THE IMPORTANCE OF THE THERMOPHYSICAL CHARACTERIZATION OF MICROENCAPSULATED PCMS FOR THE NUMERICAL ANALYSIS OF THE HEAT TRANSFER WITH SOLID-LIQUID PHASE CHANGE

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Abstract *This work presents the development of two-dimensional numerical models based on the "additional heat source" and the "effective heat capacity" methods to simulate the thermal behaviour of a microencapsulated phase change material (PCM) - Micronal® DS 5001 X. A purely diffusive, transient model was used, where conduction is the only heat transfer mechanism during phase change. Different ways are evaluated to specify the variation of the equivalent heat capacity with temperature during the solid-liquid phase change: triangular and rectangular profiles, and also the experimentally measured specific heat as a function of temperature. The formulation of the triangular profile was based on previous studies of the authors, where a deficit of total stored/released energy was observed although predicting reasonably well the phenomena kinetics. This time, a new, consistent triangular profile method is used and its application can be generalized to different materials, by a single adjustment to the thermophysical characteristics of the PCM. This new formulation, designated as "triangular adjusted profile", proved to be the most effective method, showing the best agreement with the previous experimental data obtained by the authors. The microencapsulated PCM is used to fill the rectangular cavities of an aluminium made thermal energy storage (TES) unit. Three different configurations of the TES unit were evaluated, in order to assess the influence of the number of aluminium fins in the PCM bulk. The melting/solidification time and the energy stored/released by the PCM were also evaluated for the different configurations. In general, the numerical results achieved are in good agreement with the experimental data previously obtained by the authors.*

1. INTRODUCTION

The incorporation of PCMs in small TES units (also called heat sinks) has been a subject of great interest and much work has been developed worldwide [1]. These TES units are typically made of a high-conductivity internally-finned container used to accommodate the PCM and to compensate the low thermal conductivity of paraffins, commonly used as PCMs. To prevent liquid leakage, the metallic container can be the only way of containment,

otherwise the PCM can be microencapsulated before filling the macrocapsule. The main advantage of using TES units filled with microencapsulated PCMs is that the problem of liquid leakage during manufacturing, assembling and operation can be significantly reduced. When dealing with microencapsulated PCMs, the numerical modelling of the heat transfer with phase change becomes simpler, as the advection phenomena in the melted domain can be neglected [2] and the energy conservation equation (in its purely diffusive form) is the only governing equation to be solved.

This paper presents the validation of 2D numerical models developed in a homemade FORTRAN program and based on the *additional heat source method* and the *effective heat capacity method* to evaluate the heat transfer with melting/solidification of a microencapsulated PCM – Micronal® DS 5001 X – contained in vertical modules of rectangular-section cavities. The experimental results found in refs. [2,3] are used to validate the numerical models. The main goal of this work is to evaluate which method is better to simulate the heat transfer with solid-liquid phase change. This study also aims to assess which kind of function for the variation of the effective heat capacity with temperature is more suitable to simulate the kinetics of the phase change processes and to determine the stored/released energy during a charging/discharging cycle.

It should be remarked that the product datasheet of the majority of PCMs does not specify all the thermophysical properties in both solid and liquid phases, which is crucial for numerical modelling. When an effort is carried out to match experimental and numerical results many uncertainties related to the measurements and several numerical errors have to be considered. This is not easy to do in standard thermal analyses, but it is even harder to do when a material changes its phase in time with the variation of temperature. Moreover, the characterization of PCMs is essential to provide reliable data for modelling. In this work, the authors also aim to experimentally evaluate the main thermophysical properties of the microencapsulated PCM used in the experiments, namely the specific heat of both solid and liquid phases, the latent heat and melting temperature, and the thermal conductivity.

2. METHODOLOGY

2.1. Experimental results used for numerical validation purposes

The experimental data obtained by Soares *et al.* [2,3] are used for the purpose of validating the numerical simulation. The temperatures on the surfaces of the TES unit measured during the experiments are considered as dynamic boundary conditions in the numerical study. In the laboratory setup shown in Figure 1, the TES unit has a fixed position and it is thermally insulated on its border smaller faces, such that only the right and left square bigger surfaces will be thermally active. On its left side, a heating module holding a 68 W electrical resistance (the hot-plate) is tightly fixed to perform charging processes. During charging, a thermal insulation board is placed on the rear (right) side of the TES unit to ensure adiabatic conditions. To carry out discharging processes, a cooling module holding a heat exchanger fed by a thermo-regulated water flow (the cold-plate – 14 ºC) is tightly placed on the right side of the TES unit, while a thermal insulation board is placed on the left side of the TES unit to ensure adiabatic conditions. Twenty-one K-type thermocouples were distributed on the right and left surfaces of the TES unit, respectively, to record the time evolution of temperature on both faces. Five K-type thermocouples are also positioned on the mid-plane of the TES unit to measure the temperature evolution within the PCM domain. Further details about the experimental setup, instrumentation and procedure can be found in refs. [2,3].

