Characterization of melting and solidification in a real scale PCM-air heat exchanger: Numerical model and experimental validation

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A B S T R A C T

This paper describes the models developed to simulate the performance of a thermal energy storage (TES) unit in a real scale PCM-air heat exchanger, analyzing the heat transfer between the air and a commercially available and slab macroencapsulated phase change material (PCM). The models are based on one-dimensional conduction analysis, utilizing finite differences method, and implicit formulation, using the thermo-physical data of the PCM measured in the laboratory: enthalpy and thermal conductivity as functions of temperature. The models can take into account the hysteresis of the enthalpy curve and the convection inside the PCM, using effective conductivity when necessary. Two main paths are followed to accomplish the modeling: the thermal analysis of a single plate, and the thermal behavior of the entire TES unit. Comparisons between measurements and simulations are undertaken to evaluate the models. Average errors of less than 12% on thermal power are obtained for the entire cycle. Once the model is validated, a series of parameters and variables is studied to verify their influence on the behavior and design of the TES unit.

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1. Introduction

Modeling is a useful tool in a viability analysis of applications that involve thermal energy storage by solid–liquid phase change materials. Therefore, there is a necessity to develop experimentally validated models that are rigorous and flexible to simulate heat exchangers of air and phase change materials (from here on PCM). When developing a model, the tradeoff between rigour and computational cost is crucial. There are many options reported in scientific literature to face the mathematical problem of phase change as well as to solve specific particularities such as hysteresis [1] phenomena or sub-cooling [2].

In the review by Zalba et al. [3], the authors present a comprehensive compilation of thermal energy storage (from here on TES) with PCM. One of the sections presented by the authors deals specifically with the heat transfer problem of the phase change. The authors gathered information from 1970 till 2003 and classified the analysis of the heat transfer problem under four different approaches: moving boundary problems, numerical solution considering only conduction, numerical solution considering also convection, and numerical simulation in different heat exchanger geometries. The authors remarked that although there is a huge amount of published articles dealing with the heat transfer analysis of the phase change, the modeling of latent heat thermal energy storage systems still remains a challenging task.

Later, Verma et al. [4] published a review on mathematical modeling of TES systems with PCM. The authors classified the models into two types on the basis of the corresponding law of thermodynamics under they were analyzed (first or second law). In the review, the authors pointed out the specific utility of all the models that have been experimentally validated. However, in their paper showed that only 8 of the 17 compiled models presented experimental validation, and they highlight that in order to accept any model such an experimental analysis should be done.

Regarding PCM-air heat exchangers especially interesting is the work carried out by Vakilaloojar and Saman [5]. They proposed a phase change TES for air conditioning applications. Through their numerical studies they concluded that the air velocity profile at the entrance does not affect the heat-transfer characteristics and the outlet air temperature considerably. They pointed out also that better performance can be obtained by using smaller air gaps and thinner PCM slabs. However, the authors considered constant thermo-physical properties of the PCM and pointed out that the experimental validation was necessary.

Later, Halawa et al. [6] presented an improved model of the one developed by Vakilaloojar and Saman [5]. The improvement consists of taking into account the sensible heat, but the model only considers constant thermo-physical properties, and it is limited to pure PCM as it considers single phase change temperature. The authors carried out the corresponding experiments to validate
the model [7] and concluded that the design of a thermal storage appropriate for air systems entails the careful consideration of some factors such as PCM with appropriate melting point, range of outlet and inlet temperature, and air flow rates.

Hed and Bellander [8] developed a mathematical model of a PCM-air heat exchanger. The authors highlighted the importance of the thermo-physical properties of the PCM as there is a completely different behavior between an ideal PCM (with phase transition at a given temperature) and a commercially available PCM. Although they analyzed specifically the thermal behavior of the PCM system under different shapes of the PCM enthalpy–temperature curve (the rest of the properties remain constant), the authors pointed out that the two central properties in such equipment are both, PCM heat conductivity and its variation with temperature, and heat capacity and its variation with temperature. The validation of the model with measurements on a prototype was carried out. It is in spite of having a good agreement in general, they remark that differences obtained for certain temperatures are due to difficulties in air flow measurements. The authors presented interesting results finding out that the heat-transfer coefficient between the airflow and PCM increases significantly when the surface is rough as compared to smooth surface. They also pointed out that in any design with PCM considerably attention needs to be taken to the time dependent behavior of the equipment.

