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Experimental and numerical simulation study of a PCM melting process without convective flows

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TOPIC: NUMERICAL SIMULATION AND MODELLING

1. Introduction

Latent heat thermal energy storage (LHTES) is a mechanism of thermal energy storage (TES) that aims to improve the efficiency of these systems by the use of phase change materials (PCMs). During the melting process (charging), the LHTTES system stores energy that can be retrieved in the solidification processes (discharge). These new systems achieve higher energy density because they can store the latent heat of a phase change in the same temperature range where another substance would only store energy in the form of sensible heat. In addition, the use of PCMs increases the thermal inertia of the system, as the phase change processes of pure substances are isothermal. The use of PCMs for thermal regulation is being applied in several applications: Heating and Domestic Hot Water (DHW) [1,2], production and building air cooling and heating circuits [3,4], thermal regulation of photovoltaic systems (PV-PCM) [5], among other applications [6,7].

A problem with PCMs is their low thermal conductivity, which causes low heat transfer and does not favour phase change requiring more time. In addition, another undesirable effect that can occur because of low conductivity is overheating in the liquid phase. A way to improve conductivity is using fins or nanoparticles, coupled with an optimized design that favours heat transfer. However, it is not always possible to implement these improvements. The extreme case, where heat transfer will be less favoured, is when the PCM is heated only from a top horizontal surface since in that configuration there will not be convective flow in the liquid phase to enhance heat transfer. Although this unfavourable situation tends to be avoided, it is still possible to find it in systems such as horizontal PV-PCM panels or floors/roofs with embedded PCM. It may also happen that due to the thinness of the PCM the convective heat transfer can be considered negligible compared to conduction [8]. Therefore, since these situations occur in real cases, their study is still necessary.

Nowadays, computational fluid dynamics (CFD) software is a highly functional tool for the careful design and optimization of LHTES systems. Although numerical studies offer a quick solution for the preliminary evaluation of PCM systems, the feasibility of the study in terms of computational cost and the accuracy of its results are heavily dependent on the selected phase

change calculation method. The main method that software such as Ansys Fluent uses to solve phase change is the Enthalpy-Porosity (EP) method [9]. This model combines latent and specific heat into an enthalpy term and assumes that the mesh domain consists entirely of a liquid whose viscosity is very high when it is below the phase change temperature (solid-state). Treating the PCM as a liquid and solving the momentum equations is a method that can be used in systems with convective flows. An alternative method is the Effective Heat Capacity (EHC) [10,11], which assumes that the PCM is a solid where the phase change is only evaluated by the variation of its thermophysical properties. When the PCM is considered as a solid, only the heat transfer by conduction will be considered, simplifying the resolve.

Several authors have tried to compare these models in different situations. Iten et al. [12] compared the EP with the EHC method using ANSYS Fluent for an air-PCM system (RT25). They considered negligible the effects of convection in the PCM because it was located inside long and narrow horizontal panels. As result, the EHC model better fitted the experimental data. The same assumption was used by Diarce et al. [8], who considered the PCM (RT35) as a solid with a variable specific heat, due to the large dimensions of the encapsulated convection. König-Haagen et al. [13] benchmarked five different methods for the modelling of melting, including the EP and EHC, where compare the numerical results with experimental measures from a case with convective flows.

In this work, using Ansys Fluent Software, two different CFD simulations based on simpler PCM melting models, Enthalpy-Porosity (EP) and Effective Heat Capacity (EHC) are compared with real experimental data. The work aims to evaluate whether, for the experiment performed, a simpler model such as the EHC model obtains similar accuracy results to the EP model. Consequently, the EHC model could be used in complex simulation systems where phase changes occur in the absence of convective flows.

2. Materials and method

The experimental study characterizes the phase change process, solid to liquid, of a volume of lauric acid as PCM when heat is supplied only from the upper surface in an isothermal process. As shown in Figure 1. a), the test was carried out in a thermally insulated square base tank of 220 mm x 220 mm sides and 67 mm in height. The downward heat flow was generated by a flat hot surface controlled by a proportional–integral–derivative controller (PID) set at 67 °C (Figure 1. b)), enough for melting lauric acid. The test was carried out in an adiabatic chamber, where, to prevent possible convective flow, the tank was perfectly levelled and thermally isolated (Figure 1. c)). Inside the PCM, 30 thermocouples were set to register the temperature at different positions getting a matrix of points of measure, as shown in figure 1.d). A small pipe in the top enclosure allowed the PCM to expand due to the changing density during the phase change.

The duration of the experiment exceeded 28 hours, which was necessary to ensure that all thermocouples indicated a temperature higher than the melting point. The results of the experimental campaign were used to define the boundary conditions of the simulations and to assess their accuracy.