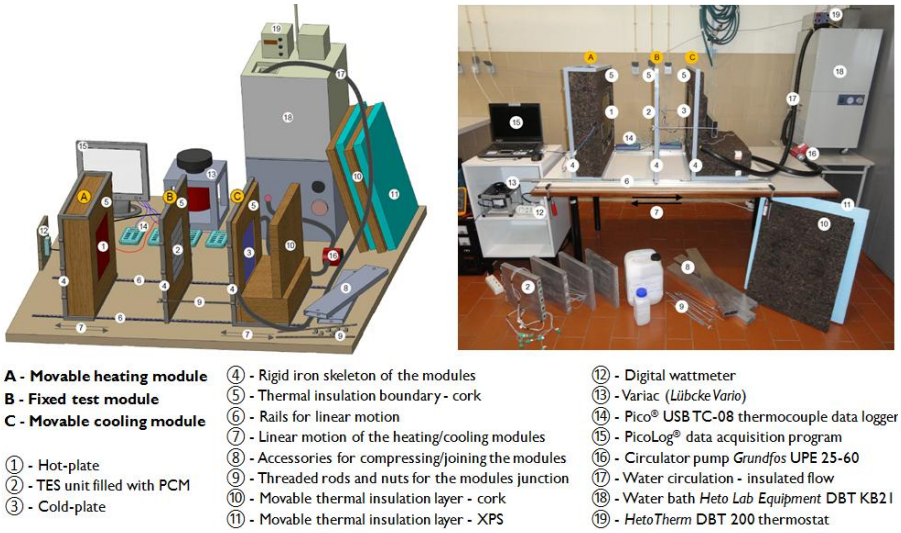
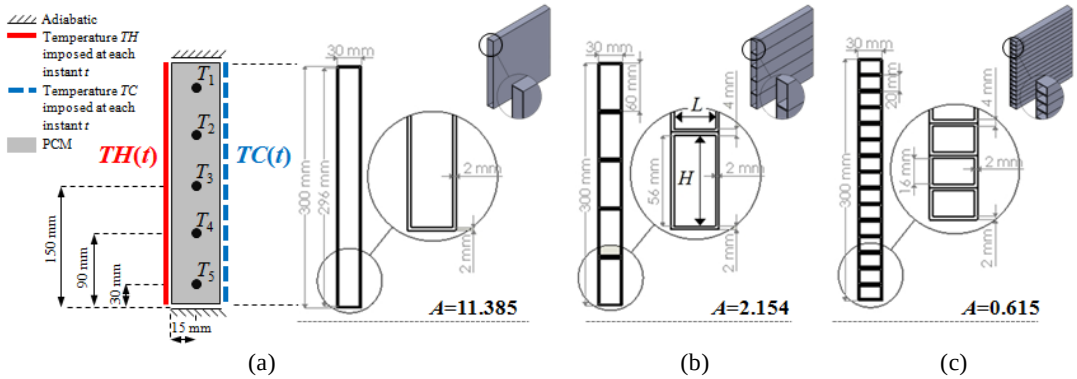


Figure 1. Sketch and photographic view of the experimental setup. Adapted from refs. [2,3].

Figure 2a shows a sketch of the 1-single cavity TES unit whose central cross section is the 2D physical model considered in the simulations. In the numerical model, the boundary conditions imposed on the vertical surfaces reproduce the time evolution of the average temperature measured on the left and right faces of the TES unit during the experiments, $TH(t)$ and $TC(t)$ respectively. The top and bottom frontiers are set to be adiabatic. T_i (i = 1 to 5, from top to bottom) are the temperatures of the PCM measured in the mid-line of the central cross section of the TES unit. The time evolution of T_i experimentally obtained is used for numerical validation purposes. To evaluate the influence of the aspect ratio of the cavities during melting and solidification processes, as well as the influence of adding metallic fins, three different configurations of the TES unit are considered, as shown in Figure 2, with the T_i temperatures measured or calculated at the same positions in every configuration.



(a) (b) (c)

Figure 2. (a) Sketch of the physical model and specified boundary conditions for the 1-single cavity TES unit (A=11.385). Sketch and dimensions of the TES units with (b) 5-cavities (A=2.154) and (c) 15-cavities (A=0.615). Figure adapted from refs. [2,3].