When working with commercially available PCM (or mixtures or impure materials), the phase change takes place over a temperature range and therefore a two-phase zone (mushy region) appears between the solid and liquid phases. In these cases, it is appropriate to consider the energy equation in terms of enthalpy [9]. When the advective movements within the liquid are negligible, the energy equation is expressed as follows:

$$\rho \frac{\partial h}{\partial t} = \nabla \cdot (\lambda \nabla T)$$  \hspace{1cm} (1)

The solution of this equation requires knowledge of the enthalpy–temperature functional dependency and the thermal conductivity–temperature curve. The advantage of this methodology is that the equation is applicable to every phase; the temperature is determined at each point and the value of the thermo-physical properties can then be evaluated. In thermal simulations of PCM, the accuracy of the model’s results relies on the material properties data [10]. In the geometry studied in this work, the main properties were enthalpy and thermal conductivity, but notice that the rate of melting/solidification can also depend on other material properties such as viscosity or density [11]. In the models developed here the variation of thermo-physical properties with temperature in all phases was considered.

The main objective of this work was to develop and experimentally validate a model that simulated the transient response of active systems of PCM-air heat exchangers. The model considered the points reported previously (h1, h2, PC1, PC2, T1, T2, t1, t2, t3, t4, t5, t6) and also fit to the particularities of the application, such as thermal interaction between the TES unit and the ambient or internal fan dissipation. Two models were developed in the numerical computing environment Matlab (R2008b version) [31]. They were based on the analysis of the heat transfer in the PCM itself by the finite differences method, with implicit formulation. This methodology has been widely used to analyze the heat transfer problem of the phase change as the work carried out by Goodrich [12], and it exponentially increased from the works done by Voller [13] up to date [14]. Due to the specific geometry and working conditions of the study system, only one-dimensional conduction was considered. Previously other models
were presented by Dolado et al. (discretized semi-analytic model, bidimensional conduction model, and fluid-dynamic model) [15,16] and a comparison showed that the models here presented a good balance between precision and computational cost when analyzing this type of heat exchanger. The PCM utilized was a commercially available organic type, melting at approximately 27 °C. The PCM was presented macroencapsulated in aluminum rigid slabs, not flat but with bulges to enhance the heat transfer and to allow the PCM volume expansion. To validate and estimate the accuracy of the models, experimental data presented previously [17] were compared with the results of the simulations. In order to obtain design conclusions, a series of parameters and variables was studied to verify their influence on the thermal performance of the TES unit.

2. Experimental setup

The experimental setup consisted of a closed loop as shown in Fig. 1.

The total amount of PCM in the TES unit was approximately 135 kg. The organic PCM utilized was macroencapsulated in aluminum rigid slabs (see Fig. 2). The slabs were located parallel to the air flow in the TES unit.

Not only the main variables that characterize the thermal behavior of the TES unit were measured, but also a single PCM plate was monitored. In this way, two different sets of data were collected: data for the entire unit performance and detailed data for a single plate.

![Fig. 1. Experimental setup.](image)

**Fig. 1.** Experimental setup.

![Fig. 2. Compact storage module panels by Rubitherm [32]: photo and 3D sketch.](image)

**Fig. 2.** Compact storage module panels by Rubitherm [32]: photo and 3D sketch.
3. The model

3.1. Basis of the model

A PCM plate model was developed with finite differences, one-dimensional, implicit formulation. Implicit formulation was selected because of its unconditional stability. The basis model assumed only conduction heat transfer inside the PCM plate, in a normal direction to the air flow. The model analyzed the temperature of the airflow in a one-dimensional way. Due to its symmetry, the analyzed system was a division of the prototype.

In the present work, the model was implemented in Matlab R2008b [31]. The software implements direct methods (variants of Gaussian elimination [18]) through the matrix division operators, which can be used to solve linear systems.

3.2. Study system

Fig. 3 shows the study system: the PCM-air TES unit. The air inlet was located on the upper side of the TES unit. The air flowed downwards in the TES unit, circulating parallel to the PCM slabs, exchanging energy with the PCM, and eventually was blown outside the TES unit by a centrifugal fan.

The system was studied from the point of view of a single slab. As the PCM zone of the TES unit was insulated as well as due to the distribution of the slabs inside the TES unit, some symmetry relationships could be considered so only the dotted domain in Fig. 4 was modeled.

The nodal distribution of the mathematical model is shown in Fig. 5. Depending on whether the encapsulation is considered, two more nodes have to be included between the PCM surface and the airflow.

In the experimental study, the heat transfer processes that take place inside the TES unit between the air flowing through the slabs and the PCM inside the slabs were: forced convection in the air, conduction in the shell of the aluminum slab, and conduction and natural convection in the PCM itself.