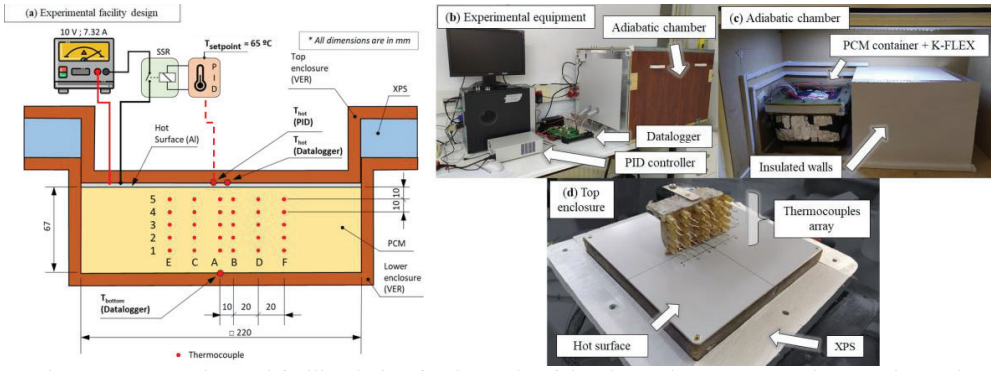

Figure 1. a) Experimental facility design for the study of the phase-change process; b) Experimental equipment; c) Position of the insulated PCM square tank in the adiabatic chamber; d) Position of the thermocouples of the top enclosure

The lauric acid (CAS 143-07-7) used in the test has a purity greater than 98%, manufactured by Sigma-Aldrich. The thermophysical properties of PCM are shown in Table 1. These properties were considered constant for the solid and liquid states, according to the values in Table 1. In the range of the phase change (316.65 K - 321.35 K), each property varies according to a temperature-dependent linear function between the solid and liquid values.

Table 1. Thermophysical properties of Lauric acid [14].

Properties	Solid	Liquid
$T_{Melting}$ (K)	316.65	321.35
ρ (kg/m^3)	940	885
C_p (J/kg·K)	2180	2390
k (W/m·K)	0.16	0.14
μ (kg/m·s)	0.08	0.008
Γ (K^{-1})	0.0008	
L (J/kg)	187210	

The numerical study, developed with Ansys Fluent, consisted of the simulation of the experimental case using two different methods, Enthalpy-Porosity (EP) and Effective Heat Capacity (EHC). Both are fixed grid methods as the mesh of the liquid and solid phase are the same.

Figure 2 shows the diagrams corresponding to each approach. From the experimental data, it was observed that all thermocouples at the same height had the same temperature values, therefore, the temperature gradient was vertical exclusively. This allowed the geometry used in the simulation to be simplified by studying a single PCM column instead of the original volume. Both the EP and EHC methods were studied using the same 2D geometry and boundary conditions, where the original 30-point measurement matrix was reduced to a single column. The upper and lower boundaries were defined as walls, whose temperature was established by UDFs from the experimental data. The two vertical sides of the geometry were defined as symmetry.

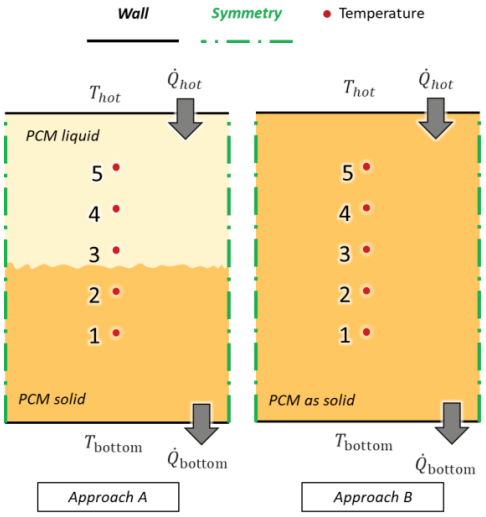

Figure 2. Diagram of the geometries and boundary conditions of each simulation.

Approach A is the case where the EP method was implemented. This method, used by default by Ansys Fluent in its solidification and melting model, resolves the phase change from the enthalpy variation of the PCM during the phase change. For this method, the energy equation is defined as [12]:

$$\frac{\partial}{\partial t}(\rho \cdot H) = K \cdot \nabla T \tag{1}$$

where ρ is the density, H the enthalpy, K the thermal conductivity and T the temperature.

