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On the use of effective thermophysical properties to predict the melting process of composite phase change materials with coarse structures

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1 **n the use of effective thermophysical properties to predict the melting process of**
2 **composite phase change materials with coarse structures**

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9 **Abstract**

10 Composite PCMs combining metallic foam and paraffin are widely used as phase change
11 materials (PCMs) to tailor the properties of pure PCMs and enhance the thermal energy
12 storage/release. For the complex composites structures, the transient thermal response
13 prediction by direct simulation (DS) is not easy in term of geometry generation and
14 computation. The volume-averaged model (1T model) considering the composite PCMs as
15 homogeneous media is sometimes used to deal with thermal transport in Composite PCMs, not
16 always with a sufficiently good local description of non-steady conditions. The paper carries
17 out a set of cases where a composite PCM modelled as an open-pore body-centred cell made
18 of Aluminium (Al) filled with paraffin (i) to investigate the combined effects of the geometry
19 of the unit cell (side length, porosity), the composite sample (sample height) and boundary
20 conditions (heat input) on the heat response; (ii) to identify the local/overall errors in
21 temperature and volume fraction of liquid PCM (and thus of stored heat) induced by the use of
22 1T model for various geometry/heat flux combinations. Analytical equations are proposed to
23 predict the maximum temperature difference between Al and PCM as well as the maximum
24 temperature difference calculated by applying 1T or DS model as a function of the open cell
25 structure geometry and heat flux. The main novelty introduced in the paper is analytical model
26 to quantify for 1T model the maximum local error on molten PCM volume fraction, and thus
27 for heat stored/released. The model supplies good local thermal response predictions for fine
28 structures and lower heat flux input. Nevertheless, errors in the volume fraction of molten
29 PCMs predicted for the whole sample are far lower and the 1T model can be easily applied in
30 a wider range of geometry/conditions.

31 **Keywords**

32 Composite Phase Change Material; effective thermophysical property; coarse structures;
33 melting process.

34 **1 Introduction**

35 The phase change materials (PCMs) used in devices for thermal energy storage and
36 management have been applied in biomedical, biomedical, electronic, textile, construction and
37 automotive industries, but often suffer a limit for applicability due to their low thermal
38 conductivity [1,2]. In order to overcome this defect, many researches on increasing thermal
39 conductivity have carried out, such as micro-encapsulation techniques [1,3], foam-stable PCMs
40 [1,4], metallic alloys [5,6].

41 Among these solutions, metal foams can have pore volume ranging in a wide range, so that the
42 composite PCM which can be obtained by filling them by the material which activates the
43 phase transition can correspondingly have a relatively large volume range of PCM. The foams
44 are typically of metallic structures, specifically those characterized by high thermal
45 conductivity, such as Al or Cu foam [7,8]. Many researchers have investigated the effect of
46 metal foam as a means to increase the effective thermal conductivity of PCM composites. Xiao
47 et al.[9] stated that the effective thermal conductivity of paraffin/copper foam characterized by
48 96.95%, 92.31%, 88.89% porosities foam are about 13, 31, 44 times larger than that of pure
49 paraffin. Ren et al.[10] carried out a comparative study to evaluate the nanoparticle-metal foam
50 combination on enhancing PCM melting, and thus its thermal storage performance. Their
51 results indicated that, in view enhancing PCM heat transfer effectiveness, the use of metal
52 foams is more effective than adding nanoparticles to PCM. Yang et al.[11] investigated the
53 effect of inclination on the thermal response of pure paraffin and paraffin/copper foam (10
54 pores per inch and the porosity of 0.96). They reported that the inclination angle has little
55 influence on the composite PCM since heat conduction dominates when the paraffin is melted
56 in open-cell metal foam. The predominance of conductive heat transport over convective one
57 in the temperature ranges where paraffin is molten has to be carefully considered for coarse
58 structures and high porosity, as shown by the Li et al. in [12].

59 The prediction of the thermal response of PCM/metal foam composites is not always an easy
60 task due to complex microstructure of foams. Therefore, direct numerical simulation (DS) is
61 considered a more precise method to predict both general and local thermal response of PCM
62 composites and in some cases they were reported to have some challenges as far as geometry
63 generation and time cost are concerned [13,14]. In recent years, the volume-averaged

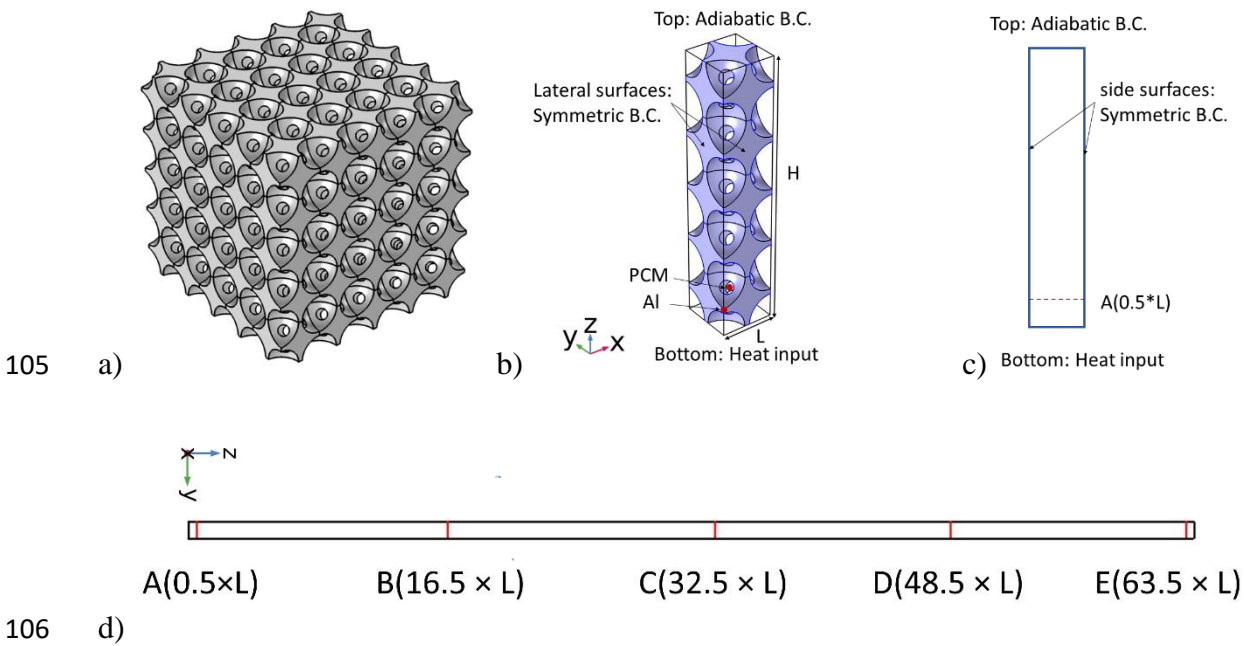
64 approaches like one-temperature (1T) [13–16] and two-temperature (2T) [13,14,17] models
65 have been proposed and experimentally validated in order to save computational time. 1T
66 model assumes that there is no temperature difference between foam and PCM while 2T model
67 considers heat transfer between PCM and porous medium [13,14]. 1T model was used to
68 predict the heat transfer behaviour in composite PCM/Cu foam system for the melting process
69 [8]. The 1T model was also applied to describe the PCM solidification process in Cu [15] and
70 multi-layer (Al, Cu and Ni) [16] open-cell metal foam. Hu et al. [13,14] stated that 1T model
71 can describe the phase change behavior during heating in constant boundary conditions, in a
72 PCM/Al foam system where the foam was represented as an ideal lattice made by Body-
73 Centered Cubic (BCC) unit cells. Sardari et al.[18] claimed that 2T model can offer more
74 accurate results compared with 1T model. However, some authors reported that 1T model can
75 predict the identical results with 2T model [13,14] and agree reasonably well with experimental
76 data [8,15,16].

77 Thus, summarizing the available scientific literature on it, among the two ‘simplified’ models,
78 1T model significantly simplifies the PCM/foam system by modelling it as a homogeneous
79 material with effective thermal properties, which offers advantages of geometrical definition
80 and computational cost for part design. Nevertheless, there is a lack of information on the foam
81 size-dependence applicability of 1T model to PCM/metallic foams, where the temperature
82 difference between the metal and PCM can become significantly high due to the low thermal
83 diffusivity of PCM compared to that of the metallic phase of this composite. On the other hand
84 2T model requires the preliminary identification of parameters such as institution heat transfer
85 coefficient and specific surface area which are related [13, 14] to the on the structural features
86 which effect is to be addressed in the present paper. The 2T model has thus not been considered
87 in the present paper.

88 The purpose of this paper is to investigate the effect of foam-size parameters as well as other
89 parameter defining boundary conditions and to identify the errors induced by the use of 1T
90 model in temperatures, volume fraction of molten phase. The models are applied under
91 assumption of only conduction heat transfer. The 1T model predictions have been compared to
92 those supplied by the computationally heavier Direct numerical Simulations (DS) model which
93 are taken as reference data. Simulations have been carried out in the temperature field where
94 PCM undergoes phase change transition, but no phase change is applicable for other material.
95 The higher-conductivity phase is an open-cell foam which can be schematically represented as
96 a BCC structure which is considered a most close real foam structure [19].

