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Evaluation of different melting performance enhancement structures in a shell-and-tube latent heat thermal energy storage system

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Abstract

Latent heat thermal energy storage employing phase change materials are widely used in energy storage systems. To further improve the low thermal conductivity of phase change materials in these systems, it is essential to investigate different thermal enhancement techniques. In this work, two principal thermal enhancement techniques, e.g. finned tubes and conductive metal foams are numerically investigated for melting processes in a shell-and-tube latent heat thermal energy storage system. For fins the topology optimised fins are used, and the simulation predictions are validated by experimental results using additive manufactured topology optimised fins. For metal foams two configurations with different filling ratios, i.e. whole-foam structure and half-foam structure are considered. Compared to the configuration without enhancement, the thermal energy storage rates are 3.3-5.8 times higher. In addition, the results show that the topology optimised fins can achieve the best performance, but can only be an economical solution when the unit price ratio between the enhancement technique and the phase change materials is less than 6. For the first time the thermal enhancement performance and economic efficiency of these two principal techniques are quantitatively analysed. The results would be useful for appropriate energy storage design solutions in practice.

Key words: Phase change material (PCM), Latent heat thermal energy storage (LHTES), Melting, Shell-and-tube device, Additive manufacturing

37 **1. Introduction**

38 Nowadays, with the increased demand for renewable energy, energy storage systems
39 are desired to deal with the mismatched supply and demand of energy, and to further
40 enhance the system performance. The latent heat thermal energy storage (LHTES)
41 techniques are attractive due to advantages of reasonable investment and high energy
42 density. In a LHTES system, phase change materials (PCMs) are used to
43 charge/discharge thermal energy during melting/solidification [1]. One of the most
44 common LHTES techniques are shell-and-tube LHTES systems, with the PCMs filling
45 in the shell while the low/high temperature heat transfer fluid (HTF) flowing through
46 the internal tubes. For this system, one main barrier that needs to be tackled is the
47 heat transfer enhancement within the low thermal conductivity PCMs.

48 Substantial investigations have been carried out to enhance the heat transfer at the
49 PCM side of the shell-and-tube LHTES device. Relevant techniques that have been
50 applied include finned tubes, PCM with metal foam and nanoparticle-enhanced PCMs
51 [1]. Fins or extended surfaces are the most common way for performance
52 enhancement. Various fin configurations have been proposed and investigated by
53 researchers, such as longitudinal fin [2], annular fin [3], helical fin [4] and bifurcated fin
54 [5]. The results have demonstrated that the discharging/charging process can be
55 significantly shortened by using fin surfaces. The effects of fin dimensions (e.g. length,
56 orientation and thickness) [6-8], pipe configurations [9] on the device performance
57 have been thoroughly investigated. Especially, previous research has showed that fin
58 configurations affect the melting performance. The optimised fin configuration angles
59 during melting were investigated by Kazemi et al. [10] and Mahood et al. [11]. Due to
60 the natural convection effect, the fins concentrate at the lower part of the shell are
61 more effective to reduce the melting time when the device is placed horizontally.
62 Nevertheless, the proposed fin configurations are limited by design freedoms and the
63 optimised selection criterion is scarce. Recently, Pizzolato et al. [12] applied topology
64 optimisation algorithm to design the fin layouts of shell-and-tube LHTES systems.
65 They firstly obtained the optimised fin layouts of the discharge process, in both two-
66 dimensional (2D) and three-dimensional (3D) domain. The topology optimised 3D
67 design shows a mixture feature of longitudinal fins, angular fins, and pin fins [12]. The
68 natural convection effect was considered for the fin designs through topology
69 optimisation. The optimised fin designs can be 37 % and 17 % faster charge and
70 discharge compared to the conventional longitudinal fins [13]. The topology optimised
71 results of multi-tube configurations were further obtained, and additive manufacturing
72 was used to demonstrate the manufacturability of topology optimised fins [14].

73 Impregnation of porous foams is another commonly used technique to improve the
74 heat transfer of LHTES device as the porous foams made of copper or aluminium have
75 high heat transfer surface areas and high thermal conductivities. The effects of various
76 influential factors of the porous foams such as inlet fluid conditions [15], configurations
77 [16], foam porosity [17, 18] and hypergravity [19] have been investigated numerically
78 and experimentally. The geometric factors of porous foams have a significant impact
79 on the performance of LHTES device. During melting, the insertion of metal foams can
80 restrict the flow motion and have passive effects on the natural convection. Recently
81 effects of porosity-variability, partial foam have been further investigated to understand

82 how this configuration affects the PCM melting. Yang et al. [20] proposed a metal foam
83 structure with linearly changed porosity. The results showed that the linear increased
84 porosity from bottom could enhance natural convection and shorten the melting
85 time. Recently, the gradient foam design design has been applied to the shell-and-
86 tube LHTES device. Pu et al. [21] numerically investigated the effect of gradient copper
87 foam on the melting performance. A radial gradient porosity (0.99-0.97-0.87) was
88 recommended that can further reduce the melting time by 23.7%. A 2D gradient
89 porosity along radial and circumferential direction is proposed by Yang et al. [22], the
90 melting time can be reduced by 32.11% compared with the uniform structure. Xu et al.
91 [23] investigated the effect of foam arrangements on the melting process, and found
92 that the optimal filling ratio of the foams is 0.7 for a horizontal shell-and-tube LHTES
93 device. Similar partial foam approach have been applied to the rectangular cavity [24].
94 In general, the partial foam concentrated in the lower part of the device would be useful
95 to enhance the heat transfer and reduce the melting time [25].

96 Recently the combination of different thermal enhancement techniques in a LHTES
97 device is also attracting attention. Yang et al. [26] numerically investigated the fin-
98 metal-foam TES device, a further heat enhancement can be achieved by combining
99 fins and metal foams. An experimental study was performed by Guo et al. [27], a
100 reduction of 83.35% melting time can be achieved compared with the conventional
101 device without thermal enhancement. An alternative methodology to enhance the
102 thermal response is the application of nanoparticles [28]. The dispersion of high
103 thermal conductivity nanoparticles can shorten the melting and solidification time.
104 However, the addition of nanoparticles can increase the fluid viscosity and cause
105 natural convection suppression [29]. Some researchers reported the use of a
106 combination fin and nanoparticles, they found that the addition of nanoparticles cannot
107 improve the melting process in the heat conduction dominated region [30], and a
108 better enhancement can be achieved by purely adding fins when using the same
109 volume materials [31].

110 As the natural convection effects during melting can be inhibited by extended fin
111 surfaces and foams, understanding how these thermal enhancement techniques
112 affect the melting performance is important. Meanwhile, there is a lack of research in
113 literature to quantitatively compare and evaluate the performance of different heat
114 transfer enhancement methods for the shell-and-tube LHTES device. Even if some
115 optimised configurations have been proposed, a comprehensive comparison and
116 evaluation of these techniques is still necessary. In this work, 2D computational fluid
117 dynamics (CFD) models were developed to evaluate the performance of the topology
118 optimised fins and porous foams for the melting process in the LHTES system. An
119 additive manufactured device was used to validate the model predictions for the
120 topology optimised fins. Different configurations, i.e. single-tube and four-tube were
121 considered. Qualitative and quantitative comparisons were made in the end between
122 different cases under same operation conditions and PCM volumes.

123

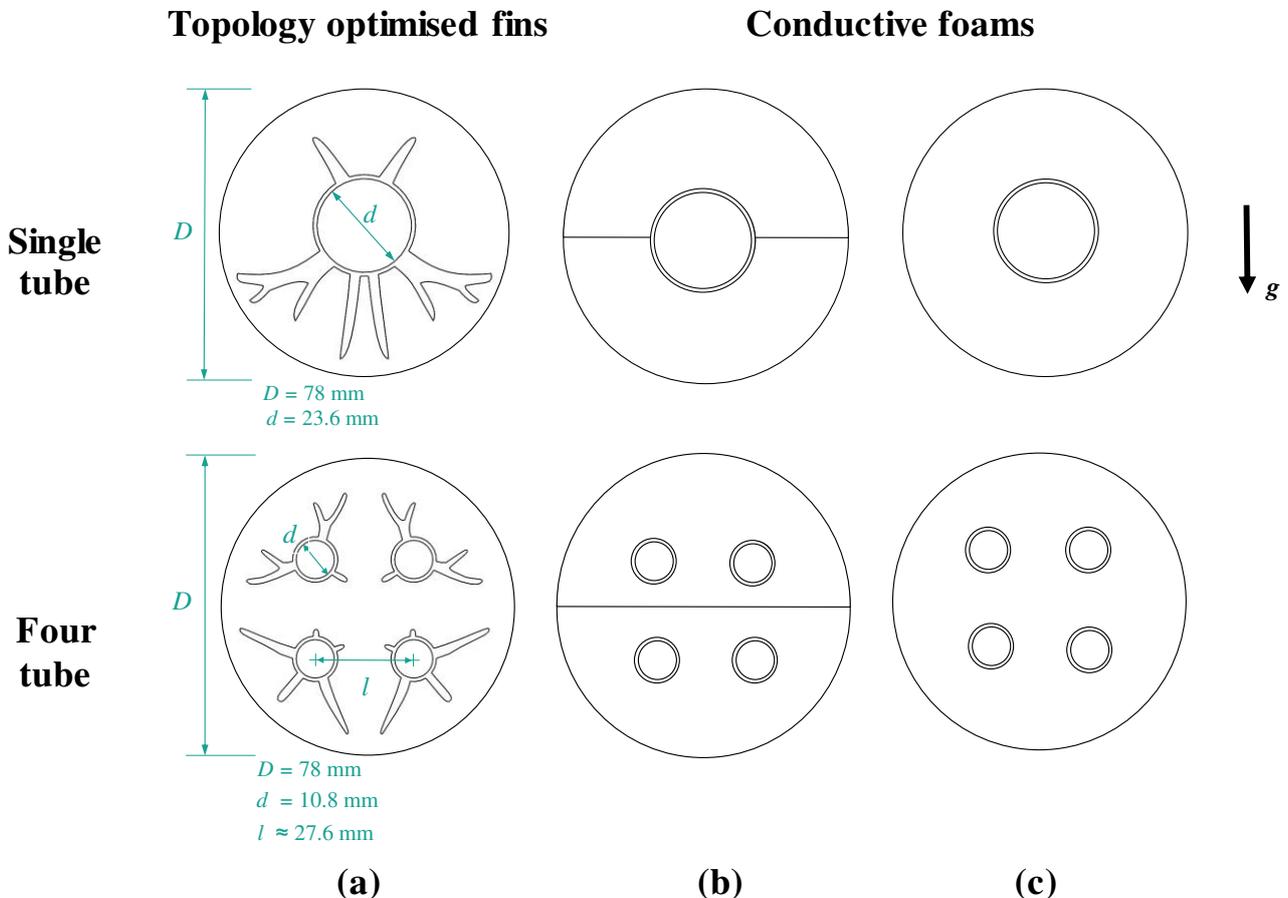
124

125 **2. Methodology**

126 2.1 System description

127 The schematic diagram of the LHTES devices and detailed dimensions used in this
 128 work are illustrated in Figure 1. The effect of tube configurations, i.e. single-tube and
 129 four-tube was considered for all cases.