The order of magnitude of the resistances was obtained as follows:

$$\frac{1}{h_{\text{air}}} = \text{from } \frac{1}{10} \text{ to } \frac{1}{40} = 0.1 - 0.025 \left[ \frac{\text{m}^2 \text{K}}{\text{W}} \right]$$

$$\frac{1}{\lambda_{\text{encap}}} = \text{from } \frac{0.001}{300} \text{ to } \frac{0.001}{200} = 3.33 \times 10^{-6} \text{ to } 5 \times 10^{-6} \left[ \frac{\text{m}^2 \text{K}}{\text{W}} \right]$$

$$\frac{1}{h_{\text{natural_conv}}} = \text{from } \frac{1}{74} \text{ to } \frac{1}{47} = 0.014 - 0.021 \left[ \frac{\text{m}^2 \text{K}}{\text{W}} \right] \quad \text{(3)}$$

The air convection coefficient was estimated in the range of forced convection for gases. According to this preliminary analysis and comparing equations, it can be stated that within the working conditions of the experiments, the thermal resistance of the encapsulation was negligible. The dominant resistance of the process could be convection on the air side and not always conduction–convection in the PCM.

In this case the thermal resistance of the encapsulation was very low, and therefore it was not necessary to consider encapsulation in the node system, as the heat transfer process was controlled by the convection on the air side and/or by the conduction–natural convection in the PCM. However, in other cases it is not always possible to disregard the thermal influence...
of the encapsulation, and therefore two models were developed: the first model did not take into account the thermal behavior of the encapsulation and the second model did, and it was developed in order to be used for general purposes.

The node equations of the two models are summarized in Tables 1 and 2.

### 3.3. Air convection coefficient calculation

In order to obtain an accurate value for the convection coefficient of the air flowing through the PCM slabs, certain considerations were required.

#### 3.3.1. Air properties

Density, thermal conductivity, and dynamic viscosity were expressed as functions of temperature for the working temperature range (0–50 °C) [20].

#### 3.3.2. Friction factor: rugosity of the encapsulation surface

As the PCM slabs manufactured by Rubitherm [32] have a special shape, rugosity had to be estimated carefully. As can be observed in Figs. 2 and 6, PCM panels were not flat but presented uniformly spread bulges over the panel surface.

In order to obtain a rugosity value, calculations were required [21]. From Fig. 6:

**Unit total surface** = 15.2 × 15.2 = 231.04 mm².

**Bulge surface** = 10.6 × 10.6 = 112.36 mm² (48.63% over unit total surface).

**Bulge high** = 0.6 mm.

Therefore depending on the shape of the bulge, the rugosity values were as follows:

- **Maximum rugosity** = 0.6 × 0.4863 = 0.292 mm, with rounded-edge bulges.
- **Medium rugosity** = 0.6 × (0.4863–0.2432) = 0.292–0.145 mm.<br>  
  - **Minimum rugosity** = 0.6 × 0.2432 = 0.145 mm, with rounded-edge bulges.

In this specific study case, rugosity was estimated to be 0.25 mm, with rounded-edge bulges.

---

**Table 1**

<table>
<thead>
<tr>
<th>Nodes</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air flow</td>
<td>( T_{air} = T_{air-1} - NTU_{air}(T_{air-1} - T_{surface}) )</td>
</tr>
<tr>
<td>PCM surface</td>
<td>( T_{surface} = \left( T_{PCM}^{air} + FoT_{PCM-1} \right) / \left( 1 + Fo + FoBi \right) )</td>
</tr>
<tr>
<td>PCM inner</td>
<td>( T_{PCM} = \left( T_{PCM}^{air} + Fo(T_{PCM-1} + T_{PCM-1}) \right) / \left( 1 + 2Fo \right) )</td>
</tr>
<tr>
<td>PCM central</td>
<td>( T_{PCM} = \left( T_{PCM}^{air} + 2Fo(T_{PCM-1}) \right) / \left( 1 + 2Fo \right) )</td>
</tr>
</tbody>
</table>

