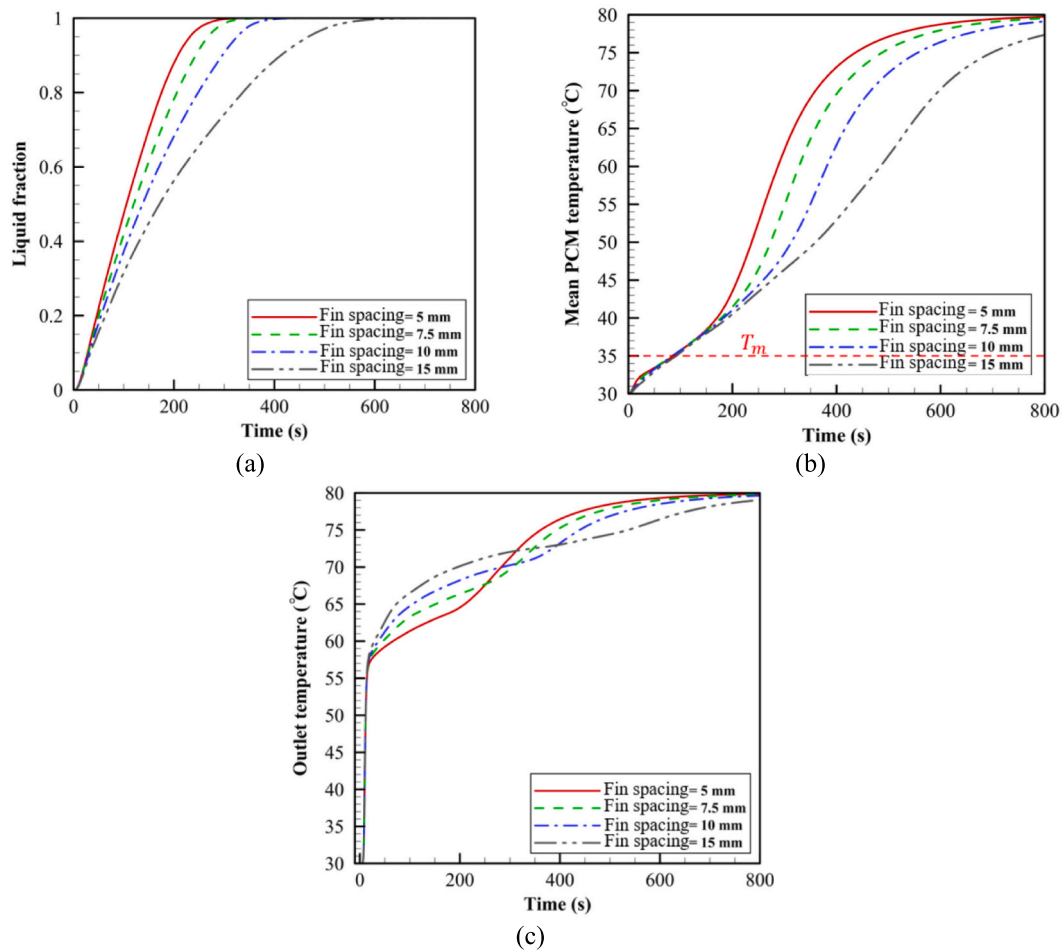


Fig. 9. Temporal response of the LHTES system for different fin spacings: (a) liquid-fraction history, (b) volume-averaged PCM temperature response, and (c) outlet-temperature evolution of the HTF. The red dashed line indicates the midpoint of the PCM melting interval, $T_m = 35\text{ }^{\circ}\text{C}$; RT35 undergoes phase change over $32\text{--}38\text{ }^{\circ}\text{C}$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 7

Effect of fin spacing on melting milestones, complete-period average heat-storage rate, and phase-resolved apparent conductance for the five-tube configuration.

Configurations	Melting time (s)				Average heat storage rate (W)	Apparent conductance $G_{10-90}(\text{W K}^{-1})$
	10%	50%	90%	100%		
Fin spacing = 5 mm	28.0	105.0	207.9	345.0	425.94	19.74
Fin spacing = 7.5 mm	29.4	120	243.3	377.0	385.48	17.19
Fin spacing = 10 mm	30.9	137.5	296.1	460.0	322.19	14.84
Fin spacing = 15 mm	33.7	171.2	412.9	695.0	222.82	12.01

the investigated range, the charging behavior therefore remains strongly dependent on the imposed thermal gradient between the HTF and PCM domains.

The effect of inlet temperature can also be expressed through the nominal PCM Rayleigh number. Based on the enclosure height and PCM properties, increasing the inlet temperature from 60 to $80\text{ }^{\circ}\text{C}$ increases Ra_H from 4.59×10^8 to 8.26×10^8 , with an intermediate value of 6.42×10^8 at $70\text{ }^{\circ}\text{C}$. These values indicate that buoyancy can contribute substantially after the molten PCM forms connected circulation pathways. Nevertheless, the early charging stage remains predominantly

conduction-controlled because the liquid layers surrounding the tube–fin surfaces are initially thin and spatially disconnected. The higher inlet temperature therefore accelerates melting through both a greater conductive temperature gradient and stronger buoyancy potential during the intermediate melting stage.

The inlet-temperature comparison was conducted using water properties evaluated at the $70\text{ }^{\circ}\text{C}$ design temperature. Therefore, the reported differences isolate the effect of the imposed thermal driving force under a common HTF property basis. In an actual variable-property system, temperature-dependent changes in water viscosity, density, thermal conductivity, heat capacity, and Prandtl number would also modify the HTF-side convection and may change the absolute magnitude of the reported improvement. Accordingly, the $60\text{--}80\text{ }^{\circ}\text{C}$ comparison should not be interpreted as a variable-property verification.

4.4. Influence of Reynolds number

The Reynolds number primarily controls forced convection within the HTF channels and therefore modifies the HTF-side component of the total thermal resistance. Increasing Re reduces the hydrodynamic and thermal boundary-layer thicknesses along the tube walls, improving heat transfer from the HTF to the copper tube–fin network. The serpentine bends may induce local flow redistribution; however, velocity-vector data were not extracted for all cases, and vortex formation is therefore not used as evidence in the present analysis. The Reynolds-number effect is instead evaluated through the resulting

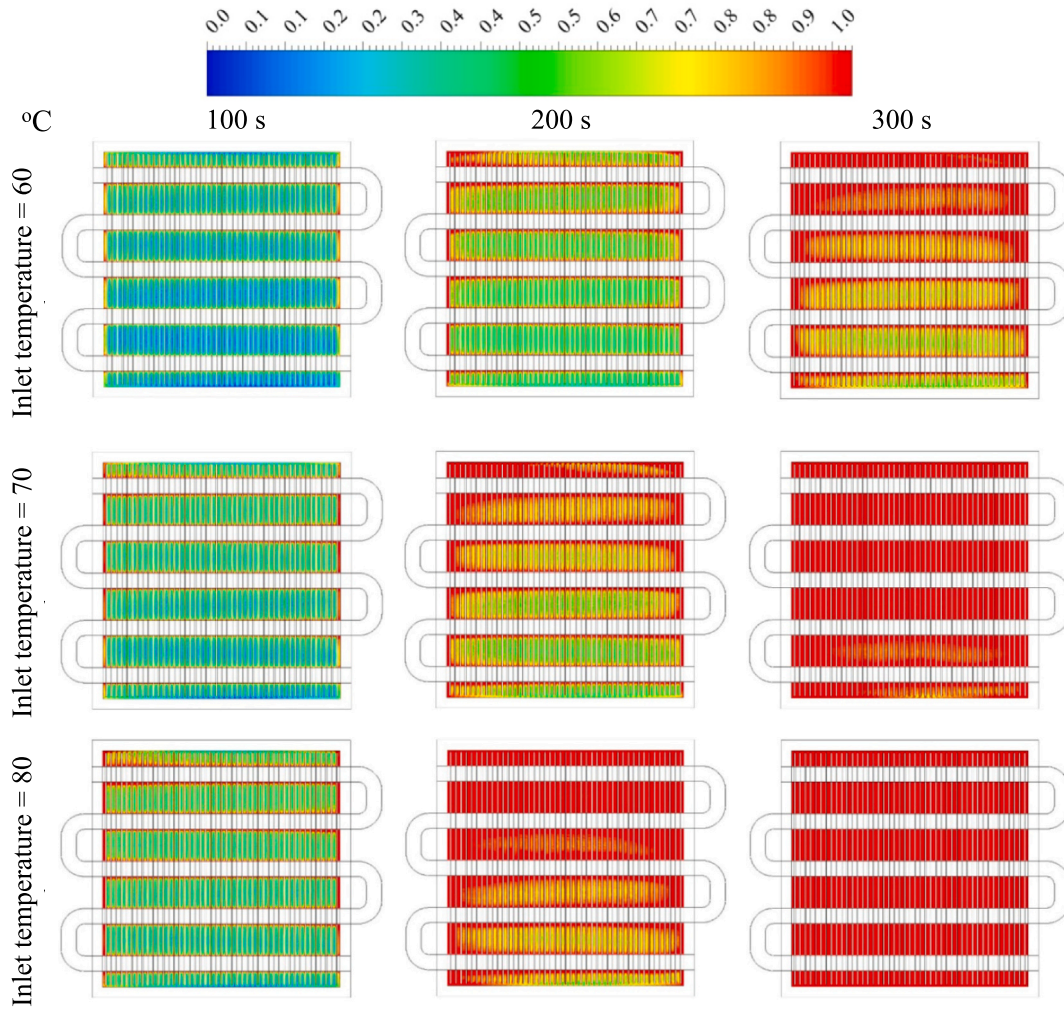


Fig. 10. Liquid-fraction contours for different HTF inlet temperatures (60–80°C) at selected charging times for the five-tube, 5 mm fin-spacing configuration.

liquid-fraction evolution, PCM temperature, HTF outlet temperature, melting time, and average heat-storage rate.

The resulting thermal response is visible in the liquid-fraction and temperature contours presented in Figs. 13 and 14. At $Re = 500$, weaker HTF-side convection limits energy transfer to the tube–fin structure, producing slower thermal penetration and larger residual low-temperature PCM regions at the same charging time. Increasing Re to 1500 and 2000 improves energy delivery to the conductive network, leading to faster expansion and interaction of the molten regions. However, Reynolds number does not directly increase the imposed temperature difference or the nominal PCM buoyancy-driving scale. All three cases have $T_{in} = 80^\circ\text{C}$ and therefore share the same nominal Rayleigh number, $Ra_H = 8.26 \times 10^8$. Their different charging responses are consequently attributed primarily to changes in HTF-side convection and the rate of energy delivery to the PCM.