2.2. Thermophysical properties of the PCM

Figure 3a shows the evolution of the thermal conductivity of the PCM with temperature, and Figure 3b shows the specific heat of the PCM measured by MDSC with a charging rate of 2 ºC/min. Regarding thermal conductivity, the values measured of about 0.08–

0.086 W·m^{-1}·ºC^{-1} are 2.3–2.5 times lower than those typically specified in the literature for organic PCMs (≈0.2 W·m^{-1}·ºC^{-1}). The peak of C_p is consistent with the temperature indicated by the suppliers. However, the phase transition occurs in a wide temperature range, which must be considered in the numerical simulations. The volumetric mass density was estimated for each experiment – about 489–538 kg/m^3. These values are 40–115% higher than those specified in the datasheet of the material (about 250–350 kg/m^3), which can significantly affect the numerical predictions.

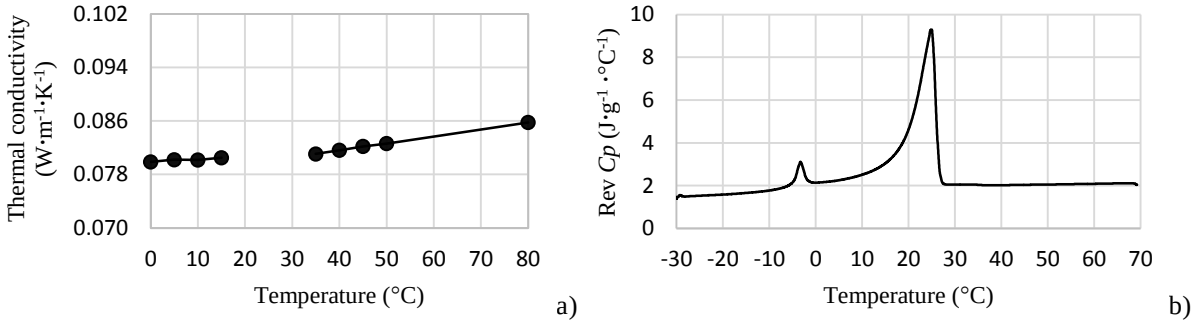


Figure 3. (a) Variation of the thermal conductivity of the PCM with the evolution of temperature – measurements with the Hot Disk TPS 2500 S equipment. (b) Specific heat of the PCM measured by Modulated Differential Scanning Calorimetry (MDSC) – the TA Instruments Q100 model was used (charging rate: 2 ºC/min).

2.3. Numerical simulation approach

The numerical models are based on the *additional heat source method* (AHS) and the *effective heat capacity method*. In the former, the latent heat is treated in the source term of the energy conservation equation in its purely diffusive form. In the second method, the latent heat is modelled in the energy conservation equation as an artificially inflated specific heat within the temperature interval where phase change occurs. Five profiles for the variation of the effective heat capacity with temperature were considered:

- Rectangular profiles (Figure 4a) – □;
- Triangular profile (Figure 4b) – Δ;
- Triangular corrected profile (2L) – Δ* (ΔT_1=7ºC, ΔT_2=2ºC); Δ** (ΔT_1=4ºC, ΔT_2=2ºC);
- Triangular adjusted profile (Figure 4c) – Δ_{adj} (varying ΔT_1 and ΔT_2 automatically).

The so-called *reverse C_p method* (RevCp) was also used, *i.e.*, the specific heat as a function of temperature obtained experimentally was considered in the simulation (Figure 3b).

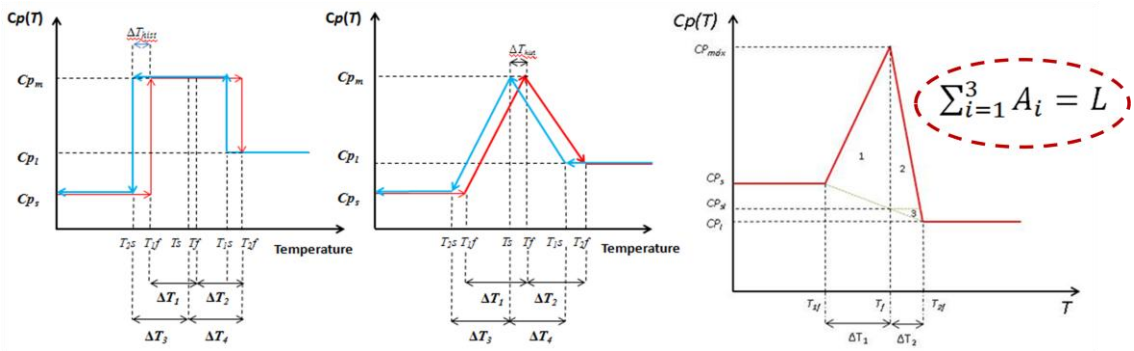


Figure 4. Sketch of the *effective heat capacity method* considering different artificial approximations for the variation of the effective heat capacity with temperature: (a) rectangular profile; (b) triangular profile; (c) triangular adjusted profile.