130 Figure 1 (a) illustrates topology optimised fins with special configurations for melting
 131 process. Both natural convection and conduction effects were considered during
 132 topology optimisation [13, 32]. This configuration could help to enhance heat transfer
 133 via both convection and conduction. The high conductivity fins mainly concentrate in
 134 the conduction dominated bottom region which is particularly obvious for the single-
 135 tube configuration. For making a better comparison with the topology optimised fins,
 136 two different conductive foam configurations are considered. In Figure 1 (b) the metal
 137 foam is only filled the lower half region, while in Figure 1 (c) the metal foam is fully
 138 filled the region. In the following, they are also named as half-foam structure and
 139 whole-foam structure, respectively. For all cases, the volume fraction of the high
 140 conductivity aluminium alloy was set to 10% of the whole domain, and correspondingly
 141 the PCM occupies 90% of the investigated domain.



142 Figure 1. Schematic diagram of the LHTES devices . (a) Topology structure. (b) Half-
 143 foam structure. (c) Whole-foam structure. The arrow shows the gravity direction.

144

145 2.2 Mathematical model

146 The enthalpy-porosity approach was used for simulation of PCM melting [33]. The
 147 temperature and the velocity of the PCM during melting can be calculated using the
 148 Navier-Stokes equations. A commercial paraffin RT25 HC (Rubitherm GmbH) was
 149 used as PCM materials, and the physical properties are listed in Table 1 [34]. In this
 150 work, the temperature-dependent function of viscosity is not considered. This is in
 151 accordance with the previous topology optimisation simulations and some relevant
 152 research works using RT 25HC PCM [14, 35]. The effect of temperature on the
 153 viscosity can be further investigated in future. The physical properties of aluminium
 154 alloy used for topology optimised fins and conductive foams are listed in Table 2 [36].

155 As the main focus of this work is on the evolutions of the liquid fraction and temperature
 156 along the radial direction, 2D domain with isothermal heating boundary of inner tube
 157 is investigated. The fluid temperature variation in the inner tubes and relevant 3D
 158 effects are not investigated in this work. The governing equations have different forms
 159 according to different systems.

160 2.2.1 Topology optimised fins

161 By using topology optimisation algorithm, the high conductive fin configurations can
 162 be optimised in the whole domain. Detailed topology optimisation procedure have
 163 been reported in previous work [13, 32]. In the following, the topology optimised fins
 164 for melting are used for performance evaluation.

165 The continuity equation is:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (1)$$

166 where u and v are the fluid velocities in x and y directions.

167 The momentum equations at two different directions are:

$$\rho_P \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = \mu_P \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - \frac{\partial p}{\partial x} + \frac{(1-\beta)^2}{(\beta^3 + \omega)} A_m u \quad (2)$$

$$\rho_P \left(\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = \mu_P \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - \frac{\partial p}{\partial y} + \frac{(1-\beta)^2}{(\beta^3 + \omega)} A_m v - \rho_P g \gamma_P (T - T_{ref}) \quad (3)$$

168 where ρ_P is the PCM density, t is time, μ_P is dynamic viscosity, p is effective pressure,
 169 T is temperature, γ_P is thermal expansion coefficient. ω is a small constant number
 170 (0.0001) to avoid division by zero which has been used by previously PCM melting
 171 simulations [13, 15]. A_m ($10^8 \text{ kg}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$) is the mushy constant that describes how
 172 sharply the velocity is reduced to zero when the PCM solidifies. β is the liquid fraction
 173 of PCM that can be given by:

$$\beta = \begin{cases} 0 & \text{if } T < T_s \\ \frac{T - T_s}{T_1 - T_s} & \text{if } T_s < T < T_1 \\ 1 & \text{if } T > T_1 \end{cases} \quad (4)$$

174 In this work, T_1 is 295 K, and T_s is 299 K (Table 1).

175 The governing energy equation of PCM phase is:

$$\rho_P C_{p,P} \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = \frac{\partial}{\partial x} \left(k_P \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_P \frac{\partial T}{\partial y} \right) - L_P \frac{\partial \beta}{\partial t} \quad (5)$$

176 where $C_{p,P}$ is the specific heat of PCM, k_P is the thermal conductivity of PCM, L_P is
177 the latent heat.

178 The governing energy equation of the topology optimised fins made of aluminium alloy
179 can be written as:

$$\rho_M C_{p,M} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k_M \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_M \frac{\partial T}{\partial y} \right) \quad (6)$$

180 where $C_{p,M}$ is the specific heat of aluminium alloy, k_M is the thermal conductivity of
181 aluminium alloy.

182 Table 1 Thermophysical properties of RT25 HC PCM [34].

Description	Parameter	
Density of solid ($\text{kg}\cdot\text{m}^{-3}$)	ρ_P	880
Melting range (K)	ΔT	295-299
Latent heat ($\text{kJ}\cdot\text{kg}^{-1}$)	L_P	232
Thermal conductivities solid/liquid ($\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$)	k_P	0.2
Specific heat ($\text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$)	$C_{p,P}$	2
Viscosity ($\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-1}$)	μ_P	0.001798
Thermal expansion coefficient (K^{-1})	γ_P	0.001

183

184

185 Table 2. Thermophysical properties of aluminium alloy [36].

Description	Parameter	
Density of solid ($\text{kg}\cdot\text{m}^{-3}$)	ρ_M	2700
Thermal conductivity ($\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$)	k_M	160
Specific heat ($\text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$)	$C_{p,M}$	0.9

186

187 2.2.2 Conductive foam

188 The conductive foam embedded in PCM phase provides a promising way to enhance
 189 heat transfer during melting process. A mathematical model has been developed to
 190 describe the whole process in porous media [15].

191 The momentum equations are:

$$\rho_P \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = \mu_P \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - \frac{\partial p}{\partial x} + \frac{(1-\beta)^2}{(\beta^3 + \omega)} A_m u + \frac{\mu_P}{a} u + \frac{1}{2} C_i \rho_P u |u| \quad (7)$$

$$\rho_P \left(\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = \mu_P \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - \frac{\partial p}{\partial y} + \frac{(1-\beta)^2}{(\beta^3 + \omega)} A_m v - \rho_P g \gamma_P (T - T_{ref}) + \frac{\mu_P}{a} v + \frac{1}{2} C_i \rho_P v |v| \quad (8)$$

192 The viscous resistance and the inertia resistance at two different directions are
 193 considered in the momentum equations. The definition of permeability a and the
 194 inertia coefficient C_i are given in the following sections. Due to the low velocities during
 195 melting process, the inertia resistance has insignificant effect on the results.

196

197 A non-equilibrium thermal model is used to describe the porous media:

$$\varepsilon \rho_P C_{p,P} \frac{\partial T}{\partial t} + \rho_P C_{p,P} \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = (k_{fe} + k_{td}) \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + h_{sf} A_{sf} (T_f - T_s) - \varepsilon \rho_P L_P \frac{\partial \beta}{\partial t} \quad (9)$$

$$(1 - \varepsilon) \rho_M C_{p,M} \frac{\partial T}{\partial t} = k_{se} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + h_{sf} A_{sf} (T_s - T_f) \quad (10)$$

198 where ε is the porosity of the conductive foam. k_{fe} and k_{se} are the effective thermal
 199 conductivities of the PCM and foam. k_{td} is used to describe the effect of thermal
 200 dispersion. A_{sf} is the surface area density, and h_{sf} is heat transfer coefficient between
 201 PCM and the porous foam.

202 (1) Permeability and inertial coefficient

203 The permeability a and the inertia coefficient C_i can be calculated by the following
 204 equations [37]:

$$a = 0.00073(1 - \varepsilon)^{-0.224} d_f^{-1.11} d_p^{0.89} \quad (11)$$

205

$$C_i = 0.00212(1 - \varepsilon)^{-0.132} \left(\frac{d_f}{d_p} \right)^{-1.63} \quad (12)$$

206 The cell ligament d_f and the pore size d_p can be defined as [37]:

$$\frac{d_f}{d_p} = 1.18 \sqrt{\frac{1 - \varepsilon}{3\pi}} \left(\frac{1}{1 - e^{-(1-\varepsilon)/0.04}} \right) \quad (13)$$

207 (2) Effective thermal conductivity and the effects of thermal dispersion

208 The effective thermal conductivities of the PCM k_{fe} and the metal foam k_{se} are
 209 calculated from a tetrakaidecahedron model [38]:

$$k_{fe} = \frac{\sqrt{2}}{2(M_A + M_B + M_C + M_D)} \Big|_{k_M=0} \quad (14)$$

$$k_{se} = \frac{\sqrt{2}}{2(M_A + M_B + M_C + M_D)} \Big|_{k_P=0} \quad (15)$$

$$M_A = \frac{4\sigma}{(2e^2 + \pi\sigma(1-e))k_M + (4 - 2e^2 - \pi\sigma(1-e))k_P} \quad (16)$$

$$M_B = \frac{(e - 2\sigma)^2}{(e - 2\sigma)e^2k_M + (2e - 4\sigma - (e - 2\sigma)e^2)k_P} \quad (17)$$

$$M_C = \frac{(\sqrt{2} - 2e)^2}{2\pi\sigma^2(1 - 2e\sqrt{2})k_M + 2(\sqrt{2} - 2e - \pi\sigma^2(1 - 2e\sqrt{2}))k_P} \quad (18)$$

$$M_D = \frac{2e}{e^2k_M + (4 - e^2)k_P} \quad (19)$$

$$\sigma = \sqrt{\frac{\sqrt{2} \left(2 - \frac{5}{8e^3\sqrt{2}} - 2e \right)}{\pi(3 - 4e\sqrt{2} - e)}} \quad (20)$$

$$e = 0.339 \quad (21)$$

210 The thermal dispersion conductivity is derived from a dimensionless thermal
211 dispersion model proposed by Georgiadis and Catton [39]:

$$k_{td} = \frac{0.36}{1 - \varepsilon} \rho_P C_{p,P} d_f \sqrt{u^2 + v^2} \quad (22)$$

212 (3) Interfacial heat-transfer coefficient

213 The heat transfer coefficient was estimated using Churchill and Chu [40] correlation:

$$h_{sf} = \frac{k_P}{d_f} \left(0.36 + \frac{0.518 Ra_d^{1/4}}{\left[1 + \left(\frac{0.599}{Pr} \right)^{9/16} \right]} \right) \quad (23)$$

$$Ra_d = \frac{g\gamma|T_f - T_s|d_f^3}{\alpha_f \nu_f} \quad (24)$$

214

215 where T_f and T_s are the temperature of fluid and solid phases, α_f is the thermal
216 diffusivity, and ν_f is the kinematic viscosity.