The quantitative trends presented in Fig. 15 and Table 9 and Table 10 indicate that increasing the Reynolds number enhances the overall charging performance, although the degree of improvement becomes progressively weaker at higher flow rates. Increasing the Reynolds number from 500 to 2000 reduces the total melting time from 695 s to 345 s, corresponding to a 50.4% decrease, while the average heat storage rate increases from 206.69 W to 425.94 W, representing a 106.1% enhancement. Although increasing Reynolds number produces a substantial reduction in melting time, its influence arises mainly from reducing the HTF-side convective resistance rather than directly modifying the PCM-side melting mechanism. The improvement is also

nonlinear: most of the reduction occurs when Re increases from 500 to 1500, whereas the additional gain from 1500 to 2000 is comparatively smaller, indicating progressive saturation of the HTF-side transport benefit. This behavior suggests that, within the investigated range, the dominant thermal resistance progressively shifts away from the HTF side toward the PCM domain itself. Once sufficient convective transport is established inside the tube network, further increases in Reynolds number produce diminishing improvement because the global charging dynamics become increasingly governed by heat diffusion and natural convection within the PCM enclosure. Increasing Reynolds number from 500 to 2000 decreases the apparent charging resistance from 0.2177 to 0.1056 K W^{-1} , corresponding to a 51.5% reduction. This global indicator is consistent with reduced HTF-side resistance and faster energy delivery, although it does not provide a local decomposition of the internal PCM heat transfer modes.

The temperature contours, shown in Fig. 14, support this interpretation. Increasing the Reynolds number produces earlier and more uniform heating of the tube–fin structure, which subsequently accelerates thermal penetration into the surrounding PCM. Nevertheless, the overall topology of the melting front remains relatively similar across the investigated Reynolds-number range, indicating that the internal PCM-side melting mechanisms are not fundamentally altered by the HTF flow intensity. The outlet-temperature histories shown in Fig. 15(c) further reflect the influence of HTF heat-capacity rate and residence time. At higher Reynolds numbers, the larger mass-flow rate allows the HTF to deliver thermal energy more effectively to the tube–fin structure,

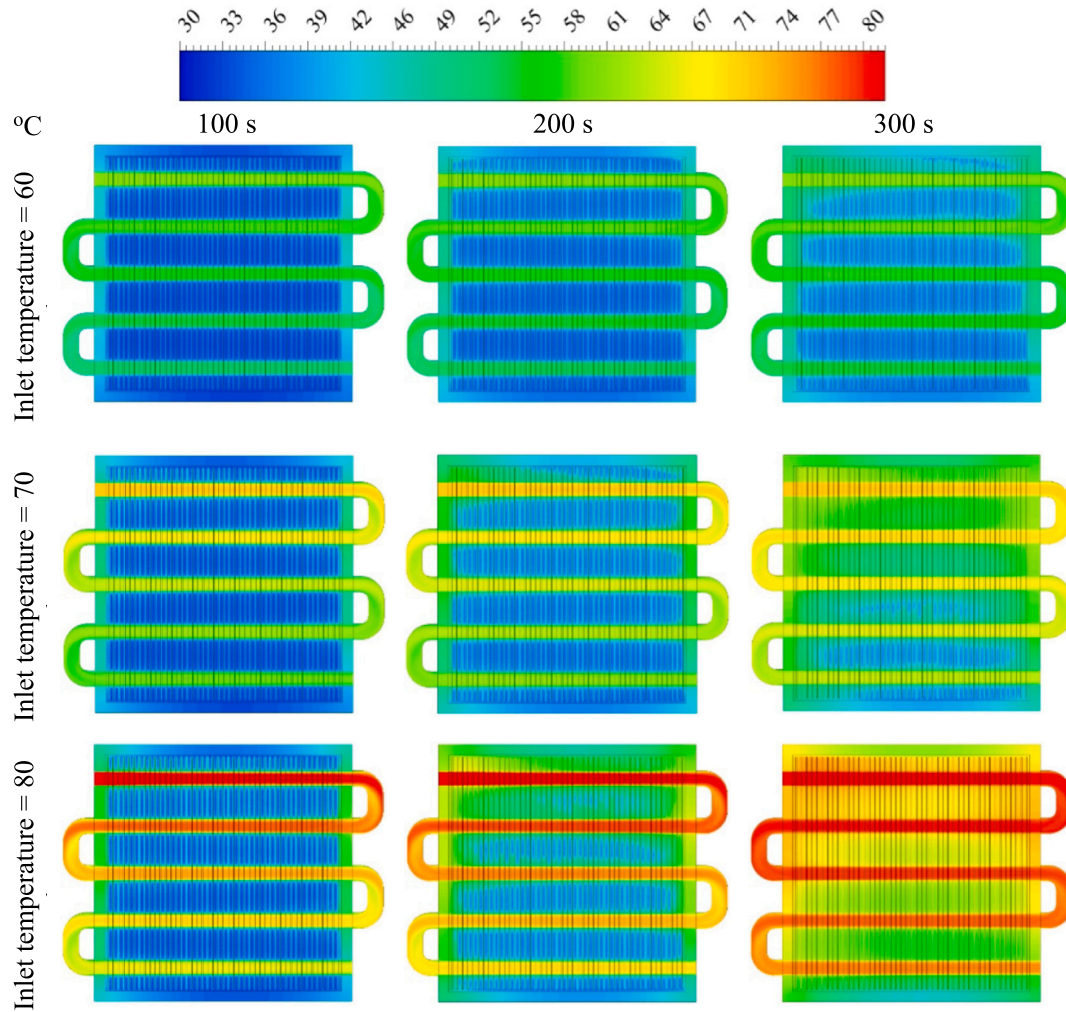


Fig. 11. Temperature contours for different HTF inlet temperatures (60–80 °C) at selected charging times, showing the influence of thermal driving potential on PCM temperature distribution. All panels use an identical temperature scale and viewing orientation to enable direct comparison at common charging times.

while the PCM continues to absorb latent heat over a substantial portion of the charging process. Therefore, the outlet-temperature response should be interpreted as a coupled indicator of HTF-side convection, flow residence time, and PCM latent heat absorption rather than as a direct measure of PCM-side melting alone.

The changes in slope in Fig. 15 result from the evolving balance between HTF-side energy delivery and PCM-side latent heat absorption. During early charging, the supplied energy primarily heats the tube–fin structure and initiates melting adjacent to the heated surfaces. The subsequent rapid increase in liquid fraction corresponds to expansion and interaction of the molten regions. Near complete melting, the liquid-fraction curves flatten, whereas the PCM and outlet temperatures continue to increase as sensible heating becomes progressively more important. Increasing Reynolds number advances these transitions by reducing HTF-side convective resistance, but the incremental shift becomes smaller from $Re = 1500$ to 2000 .

The diminishing thermal improvement from $Re = 1500$ to 2000 indicates progressive saturation of HTF-side enhancement. The newly extracted pressure results summarized in Table 9 permit this thermal benefit to be compared quantitatively with its hydraulic requirement. Because the HTF travels downward through the serpentine passage, the raw outlet-to-inlet static-pressure difference represents the remaining gravitational pressure rise after irreversible losses and is not itself the pressure drop. The elevation-corrected mechanical pressure loss increases from 1498.85 Pa at $Re = 500$ to 1552.72 Pa at $Re = 1500$ and

1584.88 Pa at $Re = 2000$, which is physically consistent with increasing flow resistance. Meanwhile, ideal hydraulic power increases from 0.00402 to 0.01251 and 0.01703 W, respectively. Thus, increasing Reynolds number accelerates charging but requires greater hydraulic power.

For the tube-number comparison at $Re = 2000$, the mechanical pressure loss increases modestly from 1506.76 Pa for two tubes to 1584.88 Pa for five tubes. However, the volumetric flow rate required to maintain the specified Reynolds number decreases as the hydraulic diameter decreases. Consequently, ideal hydraulic power decreases from 0.02191 W for two tubes to 0.01703 W for five tubes. Combined with the shorter melting period and higher average heat-storage rate, this increases ψ_{pump} from 8469 to 25,006. The five-tube configuration therefore provides the largest thermal-storage gain per unit hydraulic work among the tube-number cases, although the four-tube case retains the shortest complete-melting time.

The Reynolds-number comparison reveals a different trade-off. Increasing Re from 500 to 2000 decreases melting time from 695 to 345 s and increases the average heat-storage rate from 206.69 to 425.94 W. However, ideal hydraulic power increases from 0.00402 to 0.01703 W, causing ψ_{pump} to decrease from 51,431 to 25,006. Thus, the lowest Reynolds number provides the highest thermal-storage gain per unit hydraulic work, whereas the highest Reynolds number provides the fastest charging and highest average charging rate. These results do not identify a global optimum; they demonstrate the trade-off between

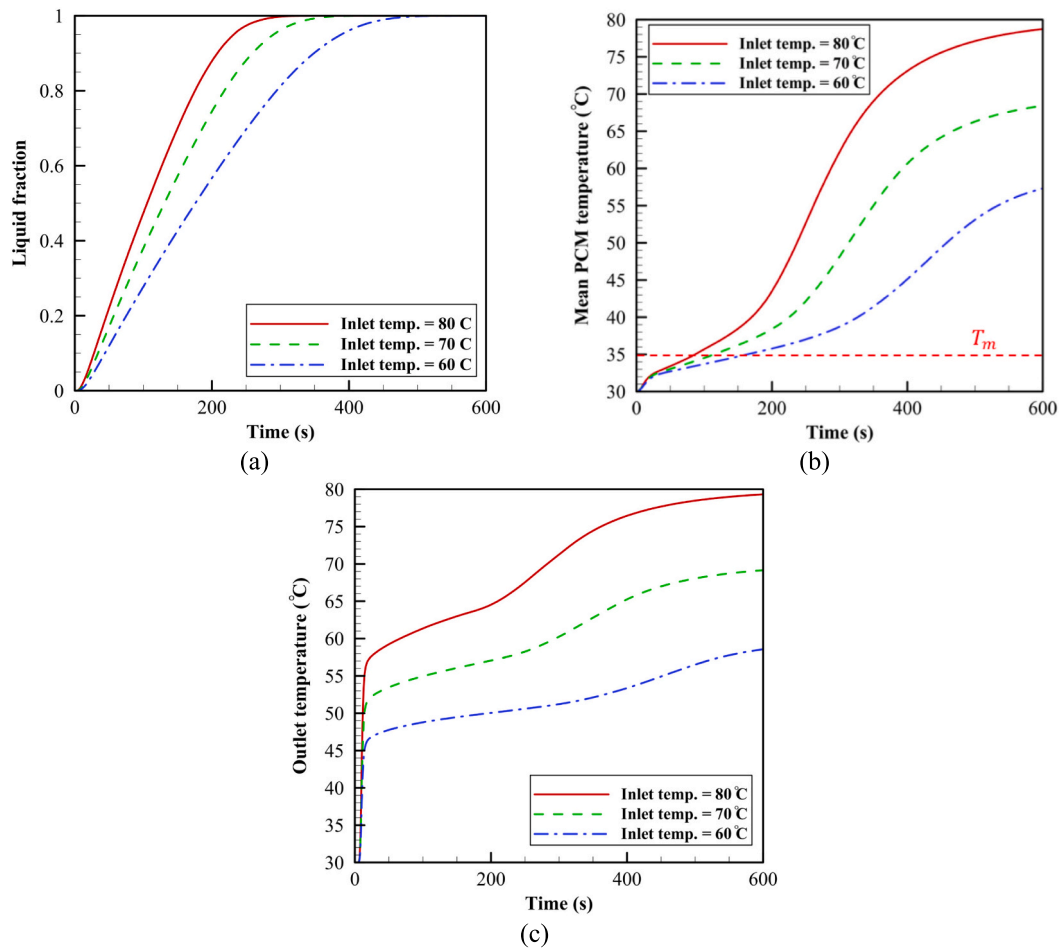


Fig. 12. Temporal response of the LHTES system for different HTF inlet temperatures: (a) transient liquid-fraction response, (b) mean PCM temperature evolution, and (c) HTF outlet-temperature variation. The red dashed line indicates the midpoint of the PCM melting interval, $T_m = 35$ °C; RT35 undergoes phase change over 32–38 °C. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 8

Effect of HTF inlet temperature on melting time and average heat storage rate for the five-tube, 5 mm fin-spacing configuration.