**Table 2**

<table>
<thead>
<tr>
<th>Nodes</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air flow</td>
<td>( T_{air} = T_{air-1} - NTU_{air}(T_{air-1} - T_{surface}) )</td>
</tr>
<tr>
<td>Surface encapsulation</td>
<td>( T_{surface} = \left( T_{surface}^{air} + 2(Fo_{enc}T_{enc} + Fo_{enc}B_{enc}T_{enc}) \right) / \left( 1 + 2(Fo_{enc}B_{enc} + Fo_{enc}) \right) )</td>
</tr>
<tr>
<td>Encapsulation PCM</td>
<td>( T_{enc} = \left( T_{enc}^{air} + 2(Fo_{enc-PCM}T_{surface} + 2Fo_{enc-PCM}B_{enc}T_{enc}) \right) / \left( 1 + 2(Fo_{enc-PCM} + 2Fo_{enc-PCM}B_{enc}) \right) )</td>
</tr>
<tr>
<td>PCM inner</td>
<td>( T_{PCM} = \left( T_{PCM}^{air} + Fo(T_{PCM-1} + T_{PCM-1}) \right) / \left( 1 + 2Fo \right) )</td>
</tr>
<tr>
<td>PCM central</td>
<td>( T_{PCM} = \left( T_{PCM}^{air} + 2Fo(T_{PCM-1}) \right) / \left( 1 + 2Fo \right) )</td>
</tr>
</tbody>
</table>
3.3.3. Convection coefficient

The study of the thermal boundary layer showed that there was no free development of the layer between the plates, therefore internal forced convection correlations had to be used. The Nusselt number can be calculated depending on the Reynolds number using the Gnielinski correlation for transition and turbulent flow \([22]\), or using straight section ducts and isothermal surface relations for laminar flow \([23,24]\).

3.4. PCM properties data: thermo-physical properties

The main input data of the model were material properties: enthalpy and thermal conductivity. As the simulation analyzed the transitory response of the PCM-air TES unit, a temperature-dependence of the properties was required.

3.4.1. Enthalpy–temperature curve

The storage capacity of the PCM is usually given by its latent heat value, but the PCM used here was a commercial type, not a pure substance, and therefore, the PCM melts and solidifies in a temperature range instead of in a set temperature; PCM also have hysteresis and some present sub-cooling phenomena. In these cases, latent heat and \(c_p\) values were not sufficient to define the storage capacity at each temperature. Nevertheless, the enthalpy vs. temperature curve of the PCM provided such information. In this work the curves were obtained utilizing the T-history method \([25]\) by means of its improved version \([26]\), obtaining typical curves as shown in Fig. 7, and then incorporated into the model.

From Fig. 7 an average phase change temperature for the PCM could be established at 26.5 °C.

3.4.2. Hysteresis

Depending on the stage of the process (heating or cooling, see Fig. 7) the models selected the appropriate enthalpy–temperature curve to be used in the simulation.

To solve the discontinuity that occurred when switching from one curve to the other (related to changing from heating to cooling, or vice versa within the phase change), transition functions were required. According to Bony and Citherlet \([1]\), during a heating step inside the phase change zone, the slope of the transition line was the same as the solid phase slope in the inferior part of the phase change; and during a cooling step it was identical to the slope of the liquid phase at the superior part of the phase change.

3.4.3. Thermal conductivity curve

Experimental results of thermal conductivity obtained by the laboratory of the Netzsch company utilizing laserflash methodology \([33]\) for the solid and liquid states of the PCM were incorporated into the model. Thermal diffusivity was measured using a NETZSCH model 457 MicroFlashTM laser flash diffusivity apparatus. To estimate the thermal conductivity within the phase change, the methodology proposed by Lazaro \([27]\) was used: a proportional mass rule based on enthalpy–temperature curve.

3.4.4. Natural convection inside the PCM

To obtain a good agreement between experimental results and simulations, it is not always sufficient to assume only conduction inside the PCM. To address this issue, effective thermal conductivity was implemented and therefore convection in the PCM liquid phase could be taken into account when necessary. Natural convection was studied in a rectangular enclosure for the geometry utilized in this work \([28]\).

The model calculated the effective thermal conductivity as \(k_{\text{eff}} = k \cdot C_{\text{PCM}}\), utilizing the expressions proposed by MacGregor and Emery \([19]\) for large rectangular enclosures. The correlation proposed by MacGregor was not strictly valid for this case (ratio \(H/e\) out of range; enclosed fluid changing phase in a temperature range, which meant a change in temperature and in PCM properties; and temperatures varying with time), but it served a first estimation.

![Image](image.jpg)
Theoretically, in this specific study case, the effect of natural convection was not crucial as the $c$ values are generally very close to 1 and always in the range $1 < c < 2$.

3.5. Thermal losses/gains of the TES unit

Also taken into account were the aspects of dissipation of the internal fan of the TES unit and ambient temperature effect over the unit. The TES unit electrical consumption was measured and the ambient temperature was monitored for each experiment.

4. Validation results

To verify the numerical models developed, a series of experiments in different working conditions were carried out. The aim was to compare simulations and experiments in the widest working range available with the experimental setup.

4.1. TES unit

The next Figs. 8–10 show how the simulations fit the experimental results for three different constant inlet air temperature curves in the melting stage.