217 The specific surface area A_{sf} of the metal foams can be calculated by [37]:

$$A_{sf} = \frac{3\pi d_f (1 - e^{-(1-\varepsilon)/0.04})}{(0.59d_p)^2} \quad (25)$$

218 2.2.3 Performance evaluation

219 Two parameters, average thermal energy storage rate, p_{ave} , and average thermal
 220 energy storage density, q_{ave} , are introduced to evaluate the performance of different
 221 structured configurations [23] :

$$222 \quad p_{ave} = \frac{Q}{t_m} = \frac{m_M \int c_{p,M} dT + m_P (\int c_{ps,P} dT + L + \int c_{pl,P} dT)}{t_m} \quad (26)$$

$$223 \quad q_{ave} = \frac{Q}{m} = \frac{m_M \int c_{p,M} dT + m_P (\int c_{ps,P} dT + L + \int c_{pl,P} dT)}{m_P + m_M} \quad (27)$$

224 where m_M and m_P are respectively the mass of enhanced structure and PCM. The
 225 p_{ave} refers to the device thermal energy storage capacity per unit charging time while
 226 q_{ave} indicates the device capacity per unit material amount. For a PCM based device
 227 particularly for these containing low temperature PCM, i.e., the paraffin in this work,
 228 the great majority of heat will be stored through the latent heat form, and the sensible
 229 heat of the enhanced structure and PCM can be ignored [23]. Therefore, the Equations
 230 (26) and (27) can be simplified as follows:

$$231 \quad p_{ave} = \frac{m_P L}{t_m} \quad (28)$$

$$232 \quad q_{ave} = \frac{m_P L}{m_P + m_M} \quad (29)$$

233 Given dimensionless transformation, the above two equations can be further changed
 234 to:

$$235 \quad p'_{ave} = \frac{p_{ave}}{p_{ave,0}} = \frac{m_P L / t_m}{m_{P,0} L / t_{m,0}} = \frac{m_P t_{m,0}}{m_{P,0} t_m} \quad (30)$$

$$236 \quad q'_{ave} = \frac{q_{ave}}{q_{ave,0}} = \frac{m_P L / (m_P + m_M)}{m_{P,0} L / m_{P,0}} = \frac{m_P}{m_P + m_M} \quad (31)$$

237 where the $p_{ave,0}$ and $q_{ave,0}$ respectively relate to the average TES rate and density of
 238 the configuration without enhancement structure.

239 A parameter of TES rate per material cost p_c is also introduced for determining the
 240 device input-output performance and its formula can be expressed as follows:

$$241 \quad p_c = \frac{Q}{t_m S} = \frac{m_M \int c_{p,M} dT + m_P (\int c_{ps,P} dT + L + \int c_{pl,P} dT)}{t_m (a_M m_M + a_P m_P)} \approx \frac{m_P L}{t_m (a_M m_M + a_P m_P)} \quad (32)$$

$$242 \quad p'_c = \frac{p_c}{p_{c,0}} = \frac{m_P L}{t_m (a_M m_M + a_P m_P)} \bigg/ \frac{m_{P,0} L}{t_{m,0} m_{P,0} a_P} = \frac{m_P}{t_m / t_{m,0} (R m_M + m_P)} \quad (33)$$

243 where S represents the total material cost of the PCM and enhancement structures. a
 244 indicates the unit price. p'_c is the dimensionless form of p_c which stands for the ratio
 245 between p_c and $p_{c,0}$. R means unit price ratio of the enhancement structures to the
 246 PCM:

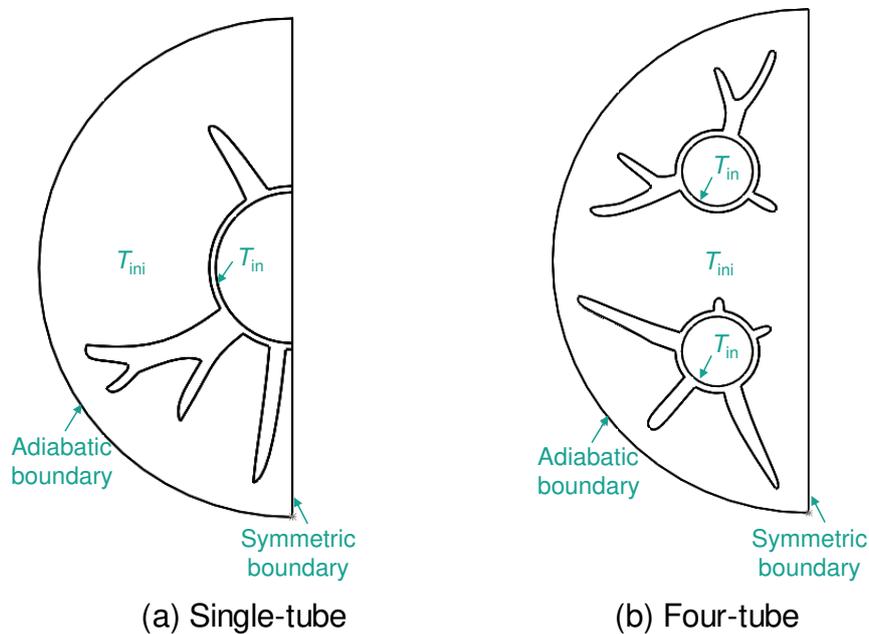
$$247 \quad R = a_M / a_P \quad (34)$$

248 where a_M is the unit price the enhancement technique, and a_P is the unit price of PCM.

249 2.3 Numerical schemes and validation

250 CFD simulations of different systems were carried out using ANSYS FLUENT 2019.
 251 A software of GAMBIT 2.2 was used for mesh building. The finite volume method (FVM)
 252 was adopted to discretise the governing equation with the PRESTO scheme and the
 253 SIMPLEC algorithm being respectively employed for the pressure correction equation
 254 and pressure-velocity coupling. A scheme of second-order upwind was used for
 255 discretising the momentum and energy terms.

256 A schematic view of the model design for CFD simulations on topology structure is
 257 illustrated in Figure 2. In simulations, due to the symmetry of the systems, only the left
 258 half of the domain needs to be considered (Figure 2). For all systems, the initial
 259 temperature of the solid PCM is $T_{ini}=294.5$ K, and the temperature of the inlet wall is
 260 $T_{in}=308$ K. Mesh independence study was performed considering different cell
 261 numbers. The liquid fraction (β) values considering different cell numbers are shown
 262 in Table 3. In this work, 1.2×10^5 cells were adopted to ensure the results reliability.
 263 Time step independence analysis is shown in Table 4. From Table 4, a time step of
 264 0.05 s is sufficient to ensure time step independence.



265
 266 Figure 2. Schematic view of the model design for CFD simulations.

267
 268
 269 Table 3. The liquid fraction (β) values considering different cell numbers.

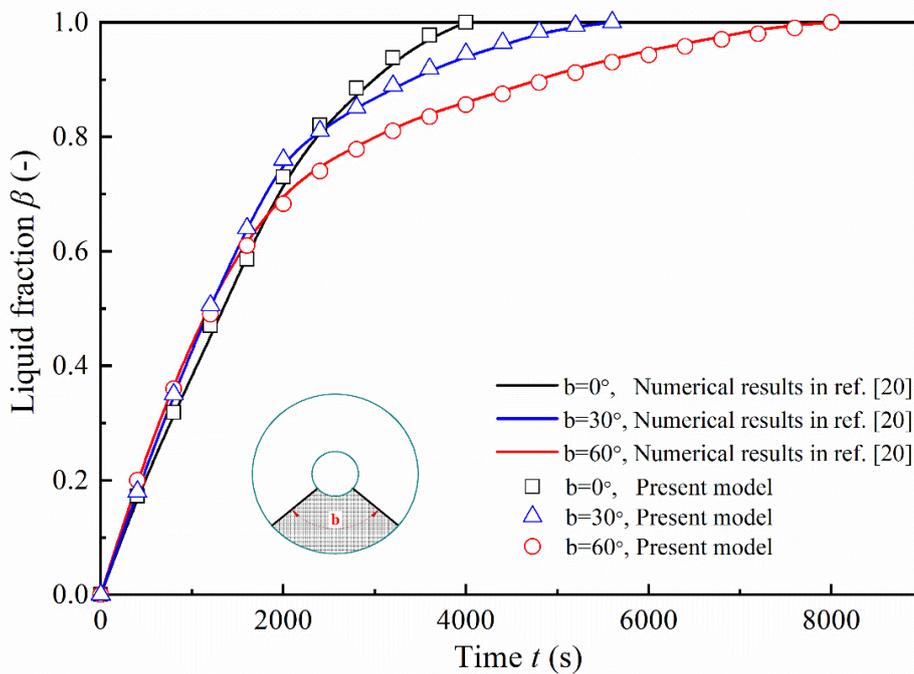
	800 s	1600 s	3200 s	4000 s
6×10^4 cells	0.396	0.614	0.939	1.0
1.2×10^5 cells	0.398	0.623	0.947	1.0
2×10^5 cells	0.394	0.618	0.946	1.0

270
 271 Table 4. Time step independence analysis.

