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1 **Experimental and numerical characterization of an impure phase change material**  
2 **using a thermal lattice Boltzmann method**

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21 **Towards experimental and numerical characterization of an impure phase change**  
22 **material using a thermal lattice Boltzmann method Abstract**

23 Of the phase change materials (PCMs) that regulate ambient temperature while reducing energy  
24 consumption, Octadecane is a good candidate because of its transparency properties and its  
25 adequate melting temperature. This study aims to characterize, through an approach combining  
26 numerical simulation and experiment, the behavior and thermo-physical properties of n-  
27 Octadecane. The approach takes into consideration the natural convection and the use of PCM's  
28 experimentally-obtained enthalpy-temperature curve that includes the supercooling and soluble  
29 impurities effects. The model uses the thermal lattice Boltzmann method based both on a partial  
30 bounce-back and an enthalpy formulation while including the experimental relationships. The  
31 numerical and experimental results exhibit good agreement. The approach adopted allows to  
32 highlight the behavior of the PCM to better characterize its thermo-physical properties.

33 **Keywords:** Phase change materials (PCMs), Lattice Boltzmann method (LBM), Convection,  
34 Supercooling, Impurities.

35

## Nomenclature

$c$	specific heat capacity (J/kg.K)
$c_s$	lattice sound speed (lu/ts)
$e_i$	streaming particle velocity in i-direction (lu/ts)
$f_i$	particle distribution function of fluid (-)
$g_i$	particle distribution function of temperature (-)
$g$	gravity's acceleration (m/s <sup>2</sup> )
$h$	specific enthalpy (J/Kg)
$k$	thermal conductivity (W/m.K)
$L$	latent heat of fusion (J/kg)
$lu$	lattice unit of length
$m$	total masse (kg)
$PCM$	phase change material
$PDF$	particle distribution function
$T$	temperature (K)
$T_a$	melting temperature of pure PCM (K)
$T_0$	initial temperature (K)
$T_m$	melting temperature of impure PCM(K)
$T_P$	imposed temperature on two faces of the sample (K)
$t$	time (s)
$ts$	lattice unit of time
$U$	macroscopic velocity (m/s)
$u, v$	x-, y-velocity component (m/s)
$x$	cartesian (m)
$X_i$	impurities' fraction
<i>Greek symbols</i>	
$\alpha$	thermal diffusivity (m <sup>2</sup> /s)
$\beta$	thermal expansion coefficient (K <sup>-1</sup> )
$\Delta t$	time step (s)
$\Delta x$	space step (m)
$\varepsilon$	liquid fraction (-)
$\nu$	kinematic viscosity (m <sup>2</sup> /s)
$\rho$	macroscopic density (kg/m <sup>3</sup> )
$\omega_i$	weight coefficient (-)
$\tau_f, \tau_h$	dimensionless lattice relaxation times
<i>Superscripts/subscripts</i>	
$eq$	local equilibria
$l$	liquid phase of PCM
$m$	melting
$s$	solid phase of PCM
$w$	wall

## 37 **1. Introduction**

38 The global population growth has led to a high energy demand and increased CO<sub>2</sub> emissions  
39 triggering a major environmental crisis. The energy use in buildings accounts for a large share of  
40 the total end use of energy, with an average consumption of about 50% of all raw materials owned  
41 in the world [1]. This percentage would differ depending on the region, and is equal to 40% in  
42 Europe, 30% in USA, and reaches 70% in undeveloped countries [2]. Energy consumption for  
43 thermal comfort in buildings rises with increasing in user demand for comfort conditions. This rise  
44 in, both, energy consumption and CO<sub>2</sub> emissions thus promoted a new policy aimed at creating  
45 more sustainable buildings [3]. Scientists all over the world are in search of new and renewable  
46 energy sources. One of the options is to develop energy storage devices, which are as important as  
47 developing new sources of energy. Thermal energy storage does not only reduce the temporal gap  
48 between supply and demand, but it also improves the performance of energy systems and plays a  
49 significant role in conserving energy [4]. Such storage can be achieved either by using sensible  
50 heat or thermo-chemical heat or latent heat. Among these different methods, the latent thermal  
51 energy storage (LTES) method, using phase change materials (PCMs), is the most preferred and  
52 the most widely used at present [5, 6] mainly for their application for heating and cooling of  
53 buildings [4, 7-11]. PCMs can be used for temperature regulation and their high storage capacity  
54 can reduce energy consumption in buildings, and thereby contribute to the reduction of CO<sub>2</sub>  
55 emissions.

56 Recently, interest in the use of Octadecane in latent heat systems and building materials has  
57 increased. Its choice is mainly due to its transparency properties and its melting temperature, which  
58 lies within the thermal comfort of human beings. The original idea is to fill Plexiglas enclosures  
59 with PCM having transparency properties, and thereby create a wall of a building façade or  
60 windows that benefits from solar gains. For PCMs in windows, paraffin-based organic materials  
61 are the most interesting since they are transparent in the liquid state and translucent in the solid  
62 state. For that, it is interesting to investigate more on Octadecane as a PCM. The main task

63 throughout this research is to develop a numerical model that matches the experimental results and  
64 helps infer some thermo-physical properties that are difficult to predict via single experiments,  
65 example: the thermal contact resistance, conductivity in liquid phase, the degree of supercooling,  
66 heat transfer coefficient, etc. Following this, the model can be also used to enhance and optimize  
67 PCM performance in practical applications. Note that, at this stage, the heat transfer by radiation  
68 is not considered since our experimental apparatus induces heat through attached plates controlled  
69 by thermo-regulated baths (see Section 4). Actually, the study of such materials will involve the  
70 characterization part, as our present study, and an application part where the experimental setup  
71 will be different and will follow appropriate climatic and external conditions and adequate  
72 geometric scales. Both tests and studies are required for this material to reach a mature state for  
73 practical applications.

74 Thus, prior to the large-scale practical application of this technology, it is crucial to consider  
75 certain issues in the stage of research and development [4]. The experimental investigation of some  
76 PCMs showed the presence of some phenomena that could affect the performance if not considered  
77 in the design, namely supercooling, convection and impurities. When supercooling occurs, the start  
78 of solidification is delayed, and the liquid solidifies at a temperature below its freezing temperature.  
79 This can lead to a mismatch between the design and the real behavior of the PCM [12]. Most of the  
80 theoretical heat transfer modeling of PCM energy storage systems is based on the conjecture that  
81 the supercooling degree is negligible or even completely absent. However, recently published  
82 researches [12-14] indicate that even a relatively small degree of supercooling might result in a  
83 significant undesirable effect on the heat release rate as a function of time, reducing the thermal  
84 efficiency of the system. Therefore, it is important to provide reliable theoretical modeling of  
85 supercooling in PCM for a more adequate design.

86 Another important phenomenon, ignored in some numerical models, is the natural convection  
87 in the liquid phase. If PCMs with high Prandtl number are used, e.g. Octadecane, it is very likely  
88 to have convection even in small samples. This is because the relative thickness of the momentum

89 boundary layer is much more than the thermal one. Hence, convection will be dominant with  
90 momentum diffusing more quickly compared to heat. In addition, soluble impurities, if they exist,  
91 may lead to depression in melting point thus altering the temperature-enthalpy curve, so that the  
92 traditional piecewise function can no longer be used. Also, the thermal contact between different  
93 materials in the system can have similar effects on the enthalpy curve. Therefore, using a simplified  
94 model may fail to successfully predict the phase change process, if the aforementioned phenomena  
95 are present. Thereby, the main aim targeted here is to provide an improved model that accounts for  
96 supercooling, convection and the modified enthalpy-temperature curve. To carry out this work, we  
97 consider the thermal lattice Boltzmann method (TLBM) [15-20] based on a partial bounce-back  
98 (PBB) approach [21-23] supplemented with an enthalpy-based model. This enhanced model  
99 provides a more accurate simulation of phase-change materials, can better predict the solidification  
100 and melting processes, and thus match the experimental results.

101 The paper is organized as follows: Section 2 provides a literature review on challenges in  
102 modeling phase-change materials. Section 3 is devoted to the lattice Boltzmann method adopted  
103 herein to achieve the numerical solution while supplementing the appropriate enhancements. The  
104 experimental setup with equipment and the measurement method is outlined in Section 4. Section  
105 5 presents the experimental determination of the thermo-physical properties of Octadecane:  
106 conductivities, specific capacities, latent heat of fusion, and the analysis of the heat flux curves.  
107 Thorough discussions of the confrontation between numerical and experimental results are  
108 presented in Section 6. Finally, Section 7 concludes the paper by providing key findings based on  
109 the dual experimental and numerical approach.

## 110 **2. Challenges of modeling of phase-change materials**

111 PCMs have various possible applications ranging from temperature stabilization to energy  
112 storage. Though many pure chemical elements can be used as PCMs, the majority often consists of  
113 a mixture, or contains at least soluble impurities. The main reason for creating a PCM as a mixture  
114 of various substances is to achieve a desirable melting temperature for a particular application.

115 However, these mixed or impure PCMs require accurate and reliable methods for determining their  
116 thermo-physical properties, which represents a significant issue that considerably affects the  
117 accuracy and credibility of the corresponding studies. Numerical modeling can help in determining  
118 some of these properties. However, other serious complexities interfere in the modeling of phase  
119 change materials, which makes it a real challenge.

120 Many macroscopic mathematical modeling schemes for solidification/melting problems can be  
121 found in the literature [23-25]. Early efforts initiated with the moving/deforming grid approach [24,  
122 25] in which independent conservation equations for each phase are initially formulated and are  
123 subsequently coupled with appropriate boundary conditions at the interfaces. However, such  
124 multiple region solutions require the existence of discrete interfaces between the respective phases.  
125 In fact, a major difficulty in their implementation [26] is associated with tracking the phase  
126 interfaces (which are generally unknown functions of space and time). Additionally, a serious  
127 limitation exists for modeling phase change behavior of multi-component systems, since they do  
128 not exhibit a sharp interface between solid and liquid phases. Moreover, solidification occurs over  
129 extended temperature ranges and solid formation often occurs as a permeable crystalline-like  
130 matrix, which coexists with the liquid phase. Otherwise, there are the fixed-grid models, using  
131 finite element (FE) or finite volume (FV) methods [24, 27]. A separate equation for the liquid  
132 fraction evolution is solved, which implicitly specifies and updates the interfacial locations with  
133 respect to space and time. The fixed grid method is relatively simple, versatile, practical, adaptable  
134 and easily programmable [11]. It can easily handle melting or solidifying materials over a range of  
135 temperatures. The latent heat evolution is accounted for in the governing equation by using, either  
136 enthalpy method [12, 23], heat capacity method [13, 28], temperature transforming model [14],  
137 heat source method [24, 25], or other methods.