The graphics plotted show the degree of agreement between experimental results and simulations. To quantify the difference between experimental data and simulated results, the relative maximum error (from here on RME) [9] and an average error were used as indicated in Eqs. (6) and (7):

$$RME(\%) = \max_{1,2,..,N} \left\{ \frac{|y_{exp} - y_{sim}|}{y_{exp}} \times 100 \right\}$$  \hspace{1cm} (6)

Fig. 8. Experimental results and simulation for a 48 °C air inlet temperature setpoint, melting stage.

Fig. 9. Experimental results and simulation for a 45 °C air inlet temperature setpoint, melting stage.
Average error (%) = \[ \sum_{i=1}^{N} \left( \frac{y_{\text{exp}} - y_{\text{sim}}}{y_{\text{exp}}} \right) \times 100 \] / N \tag{7}

The RME was always less than 15% for the 40 °C case. For the other two cases, specific errors of up to 30% could be found when the PCM in the TES unit was almost melted at low power rates. However, the average error for the melting process was less than 12% in all cases; furthermore, for the 40 °C case the average error was less than 4%.

A full cycle experiment and its corresponding simulation are shown in Fig. 11.

The average difference between measurements and simulations was 160 W, although differences of up to 400 W were found in specific locations of the curve.

The differences between the power curves could possibly exist due to the air inlet temperature input data used in the model:

- The experimental power values were obtained by the temperature difference measured with the thermopile [17,27] which takes into account the temperature distribution in the section of the duct.
- The model used as input the air temperature measured by a single Platinum resistance temperature detector PT100 located in the middle of the inlet section, which did not take into account that temperature distribution, so thermal power is calculated with slightly greater imprecision.
4.2. Single plate

To compare simulation results with the single plate experiments, encapsulation thermal equations were considered in the model. The location of the temperature sensors over and inside the single plate is shown in Fig. 12.

Fig. 13 shows the experimental measurements and the simulation results.

The differences in temperatures between the measured data and the simulated results are shown in Table 3.

Although there was an acceptable agreement between measurements and simulations for the entire heat transfer process (average differences of less than 1 °C), it could be observed that at the end of the melting stage, experimental temperature data evolved smoother than in the simulations. Some of the differences between experimental data and simulations were due to the non-exact matching of the location of the temperature sensors and monitored positions in the simulations. The temperature sensors of the PCM also might not be exactly in the middle of the PCM thickness and could make contact with the encapsulation.

5. Model sensitivity

Different situations were simulated by varying PCM properties and operating conditions to analyze the sensitivity of the model. All simulation results plotted here used the same experimental air inlet temperature curve, fan dissipation, and ambient temperature evolution.

The power curve plotted in the next figures corresponds to \( Q_{\text{TES}} \), detailed in:

\[
Q_{\text{TES}} = \dot{Q}_{\text{PCM}} + \dot{W}_{\text{fan TES}} + \dot{Q}_{\text{ambient TES}} = \dot{m} \cdot c_p \cdot (T_{\text{out}} - T_{\text{in}}) \quad (8)
\]

5.1. PCM properties input data

As the calculation results relied on the precision of the input data, the effect of a series of variations in the PCM thermo-physical properties was analyzed.

5.1.1. PCM enthalpy–temperature curve

The main input data of the model was the enthalpy–temperature curve of the PCM. The effects of varying the enthalpy values and the average phase change temperature were studied in this section.

For the experimental data used as reference, the temperature difference between the inlet air and the average phase change of the PCM had two different values according to the thermal cycle stage: it was 5 °C until complete melting, and 9.5 °C until complete solidification.

5.1.1.1. Enthalpy. The effect on the TES unit power curve of an energy variation from −30% to +30% on the enthalpy values of the enthalpy–temperature curve, was studied (Fig. 14).

The simulations showed an expected result: as the PCM enthalpy values increased, the energy delivered increased, also increasing the power peak and the duration of the process. It was also observed that in the melting stage there was a change in the shape of the curve as the enthalpy values increase, but this change in shape did not occur in the solidification stage. This behavior depended on the temperature difference between the inlet air and the average phase change of the PCM: greater the difference, faster the process.

Within the working range, a 10% increment in the value of the PCM enthalpy from its measured value led to differences in the simulation results: of 250 W in the high temperature plateau in melting, and of 100 W in the high temperature plateau in solidification. The time elapsed until full melting extended by 20 min and the time elapsed to fully solidify extended by 15 min.