	Time step (s)	Melting time (s)	Deviation from reference case (%)
Test 1	0.1	4222	13
Test 2	0.05	3753	0.48
Reference case	0.025	3735	-

272

273 The validation for the partial-porous model by comparing the present model
 274 predictions with modelling results from [25] under the same operation and geometrical
 275 conditions is shown in Figure 4. A horizontal shell-and-tube configuration with external
 276 diameter of 62.5 mm and internal diameter of 20 mm was modelled with a binary salt
 277 of $\text{Li}_2\text{CO}_3\text{-K}_2\text{CO}_3$ with mole ratio of 62:38 used as PCM. A parameter of the angle
 278 between neighbouring metal foam (b) was employed to investigate the metal foam
 279 volume effects on the melting process. One can see from Figure 4 that, for the selected
 280 different b (0° , 30° and 60°), reasonably well agreements between the current model
 281 and numerical results have been achieved with an average deviation less than 5%
 282 observed, demonstrating the reliability in the present model for partial-porous case
 283 modelling.

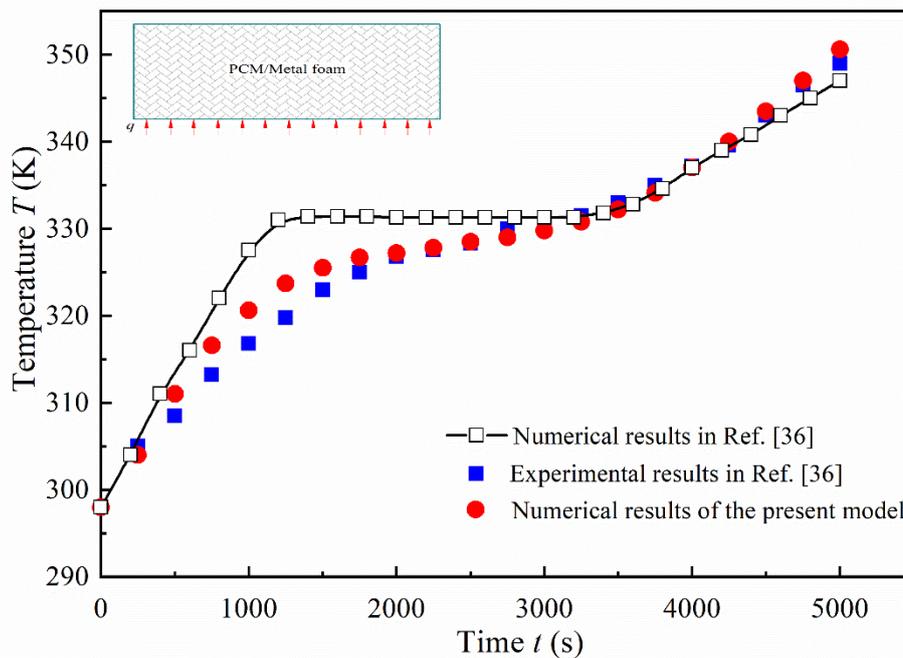


284

285 Figure 4. Model reliability for the partial-porous case.

286 Figure 5 presents the verification and validation of the full-porous model with the
 287 experimental results obtained from [41]. A copper foam mixed with paraffin wax was
 288 used as storage medium and fully filled into a rectangular tank with dimensions of 200
 289 mm in length and 50 mm in height. A constant heat flux is given from the bottom
 290 surface and the temperature variation at position of 8 mm above the heating surface
 291 is recorded for comparison. It can be seen from Figure 5 that both the present

292 modelling results and experimental data show the PCM starting to melt around 1100
 293 s and completing the charging process around 3900 s. A small deviation between the
 294 present model and experimental results has been obtained, thus establishing the
 295 reliability in the current model for the full-porous case simulation. The deviation
 296 between the present predictions and numerical results in [41] is associated with the
 297 paraffin melting temperature difference used in these two models. In [41], the melting
 298 point of PCM was taken as a constant value, whereas a melting range of 321-335 K
 299 was adopted in the present simulation. This leads to a relatively slant temperature
 300 curve over the melting process, and thus a reasonably good consistence of the present
 301 model with experimental results.



302

303

Figure 5. Model reliability for the full-porous case.

304 3. Results and discussion

305 3.1 Additive manufactured topology optimised device and experiment validation

306 In this work, selective laser melting (SLM) metallic additive manufacturing technique
 307 was applied to manufacture the topology optimised fins. The additive manufactured
 308 device is used to validate numerical simulations and demonstrate the
 309 manufacturability of topology optimised fins in reality. As illustrated in Figure 6, by
 310 extruding the 2D topology optimised single-tube design along axial direction and
 311 connected by pipes at both ends, the design is converted to a 3D device that can be
 312 manufactured. An aluminium alloy (Al-5 % Cu) with high thermal conductivity was used
 313 as the fin material. Figure 7 (a) demonstrates the final product of additive
 314 manufactured topology optimised fins. The features of fin structures can be well
 315 reproduced by additive manufacturing, and ready for experimental testing. As

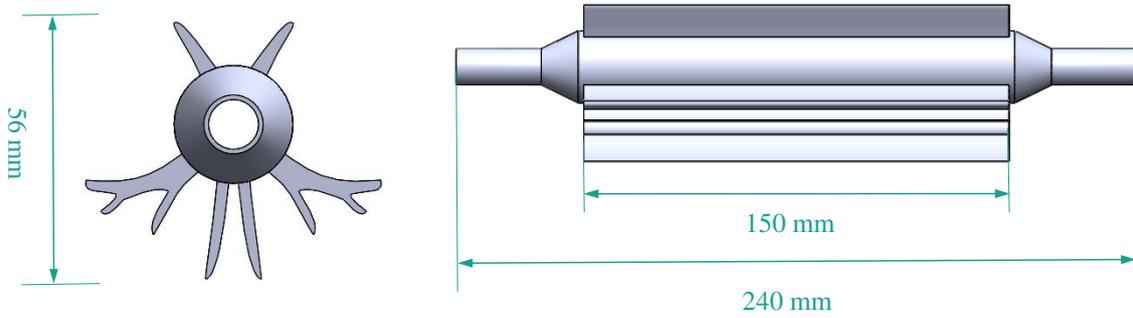
316 illustrated in Figure 7 (b), the additive manufactured device is inserted into an acrylic
317 shell for experimental tests.

318 The materials and parameters in experiments were kept the same with simulations.
319 For running experiments, the shell was filled up with liquid PCMs (RT25 HC). The PCM
320 was solidified to $T_{ini}=294.5$ K by connecting to a chiller with a temperature stability of
321 ± 0.2 °C. During experiments, the high temperature fluid with a constant temperature
322 ($T = 308$ K) flow through the central pipe, and the PCM is gradually melted. The
323 temperature at different positions within PCM is recorded during the whole process.
324 Detailed descriptions of this experimental system and test procedure have been
325 presented in our previous work [36].

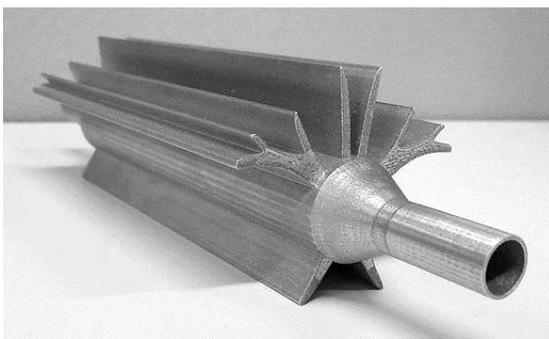
326 Figure 8 depicts the temperature evolutions at different measurement positions during
327 the whole melting process. The four temperature measurement points in Figure 8 (a)
328 are numbered by 1, 2, 3 and 4 and annotated by different colours in accordance with
329 the curves in Figure 8 (b). In this figure, the CFD simulation results are compared with
330 experimental measurements. The temperature evolutions of numerical simulations
331 and experimental measurements show same tendency. The slight difference between
332 experiments and simulations is likely because of the average physical properties
333 adopted in simulations.

334 It is worthy to notice that the temperature values at these four measurement points
335 have different trends. As illustrated in Figure 8 (b), the temperature at point 1 and 2 in
336 the lower region rises sharply to the melting range at the beginning. After 500 s, the
337 PCM at these two points are in fully melted states with slowly rising temperature trends
338 afterwards. In the upper region, the temperature evolutions at point 3 and 4 are slower
339 and have three distinguished stages. For point 3, at the initial stage (0-1200 s), the
340 PCM is solid with a constant temperature of around 295 K. After that, the temperature
341 gradually rises to 303 K, and it transforms from solid phase to liquid phase. This is
342 followed by a relatively constant temperature stage as the PCM is totally melted. The
343 temperature at point 7 shows a similar tendency with point 3 but a slower process to
344 be fully melted.

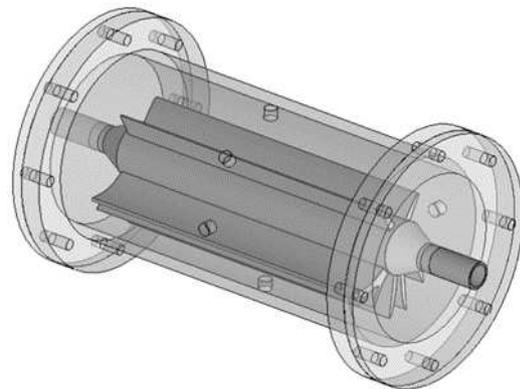
345 The PCMs of point 1 and 2 in the lower region are near the conductive fins that can
346 be rapidly melted, while point 3 and 4 in a convection dominated region have different
347 heat transfer mechanisms and temperature profiles. The results in Figure 8 testify that
348 the modelling assumptions adopted here can be used to predict the melting process
349 in the system. In the following, CFD simulations were used to further analyse the
350 temperature and liquid fraction evolutions during melting and to compare the
351 performance of different systems.