Configurations	Melting time (s)	Average heat storage rate (W)
Inlet temperature = 60 °C	558	235.65
Inlet temperature = 70 °C	421	330.94
Inlet temperature = 80 °C	345	425.94

charging speed and ideal component-level hydraulic demand within the investigated cases.

Table 11 summarizes the principal thermal performance metrics obtained for all investigated configurations and operating conditions considered in the present study. The results collectively demonstrate that the melting behavior of the flat-plate LHTES system is governed by a coupled interaction between geometric heat-distribution characteristics and externally imposed thermal operating conditions. Parameters associated with the spatial distribution of thermal energy inside the PCM domain, such as tube number and fin spacing, exhibit the strongest influence on the charging dynamics because they directly modify the conductive heat transfer pathways and the formation of buoyancy-driven melting regions. In contrast, operating parameters including inlet temperature and Reynolds number primarily regulate the intensity and delivery rate of thermal energy from the HTF side. The summarized results further indicate that the enhancement mechanisms are highly nonlinear, since the reduction in melting time and increase in heat storage rate do not scale proportionally with parameter variation. This

behavior reflects the gradual transition of the dominant thermal resistance from HTF-side convection toward conduction and natural convection within the PCM domain as the charging process progresses. Overall, Table 11 provides a consolidated overview of the thermo-hydrodynamic trends observed throughout the parametric investigation and highlights the strong sensitivity of melting dynamics to the coupled interaction between geometrical configuration and operating conditions.

Collectively, the preceding parametric analyses reveal that the thermal response of the present LHTES system cannot be interpreted through isolated parameter effects alone. Instead, the melting dynamics emerge from a continuous redistribution of the dominant thermal resistance among three coupled mechanisms: (i) HTF-side forced convection inside the serpentine tube network, (ii) conductive heat spreading through the copper tube–fin structure, and (iii) buoyancy-driven thermal transport within the molten PCM region. Geometrical parameters such as tube number and fin spacing primarily modify the conductive transport pathways and thermal diffusion length inside the PCM domain, whereas operating parameters including inlet temperature and Reynolds number regulate the intensity and delivery rate of thermal energy from the HTF side. As melting progresses, the relative importance of these mechanisms evolves continuously due to the growth of molten regions and the strengthening of natural convection. Consequently, the observed nonlinear variation in melting time and heat storage rate originates from the dynamic interaction between conduction enhancement, thermal energy redistribution, and convection-driven transport throughout the charging process. The apparent

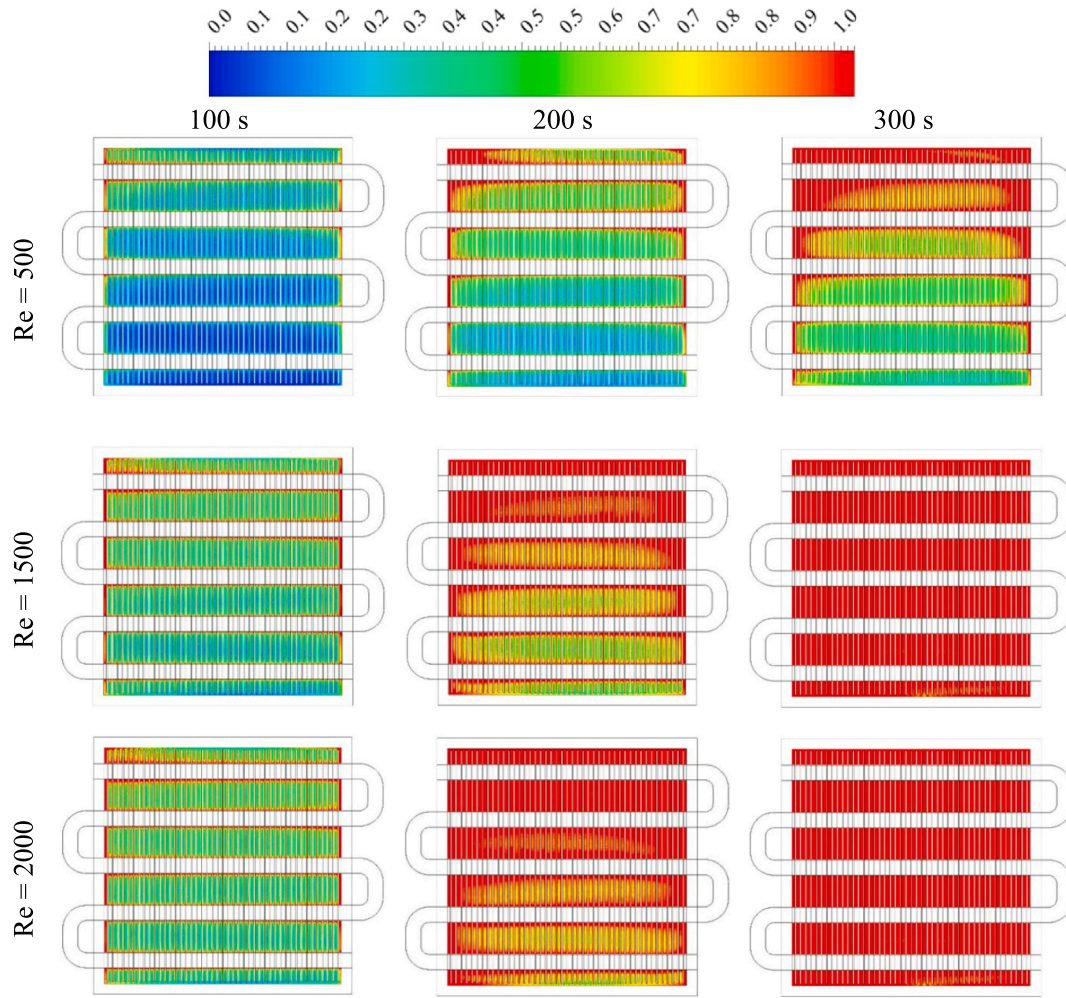


Fig. 13. Liquid-fraction contours for different Reynolds numbers ($Re = 500$ – 2000) at selected charging times for the five-tube, 5 mm fin-spacing, 80°C inlet-temperature configuration.

charging-resistance results quantitatively support the observed redistribution of the overall thermal limitation: $R_{ch,app}$ decreases by 56.5% from two to five tubes, by 47.7% when fin spacing decreases from 15 to 5 mm, and by 51.5% when Reynolds number increases from 500 to 2000. These values quantify the combined global response rather than individual local resistance components. Because wall-resolved heat-flux integrals and separate conductive and convective PCM contributions were not retained, an exact thermal-resistance decomposition is outside the scope of the present dataset.

From a practical design perspective, the constant-volume comparison represents redistribution of a limited copper inventory rather than unrestricted addition of heat transfer material. It therefore helps identify whether improved charging can be achieved through more effective placement of approximately the same amount of copper. Practical selection must also consider commercially available tube diameters and fin thicknesses, joining and fabrication requirements, structural integrity, and manufacturing cost. The present elevation-corrected pressure-loss analysis quantifies the ideal hydraulic demand of the modeled serpentine passage, but does not include pump and motor efficiencies, connecting-pipe losses, auxiliary-system power, or economic cost. Consequently, the investigated configurations provide comparative thermal and component-level hydraulic results rather than fabrication-ready or globally optimized designs.

4.5. Cross-parametric interaction analysis

The existence of parameter coupling was evaluated using a relative-effect interaction index. For two parameters A and B, the relative effect of changing A from A_1 to A_2 at a fixed level B_j was calculated as:

$$E_A(B_j) = \frac{Y(A_2, B_j) - Y(A_1, B_j)}{Y(A_1, B_j)} \times 100 \quad (18)$$

where Y denotes complete melting time. The corresponding interaction index was calculated as:

$$I_{A,B} = E_A(B_2) - E_A(B_1) \quad (19)$$

The magnitude $|I_{A,B}|$ represents the change in the relative effect of parameter A between two levels of parameter B. Therefore, $|I_{A,B}| = 0$ indicates no interaction on the adopted relative-change scale, whereas a nonzero value indicates that the effect of A depends on B. The sign indicates the direction of the interaction, while its magnitude is used to compare interaction strength.

Fig. 16 and Table 12 integrate the geometrical and operating parameters into a single performance map. Geometry is distinguished by marker shape, Reynolds number by marker size, and HTF inlet temperature by marker colour. The auxiliary curves represent constant stored-energy levels according to $Q_{st} = \dot{Q}_{avg} t_m$, providing a physics-based reference rather than an empirical mathematical fit. The five-tube, 5 mm cases are concentrated toward shorter melting times and