97 **2. Geometry and thermophysical properties of composite PCMs**

98 The composite PCMs here considered are made of a metallic, open-pore structure filled by a
 99 PCM. These composites are modelled considering the porous structure (a foam, for example)
 100 as an orderly lattice of inverse Body Centered Cubic cells of the same geometry (see Fig. 1a).
 101 The unit cells are characterized by their side length L and sphere diameters d (or, alternatively
 102 by the pore volume fraction, ϵ [12]). The foams are made of commercially pure Al. And the
 103 PCM embedded in Al foam is docosane (paraffin wax with $C_{22}H_{46}$), which is characterised by
 104 the melting temperature $T_m = 317K$ and the latent heat (LH) of 260 kJ/kg [13,14].



107 Figure 1 a) Physical model of inverse BCC lattice. Geometrical features and boundary
 108 conditions for DS (b) and 1T (c) models. d) z-axis coordinate corresponding to section planes
 109 where Al and PCM reference points are taken.

110 The properties of the Al and PCM phases are shown in Table 1. They have been selected as
 111 those in [13,14] to obtain results comparability. In the case of PCM phases, their heat capacity
 112 can be described including both specific heat and latent heat of melting, so that the phase
 113 transition can be accounted easily. These C_p description can be derived by differential scanning
 114 calorimetry measurements [20], or can be simplified by separating the fully solid, fully liquid,
 115 and transition temperature range [21]. In the present study, $C_{p,paraffin}$ has been described using
 116 the triangular peak description with same value of specific heat $C_{p,sol/liq}$ for the fully solid phase
 117 and fully liquid phase described by following Eq.1 [21] and shown in Fig 2a. The

118 corresponding volume fraction of liquid paraffin with temperature can then be derived and
 119 plotted in Fig.2a as well.

$$120 \quad C_{p, \text{paraffin}} = \begin{cases} C_{p, \text{sol/liq}} & T < T_m - b \\ C_{p, \text{sol/liq}} + \frac{2 \times LH}{b} \left(\frac{T + b - T_m}{b} \right) & T_m - b \leq T \leq T_m \\ C_{p, \text{sol/liq}} & T > T_m \end{cases} \quad (1)$$

121 where $(T_m - b)$ to T_m is the melting temperature range of the PCM, b is assumed as 2K in the
 122 present study. For the specific paraffin considered in the paper, the modelled melting
 123 temperature range is thus 316K-318K. By this model the C_p of paraffin assumes a peak value
 124 $C_{p, \text{peak}}$ at $T_m = 318\text{K}$, which is 262.89 kJ/(kg·K).

125 Different sets of composite PCMs have been considered by varying cell length L or porosity ε .
 126 Cell length L is considered to be 0.4, 1, 2, 3, 5 mm, while the volumes fraction of pore ε
 127 (corresponding to the volume fraction of PCM) considered is 0.757, 0.8, 0.85, 0.9 and 0.95.

128 Table 1. Thermophysical properties of interest for Al and PCM phases and the corresponding
 129 effective properties for the composite PCMs with the porosity ε used in the article. The first
 130 ones are used in DS model, the effective ones are used in 1T model. a) from [13,14], b)
 131 calculated.

Material	ρ [kg/m ³]	λ [W/(m·K)]	$C_{p, \text{sol/liq}}$ [kJ/(kg·K)]	$C_{p, \text{max}}$ [kJ/(kg·K)]	T_m [K]
Paraffin (PCM)	785 ^a	0.4 ^a	2.89 ^a	262.89 ^b	317 ^a
Al (foam)	2719 ^a	202.4 ^a	0.871 ^a	/	/
Composite PCMs ($\varepsilon=0.757$)	1254.962 ^b	31.157 ^b	1.827 ^b	124.927 ^b	317 ^a
Composite PCMs ($\varepsilon=0.8$)	1171.800 ^b	24.136 ^b	1.953 ^b	141.294 ^b	317 ^a
Composite PCMs ($\varepsilon=0.85$)	1075.100 ^b	16.586 ^b	2.124 ^b	163.490 ^b	317 ^a
Composite PCMs ($\varepsilon=0.9$)	978.400 ^b	9.836 ^b	2.329 ^b	190.074 ^b	317 ^a
Composite PCMs ($\varepsilon=0.95$)	881.700 ^b	4.150 ^b	2.579 ^b	222.489 ^b	317 ^a

132 3 Mathematical formulation of 1T and DS models

133 In present study, only heat conduction is considered for both 1-T and DS models. Thus, both
 134 1T and DS models for a composite material made of Al and paraffin phases are based on the
 135 energy balance equation:

$$136 \quad \rho_i C_{p,i} \frac{\partial T_i}{\partial t} - \lambda_i \nabla^2 T_i = 0. \quad (2)$$

137 where ρ , C_p , λ are the density, specific heat and thermal conductivity of the i phase, respectively.
138 In DS model, two different phases, Al and PCM, are considered (Table 1), with no thermal
139 resistance at their interface. The temperature and heat flux is continuous at the interfaces
140 between phases.

141 On the other hand, the composite PCM is considered as a homogeneous material by 1T model,
142 and the effective thermal properties are used for it and described in the following paragraph.

143 *3.1 Effective properties of the composite PCM used in 1T model*

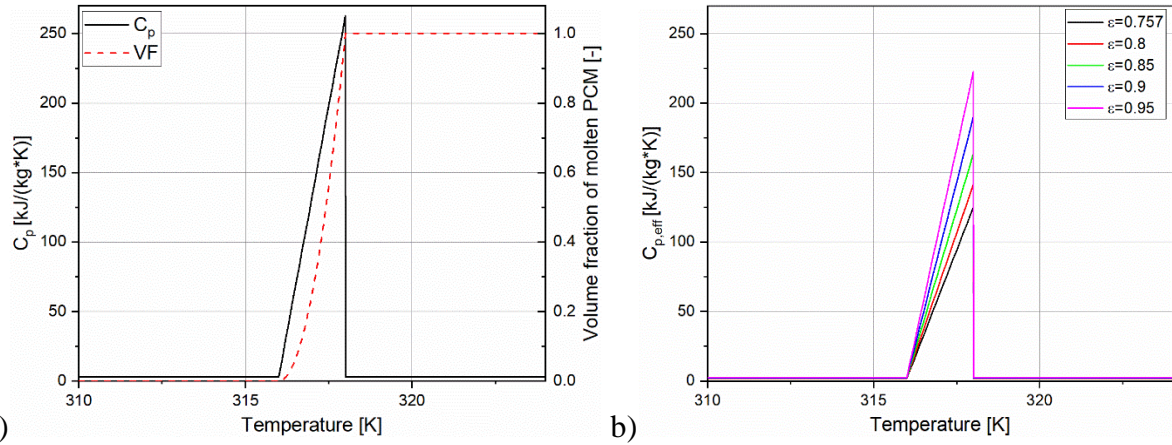
144 The effective properties used for the homogeneous phase considered in 1T model are calculated
145 as follows for thermal conductivity, density and specific heat. For Al-paraffin composites
146 characterized by inverse BCC structure considered in present study, all the effective properties
147 are only related to the phase volume amount (thus to the porosity of the composite PCM), not
148 to the size of unit cells. Thus, values are summarized in Table 1 for each set of porosity values.

149 For the composite materials, effective thermal conductivity (λ_{eff}) depends on the thermal
150 conductivity, the geometric distribution and the volume fraction of each component [22]. Since
151 λ_{eff} plays a critical role in the thermal response of composite materials [13,14], analytical
152 models for different lattices [14,23] and more general numerical methods like direct simulation
153 (DS) or Lattice Monte Carlo (LMC) [24–26] have been proposed to predict λ_{eff} . Among them,
154 the modified Progelfhof model (Eq.3) is presented to estimate λ_{eff} for the Al-paraffin composites
155 characterized by inverse BCC structure and porosity ranging from 0.69 and 0.98 [18].

$$156 \lambda_{\text{eff}} = \varepsilon \times \lambda_{\text{PCM}} + (1 - \varepsilon)^{1.3296} \times \lambda_{\text{Met}} \quad (3)$$

157 The values of λ_{eff} calculated by Eq.3 are listed in Table 1 for the considered set of porosity
158 values. It decreases from 31.157 W/(m·K) to 4.150 W/(m·K) as porosity increases from 0.757
159 to 0.95. The λ_{eff} values calculated from the analytical formula Eq.3 are very close to that
160 calculated in Z direction by DS method. As an example of $\varepsilon=0.757$, the values are 31.157
161 W/(m·K) and 31.229 W/(m·K), respectively.

162 For a composite PCM, the effective density (ρ_{eff}) can be simply derived by the volume-
163 weighted average of the components' density, while the effective specific heat ($C_{p,\text{eff}}$) can be
164 calculated by the mass-weighted average [24]. By using the aforementioned temperature-
165 dependent C_p description for paraffin, the temperature description of $C_{p,\text{eff}}$ for composite PCMs
166 can be derived. They are shown in Fig. 2b for the porosity sets considered, and the
167 corresponding $C_{p,\text{max}}$, is given in Table 1.



168 a) 169 Figure 2 (a) Modelled specific heat and volume fraction (VF) of molten PCM as a function of
 170 temperature for the paraffin used as PCM. (b) Effective specific heat of Al-paraffin composite
 171 PCMs at varying pore volume fraction of the metallic structure.