352 Figure 6. Schematic of the additive manufactured energy storage device with
 353 topology optimised fins.



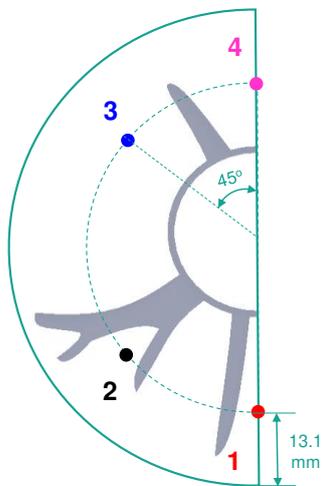
(a) Additive manufactured fins



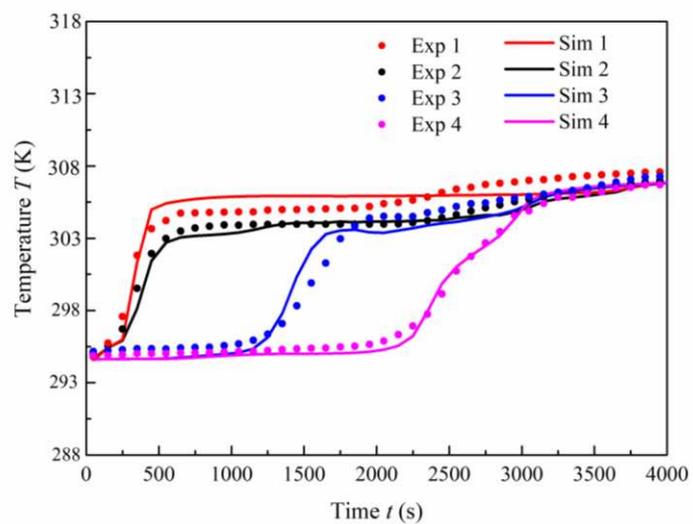
(b) 3D design of the device

354

355 Figure 7. Additive manufactured topology optimised fins and 3D design of the energy
 356 storage device.



(a) Measurement points



(b) Temperature profiles

357

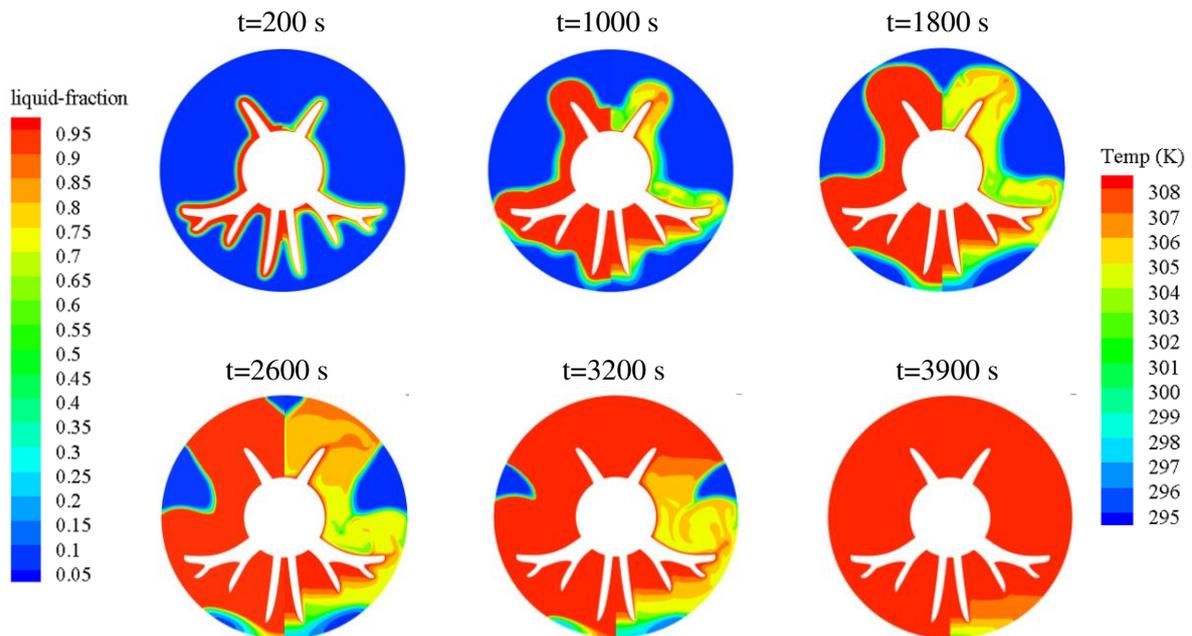
358 Figure 8. Comparison of the experimental results and numerical simulations of the
359 measured temperatures.

360 3.2 Numerical simulation results

361 3.2.1 Topology optimised fins

362 Figure 9 presents the temperature and liquid fraction profiles of the topology optimised
363 fins for single-tube configuration. At the beginning stage, the melting region occurs
364 around the fins and it gradually grows. After 3200 s, the solid phase only remains in
365 the bottom and central near wall region. The PCM is completely melted at about 3900s.
366 Figure 10 illustrates the corresponding velocity profiles. It is clear to see that the
367 convection eddies occur in the upper region and the optimised fin configurations are
368 helpful to redirect the flows, while in the region below the pipe the velocity is negligible
369 and the melting is dominated by conduction.

370 The temperature and liquid fraction profiles of the four-tube topology optimised fins
371 are illustrated in Figure 11. The melt fronts initiate along the fins of the four pipes, and
372 gradually spread to the whole region. After 1600 s, the solid PCM mainly remains in
373 the bottom region and is completely melted at about 2400 s. As shown in Figure 12,
374 high velocities can be observed near the fin regions at the beginning. Due to the strong
375 natural convection, the PCM in the upper region has been melted completely after
376 1600 s. At this time point, the melting front reaches the bottom regions, and liquid PCM
377 start to move upwards as illustrated in Figure 12. In the following section, the liquid
378 fraction variations are obtained and compared with the metal foam system.

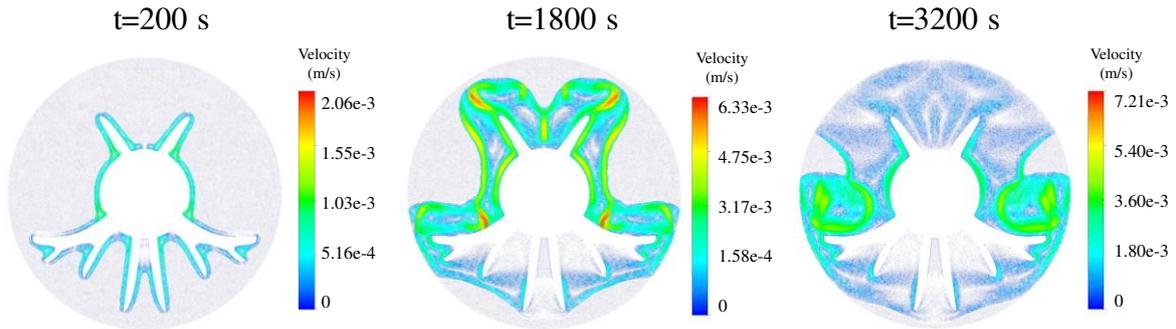


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380 Figure 9. Liquid fraction (left side) and temperature (right side) profiles of the
381 topology optimised fins for single-tube device.

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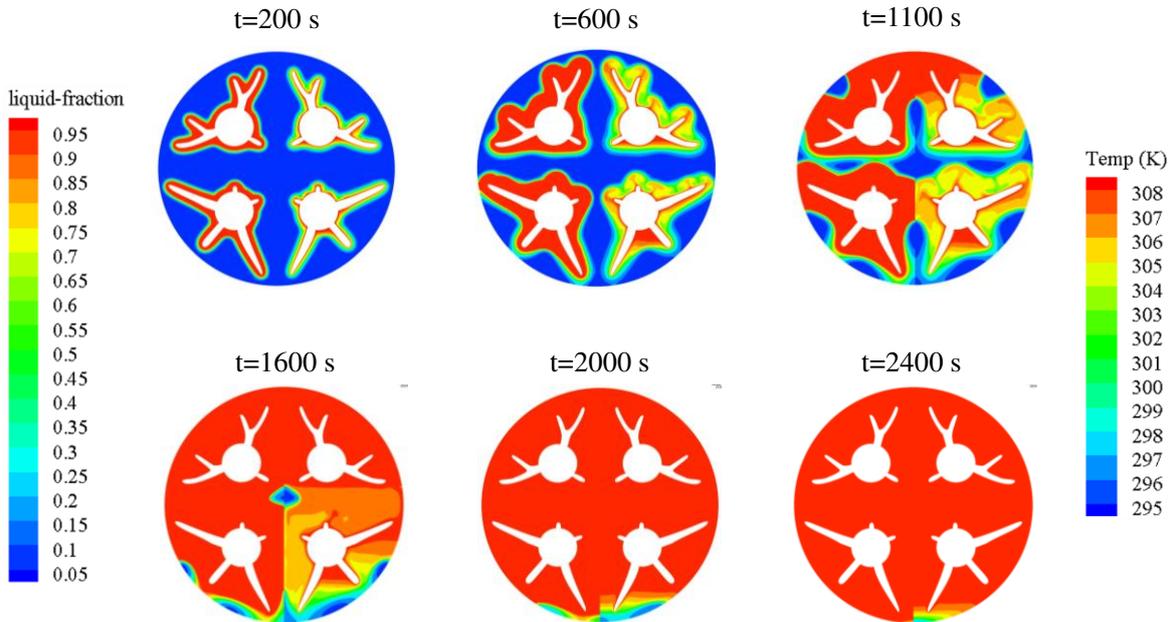
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385 Figure 10. Velocity profiles of the topology optimised fins for single-tube device.

386



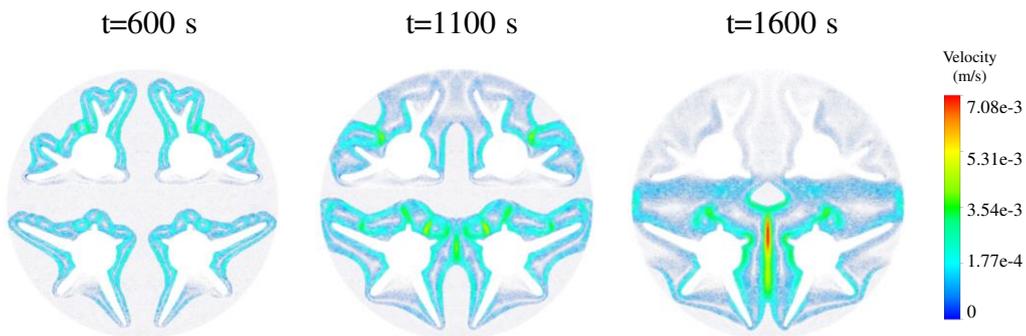
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388 Figure 11. Liquid fraction (left side) and temperature (right side) profiles of the

389

390 topology optimised fins for four-tube device.