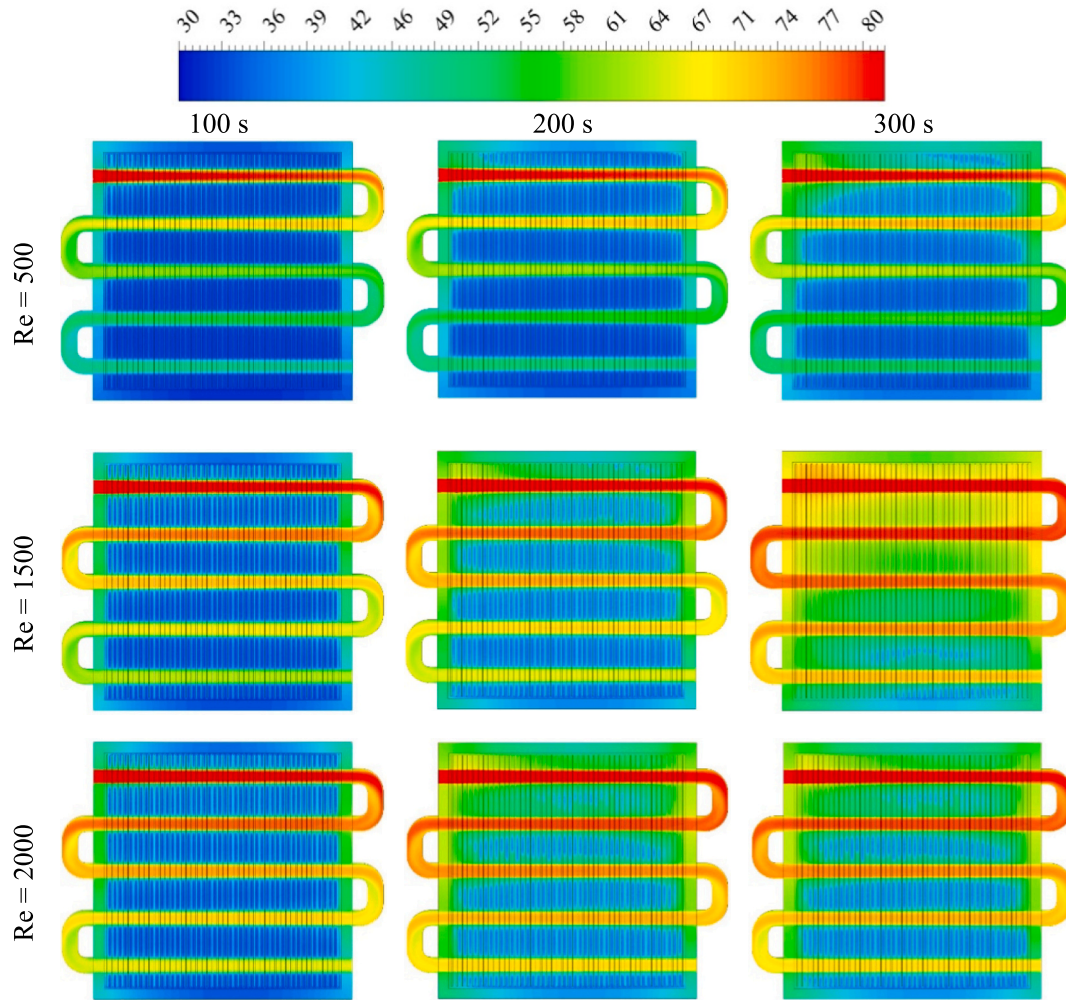


Fig. 14. Temperature contours for different Reynolds numbers ($Re = 500$ – 2000) at selected charging times, showing the influence of HTF-side convective resistance on PCM thermal response. The identical temperature scale used for all panels shows that increasing Re accelerates thermal penetration into the PCM, while the location of the remaining low-temperature regions continues to be controlled by the tube–fin distribution.

higher heat-storage rates; therefore, this region is identified as thermally favorable within the investigated parameter space rather than as a global optimum.

The interaction indices in Table 13 quantitatively demonstrate that the investigated parameter effects are not uniformly additive. The strongest interaction was observed between fin spacing and tube number, with a magnitude of 17.53 percentage points. Reducing fin spacing from 15 to 5 mm decreased melting time by 11.94% for the two-tube configuration but by 29.47% for the five-tube configuration. Geometry also modified the effects of operating conditions: increasing inlet temperature from 60 to 80°C reduced melting time by 56.42% for two tubes and 42.11% for five tubes, producing an interaction magnitude of 14.31 percentage points. Similarly, increasing Reynolds number from 500 to 2000 produced an interaction magnitude of 8.84 percentage points with tube number.

The Reynolds number–inlet temperature interaction also reached 9.43 percentage points, indicating that the benefit of increasing flow rate decreased at the higher inlet temperature. In contrast, the inlet temperature–fin spacing and Reynolds number–fin spacing interactions were only 0.97 and 1.52 percentage points, respectively, under the selected conditions. Thus, some parameter combinations exhibited meaningful coupling, whereas others behaved approximately independently on the adopted relative-change scale. These interaction indices apply only to the selected parameter levels and should not be interpreted as global sensitivity measures.

The interaction magnitudes can be interpreted through the changing balance of PCM-side and HTF-side thermal limitations. The stronger fin-spacing effect at five tubes arises because the more distributed tube network works together with closely spaced fins to shorten the conductive path and promote earlier connection of neighboring molten regions; with only two tubes, larger regions remain remote from the heated surfaces, limiting the benefit of decreasing fin spacing. Conversely, increasing inlet temperature or Reynolds number produces a smaller relative melting-time reduction at higher tube number because the distributed tube–fin network has already reduced a substantial part of the PCM-side resistance. The Reynolds number–inlet temperature interaction similarly reflects diminishing HTF-side benefit at the higher thermal driving force. The weak interactions involving fin spacing with inlet temperature or Reynolds number indicate that their relative effects remain comparatively similar at the selected endpoint conditions.

From a design perspective, the cross-parametric results show that isolated parameter sweeps provide useful trends but may not fully represent the thermal behavior of fin-enhanced LHTES systems under combined geometrical and operating variations. The same increase in Reynolds number or inlet temperature, or the same reduction in fin spacing, can produce different performance gains depending on the accompanying tube arrangement and fin distribution. Therefore, the melting behavior of the present flat-plate LHTES system is better interpreted as the result of an evolving balance between HTF-side convection, conductive heat spreading through the tube–fin network, and

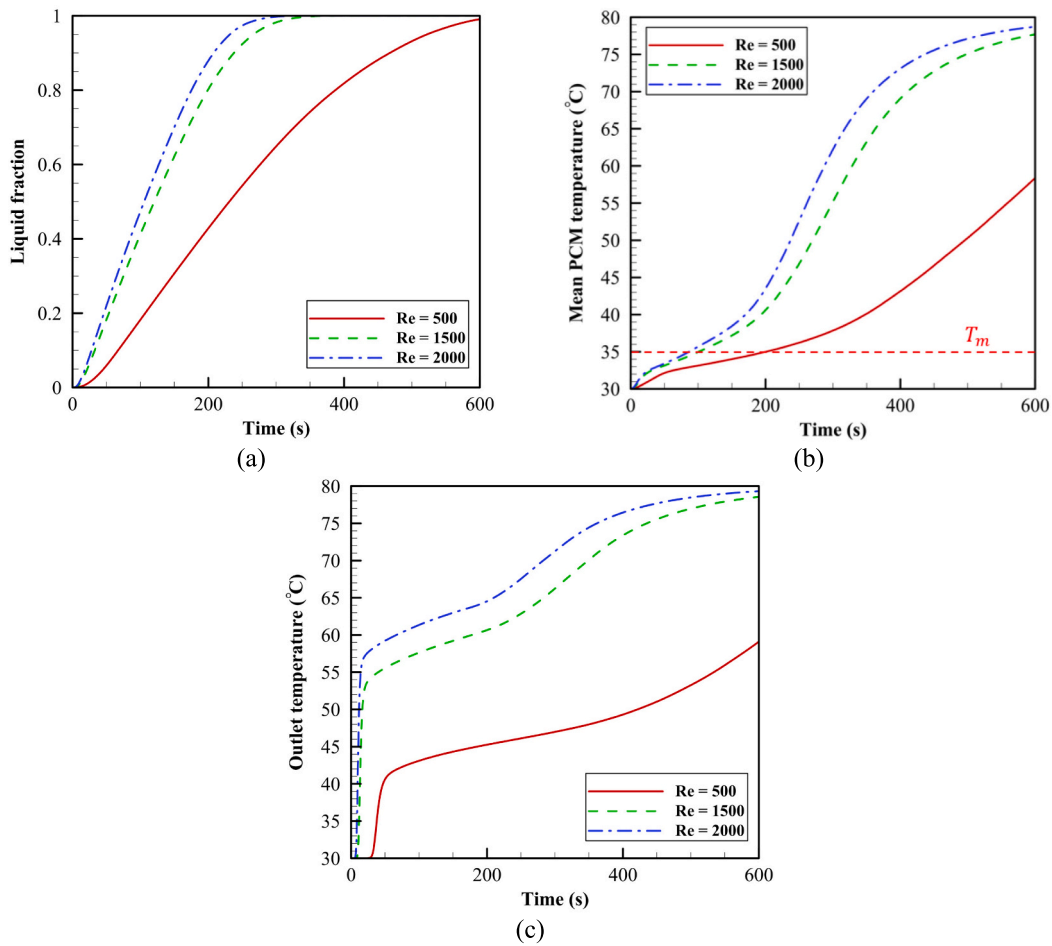


Fig. 15. Temporal response of the LHTES system for different Reynolds numbers: (a) time evolution of liquid fraction, (b) variation of volume-averaged PCM temperature, and (c) outlet-temperature evolution of the HTF. The red dashed line indicates the midpoint of the PCM melting interval, $T_m = 35$ °C; RT35 undergoes phase change over 32–38 °C. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 9

Thermo-hydraulic performance of the tube-number and Reynolds-number configurations based on elevation-corrected mechanical pressure loss.

tube	Re	Mechanical loss (Pa)	$\dot{V}(\text{m}^3\text{s}^{-1}) \times 10^{-5}$	P_{hyd} (W)	T_m (s)	W_{hyd} (J)	ψ_{pump}
2	2000	1506.76	1.4541	0.02191	749	16.411	8469
3	2000	1532.52	1.3819	0.02118	391	8.281	16,540
4	2000	1550.15	1.2287	0.01905	332	6.323	21,864
5	2000	1584.88	1.0747	0.01703	345	5.877	25,006
5	1500	1552.72	0.8059	0.01251	390	4.88	30,009
5	500	1498.85	0.2681	0.00402	695	2.793	51,431

Table 10

Effect of Reynolds number on melting time and average heat storage rate for the five-tube, 5 mm fin-spacing, 80 °C inlet-temperature configuration.

Cases	Melting time (s)	Average heat storage rate (W)
Re = 500	695	206.69
Re = 1500	390	375.50
Re = 2000	345	425.94

buoyancy-driven redistribution within the molten PCM. This interaction-oriented interpretation provides a more physically meaningful basis for design assessment than single-factor comparison alone, particularly for systems operating under variable thermal and flow conditions.

Since the present cross-parametric comparison is based on melting time and average heat storage rate, the identified favorable cases should

be interpreted as thermally advantageous configurations rather than globally optimized thermo-hydraulic designs.

The CFD analysis identifies the physical mechanisms governing the charging response but remains restricted to discrete simulated cases and stored transient outputs. The subsequent surrogate-model stage converts these CFD results into a rapidly queryable input–output mapping linking tube number, fin spacing, inlet temperature, Reynolds number, and time to liquid fraction and stored energy. Its engineering role is therefore not to replace CFD validation or discover a global optimum, but to support rapid in-domain response evaluation, response-surface generation, and preliminary screening before selected cases are examined using CFD.

4.6. Machine-learning dataset and modeling framework

The machine-learning dataset was generated from the transient outputs of 41 CFD cases. Each retained row corresponds to one stored

Table 11

Summary of melting performance across the single-parameter studies. Percentage changes are calculated relative to the reference configuration identified within each parameter group.