172 3.2 1T and DS implementation

173 Both DS and 1T models have been implemented in a finite element software. DS model
 174 considers 2-phase (the Al and paraffin) system, and its boundary conditions are shown in Fig.
 175 1b. The homogeneous system with effective material properties for 1T model is presented in
 176 Fig. 1c, with corresponding boundary conditions. The considered structure is considered to
 177 consist in N_c stacked unit cells of side L , where different height $H = N_c \times L$ have been considered,
 178 with $N_c = 5, 10, 17, 25, 32, 41, 49, 64$. For both models, in all the simulated tests performed
 179 during the present study, symmetric boundary at lateral surfaces is considered and a
 180 homogeneous heat flux is applied at the bottom surface of the modelled structures, while the
 181 top surface is thermally insulated (adiabatic).

182 Due to simple phase arrangement, mapped mesh has been selected for 1T model. The mesh
 183 sensitivity analysis has been carried out by considering number of elements for unit cell length
 184 of 5, 10, 20. Time sensitivity has been carried out considering time steps of 1, 0.1 and 0.01s.
 185 The optimal combination is 10 elements per unit cell length (total mesh number is $10 \times 10 \times N_c$)
 186 and time step of 0.1s.

187 The complex porous structure of Al requires a kind of element type able to mesh regardless of
 188 structure shape in DS model, that is obtained by the use of free tetrahedral element. The mesh
 189 size optimization is carried out for the lower side length and porosity ($L=0.4\text{mm}$, $\epsilon=0.757$) by
 190 fixing minimum mesh size, maximum element growth rate, curvature factor and resolution of
 191 narrow regions (1.6×10^{-6} m, 1.4, 0.4, 0.7 respectively) and optimizing the maximum element

192 size in the range $d/50$ - $d/5$. Results independent from mesh-size and time step have been
193 obtained when the latter is equal to 0.1s and the maximum mesh size is equal or lower than
194 $d/20$. These values have been considered for all the simulations for the DS model.

195 **4 Simulation**

196 In order to reach the targets of the present article, 4 sets of simulated tests have been performed,
197 with specific aims, thus each of them has considered one or more specific combinations of
198 porosity, cell coarseness, heat flux, sample height.

199 In Case 1, a set of tests are to check how, in nonequilibrium conditions, the maximum thermal
200 difference between Al and PCM phases at a specific height is affected by the overall height of
201 the sample. For this reason, tests have been performed by using the only DS model (at the same
202 height, 1T model predicts only 1 temperature, to be considered for both phases). For tests, 4
203 samples built with the same BCC structure characterized by $L = 2\text{mm}$ and $\varepsilon=0.757$ are used.
204 They differ for their overall length H along the Z -direction corresponding to N_c equal to 17, 33,
205 49, 64 times the cell side L . The boundary conditions are the ones described in paragraph 3.2,
206 where the heat flux $q = 10 \text{ W/cm}^2$ is homogeneously supplied at the bottom surface (where
207 $Z=0$). Reference section planes have been considered at representative sections located at the
208 A ($0.5\times L$), B ($16.5\times L$), C ($32.5\times L$), D ($48.5\times L$) and E ($63.5\times L$). As N_c increases (and thus
209 sample height), the other points C-E are progressively included in the samples. Each of these
210 heights corresponds to a mid-section of the BCC cell, which includes the central point of a
211 PCM sphere (point referred as 'PCM' in Fig. 1b). At these representative sections, the distance
212 from the point PCM to Al/PCM interface is maximum, and the maximum temperature
213 difference within PCM phase is expected. Focusing the attention on Al, the 3- order of
214 magnitude higher thermal conductivity with respect to paraffin makes it possible to consider
215 that in this phase the temperature is homogeneously distributed, so that the maximum
216 temperature at the PCM/Al interface is equal to the one at the core of the Al structure (point
217 referred as 'Al' in Fig. 1b). The temperature difference measured in points Al and PCM in each
218 of the above sections ($T_{\text{Al}}-T_{\text{PCM}}$) defines the thermal inhomogeneity in it.

219 Case 2 is aimed at checking the single and combined impact of heating conditions and
220 coarseness of porous structure on local thermal difference among the reference points identified
221 as Al and PCM. Calculations have been performed by DS model, considering only the highest
222 sample height $H=64\times L$ of Case 1, while the cell side L is selected as 0.4mm, 1 mm, 2 mm, 3
223 mm and 5 mm and the heat flow q is selected as 2 W/cm^2 , 4 W/cm^2 , 7 W/cm^2 and 10 W/cm^2 .

224 Furthermore, a set of pore volume fractions (porosity) are considered for the metallic structure:
225 $\varepsilon = 0.757, 0.8, 0.85, 0.9, 0.95$.

226 Case 3 is performed to check if and to what extent the thermal difference at section A, the one
227 closer to the heating surface, is affected by the sample height H , heat flux q and cell side length
228 L . Thus, DS simulated tests have been performed on samples with the same porosity $\varepsilon=0.757$,
229 different side L , (ranging from 0.4mm to 10mm) and different stacked number of unit cells N_c
230 (varying from 5 to 64). In some cases, $\varepsilon=0.8, 0.85, 0.9$ are additionally considered. Similarly,
231 only DS models are carried out. The simulated tests are carried out considering heat flux in the
232 range 1 W/cm^2 to 10 W/cm^2 .

233 Case 4 is aimed at comparing the thermal response of the composite PCMs simulated by DS
234 and 1T models. Simulated tests are thus carried out for both models on sample with porous Al
235 structure having the same porosity $\varepsilon=0.757$ and different coarseness, ($L=0.4\text{mm}, 1\text{mm}, 2\text{mm},$
236 3mm and 5 mm). The sample height is $H=64 \times L$. For each sample, simulated tests are run for
237 heat flux $q= 1 \text{ W/cm}^2, 2 \text{ W/cm}^2, 4 \text{ W/cm}^2, 7 \text{ W/cm}^2, 10 \text{ W/cm}^2$ (i.e., in positive Z -direction).
238 For each of them, the thermal profiles in sections A-E are derived at reference points for Al
239 and PCM in DS model, while a single temperature profile is obtained in 1T model.

240 For some simulated DS cases, the local and overall molten PCM volume fraction is calculated
241 as follows. A cubic lattice of $100 \times 100 \times 100$ points is overlapped to each unit BCC cell. The
242 points belonging to PCM phase are identified as points NPCM and a temperature profile is
243 derived for each of them. Correspondingly, by means of the correlation between temperature
244 and volume fraction of molten paraffin shown in Fig. 2a, the volume fraction profile of molten
245 PCM is calculated for each point PCM. In 1T model, the calculation of time-dependent volume
246 fraction of molten PCMs is obtained by considering 100 points along the z -direction for each
247 cell side L . And molten PCM volume fraction profiles of each point is derived from its
248 temperature profile by means of the correlation shown in Fig. 2a.

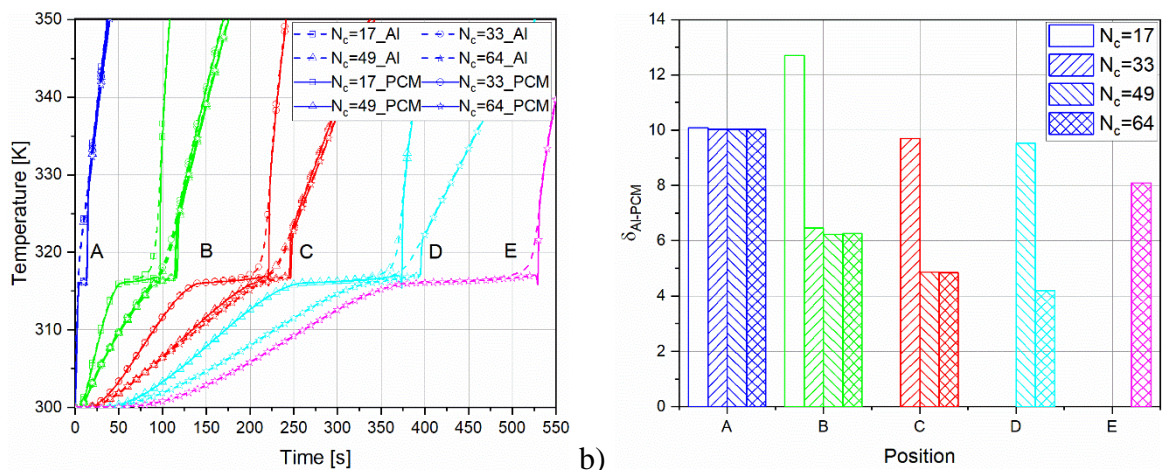
249 **5 Results and discussion**

250 5.1 Case 1: local thermal difference in sections at different height

251 Simulation results of thermal response have been analyzed at the representative sections
252 mentioned before, located at the A($0.5 \times L$), B($16.5 \times L$), C($32.5 \times L$), D($48.5 \times L$) and E($63.5 \times L$).
253 Due to the different height, only sections A and B are presented in the shortest sample.

254 Fig.3a displays that temperatures profiles obtained by DS simulations in points Al and PCM at
 255 sections A-E for different sample heights referred by the number of stacked cells (17, 33, 49
 256 or 64). In section A that far from the far-boundary for all the samples, the temperature of Al-
 257 foam, and PCM for different sample heights are close. In section B, the far-boundary effect is
 258 clearly visible for the shortest samples, for which the temperature increase is faster during the
 259 heating stage up to the PCM melting temperature range (316K-318K), point PCM stays melting
 260 temperature range for a longer time than for other samples, after that increase faster. For the
 261 higher samples, the thermal profiles of points Al and PCM in section B are far closer.