138 On the other hand, the multi-scale mesoscopic lattice Boltzmann method (LBM) has emerged  
139 to offer huge potential for solving complex thermo-fluidic problems involving morphological



140 development of complicated phase boundaries [21-23, 29-33] and recovers the Navier-Stokes and  
141 energy equations. In addition, it has been witnessed that the LBM stands out in major fields of  
142 classical fluid dynamics: multiple-scale flows and heat transfers with or without phase change  
143 process. Its advantage, compared to a classical based-continuum formulation, is that it operates at  
144 a mesoscopic level, which incorporates micro and meso-scale physics of phase transitions, and  
145 bypasses the explicit calculation of the pressure equation, leading to time-efficient computational  
146 simulations. Further, LBMs are inherently transient and parallelizable, which renders their  
147 suitability to address phase change processes over large-scale computational domains [34].  
148 Moreover, by adopting partial bounce-back approach with enthalpy formulation [15], LBM treats  
149 phase-change as flow in porous medium. Extensive work has been done to simulate fluid and heat  
150 flow in porous media using LBM [35, 36]. The liquid fraction calculated through an enthalpy  
151 formulation designates the porosity in the mushy zone and helps tracking fusion front and  
152 simulating convection. The local nature of the method allows adding local complexities where  
153 necessary.

### 154 **3. Numerical Model**

#### 155 **3.1. Enthalpy-temperature relationship**

156 The most common enthalpy/temperature relationship is often translated as a piecewise function  
157 in the case of pure materials. However, even a small amount of impurities can lead to a significant  
158 change in the enthalpy curve shape, with a depression of the melting temperature followed up by a  
159 melting range. Hence, melting point analysis can provide information on the sample purity [37]. In  
160 other words, a substance including soluble impurities will be prone to “melting point depression”.  
161 This is related to the intermolecular forces within the material. As the solid impurity increases, its  
162 structure will be more disrupted, and hence will result in a greater variation in intermolecular forces  
163 throughout different areas of the solid. The effect will be that the melting temperature is lower than

164 that of a pure material, and the solid melts over a wider range of temperatures. Note that this is not  
 165 the case for insoluble impurities. The latter will have no effect on the compound's melting point.

166 When soluble impurities exist, the model can be dealt as a binary mixture, with one component  
 167 having very small portion compared to the other. Thereby, we can calculate the depression in the  
 168 melting temperature ( $\Delta T_{am}$ ) as follows [37]:

$$169 \quad \Delta T_{am} = T_a - T_m = RT_a^2 X_i / L_f \quad (1)$$

170 where  $T_a$  is the melting point of a 100% pure material,  $T_m$  is the lowered melting point of the impure  
 171 material,  $L_f$  ( $J/mol$ ) is the molar heat of fusion,  $R$  ( $= 8.314 J/mol/K$ ) is the ideal gases universal  
 172 constant, and  $X_i$  is impurities' fraction in the considered material. In this work, this can be used as  
 173 a pre-estimate of the real melting temperature of the studied sample with respect to the expected  
 174 melting temperature in literature.

175 It seems obvious that impurities' percentage in a material alters the enthalpy curve of a substance  
 176 and consequently affects the resulting heat flux. The peak of the heat flux curves becomes wider  
 177 and shorter as the impurity increases while maintaining the same underlying area (under it), which  
 178 is related to the melting enthalpy.

179 **• Enthalpy-temperature relationship for pure PCMs**

180 The variation of enthalpy vs. temperature of a pure material is:

$$181 \quad \frac{dh_{pcm}}{dT} = \begin{cases} c_{s,pcm} & \text{for } T < T_a \\ c_{l,pcm} & \text{for } T > T_a \end{cases} \quad (2)$$

182 It should be noted that  $dh_{pcm}/dT$  tends to infinity when T approaches  $T_a$ .

183 **• Enthalpy-temperature relationship for non-pure PCMs, i.e. with soluble impurities**

184 For an impure material, the variation of the enthalpy vs. temperature can be written as [38-40]:

$$185 \quad \frac{dh_{pcm}}{dT} = \begin{cases} c_{s,pcm} - (c_{s,pcm} - c_{l,pcm}) \frac{T_m - T_a}{T - T_a} - L_f \frac{T_m - T_a}{(T - T_a)^2} & \text{for } T \leq T_m \\ c_{l,pcm} & \text{for } T > T_m \end{cases} \quad (3)$$

186 The resulting expression of the enthalpy becomes:

$$187 \quad h_{pcm} = \begin{cases} c_{s,pcm}(T - T_m) + (c_{l,pcm} - c_{s,pcm})(T_a - T_m) \ln \left[ \frac{T - T_a}{T_m - T_a} \right] + L_f \left[ \frac{T_m - T_a}{T - T_a} \right] + H_0 & \text{for } T \leq T_m \\ c_{l,pcm}(T - T_m) + L_f + H_0 & \text{for } T > T_m \end{cases} \quad (4)$$

188 where  $T_a$  and  $T_m$  are the melting temperatures of pure and impure PCMs, respectively. However,  
189  $L_f$  is the latent heat of fusion,  $H_0$  is the enthalpy at  $T_E$ , which denotes the onset of melting.

### 190 3.2 Thermal lattice Boltzmann model (TLBM)

191 The Lattice Boltzmann method (LBM) is a mesoscale discrete model that has become an  
192 increasingly popular tool for simulating fluid flows with and without heat transfers [15-20]. It  
193 consists of simulating the statistical behavior of a set of particles on a lattice with finite velocities.  
194 This evolution is carried out in a cycle of “streaming” (advection) and “collision” steps. The  
195 essential interpretation of such an approach is that it is a special finite difference form of the  
196 continuous Boltzmann equation. Furthermore, it allows providing macroscopic fluid properties,  
197 such as density, velocity, pressure, etc., through weighted averages, or moments, of the particle  
198 distribution for all discrete lattice velocities. The single relaxation time (SRT) lattice Boltzmann  
199 model (also called the lattice Bhatnagar-Gross-Krook (LBGK) model) [41, 42] for incompressible  
200 thermal flows leans on two distribution functions (DFs) with their corresponding evolution  
201 equations to solve the evolution of the two mesoscopic particle distribution functions,  $f_i$  and  $g_i$ ,  
202 via the discretized lattice Boltzmann equation as following:

$$203 \quad f_i(x + e_i, t + I) = f_i(x, t) - \tau_f^{-1} (f_i(x, t) - f_i^{eq}(x, t)) - \tau_f \beta g(T - T_0) / \rho \Delta T \quad (5)$$

$$204 \quad g_i(x + e_i, t + I) = g_i(x, t) - \tau_h^{-1} (g_i(x, t) - g_i^{eq}(x, t)) + S_h^g \quad (6)$$

205 where  $e_i$  is the microscopic particle velocity in the  $i$ -direction,  $\tau_f$  and  $\tau_h$  are the dimensionless  
206 relaxation times, and  $f_i^{eq}$  and  $g_i^{eq}$  are local equilibrium distributions functions that can be  
207 computed from:

208 
$$f_i^{eq} = \rho \omega_i \left[ 1 + \frac{3(\bar{e}_i \cdot \bar{U})}{c_s^2} + \frac{9(\bar{e}_i \cdot \bar{U})^2}{2c_s^4} - \frac{3(\bar{U} \cdot \bar{U})}{2c_s^2} \right] \quad (7)$$

209 and 
$$g_i^{eq} = T \omega_i \left[ 1 + \frac{\bar{e}_i \cdot \bar{U}}{c_s^2} \right] \quad (8)$$

210 where 
$$\omega_i = \begin{cases} 4/9 & \text{for } i = 0 \\ 1/9 & \text{for } i = 2, 4, 6, 8 \\ 1/36 & \text{for } i = 1, 3, 5, 9 \end{cases} \quad \text{and} \quad e_i = \begin{cases} (0, 0) & \text{for } i = 0 \\ (0, \pm 1) & \text{for } i = 2, 4 \\ (\pm 1, 0) & \text{for } i = 1, 3 \\ (\pm 1, \pm 1) & \text{for } i = 5, 6, 7, 8 \end{cases} \quad (9)$$

211 are, respectively, the weight coefficient and the velocity vector of the  $D_2Q_9$  model;  $\bar{U}(u, v)$  is the  
 212 macroscopic velocity, with,  $u$  and  $v$  representing velocities in the  $x$ - and  $y$ -directions,  
 213 respectively. Note that the relaxation times  $\tau_f$  and  $\tau_h$  can be determined via  $v_{lattice} = c_s^2 \Delta t (\tau_f - 0.5)$   
 214 and  $\alpha_{lattice} = c_s^2 \Delta t (\tau_h - 0.5)$ ,  $c_s$  being the lattice sound speed. It should be noted that, the lattice  
 215 viscosity and thermal diffusivity are selected so as to conform to the intended Prandtl number  $Pr$   
 216 ( $= v_{lattice} / \alpha_{lattice}$ ). Likewise, the additional force term related to Boussinesq force  $F_b$  is incorporated  
 217 in the model by shifting the velocity field by a term of  $F_b \tau_f / \rho$  as proposed by Shan and Chen [43],  
 218 where  $F_b$  ( $= -\beta g (T - T_0) / \Delta T$ ). By this treatment, there is no need to add a force term to the  
 219 collision operator. On the other hand, in  $g$ -distribution function, the source term is treated as per  
 220 the method proposed by Luo [44]. Hence, the resulting force in the LBM frame will be:  $S_h^g = -\omega_i S_h$   
 221 with  $S_h$  ( $= Ste^{-l} \partial \mathcal{E} / \partial t$ ) being the source (or sink) term that handles the phase-change. Note that,  
 222 we performed tests on the temperature and liquid fraction to insure that they converge within an  
 223 acceptable tolerance after one iteration for the parameters set considered in this study.