5.1.1.2. Average phase change temperature. Another study analyzed the effect of moving the average temperature phase change of the PCM in the enthalpy–temperature curve (Fig. 15). This variation could be related to the imprecision regarding the association of the enthalpy–temperature data pairs of the PCM input curve.

The effect of decreasing the average phase change temperature depended on the ongoing stage:

- In the melting stage it led to higher power peaks and shorter times till full melting; there was a change in the shape of the power curve: as the average phase change temperature was lower, the energy could be absorbed faster at high power values.
- In the solidification stage, decreasing the average phase change temperature had the opposite effect. As this temperature moved to lower values it made the solidification of the PCM more difficult, thereby requiring more time to accomplish full solidification and lowering the power delivered.

Table 4 summarizes the relative errors obtained in the power curve for different imprecisions in the enthalpy–temperature association.

The table showed that a mismatching in temperature of only 1 °C in the PCM enthalpy–temperature values could lead to relative errors of up to 20% in the power curve of the TES unit and up to 14% in elapsed times till full melting. This point highlighted not only the importance of the accuracy in the measurements of input data but also of selecting the proper phase change temperature of the PCM according to the operating conditions of the TES application. Choosing a good performance in only one of the stages, avoiding the analysis of the full cycle, could lead to important drawbacks in the performance of the entire TES unit.

5.1.2. PCM effective thermal conductivity

Natural convection can be studied by means of the effective thermal conductivity. As stated previously, in this specific study...
case the effect of natural convection in the PCM itself was negligible in the entire thermal process, although it is interesting to study the effect of the PCM thermal conductivity on the TES unit thermal performance.

In Fig. 16 power curve evolution was compared for a set of different fixed PCM thermal conductivity values and for the real thermal conductivity (as a function of temperature). An increment in the PCM thermal conductivity led to a higher power peak and to a faster process. However, while decreasing thermal conductivity, for very low values a different shape of the power curve could be obtained as the process controlling the heat transfer began to be conduction in the PCM.

### Table 3
Differences in temperatures between measurements and simulations.

<table>
<thead>
<tr>
<th>Position</th>
<th>Outlet air</th>
<th>PCM_{down}</th>
<th>PCM_{mid}</th>
<th>PCM_{up}</th>
<th>Enc_{down}</th>
<th>Enc_{mid}</th>
<th>Enc_{up}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average</td>
<td>−0.3</td>
<td>0.1</td>
<td>−0.7</td>
<td>−0.7</td>
<td>0.5</td>
<td>−0.2</td>
<td>−0.4</td>
</tr>
<tr>
<td>Maximum</td>
<td>−0.9</td>
<td>1.7</td>
<td>−1.9</td>
<td>3.5</td>
<td>1.3</td>
<td>−2.1</td>
<td>−1.6</td>
</tr>
</tbody>
</table>

Fig. 13. Experimental data (a) and simulation results (b).
Fig. 14. Simulations for different PCM enthalpy–temperature curves.

Fig. 15. Simulations for different PCM average phase change temperature.

<table>
<thead>
<tr>
<th>$T_{pc}$ (°C)</th>
<th>+5</th>
<th>+2</th>
<th>+1</th>
<th>Ref.</th>
<th>-1</th>
<th>-2</th>
<th>-5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relative error range in power (%)</td>
<td>22–78</td>
<td>6–37</td>
<td>3–20</td>
<td>0–7</td>
<td>5–10</td>
<td>8–18</td>
<td>41–79</td>
</tr>
<tr>
<td>RE in time till full melting (%)</td>
<td>-38</td>
<td>-21</td>
<td>-14</td>
<td>4</td>
<td>14</td>
<td>24</td>
<td>57</td>
</tr>
<tr>
<td>RE in time till solidification (%)</td>
<td>24</td>
<td>10</td>
<td>7</td>
<td>5</td>
<td>-2</td>
<td>-5</td>
<td>-14</td>
</tr>
</tbody>
</table>
The same effect was reported when simulating the PCM with thermal conductivity as a function of temperature. No significant difference was appreciated while increasing the PCM thermal conductivity from its real value, as in this case the limiting resistance was not the conduction in the PCM but the convection in the air flow. However, when decreasing the PCM thermal conductivity, the simulated power curve changed its shape clearly due to the fact that the new resistance controlling the heat transfer process was the conduction in the PCM.

For design purposes, within the working conditions, using a fixed thermal conductivity value in the range of 0.1–1 W/(m K) led to no significant differences in the performance of the TES unit.

Fig. 16. Simulations for different PCM thermal conductivity set values.

