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An experimental and numerical method for thermal characterization of Phase Change Materials for Cold Thermal Energy Storage

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Abstract

This paper seeks to establish a methodology which predicts the phase change duration and this assists the design of an optimized container sizing for cold thermal energy storage systems. The thermal characterization with numerical methods is widely used due to their versatility and low cost when compared to the experimental methods, but, to obtain reasonable results, the numerical model needs to be calibrated and validated with real data. In this work an experimental rig has been designed for phase change materials with low temperature applications. The results, obtained with pure water as PCM, have been used to validate a 1-D numerical model based on the effective capacity method and solved by MATLAB software.

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Keywords: Phase Change Materials; Numerical Model; Cold Thermal Energy Storage;

1. Introduction

Cold Thermal energy storage (CTES) is fundamental to improve the efficiency of energy systems that involves cold energy. The integration of Phase Change Material (PCM) as storage medium in a Thermal Energy Storage attracts in the recent years many researchers due to their high storage density and isothermal behavior. A review of the phase

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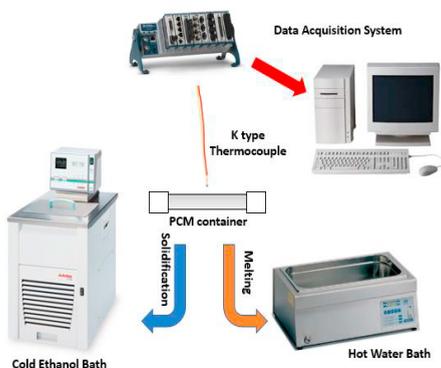
Nomenclature		Greek symbols	
D	Diameter	α	Thermal diffusivity
L	Latent Heat	β	Thermal Expansion Coefficient
Q	Heat Transfer	ν	Kinematic viscosity
T	Temperature		
V	Velocity	Abbreviations	
c	Specific heat capacity	eff	Effective
f_l	Liquid fraction	pc	Phase change
k	Thermal conductivity		
g	Gravitational acceleration	Adimensional Numbers	
h	Heat transfer convection coefficient	A, B, M, N	Constant
r	Radius	Nu	Nusselt Number
t	Time	Ra	Rayleigh Number
		Re	Reynolds Number
		Pr	Prandtl Number

change materials used for cold thermal energy storage has been reported in the literature by Oro [1], Li [2] and Sze [3]. To select a proper PCM is fundamental the understanding of the solidification and the melting process characterized by the heat transfer inside the material. This paper presents an experimental rig used to measure the thermal response of phase change materials for low temperature application. The data obtained for the melting and solidification process are then used to validate numerical 1-D. Due to the well-known thermal behaviour and the easy availability of thermal properties, pure water has been chosen as phase change material for the tests.

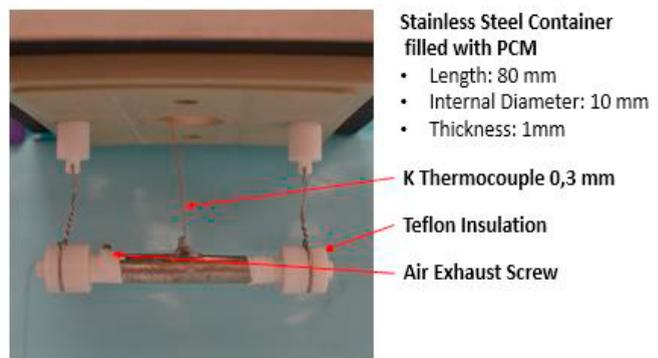
2. Materials and Methods

2.1. Experimental Rig

Fig.1 reports a scheme of the experimental-rig (Fig.1a) and the container (Fig.1b) used for the thermal characterization at low temperature of the process of solidification and melting for phase change materials. The set-up consists of a PCM container to be placed alternately between a Julabo low-temperature refrigeration system with ethanol as the heat transfer fluid (solidification) and a hot water bath (melting). The temperature is recorded with a k-type thermocouple (0.3 mm) connected to a National Instrument data acquisition system (NI cDAQ 9133 with temperature module NI 9213) at time interval of 0.5 s.



(a)



(b)

Fig.1 Experimental-rig used for low temperature thermal characterization (a), PCM container (b)

The stainless-steel container (grade 316L), showed in Fig.1b has been designed with a cylindrical shape and an internal diameter of 10mm with a wall thickness of 1mm. In order to obtain a similar behaviour of a 1-D heat transfer process, some details are added in the design of the container. In particular, the design specifics are adopted to:

- Enhance the conduction on the lateral surface of the container
- Limit the conduction and the nucleation effect of the thermocouple
- Avoid internal pressurization

The heat conduction on the end of the container has been limited by PTFE (thermal conductivity ≈ 0.25 (W/m*K)). A small screw (Fig.1b) is used to exhaust the volume of air that would pressurize the container when the cap is pushed in to close the container. During the test, the temperature has been measured with a 0.3 mm type K thermocouple funnelled through a plastic guide and secured in place with an epoxy resin. The small dimensions of the thermocouple allow to reduce the effect of the thermal conductivity and nucleation that would be present during the phase of melting and solidification. The thermocouple has been positioned in the middle of the container with the tip placed in the axis of the cylinder (5mm from the inner wall), that corresponds to the point with the longest duration of phase change and charging time. The temperature of the thermocouple is logged by a National Instrument data logger (NI cDAQ 9133 with a temperature module NI 9213).