262 A behavior similar to points in section B can be observed for the temperature profiles of
 263 reference points at sections C-E for the shortest sample where the reference point (C-E) exists.
 264 Lastly, Fig.3a shows that the temperature difference between the reference points Al and PCM
 265 reaches maximum close to the end of PCM phase transition, at 318 K, then temperature of point
 266 PCM increases sharply. The maximum temperature difference $\delta_{Al-PCM} = \max(T_{Al} - T_{PCM})$ in a
 267 given section can be considered as a measure of the thermal inhomogeneity. δ_{Al-PCM} at points
 268 A-E is here shown in Fig.3b. It is obvious that, with the exception of the cases for which the
 269 reference point (B-E) lays in the BCC cell closest to the adiabatic far-boundary, δ_{Al-PCM} differs
 270 less than 1 K for different sample height. At point A, δ_{Al-PCM} is maximum and close to 10 K for
 271 all the sample height. This means that for the relatively high heat flux considered, the
 272 temperature differences at the mid-section (A) of the cell closer to the surface where heat flux
 273 is applied are not affected by the boundary conditions at the far-end section.



274 a) Comparison between thermal profiles in the centre of the PCM sphere and the core
 275 of Al structure at reference section planes A-E supplied by DS model for samples of different
 276 height (17, 33, 49, 64 times L) and a constant heat flux of $q=10W/cm^2$ b) The maximum
 277

278 temperature difference between Al and PCM at sections A-E ($\delta_{\text{Al-PCM}}$) for samples of different
 279 sample height, characterized by the number N_c of stacked cells.

280 5.2 Case 2: Effect of heat flux and porous material coarseness on local temperature differences.

281 The results of DS simulated tests performed in case 2 have been analyzed and the maximum
 282 temperature difference $\delta_{\text{Al-PCM}} = \max(T_{\text{Al}} - T_{\text{PCM}})$ between the Al and PCM reference points in
 283 each section are shown in Fig.4a at reference points of samples with different side length L (in
 284 mm), but a common porosity value $\epsilon = 0.757$. Curves referring to the 4 different values of heat
 285 flux considered for this case are presented in different color. The boundary effects at the section
 286 closer to the heating and adiabatic ones can be observed, while a roughly linear decrease of $\delta_{\text{Al-}}$
 287 PCM with z - values of considered section can be noted.

288 The effect of the coarseness of the porous structure on $\delta_{\text{Al-PCM}}$ at given q values is clear, as well
 289 as the increase of $\delta_{\text{Al-PCM}}$ with q and L . It has been observed that when $\delta_{\text{Al-PCM}}$ in reference
 290 section A is plotted in terms of the product between q and L , an almost linear correlation is
 291 observed, as shown in Fig. 4b. The correlation can be written as:

$$292 \quad \delta_{\text{Al-PCM}} = q \times L / \lambda_{\text{melting}} - \theta \quad (4)$$

293 where $1/\lambda_{\text{melting}}$ is the slope of the fitting line and the parameter λ_{melting} has been referred as a
 294 thermal conductivity due to its unit $\text{W}/(\text{m} \cdot \text{K})$. And the unit of $\delta_{\text{Al-PCM}}$, L and heat flux q is K ,
 295 m and W/m^2 , respectively. In addition to the above correlation, calculated for $\epsilon = 0.757$, similar
 296 ones have been derived for PCM/Al composites characterized by different porosity, as shown
 297 in the same Fig. 4b. The fitting constant θ is identified as -0.85 and the calculated λ_{melting} range
 298 from 20.24 to $9.10 \text{ W}/(\text{m} \cdot \text{K})$ for ϵ varying from 0.757 to 0.95 (Fig. 4c), their best-fit correlation
 299 being:

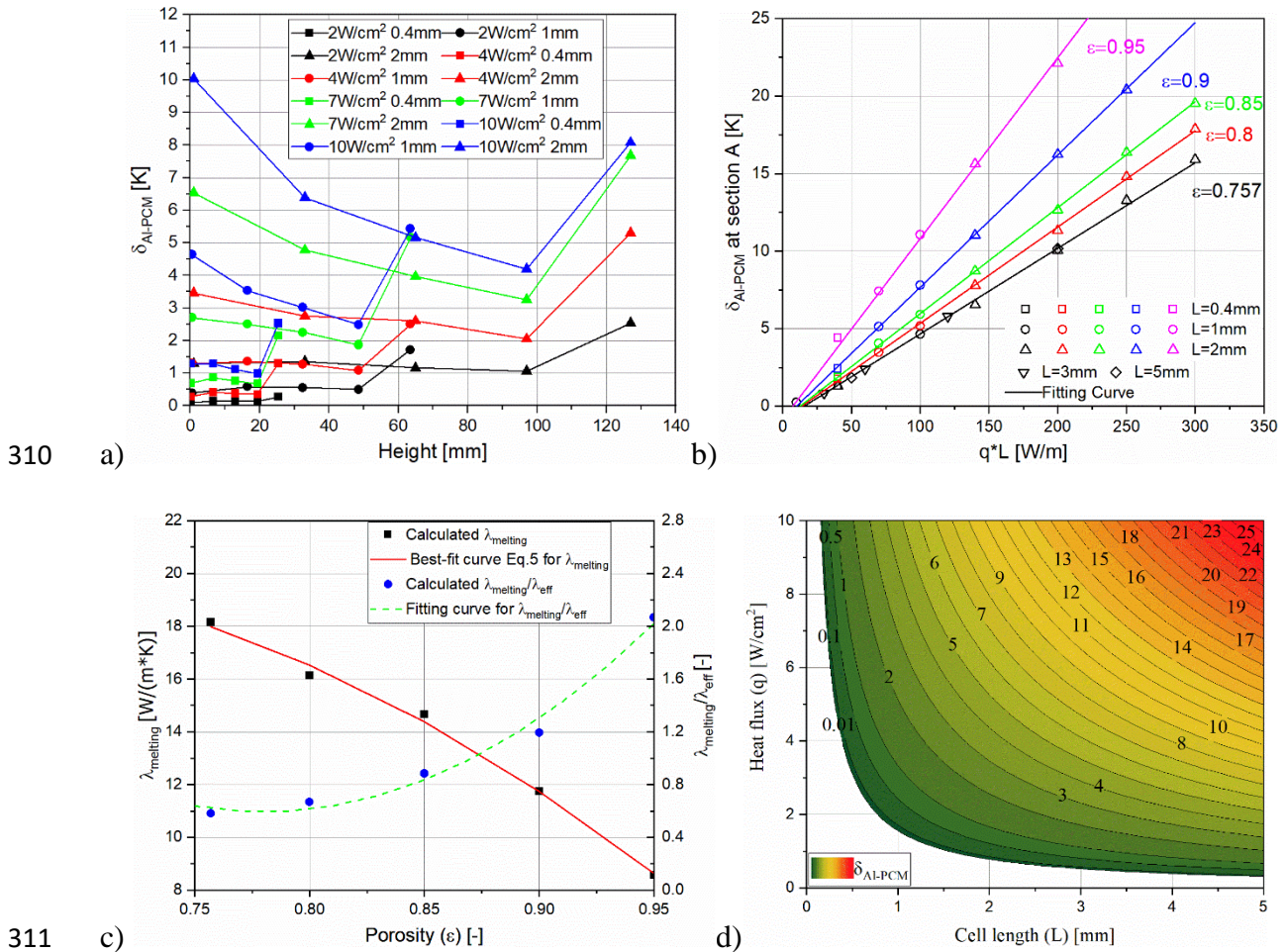
$$300 \quad \lambda_{\text{melting}} = -97.874\epsilon^2 + 118.55\epsilon - 15.671 \quad (5)$$

301 Even if λ_{melting} decreases as porosity increases, it is not directly correlated to the decrease of
 302 λ_{eff} with porosity, since the $\lambda_{\text{melting}}/\lambda_{\text{eff}}$ ratio varies with ϵ , as shown in the same Fig. 4c.

303 The combination of Eq. 4 and Eq. 5 results in the following equation, which enables to derive
 304 the maximum temperature difference $\delta_{\text{Al-PCM}}$ at section A as a function of geometrical features
 305 (L , ϵ) and heat flux.

$$306 \quad \delta_{\text{Al-PCM}} = q \times L / (-97.874 \epsilon^2 + 118.55\epsilon - 15.671) - 0.85 \quad (6)$$

307 The equation allows to build maps where the iso-temperature difference (δ_{Al-PCM}) are plotted
 308 as a function of the Al material coarseness (L) and the service conditions (q) for a PCM/porous
 309 Al structure of a given porosity ϵ . The map corresponding to $\epsilon=0.757$ is given in Fig. 4d.