Fig. 17. Simulations for different air flows.
5.2. Geometrical issues and operating conditions

There are two main paths to improve the performance of the PCM-air heat exchangers: enhance the PCM properties or optimize the heat exchanger design [29]. The latter is generally cheaper than the first option, and therefore it is interesting to study the effect of a series of operating conditions and geometrical parameters on the TES unit.

5.2.1. Air flow

Five airflows were simulated. Fig. 17 shows a clear difference behavior depending on the heat transfer phenomenon controlling the process:

- With low airflows, convection on the air side controlled and the process presented lower power peaks, required longer times to reach full melting or solidification, and the TES unit could release almost constant power for several hours.
- With high airflows, the bottleneck of the heat transfer process was due to the conduction within the PCM: the power curve had higher power peaks and the process required shorter times to fully melt or solidify.

The drawback of increasing the airflow was the electrical consumption and dissipation that originated from its corresponding fan. The pumping power of the simulated cases was calculated according to:

\[
y = 4.4682E-09x^3 + 5.3908E-06x^2 - 0.011418x + 7.0060
\]

\[
R^2 = 0.99965
\]

Fig. 18. Calculated pumping power vs. air flow.

Fig. 19. Simulations for different shapes of bulges over the plate surface.
The pressure drop of the TES unit was first estimated in accordance to the expressions proposed by Idel’cik [30] for tubes of rectangular cross section, rectangular section elbows with sharp corners, and discharge from straight walled elbow with sharp corner in the turn. The expression was then corrected by means of a multiplication factor to fit the experimental data gathered in previous works. Fig. 18 shows the pumping power potential dependence on the air flow, assuming a performance of 80%. Experimental data for pressure drop fitted to a second order...
polynomial equation so an expected third order polynomial dependence was obtained for the pumping power as turbulence is favored by higher airflows and by the plate bulges.

5.2.2. Encapsulation rugosity (bulge shape)

Due to the shape of the plate and the existence of bulges over its surface, there was an important effect on heat transfer. See Section 3.3.2 for the calculation of rugosity. In Fig. 19 the rugosity is arranged from a maximum value (square bulge shape) to a minimum value (no bulges).

As shown in the figure, bulges can significantly enhance heat transfer as they are related to the improvement of the convection coefficient value: the higher the encapsulation rugosity, the higher the power peak and the shorter the melting and solidification times.

5.2.3. Encapsulation thermal conductivity

In Fig. 20 the simulations considered a set of different thermal conductivity values for the encapsulation material.

Depending on the nature of the encapsulation material, the thermal resistance of the encapsulation was negligible compared to those of convection on the air side or conduction within the PCM: if $k_{\text{enc}}$ was in the range of $k_{\text{PCM}}$ or higher, the power curve was in all cases the same. If $k_{\text{enc}}$ was inferior to $k_{\text{PCM}}$, then the power peak was lower and the time required to fully melt or solidify extended.

![Fig. 22. Simulations for different lengths of the PCM system.](image)

![Fig. 23. Calculated pumping power vs. PCM system length.](image)
No compatibility issues between the PCM and the encapsulation material were considered; only thermal phenomena were taken into account.

5.2.4. PCM thickness

In Fig. 21, simulations with different PCM thickness values are reported.

The total mass of PCM in the TES unit was maintained constant (135 kg), but the width of the system had to fit the volume: as the PCM thickness increased, the width of the system decreased. Two opposite consequences then appeared: firstly, the heat transfer surface of the TES unit decreased as the slabs’ volume enlarged; and secondly, the air velocity increased as the slabs’ volume enlarged, which was linked to an increase of the air convection coefficient values.

When the thickness of the PCM slab increased, the power peak decreased and the time elapsed for the process to complete the melting or the solidification increased.

When the thickness decreased, the absorption/release of heat was faster, which meant that the effect of increasing the heat transfer surface was greater than the effect of the reduction of the air convection coefficient values due to the air velocity decrease.

![Air Gap](image1)

Fig. 24. Simulations for different air gaps between the slabs.

![Calculated pumping power vs. air gap](image2)

Fig. 25. Calculated pumping power vs. air gap.
5.2.5. PCM system length

The next simulations were carried out maintaining both the total mass of PCM and its thickness constant. The heat transfer surface was maintained constant: an increment in length was compensated by a reduction in width.

In Fig. 22 it is observed that as the length increases, the power peak raises and the process requires shorter times to complete melting or solidification. This increment in length meant higher air velocities, as the width was reduced and the airflow was maintained constant and thereby the convection coefficient increased.

Again, as the length increases there is a drawback in the pressure drop and so in the electrical consumption of the fan.

Fig. 23 shows the pumping power dependence on the PCM system length, assuming a performance of 80%.