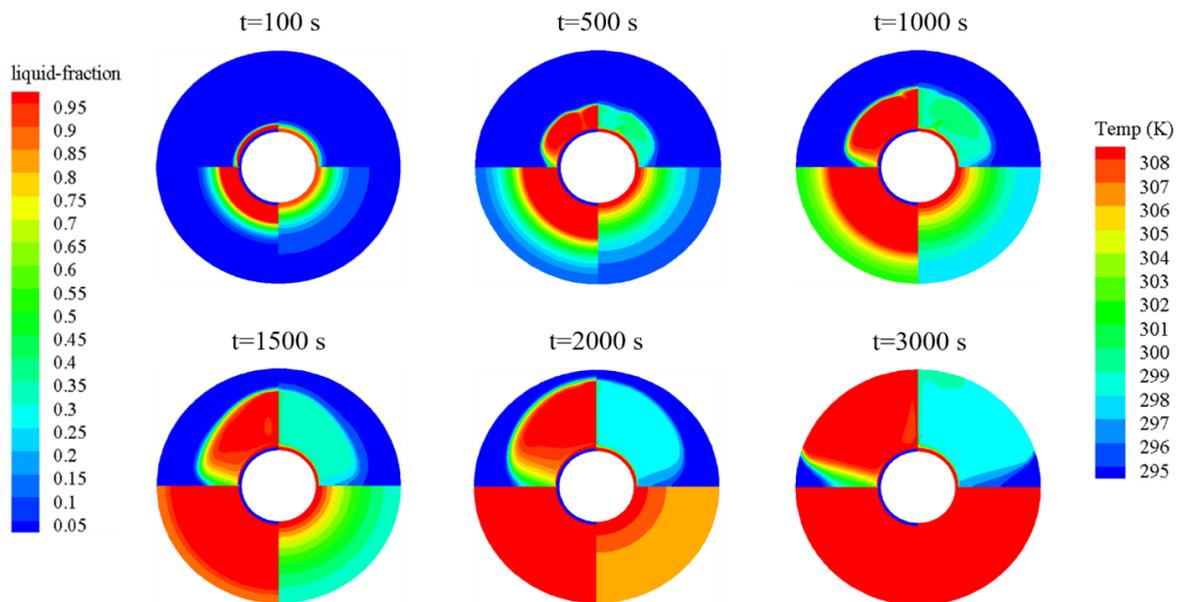
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391 Figure 12. Velocity profiles of the topology optimised fins for four-tube device.

392 3.2.2 Conductive foams

393 Figure 13 shows the contours of temperature and liquid fraction for single-tube device
394 containing half-foam structure. One can see that the natural convection and thermal
395 conduction respectively dominates the heat transfer process in the upper and lower
396 parts of the device. At the initial melting stage ($t=100$ s), the melting process within the
397 device is mainly governed by thermal conduction and only a small amount of PCM
398 close to the heating tube melts. As the melting process evolves, more solid material
399 melts, leading to the increase of liquid phase in the device. Owing to the existed
400 density between the solid and liquid phases, natural convection starts to play an
401 important role in driving the material melting, which in turn leads to the acceleration of
402 material melting in the upper part. Over the melting duration of 500-2000 s, intense
403 natural motion is apparent, achieving fast melting rate in the non-foam zone. From
404 Figure 13, it can also be seen that, due to the implementation of metal foam, the
405 effective thermal conductivity in the lower part is higher than that in the upper part,
406 which leads to a faster melting rate in the foam filled field.

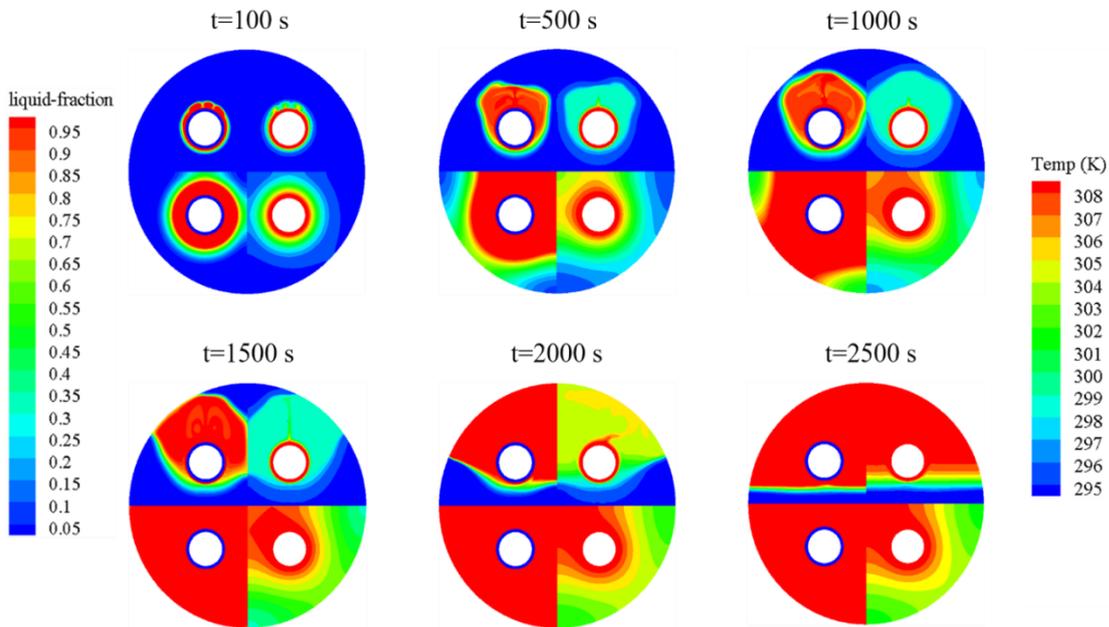


407

408 Figure 13. Contours of liquid fraction (left side) and temperature (right side) for
409 single-tube device containing half-foam structure.

410 Figure 14 displays the contours of temperature and liquid fraction for four-tube device
411 containing half-foam structure. It can be seen that, similar to single-tube device, the
412 melting process in the lower part of the four-tube device is mainly governed by thermal
413 conduction while that occurred at the upper part is first dominated by thermal
414 conduction and later by natural convection. Because of the high effective thermal
415 conductivity, the average temperature in the lower part increases faster than that in
416 the lower part. Giving the contrastive analysis of the contours shown in Figures 13 and

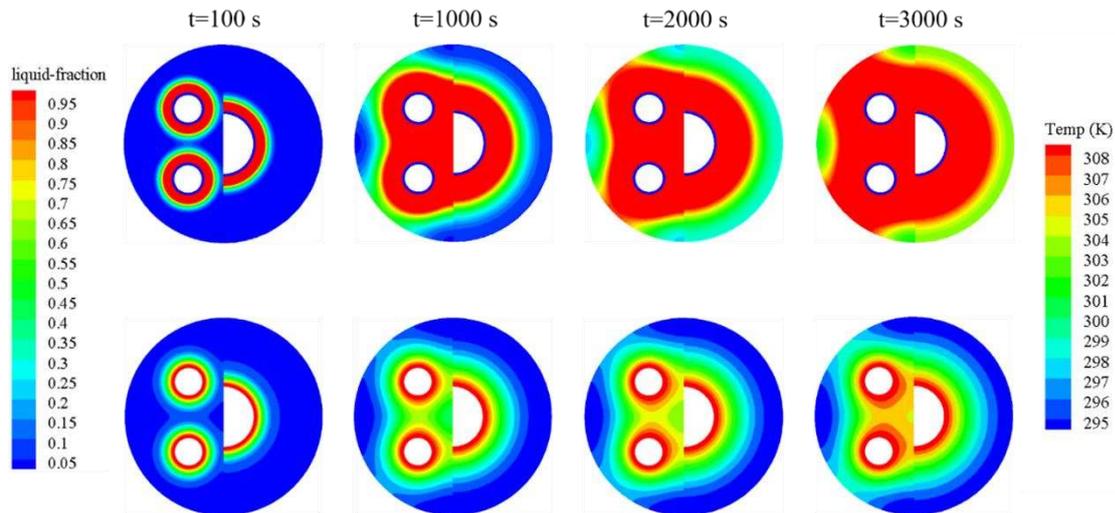
417 14, one can see a relatively faster melting process and a low extent of thermal
 418 stratification in the four-tube device than that in single-tube device. At the same melting
 419 moment, i.e., $t=500$ s and $t=2000$ s, the average temperature and liquid fraction in the
 420 four-tube configuration are apparently higher than that in the single-tube configuration,
 421 which implies a higher heat transfer rate in the four-tube device in comparison with the
 422 single-tube device. This observation indicates, for a given heat transfer surface and
 423 same volume of metal foam implemented in the lower zone, the four-tube configuration
 424 achieves a faster melting rate and hence a shorter duration for completing the charging
 425 process.



426
 427 Figure 14. Contours of liquid fraction (left side) and temperature (right side) for four-
 428 tube device containing half-foam structure.

429 For the device containing whole-foam structure, the modelling results are presented
 430 in Figure 15. One can see that the natural motion influence is not as evident as that in
 431 pure PCM because of the existence of metal foam. For both the single and four-tube
 432 devices, the melting process is conduction dominant and there is no large temperature
 433 swing existed across the melting front, leading to a broader and uniform mushy zone
 434 inside the device. From Figure 15, it can also be observed that, due to the difference
 435 in heat transfer tube arrangement, the melting rate between the single and four-tube
 436 device is also different. For a fixed heat transfer surface area, an even array of heat
 437 transfer tube in the four-tube configuration achieves a more homogeneous heat
 438 transfer and hence a higher melting rate than that in the single-tube configuration. To
 439 sum up the Figures 13-15, it can be concluded that the insert of the metal foam can
 440 be confirmed to enhance the heat transfer performance of the PCM based device, and
 441 the performance enhancement caused by implementation of metal foam is far larger
 442 than that could be achieved through natural convection.

