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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Seminar - PCMs4Buildings

PCMs: Thermophysical characterization and buildings' applications

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Framework

1 The incorporation of PCMs in small TES units has been a subject of great interest

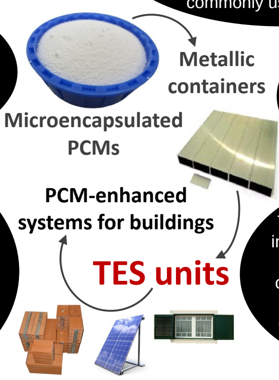
2 TES units are typically made of a high-conductivity internally-finned container used to accommodate the PCM and to overcome the low thermal conductivity of paraffins, commonly used as PCMs

3 To prevent liquid leakage, the metallic container can be the only way of containment, or the PCM can be further microencapsulated

4 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

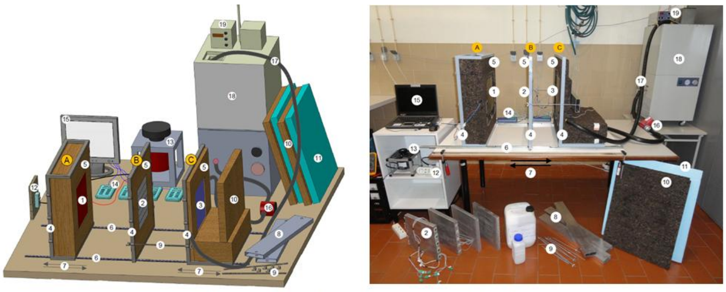
5 When dealing with microencapsulated PCMs, the numerical modelling of the heat transfer with phase change becomes simpler

6 The advection phenomena in the melted domain can be neglected and the energy conservation equation in its purely diffusive form is the only governing equation to be solved



Experimental campaign

Experiments *vs.* numerical physical domain and boundary conditions



A - Movable heating module
B - Fixed test module
C - Movable cooling module

① - Hot-plate
② - TES unit filled with PCM
③ - Cold-plate
④ - Rigid iron skeleton of the modules
⑤ - Thermal insulation boundary - cork
⑥ - Rails for linear motion
⑦ - Linear motion of the heating/cooling modules
⑧ - Accessories for compressing/joining the modules
⑨ - Threaded rods and nuts for the modules junction
⑩ - Movable thermal insulation layer - cork
⑪ - Movable thermal insulation layer - XPS
⑫ - Digital wattmeter
⑬ - Variac (*Lübcke Vario*)
⑭ - Pico® USB TC-08 thermocouple data logger
⑮ - PicoLog® data acquisition program
⑯ - Circulator pump *Grundfos* UPE 25-60
⑰ - Water circulation - insulated flow
⑱ - Water bath *Heto Lab Equipment* DBT KB21
⑲ - *HetoTherm* DBT 200 thermostat

Figure 1. Sketch and photographic view of the experimental setup previously developed by the authors.

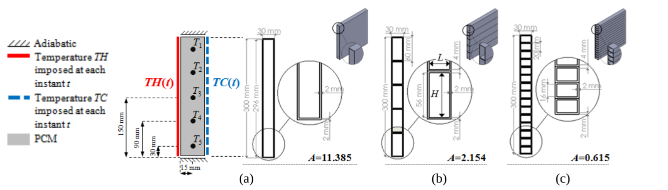


Figure 2. (a) Sketch of the physical model and imposed boundary conditions for the 1-single cavity TES unit. Sketch and dimensions of the TES units with (b) 5-cavities and (c) 15-cavities.

- 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;
- 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 (A) during melting and solidification processes, as well as the influence of adding metallic fins, three different configurations of the TES unit are considered.

Acknowledgment

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Main Goals

- To develop 2D numerical models 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 rectangular-sectioned vertical cavities;
- To validate the numerical results against previous experimental results;
- To evaluate which method is better to simulate the heat transfer with phase changes;
- 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 solid-liquid phase change processes and to determine the stored/released energy during a charging/discharging cycle;
- To experimentally evaluate the main thermophysical properties of the microencapsulated PCM used in the experiments, which are necessary for the numerical modeling.

Thermophysical properties of the PCM

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).

Volumetric mass density – the TES units were weighed empty and filled in order to determine the weight of the PCM. As the volume of the cavities is known *a priori*, the ρ-value was estimated for each experiment (489–538 kg/m³). These values are 40–115% bigger than that specified in the datasheet of the material (250–350 kg/m³), which can significantly affect the numerical predictions.

Heat capacity – the position of 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.

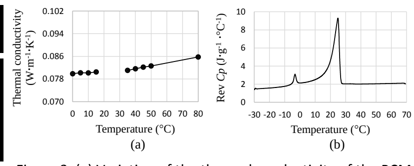


Figure 3. (a) Variation of the thermal conductivity of the PCM with the evolution of temperature – measurements with the Hot Disk TPS 2500 S equipment. (b) Specific heat of the PCM measured by MDSC (charging rate: 2 ºC·min⁻¹).

Numerical approach

Methods used:

➡ **Additional heat source method**

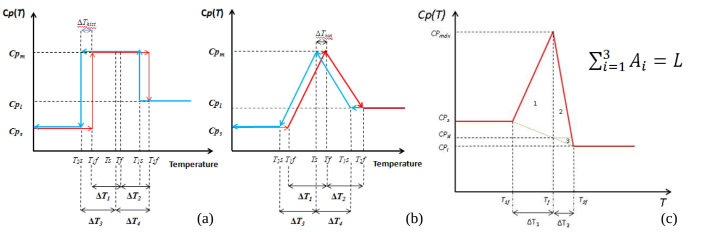
$$\frac{\partial(\rho C_p T)}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + S(f)$$

$$S(f) = -\rho\frac{\partial f}{\partial t}L$$

➡ **Reverse *Cp*** - specific heat as a function of temperature (Figure 3b)

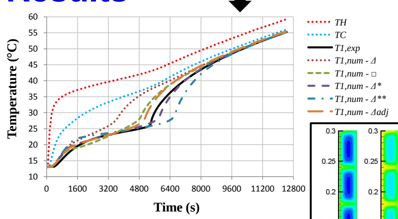
➡ **Effective heat capacity method** – the latent heat is modeled in the energy conservation equation as an artificially inflated specific heat within the temperature interval where phase change occurs

- Rectangular profiles (a) – □
- Triangular profile (b) – Δ
- Triangular corrected profile (2L) – Δ* and Δ** (varying ΔT_1 and ΔT_2)
- Triangular adjusted profile (c) – Δ_{adj} (varying ΔT_1 and ΔT_2 automatically)



Results

1D model



	Approximations of the effective heat capacity				
	Δ	□	Δ*	Δ**	Δ_{adj}
Stored Energy - E (kJ)	7.70	10.10	11.40	12.40	9.50
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

Figure 4. **One-dimensional model** – time evolution of the boundary conditions specified during charging. Evolution of $T_{1,num}$ calculated with different approximations of the effective heat capacity in comparison with $T_{1,exp}$.

2D model – 5-cavities TES unit

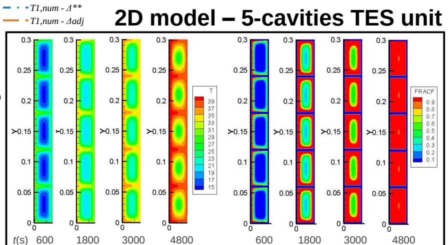


Figure 5. Time evolution of both the temperature distribution and the melted fraction of PCM during charging – Triangular adjusted profile – Δ_{adj}.

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