312 Figure 4 a) Maximum temperature difference $\delta_{Al-PCM}=\max(T_{Al}-T_{PCM})$ between the
 313 representative points for Al and PCM in sections A-E as a function of points distance from the
 314 heated surface ($Z=0$) for different combinations of cell side length L and heat flux q and the
 315 same porosity $\epsilon=0.757$. b) Maximum temperature difference δ_{Al-PCM} at point A as a function of
 316 the product of cell length L and heat flux q obtained for different porosity values, for each of
 317 which a best-fit curve with slope $(1/\lambda_{melting})$ has been derived. c) Correlation of $\lambda_{melting}$ and of
 318 $\lambda_{melting}/\lambda_{melting}$ with porosity ϵ . d) Iso- δ_{Al-PCM} curves as a function of the cell side L and heat
 319 flux q for PCM/Al porous structures characterized by $\epsilon=0.757$. Different colors refer to regions
 320 where the same maximum difference between Al and PCM temperature is expected. Only
 321 situations where $\delta_{Al-PCM}>0.01K$ are colored.

322 5.3 Case 3: Effect of sample height, structure coarseness and heat flow on local thermal
323 differences

324 Maximum temperature difference δ_{AI-PCM} is plotted (in a logarithmic scale) vs. the number of
325 stacked cells N_c for different combinations of L , q , and a fixed porosity 0.757 in Fig. 5a. It can
326 be observed that δ_{AI-PCM} reduces progressively as N_c (and thus the sample height) increases,
327 reaching a stable value above a number hereafter referred as N_s . For a given porosity $\epsilon=0.757$,
328 the curves corresponding to the same product of $q \times L$ (or δ_{AI-PCM}) are overlapped (see for
329 example the cases of $L=0.4\text{mm}$, $q=10\text{W/cm}^2$ and $L=2\text{mm}$, $q=2\text{W/cm}^2$), and N_s values are
330 shown for each value of δ_{AI-PCM} as red star points in Fig. 5a. As a result, N_s can be correlated
331 to δ_{AI-PCM} . The best-fit curve shown in Fig. 5a has the following equation:

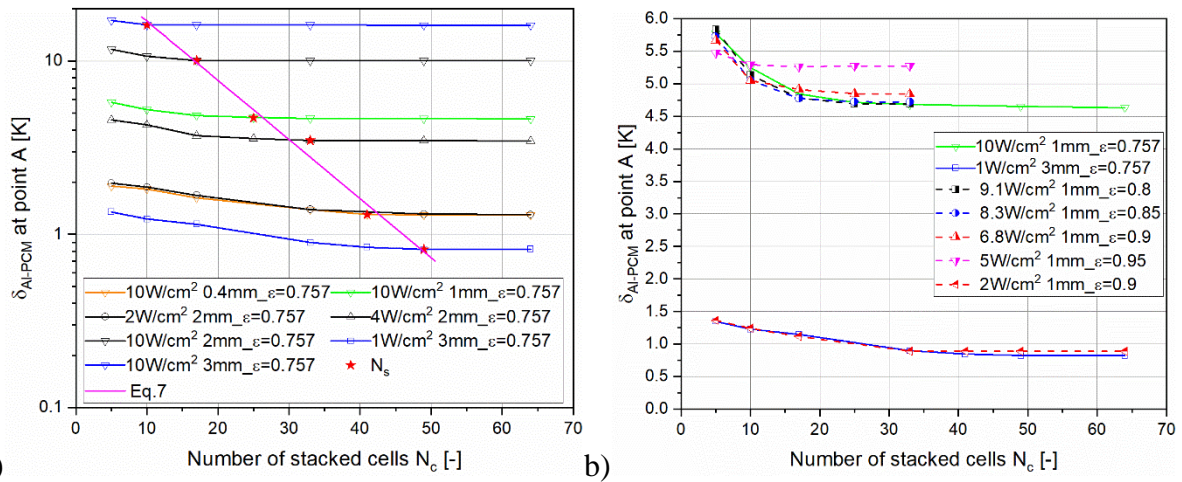
332
$$N_s = -12.72 \times \ln(\delta_{AI-PCM}) + 46.02 \quad R^2 = 0.9876 \quad (7)$$

333 The impact of porosity on δ_{AI-PCM} , shown in Fig.5b, presented that the curves corresponding to
334 the δ_{AI-PCM} of about 5 are close for porosity ranging from 0.757 to 0.9, and the same observation
335 is found in the curves corresponding to the δ_{AI-PCM} of about 1 for porosity 0.757 and 0.9. It also
336 can be observed that the sample height has a limited effect on δ_{AI-PCM} for $\epsilon=0.95$ and N_s obtained
337 for $\epsilon=0.95$ is lower than the N_s obtained for the porosity of 0.757 to 0.9. Therefore, δ_{AI-PCM} for
338 $\epsilon=0.8$ to 0.95 can surely reach a stable value when N_c above N_s derived on a basis of $\epsilon=0.757$.

339 Thus, Eq.7 also can be used to estimate the N_s for $\epsilon=0.757$ to 0.95. By combining Eq.6 and
340 Eq.7, N_s can be described as a function of geometrical features (L , ϵ) and heat flux q , as follows:

341
$$N_s = -12.72 \times \ln(q \times L / (-97.874 \epsilon^2 + 118.55 \epsilon - 15.671) - 0.85) + 46.02 \quad (8)$$

342 Eq.8 indicates that Eq.6 derived on the basic of $H=64 \times L$ also can be applied to estimate the
343 maximum temperature difference at section A near the heating surface of a sample of $H=N_c \times L$
344 when the N_c above N_s .



345 a)

b)

346 Figure 5 Maximum temperature difference between the reference points of Al and PCM in
 347 section A as a function of number of stacked cells for different cases of L and q in the case of
 348 a) a fixed porosity $\epsilon=0.757$. Red stars indicate the number of stacked cells (N_s) above which a
 349 constant value of δ_{Al-PCM} is reached. Best-fit curve for correlation between N_s and δ_{Al-PCM} is
 350 given by Eq.7. b) porosity ranging from 0.757 to 0.95.

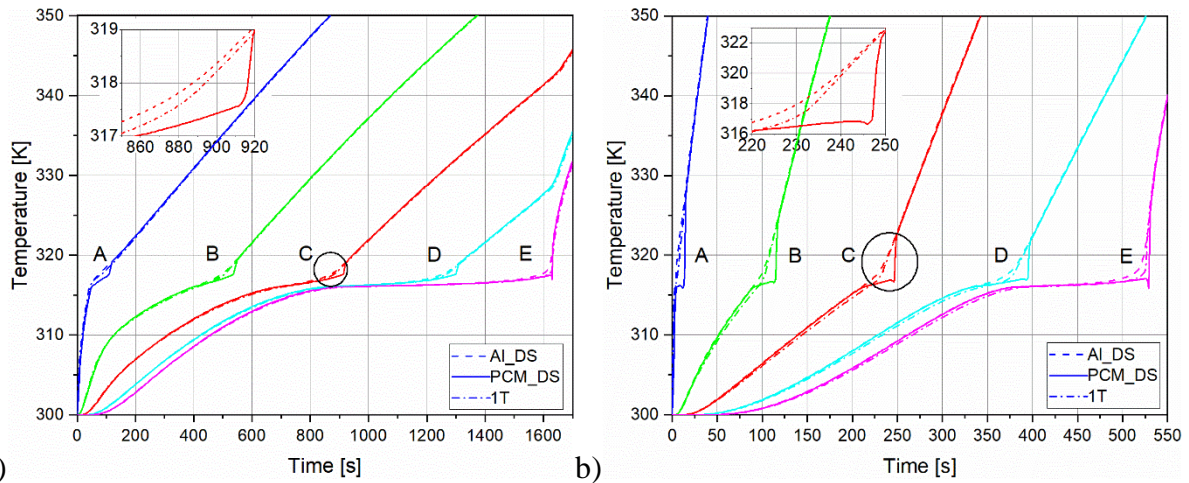
351 5.4 Case 4 Comparison between results obtained using DS and 1T models.

352 Comparisons between the results of thermal response of differently modelled composite PCMs
 353 have been presented in literature by comparing the progressive increase of the overall volume
 354 fraction of molten PCM obtained imposing both constant temperature or constant heat flux on
 355 one surface of the samples [13,14] or by comparing the obtained thermal profiles in specific
 356 sections [13,14].

357 5.4.1 Thermal profiles

358 In the present case 4, comparisons between thermal profiles of differently modelled PCM
 359 structures working in different conditions has been considered also for presenting the results
 360 of simulated tests in case 4. Fig. 6a and 6b show examples of the thermal profiles in sections
 361 A-E obtained at the two reference points referred as Al (T_{Al}) and PCM (T_{PCM}) considered also
 362 for previously cases. On the same figures the temperature profiles (T_{1T}) obtained at the same
 363 section plane for 1T model are plotted. Since the 1T model considers a homogeneous material,
 364 the temperatures are homogeneous within each section plane, due to adopted boundary
 365 conditions. Both figures refer to a sample with $L=2$ mm, $\epsilon=0.757$, but $q = 2$ W/cm² and 10
 366 W/cm², the latter (Fig. 6b) used in case 1. Both figures show that the predictions of the 2 models
 367 substantially differ when the temperature at which the PCM starts melting and in a melting

368 temperature range this difference increases with the heat flux. Looking at the insets of Fig. 6a
 369 and 6b, it is clear that the temperature simulated by 1T model lays not only within T_{Al} and T_{PCM}
 370 from DS simulations, but that it is closer to T_{Al} .