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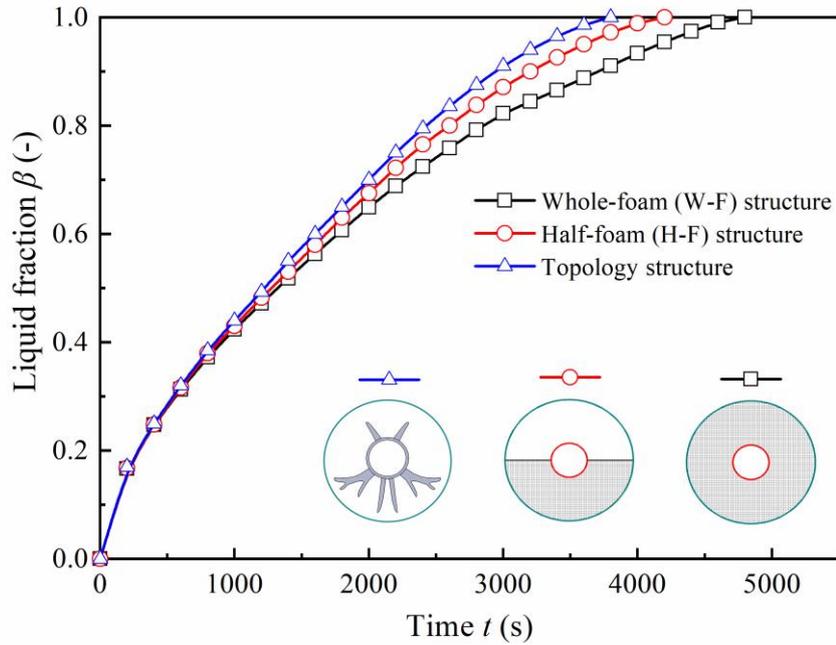
446 Figure 15. Contours of and liquid fraction (up) and temperature (bottom) for the
 447 device containing whole foam structure. The four-tube device results are shown on
 448 the left side, and the single-tube device on the right side.

449 3.3 Comparison analysis

450 In this section, for making a better quantitative analysis, the charging time of
 451 conventional devices without any enhancement structures is also calculated by
 452 numerical simulations. The conventional device has the same shell-and-tube
 453 configuration as shown in Figure 1. This device is numerically analysed to benchmark
 454 the performance of different thermal enhancement techniques in this work. As the
 455 conventional device has relative long melting time, the results are not directly
 456 illustrated in the following figures. Figure 16 shows the variation of liquid fraction
 457 with time for the single-tube device containing different enhancement structures. One can
 458 see that, compared with the device containing no additional structure, the melting rate
 459 inside the device can be significantly increased with the use of enhanced structures.
 460 For the device containing topology structure, the whole charging process is finished
 461 around 3800 s, which achieves the reduction of total charging time by more than 88%
 462 in comparison with the conventional device without enhanced structures whose
 463 charging time is 33000 s. For the half-foam structured device, a rapid melting rate is
 464 also observed in which the melting process is completed around 4250 s, denoting 86%
 465 of melting time could be saved. The melting process in the whole-foam structured
 466 device lasts 4850 s, suggesting only 84% melting time reduced compared to the
 467 device with no enhanced structure.

468

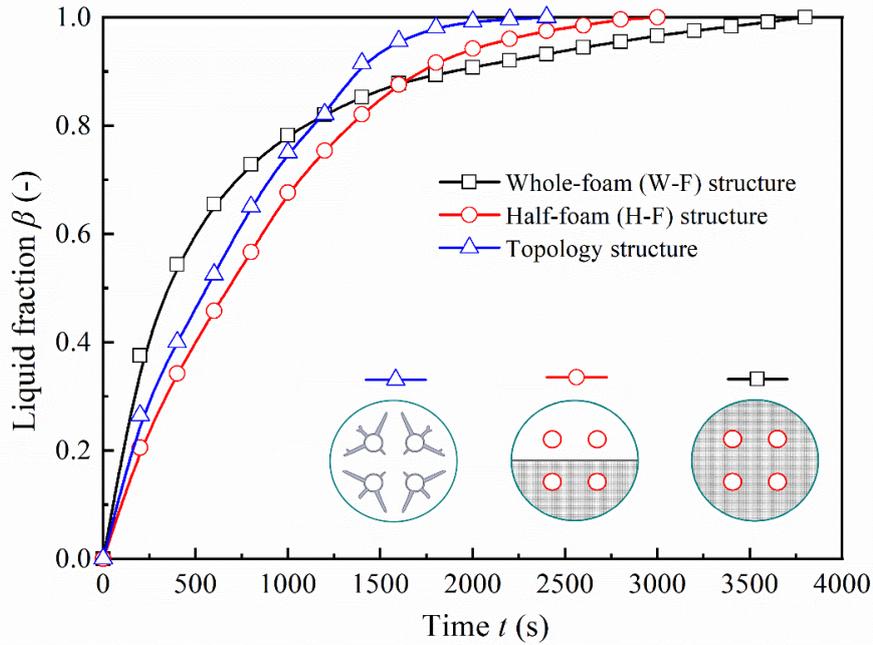
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470

471 Figure 16. Time evolutions of the liquid fraction for the single-tube configuration
 472 containing different structures.

473 Figure 17 presents the time evolution of the liquid fraction in the four-tube device with
 474 the use of different enhancement structures. One can see a similar trend in the liquid
 475 fraction as a function of time at different structured devices to these shown in Figure
 476 16 as describe above. The melting rate in the topology structured device is the highest
 477 while that in the whole-foam structured device is the lowest. Compared with the
 478 conventional device, the whole melting process for the device containing topology,
 479 half-foam and whole-foam structures is respectively reduced 88.5%, 86.8% and 83.4%.
 480 An inspection of Figure 17 also finds that, although the whole melting process in whole-
 481 foam structured device is the longest, it has the highest melting rate at initial melting
 482 stage over 0-1200 s among all the three structured devices. The main reason lies in
 483 the heat transfer domination mechanism difference among the three devices. Unlike
 484 other two structured devices where natural convection plays an important role in
 485 melting process, the heat transfer in the whole-foam structured device is completely
 486 dominated by the thermal conduction. In the initial stage, a large temperature
 487 difference is apparent and hence a high heat transfer rate is observed in the W-H
 488 structured device. With the evolve of the melting process, the temperature difference
 489 is gradually diminished, leading to a low heat transfer rate in the device and hence a
 490 slow melting process at the late charging stage.



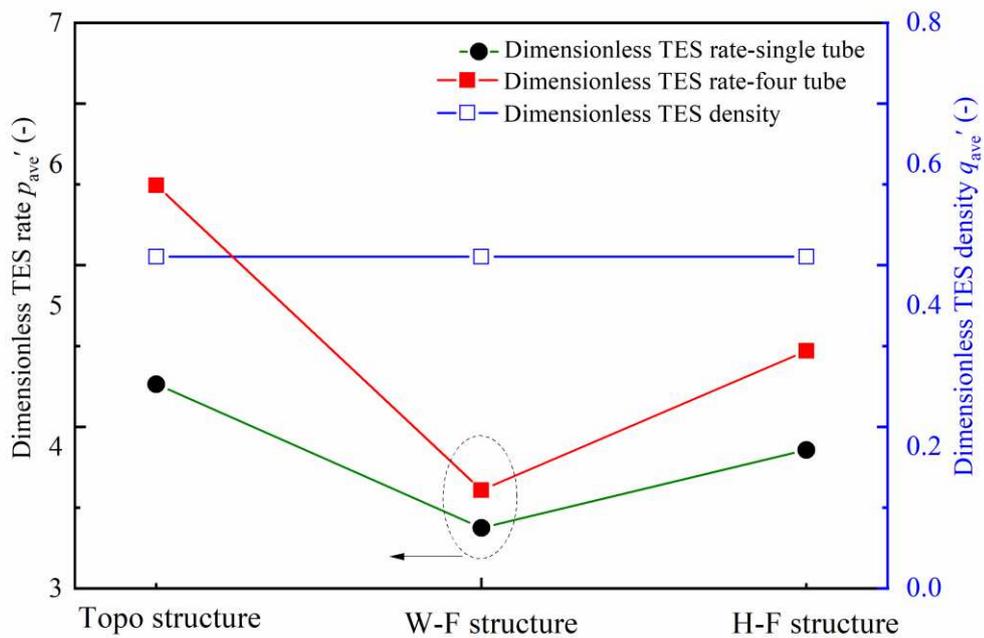
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492 Figure 17. Time evolutions of the liquid fraction for the four-tube configuration
 493 containing different structures.

494 The preliminary observations of the Figures 16 and 17 indicate that the acceleration
 495 of melting process with the use of topology structure is the highest while that with the
 496 use of whole-foam structure is the lowest, denoting the highest heat transfer rate in
 497 the topology structured device and the lowest heat transfer rate in the whole-foam
 498 structured device. The use of topology structure seems to be the optimal enhancement
 499 approach for both the sing-tube and four-tube devices. However, using the reduction
 500 extent of melting time as the output performance is not enough to disclose the
 501 superiority of the enhancement configuration. As reported in Xu's work [23, 25], the
 502 indicator of charging time can only give partial appraisalment for the enhancement
 503 approach and is insufficient to give a full evaluation. Other criteria are therefore
 504 required to achieve comprehensive assessment for a PCM based device with different
 505 performance enhancement methods.

506 Figure 18 presents the dimensionless average TES rate and TES density of different
 507 enhancement structures. One can see that due to the constant volume of the
 508 enhancement additive, the q'_{ave} in single-tube configuration is equal to the four-tube
 509 configuration, which is decreased to 0.46 times in comparison with the non-
 510 enhancement configuration. For p'_{ave} , the value in the single-tube and four-tube
 511 configurations containing topology, whole-foam and half-foam structures can be
 512 respectively increased to 4.3, 3.3 and 3.9 times, and 5.8, 3.6 and 4.7 times compared
 513 to the configuration with no enhancement. This indicates that all these three
 514 enhancement approaches in both configurations can effectively accelerate the TES
 515 rate with the highest p'_{ave} appearing in the topology structure and the lowest p'_{ave}
 516 in the whole-porous structure. For a fixed amount of additive, the p'_{ave} in four-tube

517 configuration is higher than that in single-tube configuration, denoting a better charging
 518 performance in four-tube configuration. An inspect of the results in Figure 18 can also
 519 find that the use of topology structure achieves the largest difference in p'_{ave} between
 520 the single-tube and four-tube configurations while the full-porous structure gives the
 521 lowest difference in p'_{ave} . The reason for the variation in the full-porous structured
 522 device is easily understood; the heat transfer in porous region is dominated by thermal
 523 conduction and hence a nearly equal heat transfer rate is achieved in both the single-
 524 tube and four-tube devices containing the same volume metal foam. The occurrence
 525 of the difference in topology structured configuration can be attributed to the
 526 topological optimization and heat transfer tube arrangements in the device. A more
 527 uniform heat transfer in the four-tube configuration is appeared due to the more even
 528 distribution of the topology structure and heat transfer tube, and hence a faster heat
 529 transfer rate can be obtained in four-tube configuration compared to the single-tube
 530 configuration.