224 It is worth recalling that the description and validation of the model adopted herein can be found  
 225 in [21, 45, 46]. The numerical model will calculate the temperature and velocity fields for both

226 conduction and convection heat transfer modes. Afterwards, the liquid fraction will be calculated  
 227 from the enthalpy while taking into consideration the impurities' presence. Hence, the enthalpy  $h$   
 228 is calculated from equation (4).

229 The liquid fraction ( $\varepsilon$ ) is computed as:

$$230 \quad \varepsilon = \begin{cases} 1 & \text{if } \varepsilon_1 = 1 \\ \varepsilon_2(h) & \text{if } \varepsilon_1 = 0 \end{cases} \quad (10)$$

231 where  $\varepsilon_1$  is an indicator parameter that is equal to 1 as long as nucleation did not occur for the  
 232 solidification phase. For nucleation to occur the temperature should fall below the nucleation  
 233 temperature  $T_{\text{nuc}}$ , where the degree of supercooling is the estimated as  $(T_m - T_{\text{nuc}})$ . Note that this  
 234 happens only in solidification, so that the solidification and melting curves are defined according  
 235 to different indicators. The above numeric indicator controls what enthalpy curve is used for the  
 236 calculation of liquid fraction according to Fig. 3, and then,

$$237 \quad \varepsilon_2(h) = \begin{cases} 0 & \text{for } h < h_s = c_{s,pcm}T_E = H_0 \\ \frac{h - h_s}{h_l - h_s} & \text{for } h_s \leq h \leq h_l = h_s + L_f \\ 1 & \text{for } h > h_l \end{cases} \quad (11)$$

238 It is useful to recall that, in the current model, the solid and liquid phases are defined according  
 239 to the liquid fraction value. Therefore, a mushy zone state is assigned when the value of  $\varepsilon$  is between  
 240 zero and one. In this case, the velocity field is partially bounced back and the macroscopic velocity  
 241 is modified [15, 45, 46]. The procedure for implementing the partial bounce-back approach is  
 242 described in [45, 46].

243 For the velocity field, the non-slip BCs are used for all the cavity walls. These are performed by  
 244 the on-grid bounce-back (BB) boundary conditions:

$$245 \quad f_i(x_w, t+1) = f_j(x_w, t) \quad (12)$$

246  $x_w$  being the fluid node adjacent to the wall, and  $i$  and  $j$  represent two opposite lattice directions  
 247 on the boundary site. Note that the BB conditions apply to the DF in non-parallel directions at a  
 248 solid wall.

249 To specify a constant temperature at the left and right walls, we use the method proposed by  
 250 Inamuro *et al.* [47]. Its principle is to substitute unknown DFs for a boundary point with local  
 251 equilibrium values using an adjusted temperature to set the defined temperature at that point.  
 252 Specifically, the adjusted temperature on the left side can be expressed as:

$$253 \quad T' = \frac{6}{1 - 3v_{w,x}} (T_h - \sum g_i) \quad (13)$$

254  $v_{w,x}$  being the computed near-wall velocity, and  $g_p$  represents a known distribution function.  
 255 Hence, the unknown DFs  $g_p$  are computed by  $g_p = T' \omega_i (1 + \vec{e}_i \cdot \vec{U} / c_s^2)$ . As for the adiabatic BCs,  
 256 the Neumann BCs are achieved using the BB boundary conditions for the distribution  $g_i$ , as  
 257 prescribed for  $f_i$ .

258 In the nearly incompressible formulation, the basic thermo-hydrodynamic properties, such as  
 259 density  $\rho$ , momentum density,  $\rho U$ , and temperature,  $T$ , are defined as moments of the DFs,  $f_i$   
 260 and  $g_i$ , as follows,

$$261 \quad \rho = \sum_{i=0}^{i=8} f_i, \quad \rho U = \sum_{i=0}^{i=8} e_i f_i, \quad T = \sum_{i=0}^{i=8} g_i \quad (14)$$

262 To simulate the presence of a mushy zone (co-existence of liquid and solid), a step is added to  
 263 mimic the bounce-back at a lattice node [23, 45, 46]. This condition redirects the incoming fluid  
 264 packets prior to the collision step, as follows:

$$265 \quad f_i^{out}(x,t) = (1 - \varepsilon) f_i^{col} + \varepsilon f_i^{in}(x,t)$$

266 where  $f_i^{in}$  and  $f_i^{out}$  denote the incoming and outgoing fluid packet densities at a node.

267 This ensures that for a completely liquid phase ( $\varepsilon = 1$ ), a normal collision is conducted.  
268 However, when it is completely solid ( $\varepsilon = 0$ ), the flow is bounce-backed and blocked, whereas for  
269 values between 0 and 1, the flux is partially bounce-backed according to the solid fraction estimated  
270 at the node. Such a scheme has been verified in our previous work compared to analytical solutions  
271 and other numerical methods [21-23, 40, 41].

272 The velocity field is then modified in the mushy zone and expressed in terms of the in-coming  
273 fluid packet densities,

$$274 \quad U^* = \varepsilon U \quad (15)$$

275 This modified velocity is in accordance with the requirements of the partial bounce-back  
276 approach [23, 45, 46]. As a result, the flow in the mushy zone will be dealt as flow in a porous  
277 medium and will therefore be governed by Darcy's law as proved by derived analytical solutions  
278 [23, 45, 46].

#### 279 **4. Experimental Setup**

280 Recall that the main task targeted here is to develop a mutually compatible experimental and  
281 numerical method to characterize the studied PCM. The major enhancement in the current  
282 numerical model is to add natural convection and supercooling, adopt variable thermo-physical  
283 properties, and use the real enthalpy curves corresponding to the considered PCM (viz.  
284 Octadecane). Let's point out that this PCM is an alkane hydrocarbon of chemical formula is  
285  $\text{CH}_3(\text{CH}_2)_{16}\text{CH}_3$  with Prandtl number is about 50. In general, for high Prandtl values, the  
286 momentum diffusivity dominates, and convection seems very efficient in transferring heat  
287 (energy).

288 To solve this physical problem, the TLBM, for phase change in multi-layered materials, is used  
289 herein. However, before confronting numerical simulations findings, we perform experiments on

290 the Octadecane to characterize its main thermo-physical properties: conductivity (solid and liquid),  
291 heat capacity (solid and liquid), and latent heat of fusion. The numerical model, hereby, helps us  
292 to determine both the real enthalpy curve and the degree of supercooling in the material. [Figure 2](#)  
293 shows the schema of the experimentally studied sample of Plexiglas containing Octadecane as  
294 PCM. Tables 1 and 2 gather the properties of Octadecane and Plexiglas, used in the numerical  
295 model, as per the literature [48, 49] and verified experimentally with an acceptable tolerance.

296 The experimental setup and its associated equipment, used in this work, are schematically  
297 depicted in [Figs. 2 and 3\(a, b\)](#). The studied phase-change material, viz. Octadecane (99% pure), is  
298 placed inside a parallelepiped Plexiglas enclosure and prone to a temperature gradient through  
299 exchange plates controlled by two thermo-regulated baths (Julabo Model 34 HE - 1kW with a  
300 precision of about  $\pm 0.01$  °C) that define thermal conditions (see specifications in [50]). The  
301 exchange aluminum plates ( $500\text{ mm} \times 500\text{ mm} \times 19\text{ mm}$ ) allow imposing temperature variations,  
302 with respect to selected time scales, on the two dominant faces (left and right faces). The upper and  
303 bottom faces, of the studied sample, are insulated by a 14.5 cm-thick polystyrene (a thermally  
304 insulating material). Such insulation also serves to minimize the heat transfer from the sample  
305 lateral faces into the surrounding medium. This is the guarded hot plate approach principle, often  
306 used when characterizing the thermal performance of PCM samples. The flux-meters used herein  
307 are “tangential gradients flux meters”. The inserted sensors (Captec, France) on the sample's both  
308 sides were pre-calibrated (using the comparative method) with a precision of about 2%, using the  
309 device described by [51]. Their surface, thickness and sensitivity are  $210 \times 140\text{ mm}^2$ ,  $0.2\text{ mm}$  and  
310  $124\text{ }\mu\text{V}\cdot\text{W}^{-1}\cdot\text{m}^{-2}$ , respectively. The various sensors are connected to a multichannel multimeter  
311 (Keithley 2700) adapted to low level signal measurements. Experimental data are scanned at  
312 regular and adjustable time steps of 10 s. The adopted experimental setup permits the simultaneous  
313 measurement of heat fluxes and temperatures through the different faces. Note that data acquisition  
314 is facilitated by a PC running LabVIEW for further analysis.



315 According to the thermal program applied to the sample, it is possible to characterize the  
316 apparent thermal conductivity, the specific heat capacity, the phase change temperature and latent  
317 heat of the sample. Indeed, the experimental set-up permits to impose temperature loading on each  
318 face of the studied sample. Simultaneous measurements of temperatures and heat fluxes exchanged  
319 during heating and cooling processes allow the determination of the apparent thermo-physical  
320 properties. The characterization also yields to the determination of conductivities and heat  
321 capacities when the PCM is in solid or liquid state. During the phase change, temperature and the  
322 latent heat can be determined via proven methods [50 - 52], to name few.

## 323 **5. Obtaining Octadecane thermo-physical properties**

### 324 **5.1. Thermal conductivity and thermal contact resistance in solid phase**

325 For the solid phase test, we impose, using the previous experimental setup, temperatures of  $T_G$   
326 = 10 °C and  $T_D = 15$  °C (below melting temperature) on the left and right faces, respectively, until  
327 a thermal steady state is reached. The heat fluxes are initially constant. At a particular time, an  
328 increase of 5°C in temperature is imposed in both thermo-regulated baths linked to the plate heat  
329 exchangers. This will induce an increase of temperature in the material, before reaching again a  
330 thermal equilibrium. The sample would thus store energy (sensible heat) between these two  
331 permanent steady states. A similar experiment is performed to determine the thermal conductivity  
332 in the liquid phase. The sample is also subjected to a temperature increase of 5°C starting from  $T_G$   
333 = 30 °C and  $T_D = 35$  °C, insuring temperatures higher than the melting temperature of the  
334 Octadecane. The subjected thermal loading ramp and the resulting heat fluxes are shown in Fig.  
335 4(a, b).