Study part	Parameter	Configuration	Melting time (s)	% Change from baseline	Average heat storage rate (W)	% Change from baseline
Part 1	Tube Number	2 tubes	749	Baseline	185.56	Reference case
		3 tubes	391	−47.8%	350.28	+88.8%
		4 tubes	332	−55.7%	416.43	+124.4%
		5 tubes	345	−53.9%	425.94	+129.5%
Part 2	Fin Spacing	5 mm	345	Baseline	425.94	Reference case
		7.5 mm	377	+9.3%	385.48	−9.5%
		10 mm	460	+33.3%	322.19	−24.4%
		15 mm	695	+101.4%	222.82	−47.7%
Part 3	Inlet Temperature	60 °C	558	+61.7%	235.65	−44.7%
		70 °C	421	+22.0%	330.94	−22.3%
		80 °C	345	Baseline	425.94	Reference case
Part 4	Reynolds Number	500	695	+101.4%	206.69	−51.5%
		1500	390	+13.0%	375.50	−11.8%
		2000	345	Baseline	425.94	Reference case

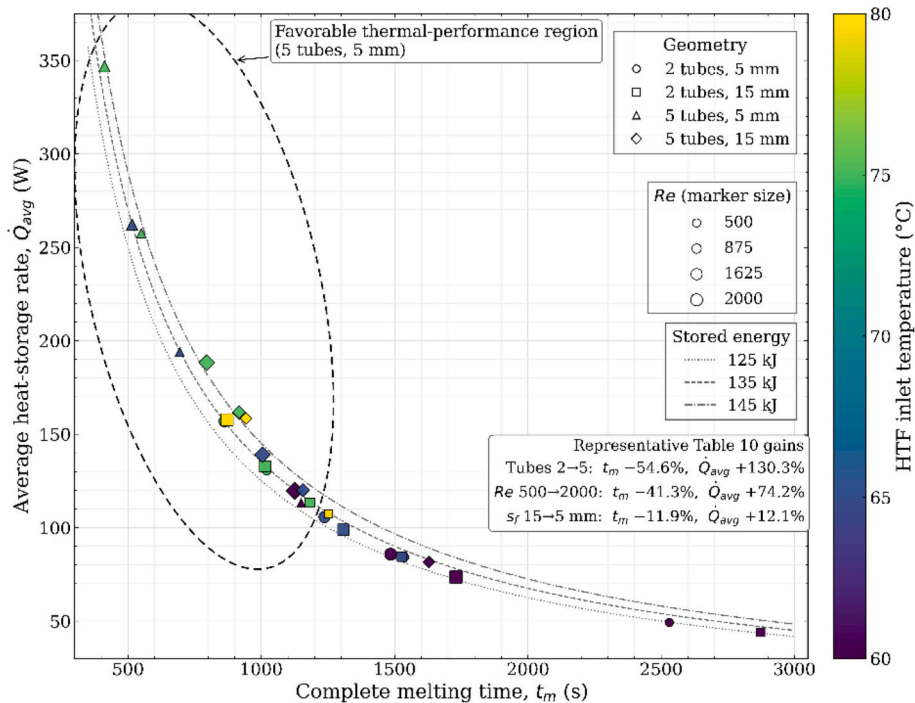


Fig. 16. Cross-parametric performance map showing melting time and average heat-storage rate. Marker shape identifies the tube-number/fin-spacing configuration, marker size represents Reynolds number, and marker colour represents HTF inlet temperature. The gray curves indicate constant stored-energy levels. The dashed oval identifies the favorable thermal-performance region within the investigated cases, while the annotation box reports representative relative performance changes.

CFD time point and combines five inputs, tube number, fin spacing, HTF inlet temperature, Reynolds number, and time, with the corresponding liquid fraction and stored thermal energy. No synthetic or experimentally measured samples were added. Rows with liquid fraction equal to unity were removed because they represent the fully melted plateau and contain limited information about the active phase-change response. This filtering also prevents long post-melting periods from disproportionately influencing model training. The resulting dataset contained 38,891 transient samples.

<http://doi.org/10.17632/mzfwpphwpf.1>

Rows corresponding to liquid fraction = 1 were removed to prevent the fully melted plateau from dominating the training process and to focus the surrogate model on the active phase-change interval, where the transient response is most sensitive to geometry and operating conditions. Five input variables were used in the learning process: Tubes, Fin spacing, Inlet Temp (°C), Reynolds number Re , and Time (s). In Scenario 1, the model had two outputs, liquid fraction and stored

thermal energy, which were predicted simultaneously. In Scenario 2, two independent single-output models were trained, one for liquid fraction and one for energy. A random row-wise split assigned 27,223 samples to training, 5834 samples to testing, and 5834 samples to validation, corresponding to 70%, 15%, and 15% of the dataset, respectively. Because the partition was performed at the transient-sample level, rows originating from the same CFD case may occur in different subsets. The resulting metrics therefore quantify interpolation accuracy for held-out transient samples within the sampled CFD trajectories and should not be interpreted as independent generalization to completely unseen geometrical-operational configurations.

Table 14 lists the variables used to construct the machine-learning models. The input set contains the main geometric, thermal, flow, and temporal descriptors of the simulations. The two output variables represent complementary aspects of the transient process: liquid fraction describes the phase-change state, while energy represents the corresponding stored thermal energy. Using the same input set for both

Table 12

Cross-parametric matrix showing the coupled effects of tube number, fin spacing, HTF inlet temperature, and Reynolds number on melting time and average heat storage rate.

Cases	Goal	Tube number	Fin spacing (mm)	Inlet temperature (°C)	Re	Melting time (s)	Average heat storage rate (W)
15	Cross parameters impact	2	5	60	500	2530	49.2
16		2	5	60	2000	1485	85.7
17		2	5	80	500	1127	118.8
18		2	5	65	875	1535	84.2
19		2	5	65	1625	1237	105.6
20		2	5	75	875	1020	130.7
21		2	5	75	1625	862	156.9
22		2	15	60	500	2873	43.9
23		2	15	60	2000	1730	73.6
24		2	15	80	500	1252	107.3
25		2	15	80	2000	872	157.8
26		2	15	65	875	1527	84.4
27		2	15	65	1625	1307	98.9
28		2	15	75	875	1182	113.3
29		2	15	75	1625	1014	132.8
30		5	5	60	500	1149	113.3
31		5	5	65	875	694	193.9
32		5	5	65	1625	515	262.2
33		5	5	75	875	550	257.6
34		5	5	75	1625	412	346.7
35		5	15	60	500	1629	81.5
36		5	15	60	2000	1125	119.6
37		5	15	80	500	943	158.4
38		5	15	65	875	1156	120.0
39		5	15	65	1625	1005	139.0
40		5	15	75	875	916	161.7
41		5	15	75	1625	795	188.3

Table 13

Quantified pairwise interactions based on complete melting time.

Parameter changed, $A_1 \rightarrow A_2$	Conditioning parameter, $B_1 \rightarrow B_2$	Fixed conditions	$E_A(B_1)$	$E_A(B_2)$	$I_{A,B}$ (pp)	$ I_{A,B} $ (pp)
Fin spacing: 15 $\rightarrow$ 5 mm	Tubes: $N = 2 \rightarrow 5$	$T_{in} = 60^\circ\text{C}$, $Re = 500$	-11.94%	-29.47%	-17.53	17.53
Inlet temperature: 60 $\rightarrow$ 80°C	Tubes: $N = 2 \rightarrow 5$	$s_f = 15$ mm, $Re = 500$	-56.42%	-42.11%	+14.31	14.31
Reynolds number: 500 $\rightarrow$ 2000	Tubes: $N = 2 \rightarrow 5$	$s_f = 15$ mm, $T_{in} = 60^\circ\text{C}$	-39.78%	-30.94%	+8.84	8.84
Inlet temperature: 60 $\rightarrow$ 80°C	Fin spacing: $f_s = 5 \rightarrow 15$ mm	$N = 2$, $Re = 500$	-55.45%	-56.42%	-0.97	0.97
Reynolds number: 500 $\rightarrow$ 2000	Fin spacing: $f_s = 5 \rightarrow 15$ mm	$N = 2$, $T_{in} = 60^\circ\text{C}$	-41.30%	-39.78%	+1.52	1.52
Reynolds number: 500 $\rightarrow$ 2000	Inlet temperature: $T_{in} = 60 \rightarrow 80^\circ\text{C}$	$N = 2$, $s_f = 15$	-39.78%	-30.35%	+9.43	9.43

Note: Here, “pp” means percentage points.

Table 14

Input and output variables of the present dataset.

Variable type	Variable	Range	Description
Input	Tubes	2 to 5	Number of tubes
	Fin spacing (mm)	5.0 to 15.0	Distance between fins
	Inlet Temp (°C)	60 to 80	Inlet temperature
	Reynolds number	500 to 2000	Flow Reynolds number
	Time (s)	0.0 to 2872.0	Simulation time
Output	Liquid fraction	0.0 to <1.0	Liquid fraction
	PCM energy	9875.69 to 251,308.4	Stored thermal energy

scenarios ensures that any difference in predictive performance is caused by the model-output strategy rather than by a change in available input information.

4.6.1. CatBoost model configuration

Gradient boosting decision tree methods are widely used for regression problems involving structured engineering data because they can represent nonlinear relationships and interactions among variables without requiring a pre-defined analytical form. This modeling choice is

supported by benchmark studies showing that tree-based models remain highly competitive for typical tabular datasets [57]. CatBoost is a robust implementation of gradient boosting that uses symmetric decision trees and ordered boosting, which improves stability and reduces prediction shift during training [58]. These characteristics make CatBoost suitable for the present dataset, where the target responses are governed by nonlinear thermal and phase-change behavior. The suitability of CatBoost for engineering prediction tasks has also been demonstrated in recent studies, such as the slope-stability early-warning model reported by [59].

The selected input variables were Tubes, Fin spacing, Inlet temperature, Reynolds number, and Time (s). The output variables were liquid fraction and stored thermal energy. These variables were selected to describe the main geometrical, thermal, flow, and transient characteristics of the melting process. All input variables and both output variables were standardized before training using the standard score transformation shown in Eq. (20).

$$z = \frac{x - \mu}{\sigma} \quad (20)$$

where x is the original variable, μ is the mean value of the training data, σ is the standard deviation of the training data, and z is the normalized variable. The scalars were fitted only on the training subset and subsequently applied to the testing and validation subsets, thereby preventing

leakage through the normalization procedure. However, because the underlying partition was performed randomly at the row level, temporal samples from the same CFD case were not necessarily isolated across subsets.

Table 15 summarizes the preprocessing settings and fixed CatBoost hyperparameters used in both modeling scenarios. No exhaustive grid, Bayesian, or evolutionary hyperparameter optimization was performed because the objective was to compare multi-output and single-output formulations under identical model complexity rather than to maximize predictive accuracy through extensive tuning. A learning rate of 0.1, tree depth of 8, maximum iteration limit of 10,000, and random seed of 42 were applied consistently to both scenarios. MultiRMSE was used for simultaneous prediction, whereas RMSE was used for each single-output model.

Several measures were used to limit and monitor overfitting. CatBoost's ordered-boosting procedure reduces prediction shift during sequential tree construction, while the tree depth was fixed to restrict individual-tree complexity. Input and output scalers were fitted only to the training subset, preventing normalization leakage. Training and validation losses were monitored separately, and their histories are reported in Fig. 20. In addition, errors are presented independently for the training, validation, and testing subsets. Nevertheless, because the dataset was divided randomly at the row level, samples from the same CFD trajectory may occur in different subsets. Consequently, the similar training and validation errors indicate an absence of evident sample-level overfitting, but they do not establish generalization to completely unseen CFD cases.