The EP defines the entire domain occupied by the PCM as a fluid, whereas the solid phase PCM zone is considered a highly viscous liquid. The temperature range where the phase change occurs, between T_s and T_l, is defined as the mushy zone and is a region where the fluid is considered as a pseudo porous medium. For the mushy zone, β is defined as the liquid fraction, a variable that indicates which fraction of the total cell volume that is in the solid state, and which is in the liquid state (Equation 2).

$$\beta = \begin{cases} 0 & T < T_s \\ \frac{T - T_s}{T_l - T_s} & T_s \leq T \leq T_l \\ 1 & T > T_l \end{cases} \tag{2}$$

The enthalpy of the material, H, is calculated as the sum of the sensible enthalpy, h, and the latent heat of the melting process, ΔH (Equation 3). Besides, the enthalpy provide as latent heat is equal to the liquid fraction multiplied by the latent heat of fusion, L (Equation 4). Finally, the sensible enthalpy is defined as the sum of the reference enthalpy of the material, h_{ref}, and the integral of the specific heat, C_p, between the temperature, T, and the temperature of the reference point of the substance, T_{ref} (Equation 5). The temperature solution is solved using an iterative process between the energy equation and the enthalpy equations.

$$H = h + \Delta H \tag{3}$$

$$\Delta H = \beta \cdot L \tag{4}$$

$$h = h_{ref} + \int_{T_{ref}}^{T} C_p dT \tag{5}$$

In the second model, Approach B, the simulation was set using the EHC method. This model simplifies the resolution of the system by considering the PCM volume as a solid, in which the phase change only manifests itself as a change in its thermophysical properties. On the one hand, simplifying the model to a solid has the advantage of not having to calculate the momentum equations. On the other hand, this model is very limited as it does not consider the convective heat transfer that occurs in the liquid phase.

The EP model evaluates the variation of the specific heat of PCM to resolve the phase change, modifying its values to consider the latent heat of fusion. For this purpose, the C_p value is defined as a piecewise function according to equation 6:

$$C_p(T) = \begin{cases} C_{p,s} & T < T_s \\ C_{p,eff} & T_s \leq T \leq T_l \\ C_{p,l} & T > T_l \end{cases} \tag{6}$$

where T_l and T_s are the temperatures for the solid and the liquid that delimit the range of the phase change, and $C_{p,l}$ and $C_{p,s}$ are the values of specific heat for these temperatures according to Table 1. $C_{p,eff}$ is the value of the specific heat for the zone of the phase change, calculated as was proposed in previous work [15,16]:

$$C_{p,eff} = \frac{L}{T_l - T_s} + \left(\frac{C_{p,l} - C_{p,s}}{T_l - T_s} (T - T_s) + C_{p,l} \right) \tag{7}$$

Both approaches were carried out in a transient regime, defining a Pressure-Based solver and SIMPLE algorithm. A Second-Order implicit discretization was selected for the transient formulation. Besides, a maximum of 250 iterations per time step was set, with 3 seconds of time-steps size for Approach A, and 15 seconds for Approach B. The convergence criteria were fixed at $10^{-5,}$ except for the energy equation, set at 10^{-10}.

After comparing several mesh sizes, a mesh composed of regular 0.5 x 0.5 mm quadrilaterals was selected for both studies. For Approach A, a smaller mesh did not improve the results, while a coarser mesh required a higher number of iterations to converge. On the other side, for Approach B the size of the cells had no relevance to the results because the EHC method is simple since it only calculates the heat transfer by conduction in a solid.

3. Results and discussion

Experimental results showed that thermocouples placed at the same height recorded the same values, confirming the absence of convective flows. As a result, during the study, the considered temperature for each depth was the average measured by the six thermocouples placed in the same row. The experimental results are represented in Figure 2.

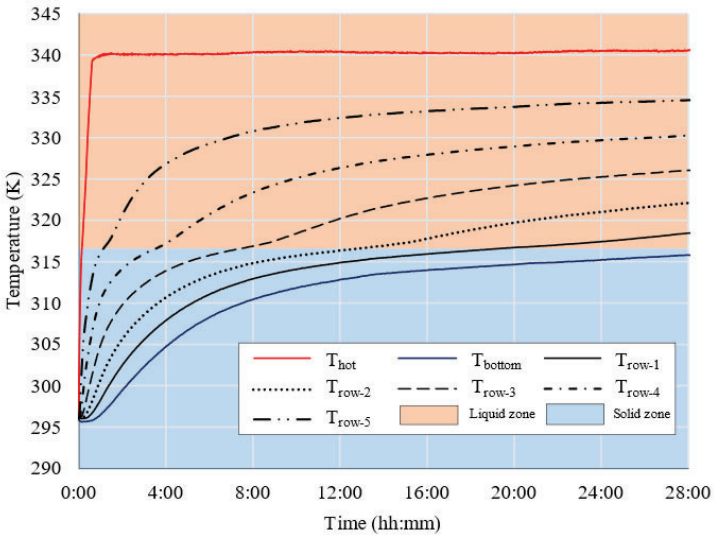

Figure 3. Experimental results of PCM temperature (K) during the melting process.

