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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Framework

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

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

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.

Microencapsulated PCMs

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

When dealing with microencapsulated PCMs, the numerical modeling of the heat transfer with phase change becomes simpler.

Metallic containers

Experimental campaign

Experiments vs. numerical physical domain and boundary conditions

A - 3D model
B - 2D model
C - Experimental

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 unit 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(s) and TC(s) respectively.
- The top and bottom frontiers are set to be adiabatic.
- The time evolution of TH 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.

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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 are about 0.081 115 0.094 0.102 m°K/W with the values specified in the literature for organic PCMs (0.15 W/m°K).

Volume mass density – the TES units were weighed in order to determine the volume of the PCM contained in the cavities. The volume mass density was calculated according to (30 35 40 55 kg/m3). These values are close to the density values obtained from the material's datasheet (250 1,2*1,2*1,2*1 m3). These values are close to the density values obtained from the material's datasheet (250 1,2*1,2*1,2*1 m3).

Effective heat capacity method

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.

Numerical approach

Methods used:

- Additional heat source method
  
  \[ \frac{\partial (\rho C_p T)}{\partial t} = \frac{1}{x} \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + f(T) \]

- Reverse C_p - specific heat as a function of temperature
  
  \[ s(T) = -\rho C_p \frac{dT}{dt} \]

- Effective heat capacity method
  
  \[ \sum_{i=1}^{\Delta T} \Delta T \left( C_{p,i} \Delta T \right) \]

1D model

2D model – 5-cavities TES unit

Results

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 MDSIC (charging rate: 2 °C/min).

Figure 4. One-dimensional model – time evolution of the boundary conditions specified during charging.

Evolution of \( T_{avg} \) calculated with different approximations of the effective heat capacity in comparison with \( T_{avg} \) experimentally obtained.

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