The prediction error was evaluated using the root mean square error (RMSE). For a single-output regression problem with N samples, RMSE is defined as:

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{N}} \quad (21)$$

where y_i and $\hat{y}_i$ are the actual and predicted values of the i^{th} sample, respectively. For the multi-output model, the MultiRMSE loss extends this definition by accounting for all target variables simultaneously. For N samples and M output variables, MultiRMSE can be written as:

$$MultiRMSE = \sqrt{\frac{\sum_{i=1}^N \sum_{j=1}^M (y_{ij} - \hat{y}_{ij})^2}{N}} \quad (22)$$

In the present study, $M = 2$ because the simultaneous-output model predicts liquid fraction and stored thermal energy together. To determine whether the surrogate captures parameter-dependent responses independently of the general transient curve shape, a fixed-time relative sensitivity analysis was performed. For the energy output, the predicted net stored energy was first calculated consistently with Eq. (8) as:

$$\hat{Q}_{st}(t) = \hat{E}(x, t) - \hat{E}(x, 0) \quad (23)$$

Table 15
Training settings used for the CatBoost models.

Setting	Scenario 1: multi-output model	Scenario 2: single-output models
Learning rate	0.1	
Loss function	MultiRMSE	RMSE
Maximum number of iterations	10,000	
Tree depth	8	
Random seed	42	
Early stopping	No	
Training/testing/validation split	70% / 15% / 15%	
Data split strategy	Random row-wise split	
Input normalization	StandardScaler	
Output normalization	StandardScaler	

The fixed-time sensitivity of output y , where y denotes liquid fraction or net stored energy, was then defined as:

$$S_x^{(y)}(t) = \frac{\hat{Y}(x_2, t) - \hat{Y}(x_1, t)}{\hat{Y}(x_1, t)} \times 100 \quad (24)$$

During each comparison, time and all inputs other than the investigated parameter were held constant. The parameter changes were defined as 2 to 5 tubes, fin spacing from 15 to 5 mm, inlet temperature from 60 to 80 °C, and Reynolds number from 500 to 2000. The enhanced endpoint corresponded to the common reference condition of five tubes, 5 mm fin spacing, 80 °C inlet temperature, and $Re = 2000$. The analysis was conducted at $t = 100$ and 175 s to represent the early and intermediate charging stages. The same indices were independently calculated from the corresponding CFD values as an in-domain consistency check.

Fig. 17 summarizes the machine-learning workflow used to

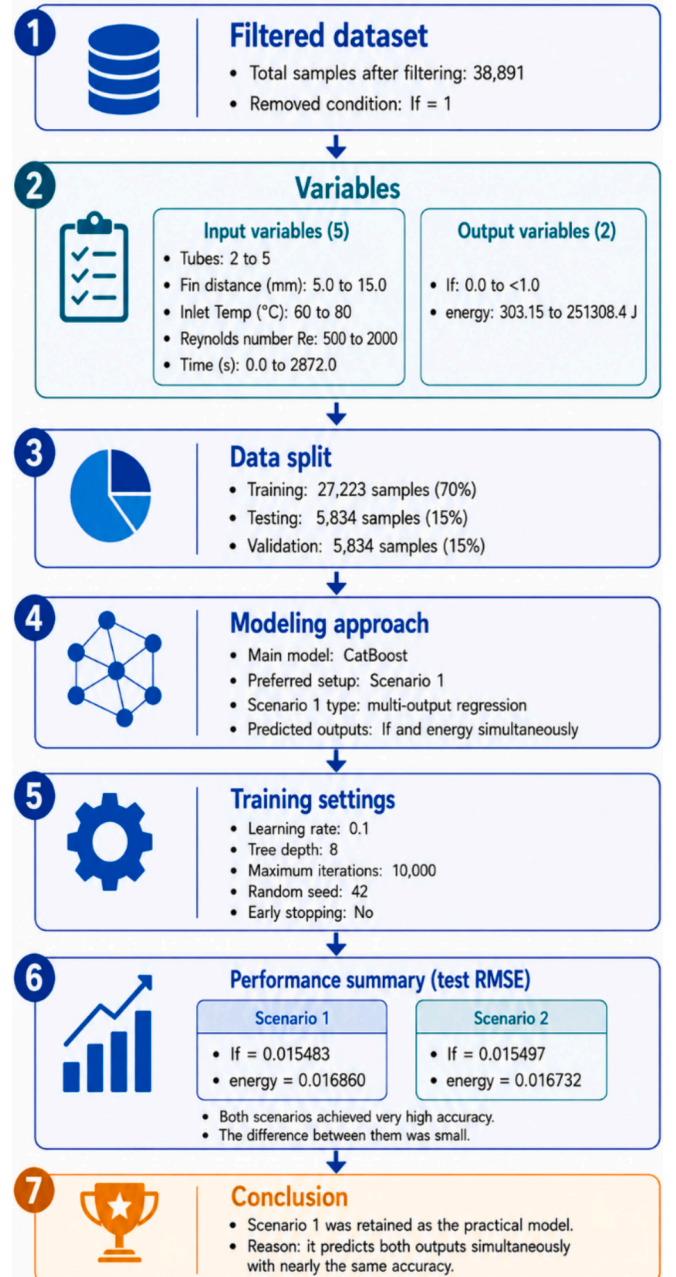


Fig. 17. Overall workflow of the CatBoost modeling approach.

interpolate the transient outputs of the investigated system. After removing the fully melted plateau, the dataset contained 38,891 transient samples from 41 CFD cases and was divided randomly at the row level into training, testing, and validation subsets. Five input features are used: number of tubes, fin spacing, inlet temperature, Reynolds number, and Time (s). These variables describe the main geometrical, thermal, flow, and transient characteristics of the system. Before model training, both input and output variables are standardized using scalers fitted only on the training data. Two CatBoost modeling scenarios are then considered. In Scenario 1, a single multi-output CatBoost model predicts liquid fraction and stored thermal energy simultaneously. In Scenario 2, two independent single-output CatBoost models are trained separately, one for liquid fraction and one for energy. The same main training settings are used for both scenarios, including a learning rate of 0.1, tree depth of 8, maximum iterations of 10,000, and random seed of 42. The final part of the workflow compares the predictive performance of the two modeling scenarios using the testing dataset. The results indicate low sample-level interpolation errors for both approaches under the adopted random row-wise split, with only marginal differences between the multi-output and single-output strategies. These errors characterize reconstruction of held-out samples within the simulated trajectories rather than prediction of entirely unseen CFD cases.

The input features included tube number, fin spacing, inlet temperature, Reynolds number, and time, while the target outputs were liquid fraction and stored thermal energy. All continuous features and target variables were normalized using parameters determined from the training subset. The reported errors were evaluated on randomly held-out transient samples and therefore represent interpolation performance within the CFD-generated dataset.

4.6.2. Scenario 1: Multi-output CatBoost model

In Scenario 1, one CatBoost model was trained with two output variables, corresponding to liquid fraction and stored thermal energy. This approach allows the model to learn a common tree structure for both responses. The normalized evaluation metrics are presented in Table 16. The model achieved low errors for both outputs across the training, testing, and validation subsets, which show strong predictions.

4.6.3. Scenario 2: Single-output CatBoost models

In Scenario 2, two independent CatBoost models were trained. The first model predicted liquid fraction, while the second model predicted

energy. This strategy removes the constraint that both outputs must share the same ensemble structure and allows each model to focus on the error characteristics of a single target variable. The normalized evaluation metrics are summarized in Table 17.

4.6.4. Comparison of multi-output and single-output modeling strategies

The comparison between Scenario 1 and Scenario 2, presented in Table 18, shows that the two strategies produced very similar errors for the filtered dataset. For the test data, the RMSE of liquid fraction changed from 0.015483 in Scenario 1 to 0.015497 in Scenario 2, corresponding to a slight increase of approximately 0.09%. For energy, the test RMSE decreased from 0.016860 to 0.016732, corresponding to an improvement of approximately 0.76%. Similar small differences were observed for the validation data, where the RMSE decreased by approximately 0.50% for liquid fraction and 0.84% for energy. These results indicate that the two modeling strategies remain quantitatively comparable for the present dataset under the adopted random row-wise data-splitting strategy.

These results indicate that, for the present dataset and random row-wise partition, the independent single-output models do not provide a decisive accuracy advantage over the multi-output model. Scenario 2 provides a small improvement for stored-energy prediction, whereas Scenario 1 is marginally more accurate for liquid fraction on the testing subset. Because Scenario 1 predicts both responses simultaneously while maintaining comparable sample-level accuracy, it offers a more compact surrogate for interpolating the transient CFD outputs. Nevertheless, the reported comparison applies to held-out sample rows within the simulated trajectories and does not establish predictive accuracy for completely unseen geometrical–operational configurations.

Figs. 18 and 19 compare the actual and predicted values for the testing dataset. Fig. 18 corresponds to the multi-output model of Scenario 1, whereas Fig. 19 corresponds to the independent single-output models of Scenario 2. These plots provide a visual assessment of the regression accuracy for energy and liquid fraction. A closer concentration of points around the ideal diagonal line indicates stronger agreement between the numerical simulation results and the CatBoost predictions.

Fig. 20 presents the training and validation loss histories of the CatBoost models. Fig. 20(a) shows the loss variation for the multi-output model in Scenario 1, while Figs. 20(b) and 20(c) show the corresponding histories for the single-output liquid-fraction and stored-energy models in Scenario 2, respectively. The curves are plotted with a logarithmic vertical axis to clarify the convergence behavior over the full training range and to verify that the validation loss remains close to the training loss during the selected iteration range.

Case C35 was selected as a representative transient case to compare the CatBoost-predicted liquid fraction and stored energy with the corresponding CFD results. This comparison provides a time-resolved assessment of whether the trained surrogate model can reproduce the evolution of the melting process for an individual operating condition.

Table 16

Normalized evaluation metrics for Scenario 1.

Data	Output	MSE	RMSE	MAE	R ²
Train	Liquid fraction	1.972780e-04	0.014046	0.009774	0.999803
	Energy	2.366236e-04	0.015383	0.010655	0.999763
	Liquid fraction & Energy	2.169508e-04	0.014729	0.010215	0.999783
	Liquid fraction	2.397199e-04	0.015483	0.010805	0.999762
Test	Energy	2.842739e-04	0.016860	0.011733	0.999719
	Liquid fraction & Energy	2.619969e-04	0.016186	0.011269	0.999741
	Liquid fraction	2.334531e-04	0.015279	0.010886	0.999768
Validation	Energy	2.769306e-04	0.016641	0.011731	0.999725
	Liquid fraction & Energy	2.551919e-04	0.015975	0.011309	0.999747

Table 17

Normalized evaluation metrics for Scenario 2.

Model	Data	MSE	RMSE	MAE	R ²
Liquid fraction	Train	1.961258e-04	0.014004	0.009732	0.999804
	Test	2.401619e-04	0.015497	0.010764	0.999761
	Validation	2.311456e-04	0.015203	0.010688	0.999771
Energy	Train	2.337434e-04	0.015289	0.010565	0.999766
	Validation	2.723051e-04	0.016502	0.011531	0.999730
	Test	2.799432e-04	0.016732	0.011613	0.999724

Table 18

Comparison of normalized RMSE values for the multi-output and single-output CatBoost modeling scenarios.