336 The thermal conductivity  $\lambda$  can be determined depending on the sum of heat fluxes and the  
337 temperature difference, using the following relation [53],

$$338 \quad \lambda = \sum \phi L / 2\Delta T \quad (16)$$

339 where  $\varphi$  is the heat flux density in  $W/m^2$  and  $L$  is the thickness of the sample.

340 It is useful to mention that the used method involved simultaneous measurements of the heat  
341 fluxes and temperatures on both sides of the differentially heated sample. Compared to  
342 conventional methods of determining the thermal conductivity in steady state, this method is four  
343 times faster [53]. The exact term for the quantity measured is “thermal transmission”, which,  
344 depending on the material being measured, can have components of convective, radiative and  
345 conductive heat transfer; it is commonly referred to as the effective or apparent thermal  
346 conductivity.

347 The heat sensor is made of a thin material with a high thermal conductivity (copper). Thermal  
348 contact resistance (or contact resistivity) may cause huge errors of thermal conductivity  
349 measurements if it is not taken into account. Moreover, when there are two different material layers,  
350 a thermal resistance exists on their interface. It is more obvious in the case of two solids. In case of  
351 thermal insulation materials (small conductivity) the sample’s thermal resistance is large and  
352 thermal contact resistance can be neglected. But, in case of higher conductivity materials ( $> 0.1$   
353  $W/mK$ ), the thermal contact resistance becomes significant compared to the sample’s thermal  
354 resistance and cannot be neglected [54]. Hence, it is important to estimate this effect for accurate  
355 results.

356 The resistance of the sample can be defined by:

$$357 \quad R_{eq} = 2R_c + 2R_{pl} + R_{oct} \quad (17)$$

358 where  $R_c$ ,  $R_{pl}$ , and  $R_{oct}$ , are respectively the thermal resistivity contact, resistance of Plexiglas and  
359 Octadecane. We first neglect the thermal contact resistivity. Then,

$$360 \quad R_{eq} = \frac{L}{\lambda_{eq}} = \frac{2L_{pl}}{\lambda_{pl}} + \frac{L_{oct}}{\lambda_{oct}} \quad (18)$$

361 Here, we apply Eq. 18 to calculate the equivalent conductivity of the sample (Plexiglas +  
362 Octadecane). The literature properties of Plexiglas are gathered in Table 1, and those for

363 Octadecane are in Table 2. The resultant conductivity in the solid case is:  $\lambda_{eq} = 0.167 \text{ W/(m.K)}$ .  
364 Hence, by applying Eq. 18, we get  $\lambda_{oct} = 0.152 \text{ W/(m.K)}$ . This value is very far from the  
365 conductivity of Octadecane reported in the literature [48, 49]. The error is probably due to ignoring  
366 the thermal contact resistivity. As stated before, when testing samples of moderate thermal  
367 conductivity ( $\lambda \sim 0.1\text{-}10 \text{ W/(m.K)}$ ) the thermal contact (or interface) resistance must be addressed,  
368 otherwise significant errors will result. Since we are not sure about  $R_c$ , we will suppose range of  
369 values of  $1/R_c = 50 - 100$ . Thus, as we change  $R_c$ , we obtain different thermal conductivities of  
370 solid Octadecane: ( $R_c = 1/100$ ;  $\lambda_{oct} = 0.219 \text{ W/(m.K)}$ ); ( $R_c = 1/70$ ;  $\lambda_{oct} = 0.27 \text{ W/(m.K)}$ ); ( $R_c = 1/60$ ;  
371  $\lambda_{oct} = 0.31 \text{ W/(m.K)}$ ); ( $R_c = 1/50$ ;  $\lambda_{oct} = 0.39 \text{ W/(m.K)}$ ).

372 From here, we can realize the major impact of considering the thermal contact in calculating the  
373 conductivity of Octadecane, which has a relatively moderate conductivity. The estimated values of  
374  $\lambda_{oct}$  are plotted versus  $R_c$  in Fig 5a. The value in the literature for the conductivity of Octadecane is  
375  $\lambda_{oct}(\text{solid}) = 0.356 \text{ W/(m.K)}$  which corresponds mostly to around  $R_c = 1/60$ . It is worth mentioning  
376 that the contact resistances here occur between the flux sensors and Plexiglas, and also between  
377 Plexiglas and solid PCM. This is applicable for the 4 faces of the enclosure. However, since we  
378 take a 2D model, we ignore the effect of resistance on the upper and lower faces.

## 379 5.2. Thermal conductivity, thermal contact resistance and convection in liquid phase

380 As in the previous procedure, we calculate the conductivity in liquid Octadecane. The Flux  
381 density and surface temperatures are plotted in Fig 4b. The estimated value by Eq. 18 is  $\lambda_{app}$  (liquid)  
382  $= 0.22 \text{ W/(m.K)}$ , which can be seen as an apparent conductivity. It is important to recall here that  
383 the quantity measured may have a convection component. Therefore, we seek to, theoretically,  
384 prove the existence of convection in the liquid state. This would check the high value of the  
385 apparent conductivity in liquid phase, and then to confirm this experimentally and numerically.

### 386 ■ Theoretical evaluation of the convection

387 We need to calculate  $Ra_H = \beta g \Delta T H^3 / \alpha \nu$  for the above problem ( $A=H/L \approx 20$ ), corresponding to  
 388 the considered sample. This gives us an idea about the mechanism of heat transfer, within the  
 389 sample, and on the effect of the fluid flow, following the scaling laws [55]. In such a tall enclosure  
 390 the convection is usually ignored. Here, our aim is to check the importance of considering  
 391 convection theoretically, numerically, and experimentally.

392 According to the scaling laws [55], the parameter  $Ra_H$  needs to be calculated and to  $H/L$ :

393  $(Ra_H)^{1/4} = (\beta g \Delta T H^3 / \alpha \nu)^{1/4} = (1.415 \times 10^{10})^{1/4} \approx 345.$

394  $(Ra_H)^{-1/4} = (\beta g \Delta T H^3 / \alpha \nu)^{-1/4} = (1.415 \times 10^{10})^{-1/4} \approx 0.003$

395  $H/L = 20.2$ , so  $(Ra_H)^{-1/4} < H/L < (Ra_H)^{1/4}$ .

396 So, the flow pattern is expected to show a boundary layer on all four walls, with one core  
 397 remaining stagnant. The dominant heat transfer mechanism is “boundary layer convection” with a  
 398 significant effect of the fluid flow. To calculate the Nusselt number, we can use an adequate  
 399 empirical formula. Since  $Ra_L = \beta g \Delta T H^3 / \alpha \nu = 3.43 \times 10^5$ , with  $10 < H/L < 40$ ,  $1 < Pr < 2 \times 10^4$ ,  $10^4$   
 400  $< Ra_L < 10^7$ , then:

401  $\overline{Nu}_L = 0.42 x Ra_L^{1/4} x Pr^{0.012} x (H / L)^{-0.3}$  (19)

402 This relationship allows to deduce  $\overline{Nu}_L = 4.33$  with  $Ra_L = \beta g \Delta T L^3 / \alpha \nu$ . This reveals that the  
 403 convective heat transfer is four times stronger than the conductive one. Once again, this shows that  
 404 the convection is the dominant mechanism in this problem. The apparent conductivity measured  
 405 by Eq. 18 has a convection contribution, and we can state that it is not the equivalent conductivity  
 406 of the sample.

407 **▪ Experimental investigation of the convection**

408 To achieve this, we perform a new experiment. We inject in the Plexiglas enclosure of  
 409 Octadecane, described in Fig. 2, silver coated hollow glass spheres, and allow them to settle down.  
 410 Using Particle Image Velocimetry (PIV) system, we trace the flow of the particles inside the  
 411 enclosure. In the case of liquid Octadecane, due to the presence of convection, and as expected, the

412 powder circulates inside liquid Octadecane. In contrary, if conduction was the dominant mode, the  
413 powder would have stayed at the bottom, and no motion would have been noticed.

414 After proving the presence of convection, we will estimate the value of the conductivity of liquid  
415 Octadecane, by the aid of the numerical simulations.

416 **▪ Numerical assessment of the convection**

417 The implemented LBM numerical model is used to evaluate the convection in liquid Octadecane  
418 within the Plexiglas enclosure. Thus, the average Nusselt number ( $\overline{Nu}_L$ ) value on the Octadecane  
419 interface is 4.81. Such a value seems close to that estimated empirically by the order of 10%.

420 The average equivalent conductivity for natural convection can be estimated via the following  
421 relationship [55]:

$$422 \frac{\lambda_{app}}{\lambda_{eq}} \approx \frac{Q_{LBM,conv}}{Q_{LBM,cond}} \quad (20)$$

423 where  $\lambda_{app}$  and  $\lambda_{eq}$  are the apparent and equivalent conductivities of liquid Octadecane. Note that,  
424 by apparent here, we mean that it contains the convection contribution. As for the equivalent, we  
425 point to the conductivity calculated for the sample (Plexiglas + Octadecane). To compute the ratio,  
426 we implement two models. The first is for convection (with a Boussinesq force evaluated by the  
427 corresponding  $Ra$  value), and the second is a pure conduction model (without the Boussinesq force,  
428 insuring a zero-velocity field). The simulation results do not depend on the selected value of  
429 conductivity, since in LBM we assign a fixed Prandtl number of 50. The main aim here is to  
430 evaluate the effect of including the Boussinesq force that designates the convection. This method  
431 is only an approximation. The calculated ratio is  $\lambda_{app}/\lambda_{eq} = 1.76$ , hence the value of the equivalent  
432 conductivity is  $\lambda_{eq} = 0.125 \text{ W/mK}$ . Here, the thermal contact resistance occurs only between the  
433 flux sensors and the Plexiglas. Now we use Eq. 18 with different trials on the thermal contact  
434 resistance to get:  $R_c = 1/100$ ;  $\lambda_{oct} = 0.123 \text{ W/(m.K)}$ ;  $R_c = 1/70$ ,  $\lambda_{oct} = 0.137 \text{ W/(m.K)}$ ;  $R_c = 1/60$ ;  
435  $\lambda_{oct} = 0.151 \text{ W/(m.K)}$ ;  $R_c = 1/50$ ;  $\lambda_{oct} = 0.162 \text{ W/(m.K)}$ .