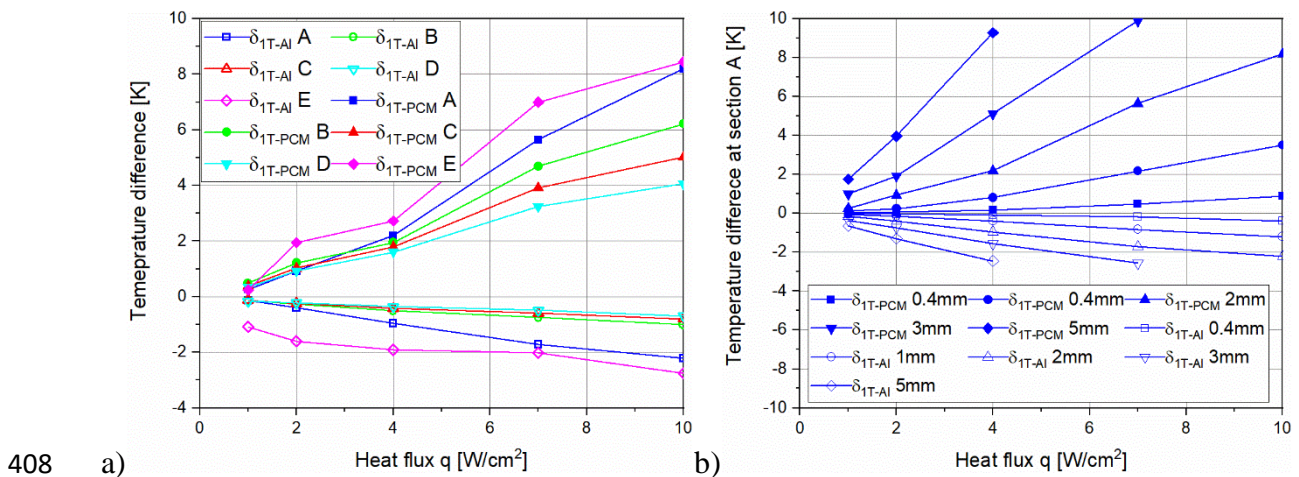


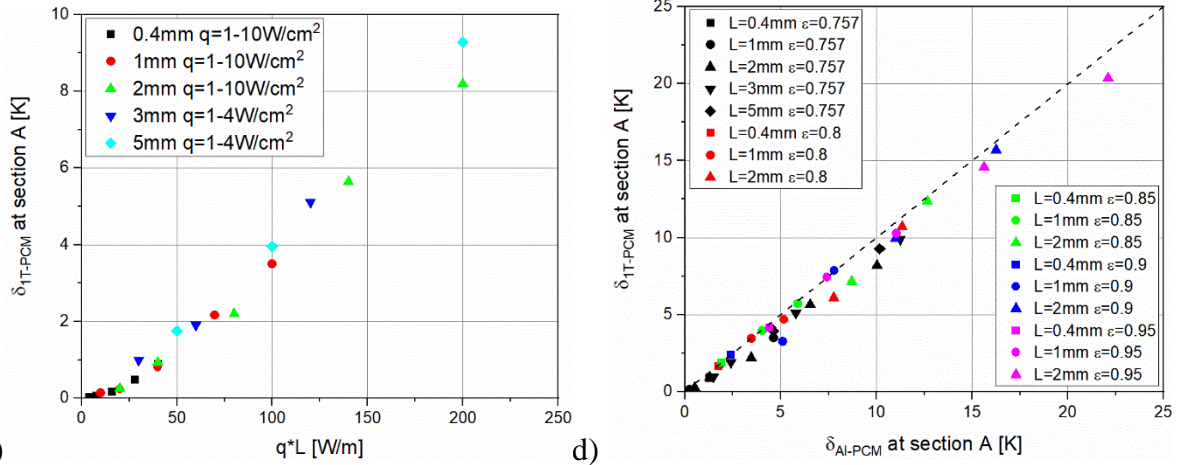
371 a) b)
 372 Figure 6 Comparison between temperatures profiles of PCM and Al reference points at sections
 373 A-E for DS model and the temperature at corresponding section planes for 1T model. a)
 374 $L=2\text{mm}$, $q=2\text{W}/\text{cm}^2$; b) $L=2\text{mm}$, $q=10\text{W}/\text{cm}^2$.

375 The situation presented for increasing q value is also observed, as expected, for coarser
 376 structures. The authors consider the need of identifying one or a set of parameters in order to
 377 compare the predictions obtained by the two models. In the previous cases, the temperature
 378 inhomogeneity at constant distance from the sample basis and passing through the center of the
 379 inner PCM sphere in BCC cell is characterized by means of parameter δ_{Al-PCM} (i.e. the
 380 maximum temperature difference between the reference points considered for Al and PCM
 381 phases).

382 In the present case, at sections A-E, the parameters δ_{1T-Al} and δ_{1T-PCM} are defined as the
 383 maximum temperature differences between the temperature at section obtained by 1T model
 384 and temperature in the representative points for Al and PCM phases from DS model,
 385 respectively. These parameters can be used to compare the differences of thermal profiles
 386 produced by the use of DS or 1T models. Fig.7a summarizes the results of the set of simulations
 387 carried out for different supplied heat flux values but a constant value of L (2mm). It clearly
 388 shows what discussed above by comparing temperature profiles shown in Fig.6, i.e., that δ -
 389 values increases as the heating flux increases and δ_{1T-Al} is lower than δ_{1T-PCM} (maximum at T_m).
 390 Further, the effects of heating flux on the δ -values increases as sections considered are closer
 391 to the heating surface. Fig.7b shows the changes in terms of δ_{1T-Al} and δ_{1T-PCM} for different side

392 length of the metallic structure, the coarser one resulting in larger absolute values of δ_{1T-AI} and,
 393 particularly, of δ_{1T-PCM} . Focusing the attention on δ_{1T-PCM} , it has been done for previous cases,
 394 the correlations shown in Fig. 7a and 7b for q and L separately have been checked also for the
 395 product of $q \times L$. The result is shown in Fig. 7c. Even these data only refer to the constant
 396 porosity ε , a clear dependence of δ_{1T-PCM} on $q \times L$ exists, similarly to what observed for δ_{AI-PCM}
 397 in Fig. 4b. Further, the closeness of δ_{1T-PCM} to δ_{AI-PCM} discussed on the basis of the results in
 398 Fig. 4 is confirmed when δ_{1T-PCM} is plotted against δ_{AI-PCM} in Fig.7d, for several $q \times L$ values as
 399 well as for several porosity ε in point A. Since δ_{1T-PCM} , which can be considered as the
 400 maximum temperature error in the description of the PCM temperature profile within the PCM
 401 phase is only slightly lower than δ_{AI-PCM} (representing the actual maximum temperature
 402 difference between the temperature of Al, assumed as homogeneous, and the minimum one in
 403 PCM phase), δ_{AI-PCM} can be used as a parameter suggesting the goodness of 1T model in
 404 different situations as far as the porous structure geometry (L , ε) and heat flux are concerned.
 405 Thus, the maps derived from Eq. 6 presenting the value of δ_{AI-PCM} for a given porosity (and
 406 thus a given λ_{eff} , i.e., similar situation in steady-state conditions) as a function of q and L also
 407 can be used to suggest the goodness of 1T model.





409 c) d)
 410 Figure 7 The maximum temperature differences δ_{1T-AI} and δ_{1T-PCM} between DS and 1T model
 411 predictions for a) $L=2$ mm at sections A, B, C, D and E; b) $L=0.4$ mm, 1 mm, 2 mm, 3 mm and
 412 5 mm at section A. C) δ_{1T-PCM} vs. $q \times L$ obtained from simulated tests at $\epsilon=0.757$. d) A
 413 correlation of δ_{1T-PCM} vs. δ_{AI-PCM} for different q , L and ϵ values.

414 From the insets of Fig. 6a and 6b, it can be further noted that, in the time range where PCM
 415 melting occurs, temperature difference between 1T and AI phase and that between 1T and PCM
 416 phase change with time, the first being maximum at the beginning of melting, the second being
 417 maximum at the end of it, at T_m . Further, it can be noticed that at times where the end of melting
 418 is reached for the reference point PCM (practically, the last point of PCM phases which melts,
 419 being located at the center of PCM sphere in the BCC structure), the δ_{1T-PCM} is slightly lower
 420 than δ_{AI-PCM} considered for previous cases. Thus, the considerations done in previous cases to
 421 predict δ_{AI-PCM} could be applied for the estimation of the goodness of 1T model in terms of
 422 temperature predictions. 1T model has more reliable temperature prediction in the case of finer
 423 foam structure and lower heat flux supply and δ_{1T-PCM} near heating surface has critical value.

424 5.4.2 Volume fraction of molten PCM.

425 Since PCMs are typically used for thermal storage application where the amount of stored
 426 latent heat where the phase transformation occurs over a narrow temperature range several
 427 times higher than the sensible heat accumulated even in a wider temperature range, the amount
 428 of heat stored can be considered as roughly proportional to the volume fraction of the molten
 429 PCM. The goodness of a model can thus be inferred by the analysis of volume fractions. This
 430 can be done also by comparing the results predicted by 1T model with those obtained by DS
 431 model, that can be considered as a detailed manner to describe what is going on.