Output	Data	Scenario 1 RMSE	Scenario 2 RMSE	Improvement
Liquid fraction	Train	0.014046	0.014004	0.29%
	Test	0.015483	0.015497	−0.09%
	Validation	0.015279	0.015203	0.50%
Energy	Train	0.015383	0.015289	0.61%
	Test	0.016860	0.016732	0.76%
	Validation	0.016641	0.016502	0.84%

Fig. 21 compares the CatBoost-predicted liquid fraction and energy trajectories with the corresponding CFD values for Case C35. The predicted responses follow the CFD trajectories throughout the active melting interval, indicating that the surrogate reproduces both the phase evolution and energy-storage history for this representative sampled configuration. Because transient rows from Case C35 may occur in different data subsets under the random row-wise partition, this comparison represents a trajectory-reconstruction check rather than independent validation for an unseen CFD case.

Fig. 22 provides a physics-based interpretation of the CatBoost-predicted response surfaces by illustrating how the dominant geometrical and operating variables jointly control the transient melting state.

At ($t = 100$) s, the liquid fraction remains relatively low, and the response is mainly governed by conductive heat penetration from the tube–fin structure into the surrounding PCM. Under this condition, smaller fin spacing increases both liquid fraction and stored energy because the conductive network becomes more densely distributed and the characteristic thermal diffusion length is reduced. Increasing inlet temperature further amplifies this effect by increasing the thermal driving force between the HTF and PCM. At $t = 175$ s, the same trends become more pronounced as the melt region expands and natural convection begins to contribute to heat redistribution within the liquid PCM. The Reynolds-number-based response surfaces show that increasing Re improves the predicted liquid fraction and stored energy by reducing HTF-side convective resistance; however, its influence is weaker than that of inlet temperature and fin spacing once the dominant resistance shifts toward the PCM side. Therefore, the response surfaces are physically consistent with the CFD-based interpretation: inlet temperature controls the thermal driving potential, fin spacing controls conductive heat spreading and diffusion length, and Reynolds number regulates the HTF-side thermal resistance.

As a bounded proof-of-concept, the trained surrogate provides rapid reconstruction and comparison of liquid-fraction and stored-energy trajectories within the CFD-generated dataset. This enables efficient visualization of the sampled response space and avoids repeated extraction of individual transient CFD outputs. However, the random

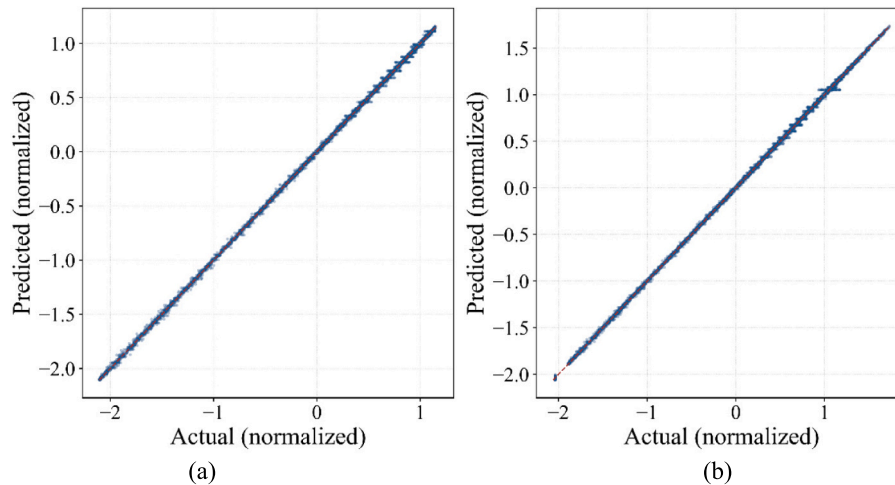


Fig. 18. Actual versus predicted values for the testing dataset of Scenario 1: (a) liquid fraction and (b) energy.

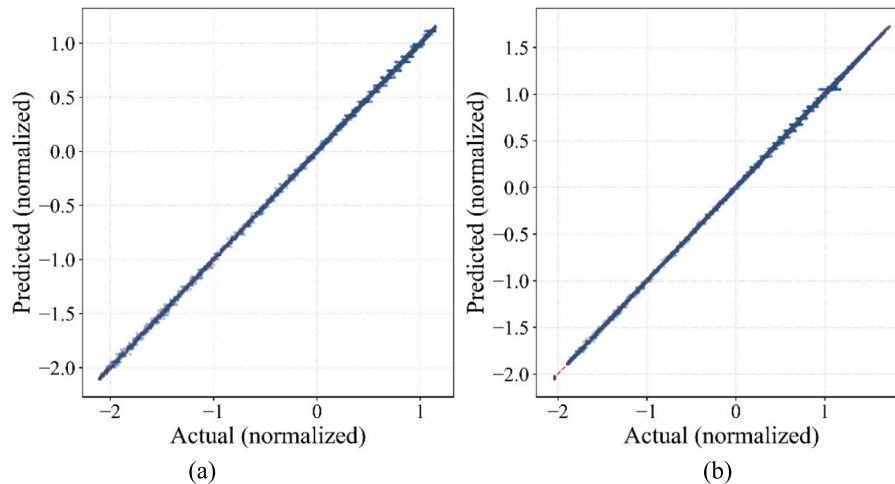


Fig. 19. Actual versus predicted values for the testing dataset of Scenario 2: (a) liquid fraction and (b) energy.

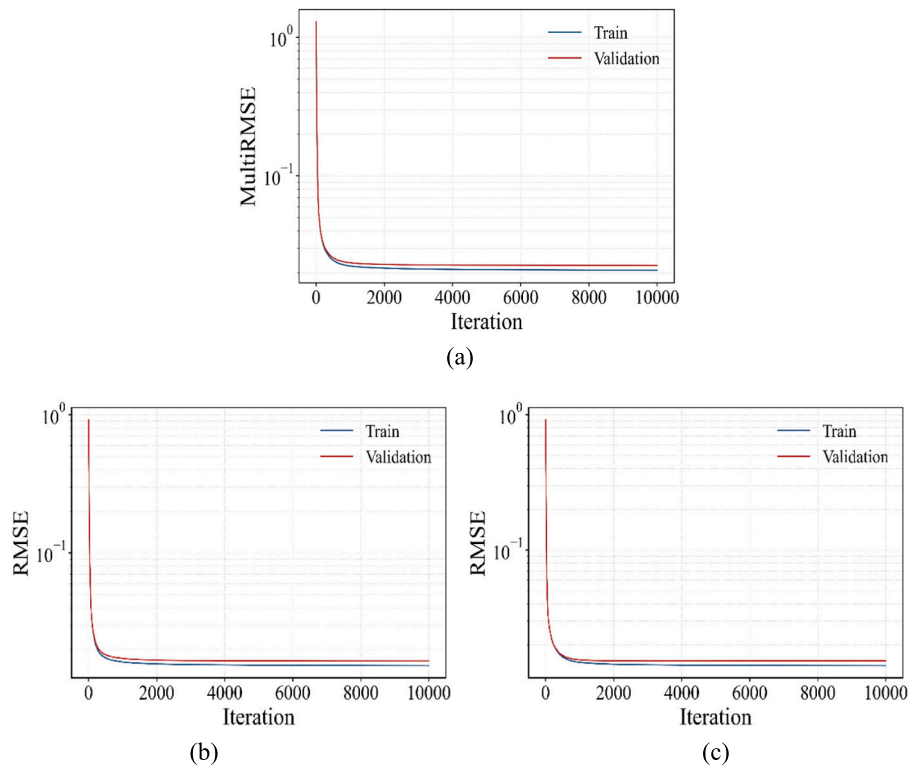


Fig. 20. Training and validation loss histories of the CatBoost models: (a) multi-output model in Scenario 1, (b) single-output liquid-fraction model in Scenario 2, and (c) single-output stored-energy model in Scenario 2.

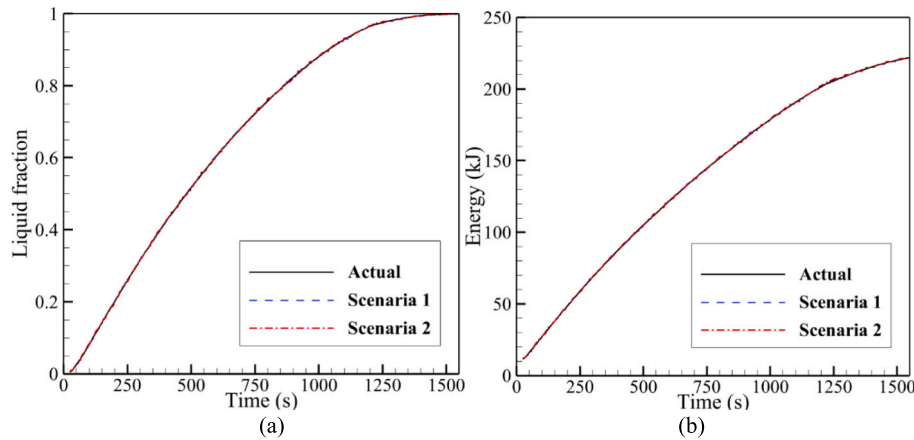


Fig. 21. A comparison of predicted and actual (a) liquid fraction and (b) stored thermal energy for Case C35.

row-wise split does not provide independent evidence of generalization to unseen CFD cases, even when their inputs lie within the nominal parameter ranges. Therefore, predictions at unsimulated parameter combinations, parameter boundaries, or outside the investigated ranges require additional CFD verification. The model is not used here for Pareto optimization, global design selection, or extrapolation.

Table 19 demonstrates that the surrogate predicts distinct parameter effects even when time is held constant. At 100 s, increasing Reynolds number produces the largest relative change because the $Re = 500$ response remains comparatively low during the early charging stage. Its relative sensitivity decreases at 175 s as melting progresses and the reference responses become larger. Conversely, the fin-spacing influence increases between 100 and 175 s, consistent with the growing importance of conductive-path distribution as heat penetrates farther into the PCM. The temperature sensitivity also changes with the melting stage,

confirming that the surrogate does not represent the transient responses through a single time-dependent curve shape.

The CatBoost and CFD sensitivity indices show close quantitative agreement. Across the 16 output–time comparisons, their mean absolute difference is 0.86 percentage points, while the maximum difference is 2.95 percentage points. This agreement confirms that the fixed-time surrogate responses remain consistent with the underlying CFD parameter effects. Nevertheless, because these comparisons use sampled CFD configurations and the adopted row-wise partition, they constitute an in-domain consistency check rather than independent validation for unseen cases or extrapolation beyond the investigated ranges.