436 The conductivity of liquid Octadecane is  $\lambda_{oct} = 0.148 \text{ W/(m.K)}$  in literature. So in both liquid  
 437 and solid cases the closest calculated value of conductivity is obtained when considering  $R_c = 1/60$ .  
 438 Fig. 5b shows the estimated values of  $\lambda_{oct}$  for the liquid Octadecane versus the thermal contact  
 439 resistance. As deduced, the effect of thermal resistivity contact is much more in the case of the  
 440 solid state, where there is a solid-solid contact. Thereby an interface of the air gap may rise in  
 441 between. From our approach, the conductivity of solid and liquid Octadecane are  $\lambda_{oct} (solid) = 0.31$   
 442  $\text{W/(m.K)}$  and  $\lambda_{oct} (liquid) = 0.151 \text{ W/(m.K)}$ , respectively with  $R_c = 1/60$ . However, we should still  
 443 consider border effects for more accuracy.

### 444 5.3. Specific heat capacity

445 The temperatures and the heat fluxes evolution on both sides of the sample, when Octadecane  
 446 is in the solid and the liquid phases are represented in Fig. 4. A symmetrical behavior of heat fluxes  
 447 and temperatures measured on both faces of the sample can be observed, which correspond to the  
 448 results classically obtained with a solid material without phase change.

449 Initially, the sample is isothermal (at a thermal equilibrium state), and then a temperature change  
 450 is imposed on its both sides. This induces a thermal evolution of the system in an asymptotic way  
 451 towards a second thermal steady state. Also, it should be noted that the heat fluxes evolve quickly  
 452 when the temperatures of the sample are increased and then converge to a second thermal  
 453 equilibrium state obtained at the end of the test. The specific heat capacities of the sample are  
 454 obtained starting from the determination of the sensible heat accumulated by the material between  
 455 the imposed temperatures. The sensible heat is calculated by integrating the difference in heat  
 456 fluxes between the initial and the final state using the following relationship:

$$457 \quad Q = \frac{1}{\rho L} \int_{T_{init}}^{T_{end}} \Delta\phi = \sum_i C_{p,i} (T_{end} - T_{init}) \quad (21)$$

458 where  $\Delta\phi$  represents the cumulative heat rate entering the sample and  $C_p$  is the apparent specific  
 459 heat capacity ( $\text{kJ/(kg.}^\circ\text{C)}$ ).

460 The calculated specific heat capacity of Octadecane in solid and liquid phases are:  $c_{oct,solid} = 1925$   
461  $kJ/(kg \cdot ^\circ C)$  and  $c_{oct,liquid} = 2365 kJ/(kg \cdot ^\circ C)$ . It is noted that these values are consistent with those  
462 available in the literature.

#### 463 **5.4. Analysis of the heat flux with phase-change**

464 To analyze the heat flux in the presence of a phase change, we use a four-hour ramp. The sample  
465 is initially at  $15.8^\circ C$ , then the both plates' temperature  $T_p$  is increased from  $15.8^\circ C$  to  $40^\circ C$  in 4  
466 hours ( $4h$ ). Then a constant loading of  $40^\circ C$  is applied followed by a decreasing ramp until  
467 reaching  $15.8^\circ C$  again, as illustrated in Fig. 6. As noted, the sample is initially in thermal  
468 equilibrium, where the heat flux is zero. This is followed by sensible heat flow when the PCM is  
469 still in its solid state. The curve then starts increasing gradually at a time corresponding to the onset  
470 of melting. The latent heat absorbed also increases gradually and the largest quantity is absorbed  
471 in the vicinity of the melting point. After complete melting, and reaching the constant heating  
472 phase, the PCM goes back to a thermal equilibrium, with no more flux variation, until the cooling  
473 ramp starts.

474 When cooling starts, the liquid PCM releases sensible heat until reaching the solidification  
475 temperature. The difference between the melting and solidification is that the majority of freezing  
476 happens directly, and the largest amount of latent heat is released at first, then the rest will solidify  
477 gradually. This behavior can be also regarded to the expected shape of the enthalpy curve. The  
478 portion around the curve at the solidification temperature is discontinuous. There is a direct energy  
479 jump from a temperature point in the liquid state to the solidification point. We note also the  
480 existence of supercooling, which is illustrated by the formation of a vertical portion or discontinuity  
481 in the curve (Fig. 1). After complete freezing, the PCM returns back to its equilibrium state with  
482 almost zero flux.

#### 483 **6. Results and discussion**

484 As previously stated, the major aim is to first estimate the main thermo-physical properties and

485 to highlight their effect on the numerical results if the supercooling, convection, and soluble  
486 impurities are ignored or not. To achieve this, we compare the numerical results, using an improved  
487 model, with the experimental ones. The properties in [Tables 1 and 2](#) and the verified thermo-  
488 physical properties (conductivities, specific heat capacities, latent heat of fusion, thermal contact  
489 resistance, etc.) are fixed in the model. It should be noted that the Boussinesq force has been varied  
490 to account for convection, the melting temperature to calibrate the enthalpy curve, and the degree  
491 of supercooling to estimate the nucleation temperature. In the following, some significant results  
492 showing effects of physical phenomena are comprehensively presented and discussed.

### 493 **6.1. Effect of enthalpy curve shape**

494 As explained before, the presence of soluble impurities in the PCM results in a melting  
495 temperature depression. Recall that, the used Octadecane is thought to be 99% pure. So, the 1% of  
496 soluble impurities can have an impact on the heat flux curve. This will be investigated theoretically  
497 and numerically. First, the depression in the melting temperature is calculated from Eq. (1) to obtain  
498  $T_m = 28.03$  °C. Thus, the PCM melts with a depression of about 0.1 °C compared to the case of  
499 pure Octadecane. Then, this melting temperature will be used in the numerical model, to check if  
500 this the numerical and experimental fluxes match. If not,  $T_m$  will be changed until they well match.

501 The enthalpy-temperature curves are plotted in [Fig. 7](#) for different values of  $(T_a - T_m)$ . As  
502 demonstrated, the curve becomes less steep as  $T_m$  deviates from  $T_a$ . This induces a melting  
503 temperature range that causes a gradual increase in latent heat instead of absorbing it at once.

504 Moreover, to show the important impact of enthalpy curve on the flux, we compare the heat flux  
505 obtained numerically for the case pure Octadecane to the experimental one (cf. [Fig. 8a](#)). In pure  
506 PCM, there is no melting range. Thus, the immediate absorption of latent heat at the melting  
507 temperature results in a sharp and high rate of heat flow at this moment, as shown in the comparison  
508 curves. However, when there exists a temperature depression, the rate of heat absorption decreases  
509 more, since there is no instant absorption and release. The accurate prediction of the onset of



510 melting and freeing is highly dependent on taking into account the real enthalpy-temperature  
511 relation.

512 By comparing the experimental and numerical curves, the best fit was obtained for  $T_m = 27.6$   
513 °C, which corresponds to a variation of about 0.5°C from the supposed pure melting temperature  
514 found in literature (Fig. 7). This shows that using Eq. (1) may not be adequate in our case but can  
515 be used as pre-estimation. Also, the supposed melting temperature [48, 49] of pure Octadecane is  
516 also questionable. If Octadecane is considered pure, the heat flux curve will show a high  
517 discrepancy when compared to the experimental one, as shown in Fig. 8a. The curve obtained  
518 numerically comes from considering the enthalpy curve as the traditional piece-wise function. This  
519 shows that such a curve cannot be used for our case.

520 The final numerical curve for melting is plotted in Fig. 11 despite the fact that this is the result  
521 from the enhanced numerical model, i.e. including also convection. In addition, we highlight that  
522 the heating rate does not influence the prediction of the melting point  $T_m$ , since the enthalpy curve  
523 is unique for a material.

## 524 **6.2. Effect of presence of supercooling and convection**

525 We show, in what follows, the discrepancy that would have resulted if we ignored the presence  
526 of convection and supercooling. The major effect of ignoring convection (cf. Fig. 9a) is on  
527 estimating the time of melting and mainly that of solidification. At first, the material is solid. So  
528 convection will start affecting the curve as soon as the liquid fraction starts increasing. It is  
529 important here to address the effectiveness of our partial bounce-back LBM model. By this method,  
530 we are able to treat the mushy zone as a porous medium, where the velocity of the fluid is restrained  
531 but not completely blocked. The Rayleigh number (Ra), corresponding to the real convection, is  
532 searched by a fitting method, and is found to be  $Ra = 1.2 \times 10^4$ . Higher values would lead to an over  
533 estimation (Fig. 9b).

534 On the other hand, if supercooling is ignored (see Fig. 10a), the solidification starts before the  
535 real instant. So, the experimental and numerical results will show a lag in time. To overcome this,

536 we have sought the degree of supercooling through a tuning (fitting) method. Hereafter, the best  
537 estimated degree of supercooling corresponds to 1.4 °C. If higher supercooling degree is used, the  
538 supercooling phenomenon will be overestimated (see Fig. 10b).

539 By this, we can combine all the enhancements to the present model: using the real enthalpy  
540 curve, including convection and supercooling, using variable thermo-physical properties for solid  
541 and liquid phases, and using a partial bounce-back LBM for phase change to better simulate the  
542 low effect of convection. The enhanced model calculated for  $Ra = 1.2 \times 10^4$ , degree of super cooling  
543 of 1.4 °C, and a melting point depression of 0.43 °C is displayed in Fig. 11, and shows a great  
544 improvement, and matches the experimental results.

545 The simplifications taken in some numerical models can result in an overall discrepancy in the  
546 real behavior of PCM. These discrepancies may lead to wrong estimation of the fusion times and  
547 the energy amount stored. Consequently, the PCM will not give the desired performance. The major  
548 enhancement to the proposed model was to take into account natural convection, supercooling, to  
549 adopt variable thermo-physical properties for solid and liquid phases, and to use the real enthalpy  
550 curves corresponding to the considered PCM. These improvements have led to better agreement  
551 with the experimental results, and showed that if the above phenomena were present, they cannot  
552 be ignored.

## 553 **7. Conclusion**

554 The main aim of this work is to characterize the thermo-physical properties and performance of  
555 Octadecane. This PCM may be promising for the usage in glass facades or other building materials  
556 and latent heat systems. To achieve such an objective, we adopted an approach based on  
557 experimental and numerical techniques. The enhanced numerical model, used here, can help  
558 estimate some properties, and can be also used as an optimization tool for any practical application.