3. RESULTS AND DISCUSSION

The results of the parametric study carried out, considering all the methods mentioned above for the three configurations of the TES unit, can be found in ref. [4]. In this section, only some representative results are presented.

Figure 5 shows the time evolution of $T_{5,num}$ calculated with the *additional heat source method* (AHS) and with different approximations of the effective heat capacity (rectangular and triangular adjusted profiles, and *reverse* C_p *method*) in comparison with $T_{5,exp}$, considering a unidirectional model. The results show that the approaches based on the *effective heat capacity method* suit better the kinetics of the charging process. In fact, it was concluded that further research has to be carried out in order to improve the AHS and RevCp numerical approaches.

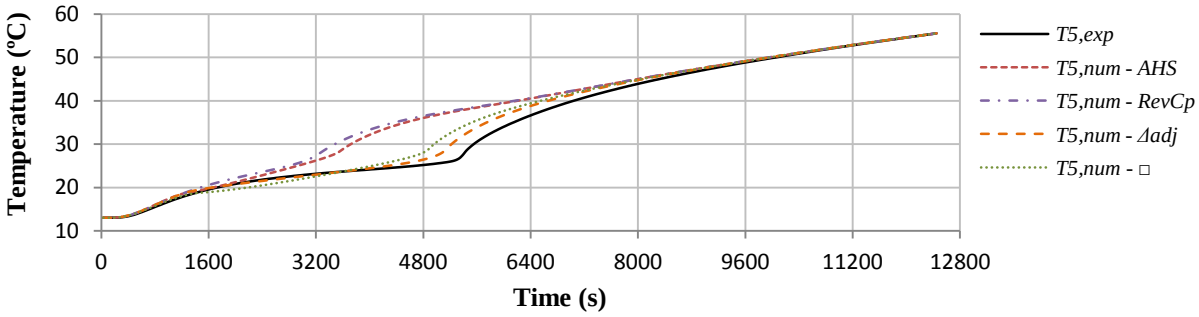


Figure 5. Unidirectional model – time evolution of $T_{5,num}$ calculated with different numerical methods in comparison with $T_{5,exp}$ (1-single cavity).

Figure 6 shows the time evolution of the boundary conditions specified during charging (*TH* and *TC*), and the evolution of $T_{1,num}$ calculated with different approximations of the effective heat capacity in comparison with $T_{1,exp}$, considering a unidirectional model. Figure 1 shows that both □, Δ* and Δ_{adj} profiles suit well the kinetics of the charging process. However, Table 1 shows that the profile that better estimates the stored energy during charging is the triangular adjusted profile.

Figure 7 shows the results of the 2D model for the 5-cavities TES unit, during charging and discharging. The triangular adjusted profile was used in the 2D simulations. Figure 8 shows the time evolution of both the temperature distribution and the melted fraction of PCM during charging and discharging.