5.2.6. Air gap

The air gap is related to the Reynolds number and to the air convection coefficient.

From Fig. 24 it can be observed that as this gap narrowed, the power peaks increased and times till full melting or solidification decreased. If the gap widened, power peaks diminished and melting or solidification times extended: this was due to the fact that the bottleneck of the heat transfer process was on the air side.

In Fig. 25 the pumping power dependence on the air gap is plotted, showing that air gaps of less than 10 mm quickly led to high pumping powers.

6. Computational issues: time step

Computational cost and precision are two important issues in PCM modeling for TES systems and its integration in building simulation tools (such as the tool Trnsys [34] used to simulate the transient performance of thermal energy systems). This section studied the time step and its effect on the accuracy of the results.

Fig. 26 shows the effect of time step size on the power curve. Results showed that typical time steps (of 1 h) in building simulation tools led to inaccurate power curves. Adequate results could be obtained using time steps up to almost 5 min, and therefore it is recommended to solve 1 h time-step simulations by means of, at the most, 5 min time-step loops if using this model.

7. Conclusions

A model was developed and experimentally validated to test the thermal behavior of a TES unit consisting of a PCM-air heat exchanger.

The model was based on one-dimensional conduction analysis, utilizing finite differences method, and implicit formulation. The phase change process was described by means of the $h_{\text{PCM}}(T)$ curve.

As the effect of hysteresis phenomenon on the TES unit thermal performance can be substantial, it has been included in the model and considered for the PCM enthalpy–temperature curve.

Natural convection within the liquid PCM has been considered in the model by means of the effective thermal conductivity.

The model is theoretically valid for every air flow under internal forced convection and it was experimentally validated for an air velocity range from 0.7 to 2.1 m/s and for an inlet air temperature range from 8 to 45 °C. As the model is one-dimensional, the length/thickness ratio in each plate must be over 10 to ensure a negligible 2D conduction.

From the comparison between simulations and experimental results it was concluded that to determine the thermal behavior of the TES unit, thermal simulation of the PCM encapsulation was not necessary. This happened in this specific study case due to the relationship between the main thermal resistances in the process. However, it is mandatory to take into account the rugosity of the encapsulation, as rugosity is related to the calculation of heat transfer between the air and the PCM slabs.

From these comparisons it could also be concluded that a 1D model was suitable to achieve good results of the thermal behavior of this type of TES unit. Average errors of less than 12% on thermal power were obtained for the entire cycle.

The analyses carried out to study the influence of the PCM thermal properties used as inputs showed that:

- A 10% increment in the value of the PCM enthalpy from its measured value led to differences in the simulation results of 6% of thermal power in the high temperature plateau in melting and of 2.5% in the high temperature plateau in solidification. It also meant that times elapsed until full melting extended by 11% and times to fully solidify extended by 10%.
A drop of the average phase change temperature in the melting stage led to higher power peaks and shorter times until full melting. In the solidification stage, decreasing the average phase change temperature had the opposite effect: as this temperature moved to lower values it made the solidification of the PCM more difficult, requiring more time to accomplish full solidification and lowering the power delivered.

A mismatching in temperature of only 1°C in the PCM enthalpy–temperature values could lead to relative errors of up to 20% in the power curve of the TES unit and up to 14% in elapsed times till full melting.

An enhancement of the PCM thermal conductivity led to minor improvements on the TES unit thermal performance, as in many cases the bottleneck of the heat transfer process was on the air side.

The hysteresis phenomenon in the enthalpy–temperature curve of the PCM was a point to consider as the thermal performance of the TES unit is greatly affected by this phenomenon.

The previous aspects stress the significance of selecting adequate PCM for the desired application and also emphasize the importance of the accuracy of the material properties’ data used as inputs of the model, as the simulations could return completely different results.

From the analyses of a series of geometrical parameters and operating conditions (airflow, encapsulation rugosity, encapsulation thermal conductivity, PCM slab thickness, PCM system length, air gap) it was concluded that the thermal power curve of the TES unit could be adapted to the corresponding application requirements without modifying the PCM properties but by modifying the heat exchanger design. For example, higher power peaks and shorter melting/solidification times could be reached by means of: increasing the air flow rate (although the drawback is in the fan’s electrical consumption), increasing the rugosity of the slab surface, reducing the PCM slab thickness, increasing the PCM system length or by reducing the air gap between the PCM slabs.

Finally, to integrate this model in building simulation tools such as Trnsys [34], which typically use time steps of 1 h, in order to obtain sufficiently accurate results, it is recommended to solve 1 h time steps of the model by means of calculation-loops of 5 min or less.

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