432 In a composite PCM, the fraction of molten PCM should be evaluated with respect to the total
 433 volume fraction of PCM (the porosity ε in the present case). The normalized volume fraction
 434 (NVF) of molten PCM is here defined as the ratio between the volume of molten PCM and the
 435 volume occupied by PCM for the composite PCM. Both a local and overall approach for the
 436 calculation of NVF profiles are possible. 1 From the practical point of view, in the case of DS
 437 model, at each time the volume fractions of molten paraffin at the points NPCM (for the unit
 438 cell A-E) have been summed up and divided by NPCM. In the 1T model at each time the
 439 volume fractions of the 100 points corresponding to the cell across the considered section A-E
 440 are averaged. The overall approach considers the whole sample as the reference volume for the
 441 calculation of NVF.

442 Fig.8a shows the comparison between the local NVF at unit cells A-E and the overall NVF for
 443 the sample in the case of $L=1\text{mm}$ and $q=4\text{W/cm}^2$ (sample height $H=64\times L$ and porosity
 444 $\varepsilon=0.757$). It is observed that when the focus is on the description of local phase transition and
 445 energy storage, the 2 models significantly differ. Specifically, at each of the unit cell A-E, 1T
 446 model predicts longer time for the onset of melting and shorter time for the melting completion.
 447 Definitely, 1T model predicts shorter phase transition times, in any case within those predicted
 448 by the more reliable DS model.

449 Fig. 8b shows the comparison between NVF profiles predicted by the two models have also
 450 been plotted for effects of q (ranging from 2 W/m^2 to 10 W/m^2) for unit cell A in the case of a
 451 sample of $L=3\text{mm}$. In order to quantify the errors induced by the use of 1T model, the maximum
 452 difference between NVF predicted by DS and 1T model at this unit cell is considered. In this
 453 location the maximum difference can occur both at the onset or offset of the phase transition
 454 predicted by 1T model. Nevertheless, since this is a peculiar situation of section A, which could
 455 be partly related to its closeness to boundary. Only the temperature difference at the end of the
 456 phase transition in 1T model is considered, that is at T_m . The error of NVF caused by 1T model
 457 has been calculated for unit cell centered at each reference section as:

$$458 \text{ NVFE} = (\text{NVF}_{1\text{T}} - \text{NVF}_{\text{DS}})_{T_m} \quad (9)$$

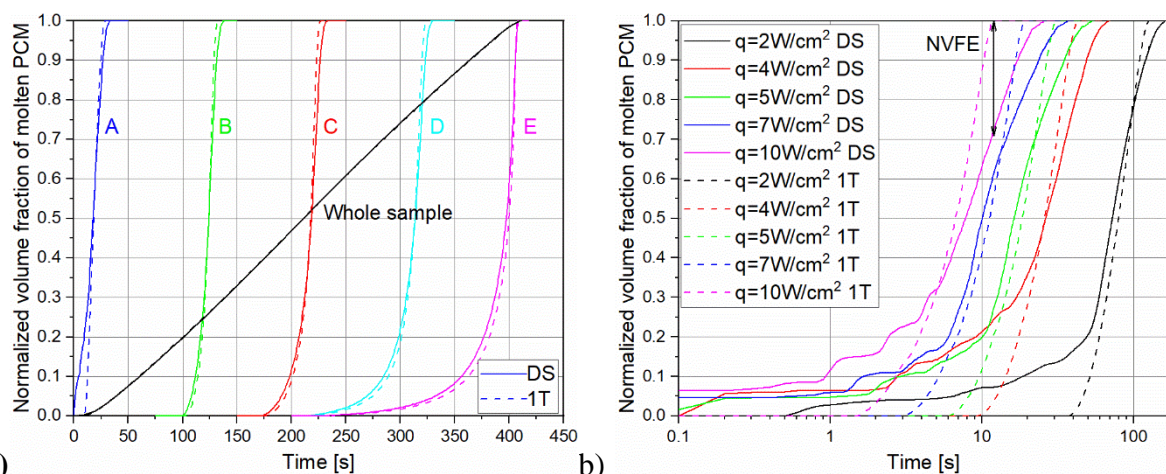
459 NVFE tends to increase with q , as shown in Fig. 8b. Further, it can be observed that when high
 460 heat flux is applied the NVF profile predicted by DS model is not smooth but shows the melting
 461 of PCM spheres, that are well visible in the case of a low porosity structure considered for the
 462 evaluation here. The volume fraction profiles tend to be smoother as the value of q decreases.

463 The same occurs when the Al structure coarseness is reduced (i.e., lower L are considered) and
 464 when the porosity level is increased.

465 These errors have been calculated for the unit cell A-E for a selected set of heat flux and sample
 466 geometry (varying L but keeping the same porosity and number of stacked cells). The results
 467 are shown in Fig. 8c, where NVFE is plotted vs. the product $q \times L$, as done for other cases. The
 468 overall trends of the NVFE with the product of $q \times L$ is increasing, even if is not linear and
 469 monotonic. Further, the differences are particularly high for the unit cell A and E, where
 470 boundary conditions effects are present. Here the difference between normalized volume
 471 fractions (and thus energy stored) can reach values just below 0.15 for $q \times L = 8 \text{ W/m}$ but
 472 increases up to 0.25 when $q \times L$ reaches 200 W/m . In internal sections the effect of $q \times L$ on
 473 NVFE is also remarkable and for the same $q \times L$ range it raises from 0.05 to about 0.25.

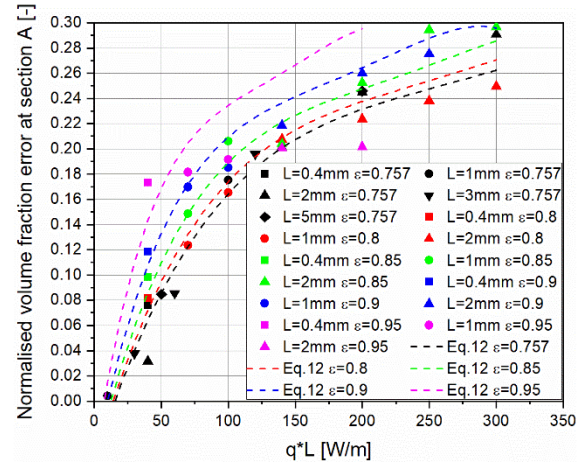
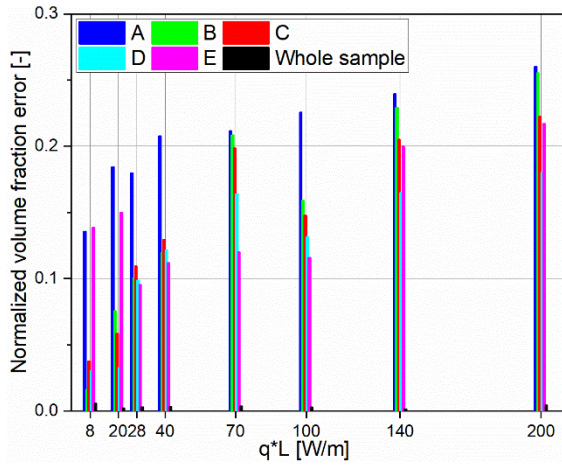
474 The overall approach, which has been used by other authors to compare results from 1T and
 475 DS models [13,14], give close profiles of NVF (referred as ‘Whole sample’ in Fig. 8a) and,
 476 correspondingly, far lower NVFE, lower than 0.06 for the $q \times L$ range considered in Fig. 8b.
 477 This confirms that once the predictions of the overall energy stored /released are needed, the
 478 1T model can be considered to supply sufficiently good results.

479 The NVFE at unit cell A for different porosity versus $q \times L$ is plotted in Fig. 8d. Even if scattering
 480 of result is noticed, a clear correlation between NVFE and $q \times L$ can be observed, with the only
 481 exception of the results for the highest porosity value ($\epsilon = 0.95$), for which NVFE reaches and
 482 holds a constant value of about 0.20 at $q \times L = 140 \text{ W/m}$.



483 a)

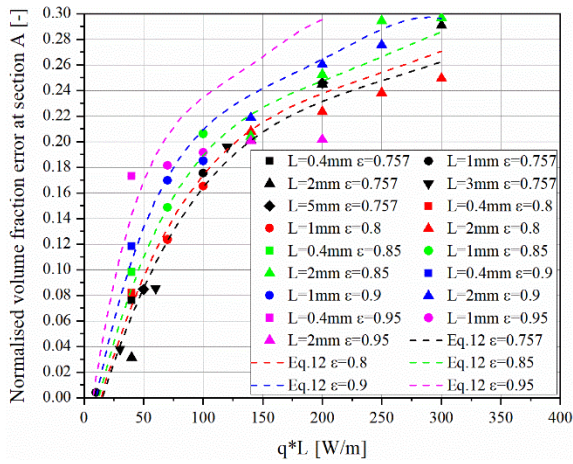
b)