5. Scope and applicability of the results

All quantitative trends and comparative conclusions reported in this

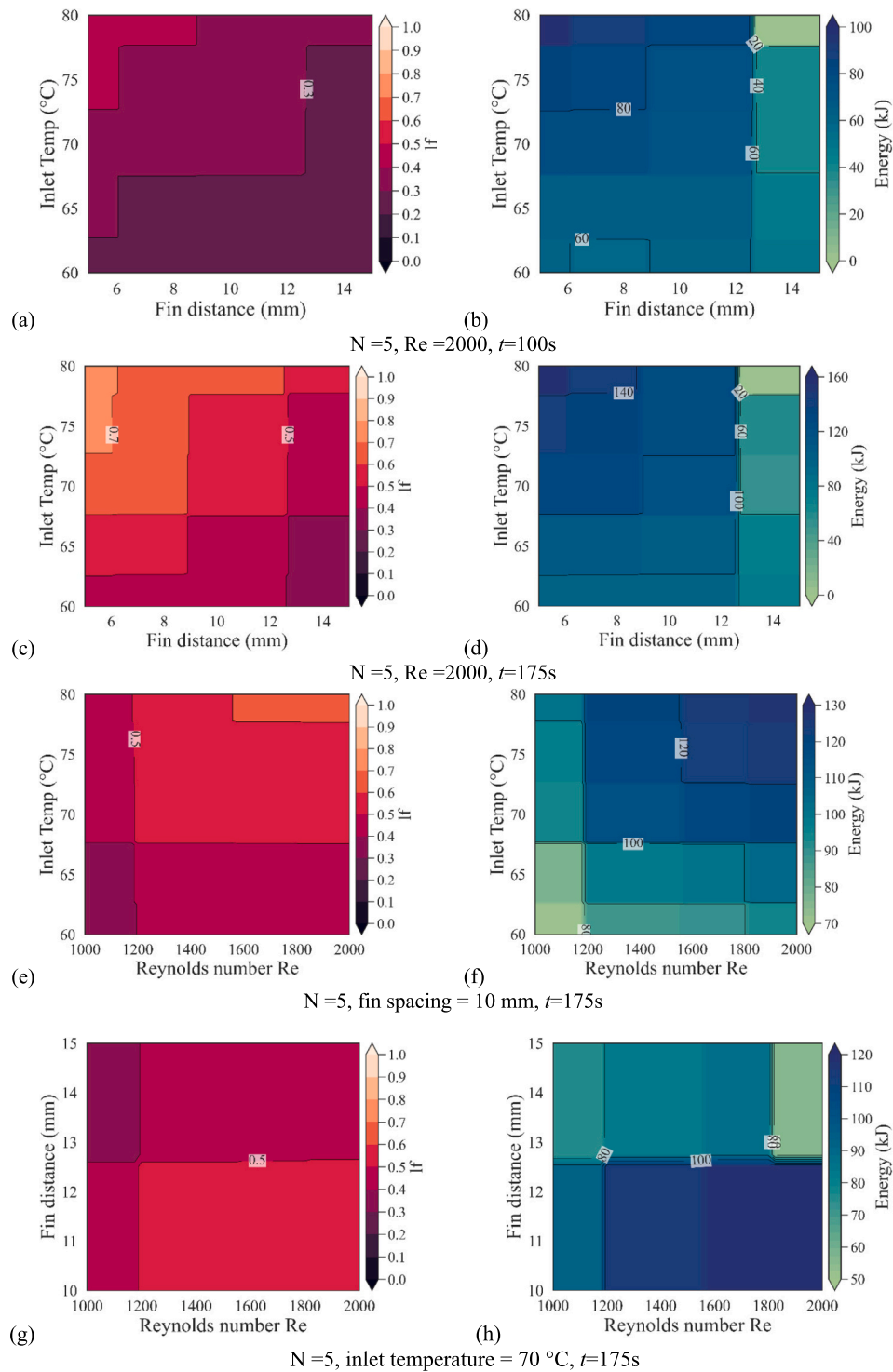


Fig. 22. Fixed-time CatBoost parameter-response surfaces for liquid fraction and stored thermal energy under selected operating conditions: (a,b) effects of fin spacing and inlet temperature at $N = 5$, $Re = 2000$, and $t = 100$ s; (c,d) effects of fin spacing and inlet temperature at $N = 5$, $Re = 2000$, and $t = 175$ s; (e,f) effects of Reynolds number and inlet temperature at $N = 5$, fin spacing = 10 mm, and $t = 175$ s; and (g,h) effects of Reynolds number and fin spacing at $N = 5$, inlet temperature = 70 °C, and $t = 175$ s.

study are restricted to the investigated parameter space: 2–5 tubes, fin spacing of 5–15 mm, Reynolds number of 500–2000, and HTF inlet temperature of 60–80 °C, using the specified PCM, water, enclosure dimensions, and tube–fin geometry. The inlet-temperature trends are additionally restricted to the adopted 70 °C reference-property basis and quantify controlled changes in thermal driving force rather than the combined influence of inlet temperature and temperature-dependent

HTF properties. Terms such as ‘favorable,’ ‘preferred,’ and ‘dominant’ describe relative performance or governing mechanisms only within these investigated conditions and should not be interpreted as evidence of a global optimum. Extrapolation beyond these ranges, or to different geometries, materials, working fluids, discharge conditions, and thermo-hydraulic constraints, requires additional CFD or experimental verification. The present CatBoost application should therefore be regarded as

Table 19

Fixed-time CatBoost-predicted and CFD-derived sensitivities of liquid fraction and net stored thermal energy.

Time (s)	Parameter change	CatBoost S_l^{lf}	CFD S_l^{lf}	CatBoost $S^{(Q)}$	CFD $S^{(Q)}$
100	N: 2 → 5	93.11%	93.21%	84.61%	85.11%
100	f_s : 15 → 5 mm	50.10%	50.04%	41.55%	42.04%
100	T_{in} : 60 → 80 °C	73.82%	70.88%	70.57%	68.41%
100	Re: 500 → 2000	157.98%	159.83%	143.74%	145.89%
175	N: 2 → 5	89.11%	89.62%	84.32%	85.39%
175	f_s : 15 → 5 mm	57.20%	57.05%	48.84%	49.13%
175	T_{in} : 60 → 80 °C	60.78%	60.48%	64.60%	65.01%
175	Re: 500 → 2000	116.48%	117.00%	118.85%	119.16%

a dataset-level interpolation proof-of-concept. No boundary-extrapolation test, physics-informed sampling strategy, Pareto-front construction, or downstream optimization task was performed.

Because the surrogate was trained exclusively on CFD-generated data, its high R^2 values measure fidelity to the numerical dataset rather than agreement with physical experiments. The model necessarily inherits the assumptions and uncertainties of the CFD framework, including constant thermophysical properties, idealized adiabatic boundaries, numerical discretization, the enthalpy–porosity formulation, and the absence of geometry-specific experimental validation. Consequently, surrogate accuracy cannot exceed the physical reliability of the underlying CFD data, and experimental measurements remain necessary before the model can be used for practical system prediction.

6. Conclusion

Efficient thermal charging in fin-enhanced LHTES systems remains challenging because PCM melting is governed by coupled conductive and convection-driven transport mechanisms that evolve continuously during phase change. In this study, a three-dimensional flat-plate LHTES system was investigated using a combined CFD-based and machine-learning-assisted framework to examine how tube number, fin spacing, inlet temperature, and Reynolds number influence melting dynamics and thermal storage performance. The results demonstrate that the thermal response is strongly interaction-driven, depending on the combined influence of heat-source distribution, conductive transport pathways, HTF-side thermal resistance, and buoyancy-driven redistribution within the molten PCM. The principal findings of the present study can be summarized as follows:

- Increasing tube number accelerated melting during the conduction-dominated stage by reducing the characteristic thermal diffusion length and promoting earlier interaction of neighboring molten regions. However, the enhancement progressively weakened at higher tube densities because of increasing overlap between thermal influence regions.
- Reducing fin spacing from 15 to 5 mm decreased the complete melting time by 50.4% and increased the average heat-storage rate by 91.2%. Although the nominal spacing-based Rayleigh number decreased by 96.3%, G_{10-90} increased by 64.3% and the principal 10–90% melting interval decreased by 52.6%. These counter-trends provide system-level evidence that the denser fin arrangement reduces the effective thermal resistance sufficiently to offset the reduced spacing-based buoyancy scale within the investigated range.
- Increasing inlet temperature intensified the thermal driving force between the HTF and PCM domains, thereby accelerating both conductive transport and convection-assisted melting within the molten PCM region.
- Reynolds number primarily influenced the HTF-side convective resistance rather than directly altering the internal PCM melting mechanisms. Consequently, its impact became progressively weaker

once the dominant thermal resistance shifted toward the PCM domain.

- The mechanical pressure loss increased from 1498.85 to 1584.88 Pa when Reynolds number increased from 500 to 2000, while ideal hydraulic power increased from 0.00402 to 0.01703 W. Accordingly, the thermal-storage gain per unit hydraulic work decreased from 51,431 to 25,006, demonstrating a trade-off between rapid charging and hydraulic efficiency. Among the tube-number cases at $Re = 2000$, the five-tube configuration provided the largest thermal-storage gain per unit hydraulic work, whereas the four-tube configuration retained the shortest complete-melting time.
- The relative-effect interaction analysis quantitatively confirmed non-additive parameter behavior. Based on complete melting time, the fin spacing–tube number, inlet temperature–tube number, Reynolds number–tube number, and Reynolds number–inlet temperature interaction magnitudes were 17.53, 14.31, 8.84, and 9.43 percentage points, respectively. By comparison, inlet temperature–fin spacing and Reynolds number–fin spacing interactions were relatively weak under the selected conditions.
- A dataset comprising 38,891 samples was developed from CFD-simulated data. The CatBoost-based surrogate model reproduced the CFD-generated transient liquid fraction and stored thermal energy with low normalized errors within the sampled design space. For the multi-output model, the normalized test RMSE values were 0.0155 for liquid fraction and 0.0169 for stored energy, with corresponding R^2 values exceeding 0.9997. Because a random row-wise partition was employed, the reported errors represent sample-level interpolation within the CFD-generated trajectories. They should not be interpreted as independent validation for unseen geometrical–operational configurations or as extrapolation to new materials, geometries, and operating regimes.

From an engineering perspective, the CFD analysis clarifies how HTF-side convection, conductive heat spreading, and buoyancy-driven transport interact during charging. The CatBoost surrogate complements the CFD analysis as a bounded proof-of-concept for rapid reconstruction and comparison of transient liquid fraction and stored energy within the sampled dataset. Because independent case-wise validation, boundary testing, and downstream optimization were not performed, its predictions should not be used for unsimulated design selection without additional CFD verification. Its use remains limited to interpolation within the investigated parameter domain and should not be interpreted as validated extrapolation or global design optimization.

The principal limitations of this study arise from its restriction to numerical charging, constant thermophysical properties, idealized adiabatic boundaries, and the absence of geometry-specific prototype validation, discharge and cyclic operation, whole-system pump and motor efficiencies, external piping losses, auxiliary-system power, economic evaluation, and local conductive–convective heat-flux decomposition. Future research should therefore prioritize experimental validation of the serpentine tube–fin unit, temperature-dependent material properties and environmental heat losses, charging–discharging cycles, and integrated thermo-hydraulic and economic assessment. Following validation with independently sampled CFD cases and experimental data, the surrogate framework could also be extended using case-wise partitioning, physics-informed sampling, and multi-objective design optimization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Dataset containing samples record of melting phase change is provided on Mendeley: <http://doi.org/10.17632/mzfwpphwpf.1>.

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