559 The thermo-physical properties obtained experimentally and, using the numerical model, match  
560 the expected values from literature. The adopted numerical model is a thermal LBM with a partial

561 bounce-back approach and an enthalpy-based model. We considered the natural convection,  
562 supercooling, variable thermo-physical properties (when necessary), and the real enthalpy curve of  
563 Octadecane. Simulations performed using the improved model corroborate the experimental results  
564 and show that ignoring these phenomena may lead to wrong estimation of the fusion times and  
565 amount of energy stored and the PCM will not give the desired performance.

#### 566 **Disclosure statement**

567 The authors declare no potential conflicts of interest regarding authorship and/or publication of this  
568 paper.

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- 718

719 **List of Tables**720 **Table 1.** *Properties of Plexiglas* [48, 49]

Property	Value
Heat capacity	1470 J.Kg <sup>-1</sup> .K <sup>-1</sup>
Thermal conductivity	0.19 W.(m.K) <sup>-1</sup>
Density	1190 Kg.m <sup>-3</sup>

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722 **Table 2.** *Properties of Octadecane from literature* [48, 49]

Property	Value
C <sub>solid</sub>	1910 JKg <sup>-1</sup> °C <sup>-1</sup>
C <sub>liquid</sub>	2230 JKg <sup>-1</sup> °C <sup>-1</sup>
Density ρ	779 Kg.m <sup>-3</sup>
λ <sub>solid</sub>	0.356 Wm°C <sup>-1</sup>
λ <sub>liquid</sub>	0.149 Wm°C <sup>-1</sup>
Enthalpy of fusion	241650 JKg <sup>-1</sup>
Temperature of fusion	28.15 °C
β	0.02 K <sup>-1</sup>
Pr	50

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725 *List of Figure Captions*

726 **Figure 1.** Enthalpy-temperature relationship for pure PCMs with soluble impurities in the presence  
727 of supercooling.

728 **Figure 2.** Two-dimensional schematic of the studied sample.

729 **Figure 3.** (a) Schematic illustration of the experimental setup, (b) Schematic illustration of the  
730 studied sample.

731 **Figure 4.** Heat flux curves with no phase-change for (a) solid state, (b) liquid state.

732 **Figure 5.** Estimated thermal conductivity vs thermal contact resistivity: (a) solid state, (b) liquid  
733 state.

734 **Figure 6.** Heat flux curves indicating the presence of supercooling.

735 **Figure 7.** Enthalpy-temperature relationship for different ( $T_a - T_m$ ) values.

736 **Figure 8.** (a) Effect of the presence of impurities on the heat flux, (b) Numerical and experimental  
737 shapes with  $T_m = 27.6$  °C.

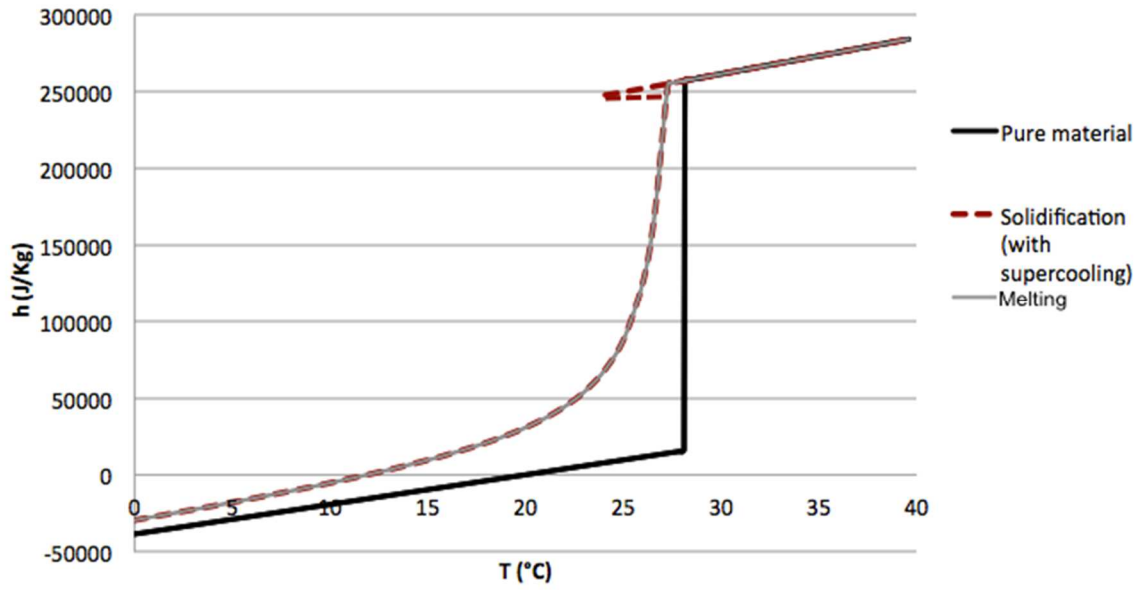
738 **Figure 9.** Effect of convection on the shape of the heat flux curve: (a) ignoring convection, (b)  
739 overestimating convection

740 **Figure 10.** Effect of supercooling on the shape of the heat flux curve: (a) ignoring supercooling,  
741 (b) overestimating supercooling

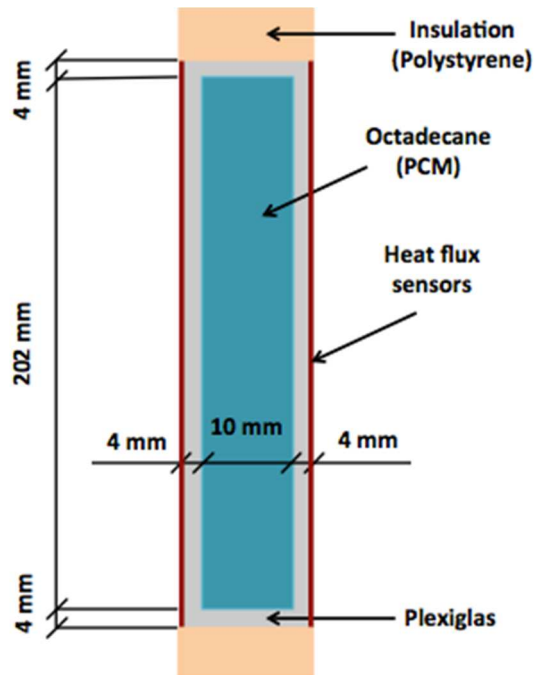
742 **Figure 11.** Experimental vs. numerical results when using the enhanced model.

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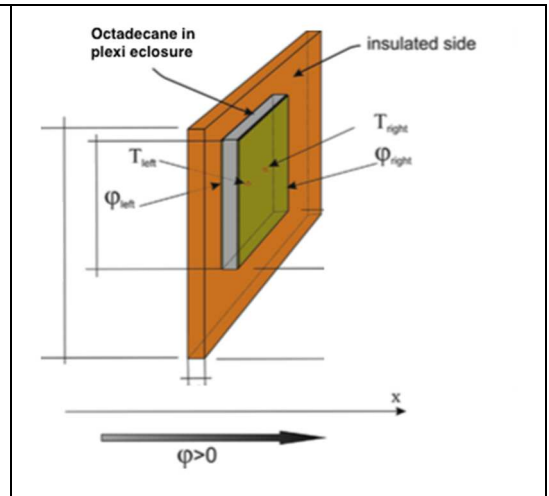
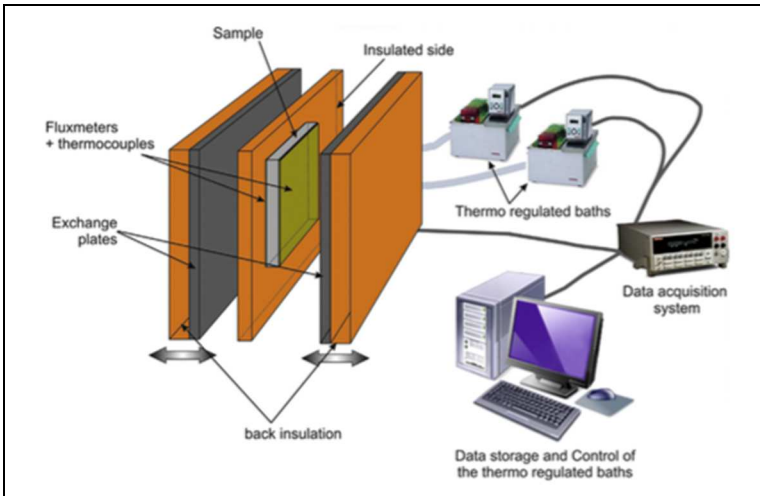


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754 **Figure 2.** Two-dimensional schematic of the studied sample  
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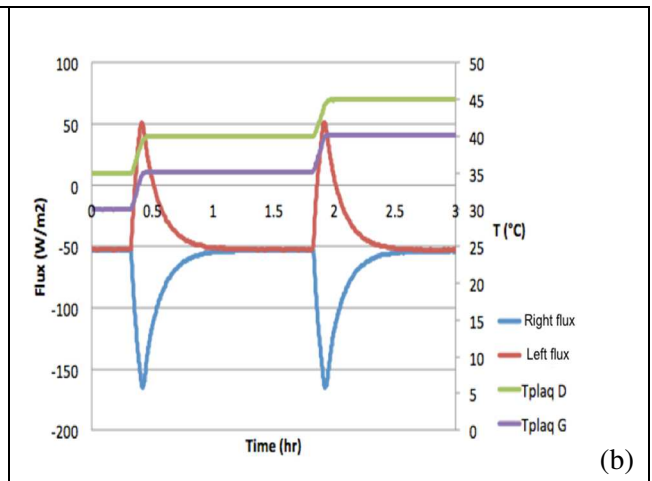
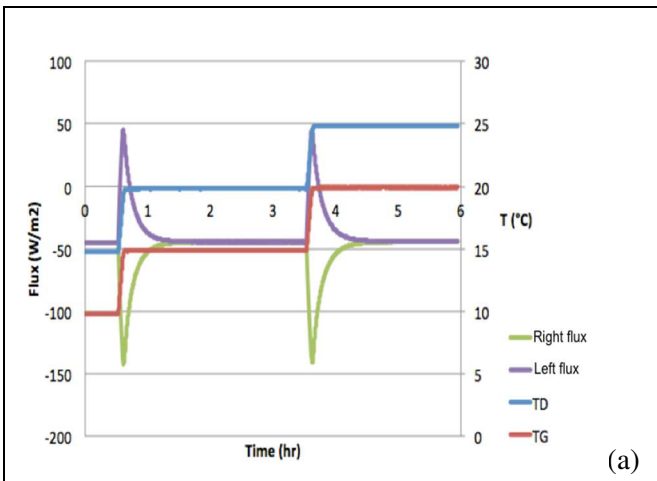
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**Figure 3a.** Schematic illustration of the experimental setup