To validate the CFD models, the results of both simulations were evaluated by comparing the experimental temperature (average of each row of thermocouples) with the simulation temperature calculated at points at the same height as the thermocouples. Figure 4 shows the results obtained for both simulation approaches and the experimental results at four specific instants of the study: hours 1, 6, 12 and 28.

A clear deviation is observed in the first hour, which decreases as the simulation progresses, due to a mismatch in the solid-state properties of lauric acid. Figure 5 represents the absolute error between the experimental results and the simulation results for each row. It shows that, in addition to the initial error observed in Figure 4, in general, both models underestimate the temperature values when the phase change occurs. It can also be seen that after the phase change, the simulations tend to show higher values than those obtained experimentally. In both figures, the results of Approach A and Approach B show small differences between them.

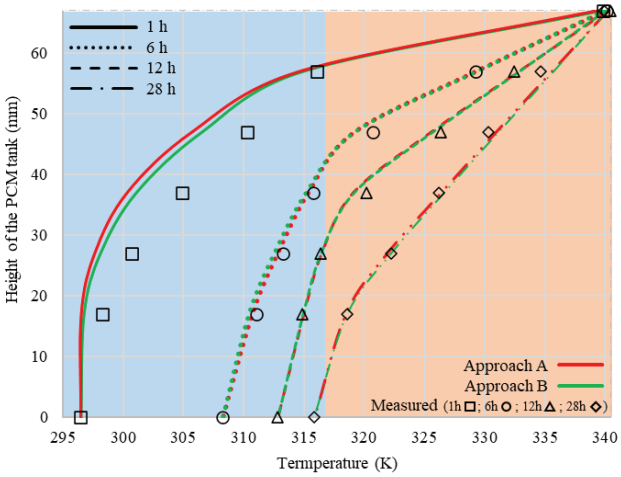

Figure 4. Temporal evolution of the melting process for experimental and simulated cases. Hours 1, 6, 12 and 28.

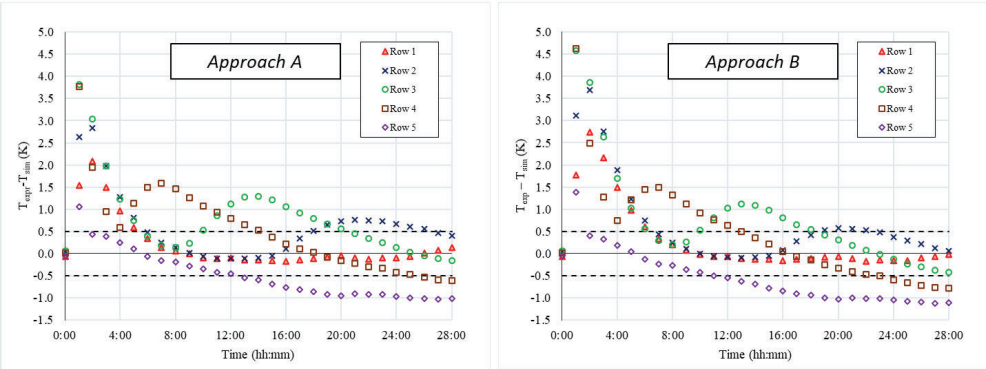

Figure 5. For both approaches, temporal evolution of the differences between experimental and simulated temperatures, $T_{exp} - T_{sim}$ (K) for each row of thermocouples in the experimental equipment (Dashed lines show the experimental error of the thermocouple probes).

The statistical parameters root-mean-square deviation (RMSD) and the coefficient of determination (R2) have been used to compare both simulation results. The RMSD obtained for Approach A and B was 0.78 K and 0.92 K respectively, while R2 was 0.9965 and 0.9951. Both models showed high accuracy, with R2 values greater than 0.99 and RMSD less than 1 K, therefore both models perform precisely.

Another relevant aspect to compare the methods is the time needed to complete the simulation since the calculation time depends on the computational cost of the model. Selecting a model with low computational cost and good accuracy will be key for more complex simulations, such as a panel PV with PCM, where phase change is not the main objective of the study. For the case studied in this paper, Approach A required about 10 hours to complete the simulation, while Approach B required only one hour, which is a great advantage of the EHC method over the EP method.

4. Conclusions

The phase change of lauric acid in absence of convective flows has been analyzed experimentally and numerically. The experimental study was carried out by heating the lauric acid, contained in an insulated tank, from its upper surface.

The experimental results were used to define the boundary conditions and to verify the results of the numerical studies. Data obtained from simulations in Ansys Fluent showed that both EP and EHC models show accurate results with low RMSE temperature values (around $1K$). However, the EHC model has clear advantages because the computational time and resources required are significantly lower. In conclusion, in cases of no convective fluxes, using the EHC model is a clear advantage as the accuracy of the result is similar with a much lower computational cost.

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