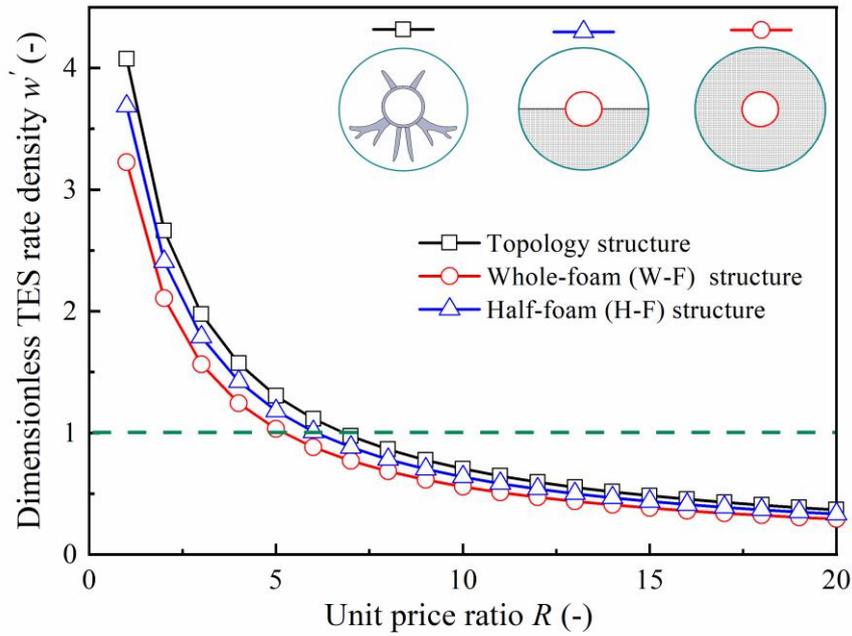


531

532 Figure 18. Dimensionless average TES rate and TES density of different structured
 533 configurations.

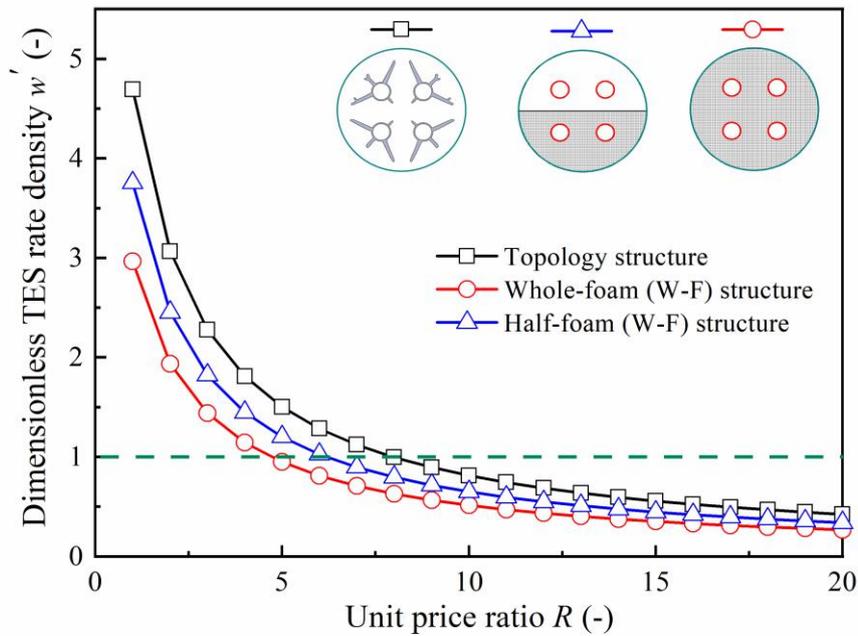
534 In Xu's work [25], a more comprehensive parameter of TES rate per material cost,
 535 relating to the ratio between the TES rate and material unit price was proposed to
 536 compare the enhancement efficiency of the PCM based device from the perspective
 537 of material cost. In general, ideal enhancement structure should not only possess the
 538 ability to endow the device with high heat transfer performance but also has the low
 539 cost. In real applications, however, the preeminent additions are either constitutionally
 540 expensive or hard to produce with high manufacture cost. Therefore, the right balance
 541 should be struck between the performance and the cost for a PCM based device
 542 containing enhanced structures. In this work, such a parameter of p_c and its

543 dimensionless form p'_c is defined by Equations (32) and (33) for determining the device
544 input-output performance. Figures 19 and 20 show the variations of p'_c with R for
545 different structures in the single-tube and four-tube configurations, respectively. One
546 can see that the unit price ratio R plays an important role in selecting the optimal
547 structure. When R is equal to 1, the economic efficiency of p'_c in the enhanced
548 configuration can be enhanced to 3-5 times in comparison with the configuration
549 containing no enhancement structure. With the increase of R , the economic efficiency
550 of all the enhanced structures in both the single-tube and four-tube configurations is
551 decreased with different extents. When R is in the range of 1-6, the economic
552 efficiency in the topology structure is the highest while that in the whole-foam structure
553 is the lowest, indicating the topology structure is the best option and the whole-foam
554 structure is always not the best solution. This is agreement with the results discussed
555 in Figures 16-18 that the topology structure achieves the best heat transfer
556 performance in the device. With the further increasing R , p'_c in both the single-tube and
557 four-tube configurations will be less than 1 when R is larger than 6. This indicates that,
558 for a given enhanced structure with price more than 6 times higher than the PCM, the
559 economic efficiency of the device with enhancement addition will be lower than that in
560 the device with no enhancement. In such cases, a desired utilization efficiency of the
561 material cost will not be realized. This observation, together with the results presented
562 in Figures 16-18, suggest that the parameter of the TES rate per unit price could be
563 quantitatively used for evaluating the device input-output efficiency and pointing the
564 optimal enhancement design from the economic perspective. The amount of
565 enhancement addition and its geometry as well as arrangement should be
566 meticulously optimized with the synthetical consideration of the heat transfer rate and
567 material cost. Although the manufacturing technology and the associated cost for
568 using porous metal foam is mature and rational at the present stage, it does not have
569 the optimal heat transfer enhancement efficiency. As the current metal additive
570 manufacturing is mainly used for customised parts, the costs are still not within a
571 reasonable range. For the implementation of additive manufacturing technology, the
572 insert of topopology structure would be an economical solution to realize the combined
573 enhancement of heat transfer performance and material utilization efficiency if the unit
574 price ratio R between the structure and the PCM can be controlled to less than 6.



575

576 Figure 19. Variation of dimensionless average TES rate per material cost p'_c with unit
577 price ratio R for different structures in single-tube configuration.



578

579 Figure 20. Variation of dimensionless average TES rate per material cost p'_c with unit
580 price ratio R for different structures in four-tube configuration.

581

582 **4. Conclusions (Add more quantitative results)**

583 In this work, different melting enhancement techniques i.e. topology optimised
584 structures and conductive foam structures for the LHTES system are investigated by
585 CFD simulations.

586 The SLM metallic additive manufactured device are used to demonstrate the
587 manufacturability of topology optimised structures and to validate the numerical
588 simulations. The temperature and liquid fraction evolutions during melting are
589 analysed considering different topology optimised fin configurations. The
590 corresponding conductive foam structures including whole-foam structure and half-
591 foam structure are further analysed. For the first time, these different structures are
592 quantitatively compared from perspectives of device performance and economy. The
593 comparison results show that the topology optimised structure can achieve the highest
594 TES storage rate. The highest dimensionless TES rate p'_{ave} is 5.8 for the four-tube
595 topology optimised structure, while the lowest p'_{ave} is 3.3 for the whole-foam half
596 single-tube configuration. However, from a perspective of material and device cost,
597 the unit price ratio between the enhance technique and PCM material has to be
598 controlled to less than 6 ($R < 6$) to become an economical solution. The results
599 presented here provide an insight to comprehensively evaluate different melting
600 enhancement techniques.

601 As a perspective it would be useful to further advance the structure design,
602 performance and economy evaluation to typical applications in future.

603

604 **Nomenclature**

605

606 *Abbreviations*

2D	Two-dimensional
3D	Three-dimensional
CFD	Computational fluid dynamics
FVM	Finite volume method
HTF	Heat transfer fluid
LHTES	Latent heat thermal energy storage
PCM	Phase change material
SLM	Selective laser melting
TES	Thermal energy storage

607 *Symbols*

A_m	Mushy constant, $\text{kg}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$
A_{sf}	Surface area density, m^{-1}

a	Permeability, m^2
a	Unit price
C_i	Inertia coefficient, $\text{W}\cdot\text{m}^{-2}\cdot\text{K}^{-1}$
C_p	Specific heat, $\text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$
d_f	Cell ligament diameter, m
d_p	Pore diameter, m
g	Gravity, $\text{m}\cdot\text{s}^{-2}$
h	Heat transfer coefficient
k	Thermal conductivity, $\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
L	Latent heat, $\text{kJ}\cdot\text{kg}^{-1}$
m	Mass, kg
Pr	Prandtl number
p	Pressure, Pa
ρ_{ave}	Average TES rate, $\text{J}\cdot\text{s}^{-1}$
ρ_c	Average TES rate per material cost, $\text{J}\cdot\text{s}^{-1}\cdot\text{\$}^{-1}$
ρ_{ave}'	Dimensionless average TES rate
ρ_c'	Dimensionless average TES rate per material cost
Q	TES capacity, J
q_{ave}	Average TES density, $\text{J}\cdot\text{kg}^{-1}$
q_{ave}'	Dimensionless average TES density
Ra	Rayleigh number
R	Unit price ratio
S	Material cost
T	Temperature, K
t	Time, s
t_m	Melting time, s
u, v	Velocity, $\text{m}\cdot\text{s}^{-1}$
w	TES rate density, $\text{J}\cdot\text{kg}^{-1}\cdot\text{s}^{-1}$
w'	Dimensionless TES rate density
x, y	Coordinates

608 *Greek letters*

α	Thermal diffusivity, $\text{m}^2\cdot\text{s}^{-1}$
β	Liquid fraction

γ Thermal expansion coefficient, K^{-1}
 ϵ Foam porosity
 μ Dynamic viscosity, $kg \cdot m^{-1} \cdot s^{-1}$
 ν Kinematic viscosity, $m^2 \cdot s^{-1}$
 ρ Density, $kg \cdot m^{-3}$
 ω Constant number

609 *Subscript*

0 Basic case without enhancement
f Fluid
fe Effective thermal conductivity of fluid
l Liquid phase
M Metal enhancement material
P Phase change material
ref Reference value
s Solid phase
sf Between solid and fluid
se Effective thermal conductivity of solid
td Thermal dispersion

610

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617

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