484

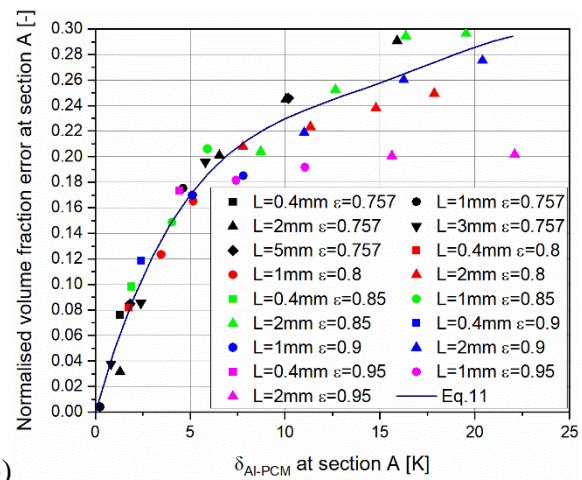
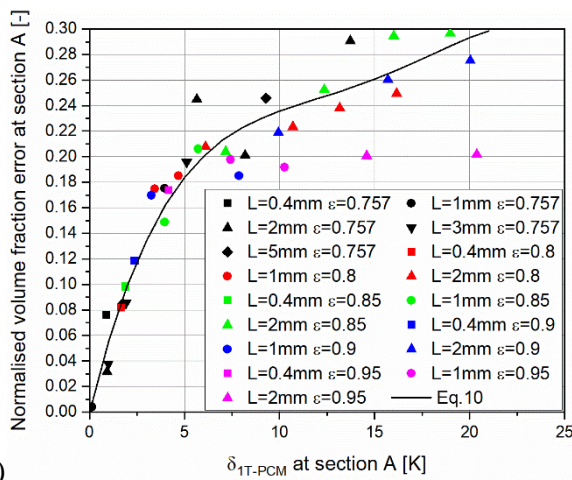
c)

d)



485

486 Fig. 8 Comparison between the melting rate of PCM at unit cell A-E and overall volume from
 487 direct simulation and the 1T simulation for a) $L=1\text{mm}$, $q=4\text{W}/\text{cm}^2$. b) $L=3\text{mm}$, a set of heat
 488 flux $q=2\text{ W}/\text{cm}^2$ to $10\text{ W}/\text{cm}^2$; c) Normalized volume fraction error for a set of $q \times L$ for porosity
 489 $\epsilon=0.757$; d) Normalized volume fraction error (NVFE) at unit cell A for a set of $q \times L$ for
 490 different porosities and NVFE predicted by Eq.12 for different porosities.



491

a)

b)

492 Figure 9. Correlation between NFVE and δ_{IT-PCM} (a) and δ_{AI-PCM} (b) for different q , L and
 493 porosity ε at section A. In each plot, data points calculated for $0.757 \leq \varepsilon \leq 0.9$ have been fitted
 494 with a polynomial line.

495 The final step is to understand the possibility to model adequately the melting of PCM filling
 496 a high-conductivity inverse BCC structure with relatively high coarseness and ε on a local scale.
 497 Correlations between NFVE and δ_{IT-PCM} or δ_{AI-PCM} for data points calculated for $0.757 \leq \varepsilon \leq 0.95$,
 498 are shown in Fig. 9a and 9b, respectively. For the porosity $0.757 \leq \varepsilon \leq 0.9$ and δ_{AI-PCM} and δ_{IT-PCM}
 499 up to 20K, the following correlations exists:

$$500 \text{ NVFE} = -4.73 \times 10^{-6} \times \delta_{IT-PCM}^4 + 2.82 \times 10^{-4} \delta_{IT-PCM}^3 - 6.04 \times 10^{-3} \times \delta_{IT-PCM}^2 + 6.05 \times 10^{-2} \times \delta_{IT-PCM};$$

$$501 \quad R^2 = 0.95 \quad (10)$$

$$502 \text{ NVFE} = -3.24 \times 10^{-6} \times \delta_{AI-PCM}^4 + 2.03 \times 10^{-4} \times \delta_{AI-PCM}^3 - 4.69 \times 10^{-3} \times \delta_{AI-PCM}^2 + 5.28 \times 10^{-2} \times \delta_{AI-PCM};$$

$$503 \quad R^2 = 0.97 \quad (11)$$

504 Since, as shown in Fig. 7d, δ_{AI-PCM} and δ_{IT-PCM} are very close, the only Eq. 11 can be considered.
 505 Furthermore, by combining Eq. 6 and Eq. 11, the description of NVFE as function of $q \times L$ and
 506 ε is obtained as follows.

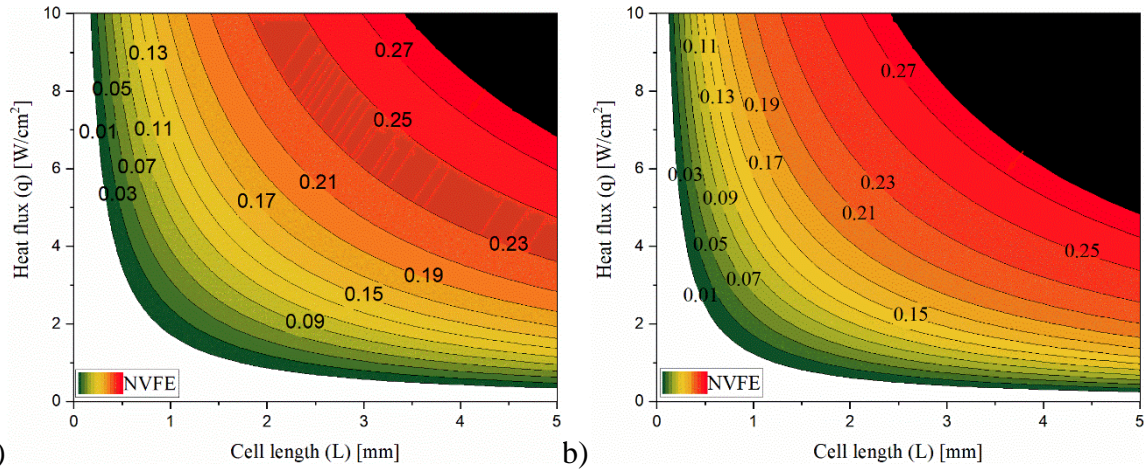
$$507 \text{ NVFE} = -3.24 \times 10^{-6} \times (q \times L / (-97.874 \times \varepsilon^2 + 118.55 \times \varepsilon - 15.671) - 0.85)^4 + 2.03 \times 10^{-4} \times (q \times L / (-97.874 \times$$

$$508 \varepsilon^2 + 118.55 \times \varepsilon - 15.671) - 0.85)^3 - 4.69 \times 10^{-3} \times (q \times L / (-97.874 \times \varepsilon^2 + 118.55 \times \varepsilon - 15.671) - 0.85)^2 + 5.28 \times 10^{-}$$

$$509 2 \times (q \times L / (-97.874 \times \varepsilon^2 + 118.55 \times \varepsilon - 15.671) - 0.85) \quad (12)$$

510 Validation of Eq. 12 has been performed by plotting the foreseen NVFE for different $q \times L$
 511 values at various porosity ratios in Fig. 8d. It can be observed that Eq. 12 can well predict the
 512 NVFE for porosity ε ranging from 0.757 to 0.9 while it overestimates the NVFE for $\varepsilon = 0.95$.

513 As shown in Case 3, the equation can be applied only when the number of stacked cells over
 514 N_s defined in Eq. 8. Eq.12 gives the possibility to draw iso-NVFE lines at fixed ε in q vs. L
 515 plots, similarly to what done with Eq. 6 in Fig. 4d. This is shown in Fig. 10a and 10b for $\varepsilon = 0.8$
 516 and 0.9, respectively. The correlation of NVFE and δ_{AI-PCM} has been simply described by
 517 parabolic law, which well predicts NVFE by δ_{AI-PCM} when δ_{AI-PCM} is less than 20K and the
 518 corresponding $q \times L$ is less than 345 W/m for $\varepsilon = 0.8$, less than 245 W/m for $\varepsilon = 0.9$. The black
 519 area in the upper-right corner of plots in Fig. 10, corresponds to areas where δ_{AI-PCM} exceeds
 520 20K. The closer iso-NVFE for $\varepsilon = 0.9$ visually suggest the stronger effects of q and L on NVFE.



521 a) 522 Figure 10. Map showing iso-NVFE curves in section A as functions of q and L for porosity $\varepsilon=$
 523 0.8 (a) and 0.9 (b) derived from Eq. 12. The black area refers to $q \times L$ more than 345W/m for
 524 $\varepsilon = 0.8$ and 245W/m for $\varepsilon = 0.9$, respectively.

525 6 Conclusion

526 The present study has investigated the effect of structure coarseness and boundary condition
 527 on local thermal response of the composite PCMs combining paraffin with Al structure
 528 modelled as inverse BCC lattice. Local temperature difference at reference points of Al and
 529 PCM phases for different height has been presented for a set of cell length L and heat flux q .
 530 The exacting correlation between the above temperature difference and the product of L and q
 531 have been modelled for pore volume fraction ranging from 0.757 and 0.95. This correlation is
 532 applied to the cell closer to heating boundary in case of sufficiently thick specimens (N_c above
 533 critical value N_s).

534 1T model considering homogeneous media with proper effective thermophysical properties,
 535 supply good local thermal response predictions for fine structures and lower heat flux input.
 536 1T model is not precise to predict the liquid PCM volume fraction of local section but it is
 537 sufficient to estimate the liquid PCM volume fraction of whole sample. A analytical model is
 538 proposed to predict the maximum local error for volume fraction of molten PCM, normalized
 539 to the overall volume of PCM in the representative unit cell induced by 1T model for the
 540 porosity ranging from 0.757 to 0.9.

541 The main novelty of the paper is the possibility to quantify the error introduced by the use of
 542 the simple 1T model in the molten volume fraction prediction (and thus on energy
 543 stored/release) for porous Al/paraffic composite PCMs with generic amount of phases,
 544 coarseness and service conditions (heat flow).

545

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