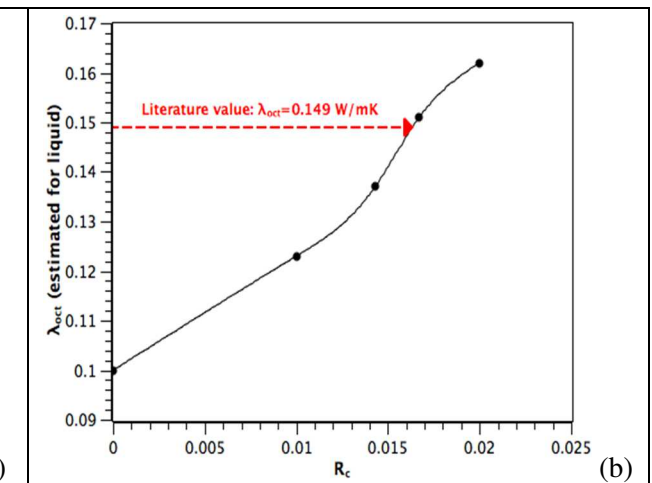
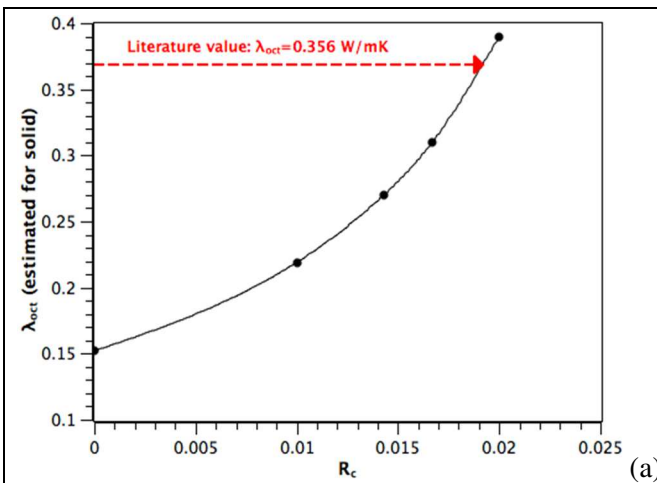
**Figure 3b.** Schematic illustration of the studied sample

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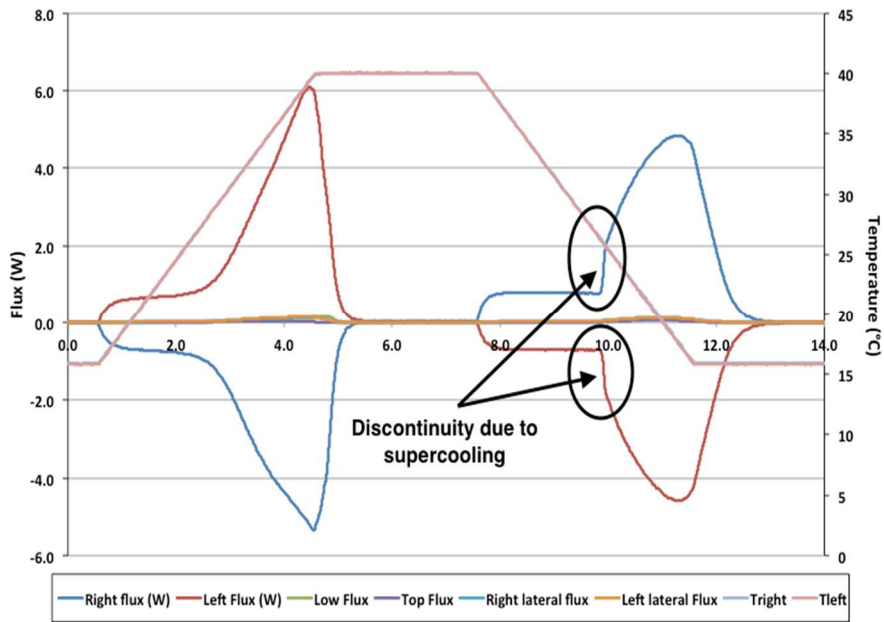
**Figure 4.** Heat flux curves with no phase-change for (a) solid state, (b) liquid state.

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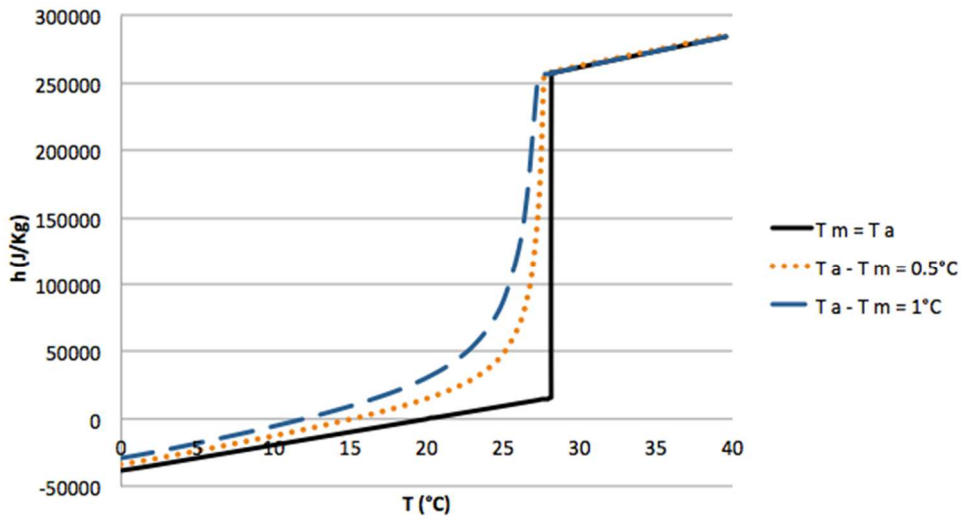
**Figure 5.** Estimated thermal conductivity vs. thermal contact resistivity: (a) solid state, (b) liquid state.

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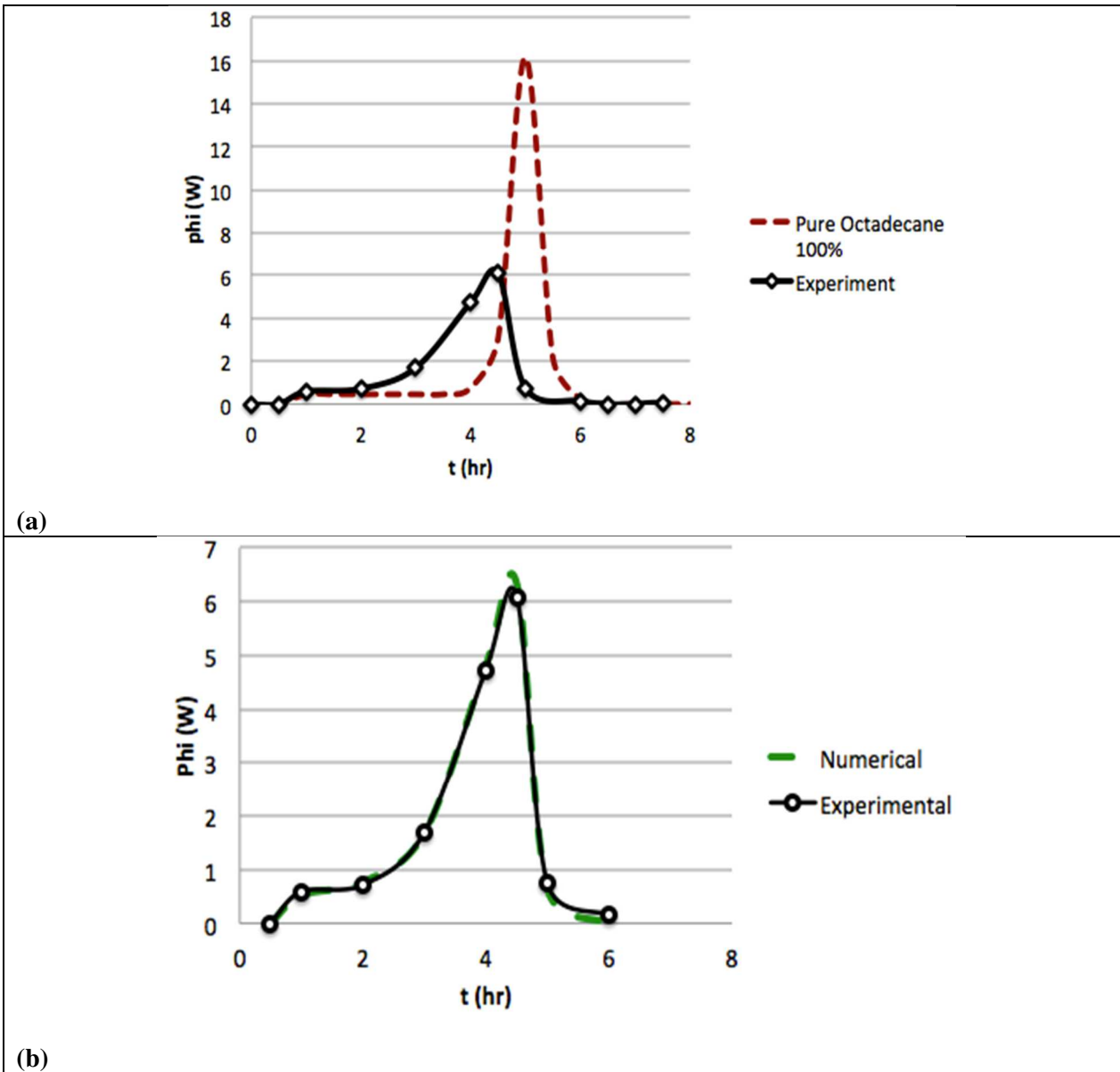
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Figure 6. Heat flux curves indicating the presence of supercooling.