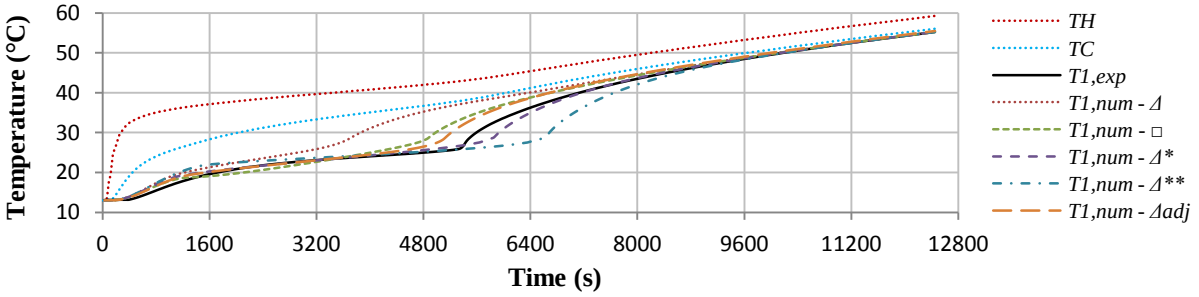
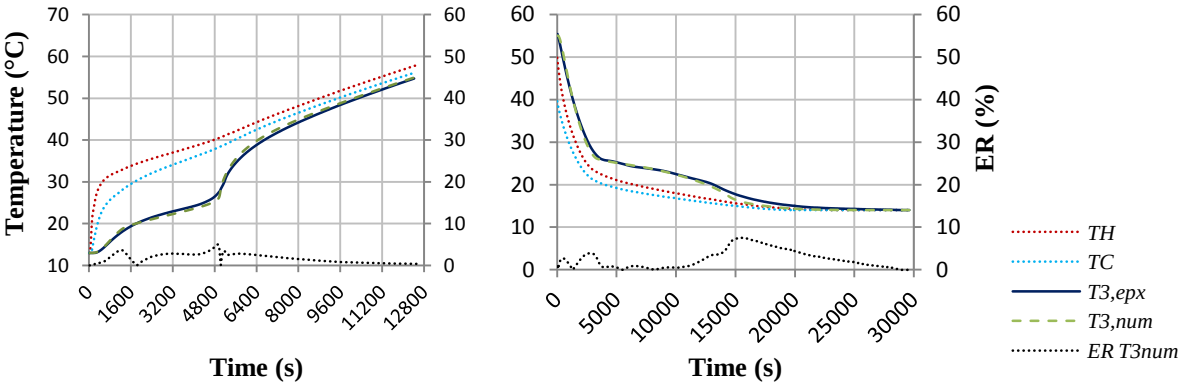


Figure 6. Unidirectional model – time evolution of the boundary conditions specified during charging; evolution of $T_{1,num}$ calculated with different approximations in comparison with $T_{1,exp}$ (1-single cavity).

Table 1. Comparison between the theoretical stored energy and the values obtained with different approximations of the effective heat capacity.

	Approximations of the effective heat capacity				
	Δ	□	Δ*	Δ**	Δ_{adj}
Stored Energy – E (kJ)	7.7	10.1	11.4	12.4	9.5
Theoretical Stored Energy (kJ)			9.8		
ER $T_{1,num}$ (%)	10.4	4.4	2.0	5.4	3.4
ER E (%)	20.9	3.7	17.0	27.5	3.1



(a) (b)

Figure 7. 2D model / 5-cavities TES unit – time evolution of the specified boundary conditions and time evolution of $T_{3,num}$ calculated with the triangular adjusted profile in comparison with $T_{3,exp}$ during (a) charging and (b) discharging.

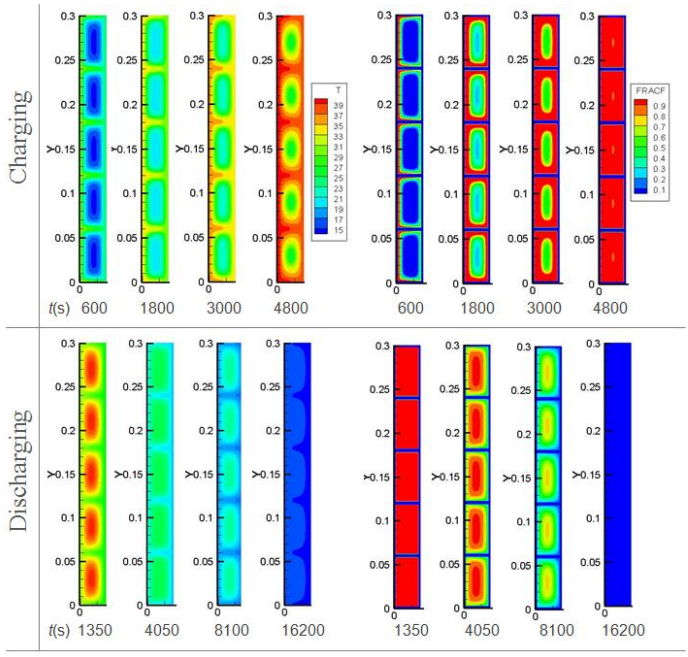


Figure 8. Time evolution of both the temperature distribution and the melted fraction of PCM during charging and discharging – 5-cavities TES unit.

3. CONCLUSION

In this paper, previous experimental results were used to validate homemade numerical

models based on the *additional heat source method* and the *effective heat capacity method* to simulate the thermal behaviour of a microencapsulated PCM - Micronal® DS 5001 X. Five approximations of the effective heat capacity were investigated: two triangular and a rectangular profile, the specific heat as a function of temperature obtained experimentally, and a new formulation designated as triangular adjusted profile. It was concluded that the last formulation is the most effective method, showing better agreement with the experimental results.

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