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Figure 7. Enthalpy-temperature relationship for different  $(T_a - T_m)$  values.



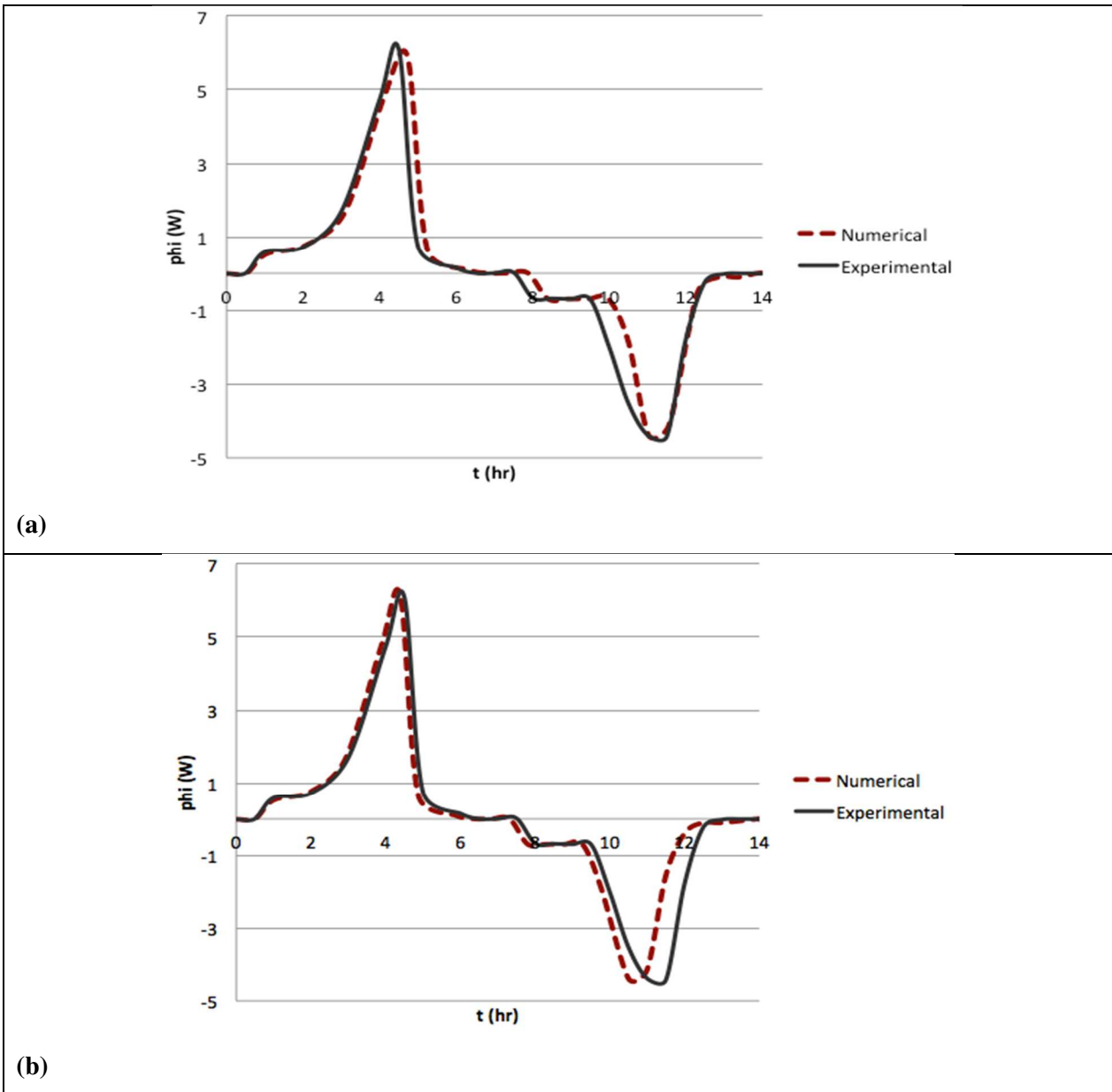
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 777 shapes (b) with  $T_m = 27.6$  °C

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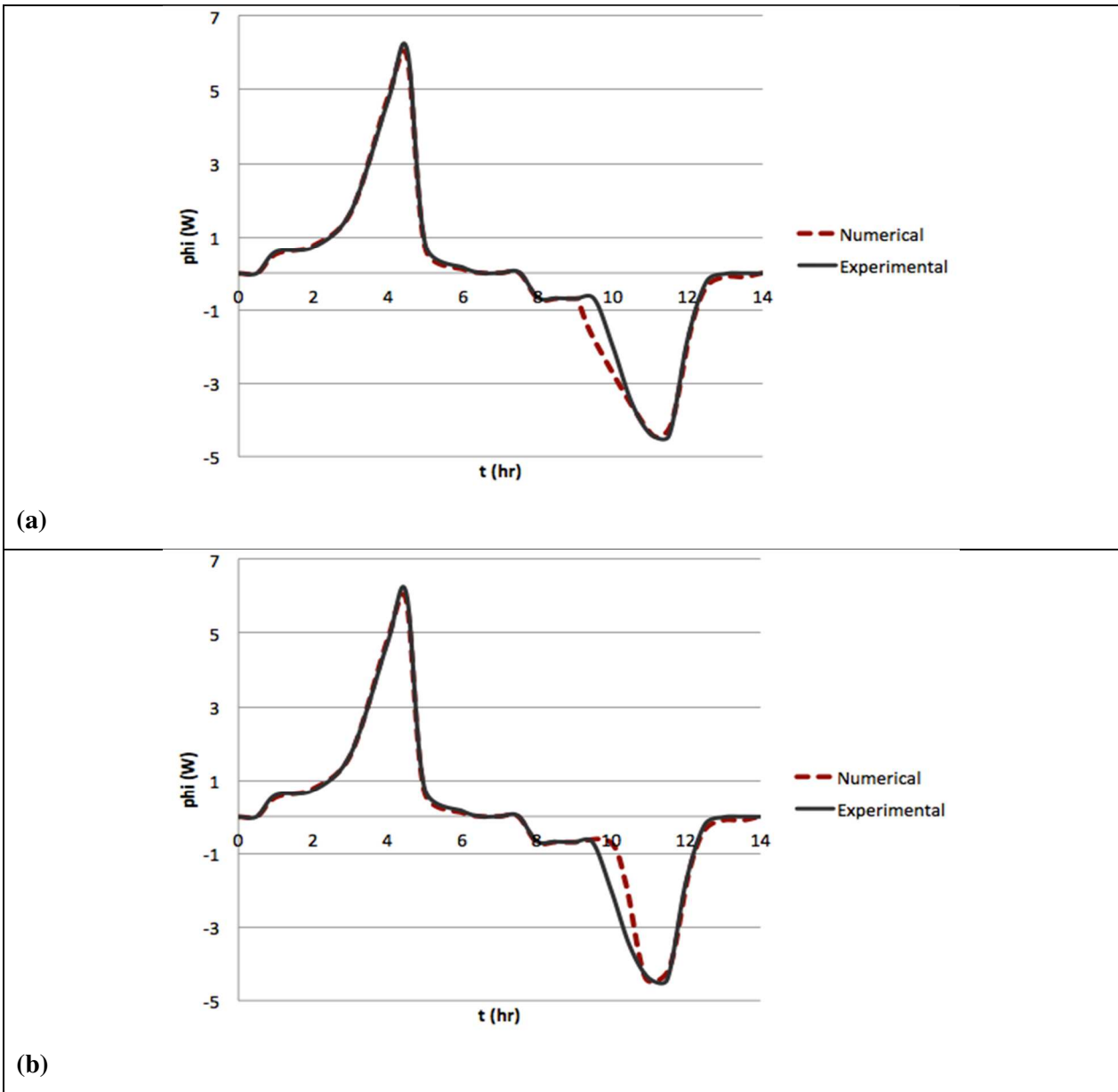
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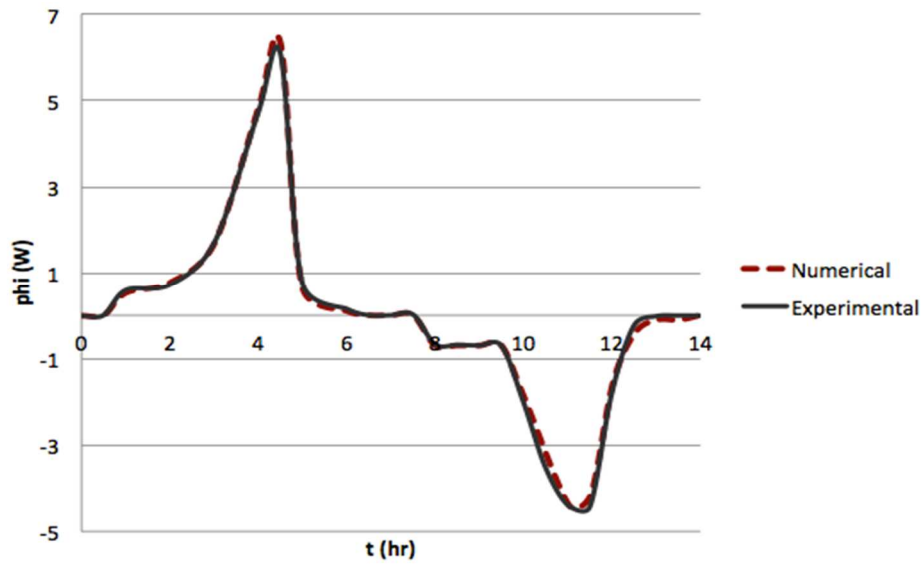
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 783 **Figure 9.** Effect convection on the shape of the heat flux curve: (a) ignoring convection, (b)  
 784 overestimating convection  
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**Figure 10.** Effect supercooling on the shape of the heat flux curve: (a) ignoring supercooling, (b) overestimating supercooling



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**Figure 11.** Experimental vs. numerical results when using the enhanced model.