Deionized water (4.5 g) was filled into the container from one end and closed with an insulation cap: the air inside the container was then exhausted by the screw and PTFE tape was sealed to prevent leakage from the container's junction. The container was then hooked by two supports placed in the thermal bath cover. Before starting the solidification process, the temperature of the material was stabilized at 24°C in the hot water thermal bath. During the solidification process, the container was placed in a cold bath cooled by a Julabo ultra-low refrigerated circulator (FP89-HL) with a lower temperature limit of -90 °C. In the case of pure water, with a freezing temperature of 0°C, the cold bath has stabilized with a temperature of -10°C that allows the liquid phase to reach the sub-cooling temperature before to start the phase change. The solidification process was ended when the temperature in the axis of the container has stabilized at the cold bath temperature, then the container is quickly placed in the static warm thermal bath (P-selectr unitronic OR) with pure water at the temperature of 24°C to proceed with the melting process. During the solidification and melting process the temperature was recorded by the data acquisition system with a timestep of 0,5 sec.

2.2. 1-D Numerical Model

The experimental rig and procedure described above, is used for the validation of a numerical 1-D model for thermal characterization of the low temperature PCM. On developing a numerical model, the mathematical representation of heat transfer involving phase change, is included in the category of moving-boundary problem. The most common approaches include the enthalpy method and the heat capacity method [4] where the conduction is the main heat transfer mechanism. The heat capacity method (or energy based method) considers the latent heat as a large heat insensible form during the phase change temperature. Therefore, is also widely used in problem involving non-isothermal behaviour of the material. In 1-D form the energy equation can be written in cylindrical coordinates as:

$$\rho c_{eff} \left(\frac{\partial T}{\partial t} \right) = k \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) \quad (1)$$

Where c_{eff} represents the effective heat capacity that can be approximated considering as a large heat capacity during the phase change (between T_1 , where the solidification/melting start and T_2 where the solidification/melting start):

$$c_{eff} = \begin{cases} c_{solid} & T < T_1 \\ c_{pc} + \frac{L}{(T_2 - T_1)} & T_1 \leq T \leq T_2 \\ c_{liquid} & T > T_2 \end{cases} \quad (2)$$

The thermal properties of the PCM [5] assumed the numerical model are resumed in Table 1. The natural convection, that results as a dominant heat transfer mechanism in the melting process, has been taken in account introducing an effective thermal conductivity k_{eff} for the liquid phase [6]. In order to have an accurate approximation, the properties of the material during the phase change (pc) are assumed to change according to the liquid fraction [7].

Table 1. PCM properties used for the 1-D numerical model

PCM Properties	Liquid $>T_2$	Phase Change	Solid $<T_1$
ρ (kg/m ³)	1000	$\rho_{pc} = (1 - f_l)\rho_{solid} + f_l\rho_{liquid}$	917.4
c (kJ/K*Kg)	4.20	$c_{pc} = (1 - f_l)c_{solid} + f_l c_{liquid}$	2.11
k (W/m*K)	0.558 ($k_{eff}=0.98$)	$k_{pc} = (1 - f_l)k_{solid} + f_l k_{liquid}$	2.108
L (kJ/kg)		334	
f_l	0	$(T - T_1)/(T_2 - T_1)$	1
T_{pc} (T1, T2) (K)	273.3		270

For the 1-D numerical model simulation the following initial and boundary conditions are assumed and resumed in Table 2:

Table 2. Initial and boundary conditions used for the 1-D numerical model

$r_i = 0$	$0 \leq r_i \leq r_1$ ($t=0$)	$r_i = r_1$
$k \partial T / \partial r = 0$	$T = T_{bath}$	$-\partial T / \partial r = Q$

Where r_1 represents the internal radius of the container (5mm) and r_2 is the external radius (6mm). Q (kW/m) represents the heat transfer from the boundary to the material and is considered as the contribution of the convection heat transfer coefficient and the thermal resistance due to the wall of the container represented by the thermal conductivity k_{cont} (≈ 13 W/m*K) [8]:

$$Q = \frac{T(r_i, t) - T_{bath}}{\left(\frac{1}{h_{conv}} + r_2 \frac{\ln(r_2/r_1)}{k_{cont}}\right)} \quad (3)$$

For the melting and the solidification solutions, the convection heat transfer coefficient can be obtained from the Nusselt number. When PCM is placed in a static water warm bath for the melting process, the convection heat transfer coefficient can be calculated considering free convection outside the container, assuming pure water as transfer fluid. In this case the Nusselt number can be related as function of the Rayleigh number assuming an empirical correlation [8]:

$$Nu_{free} = \frac{h_{free} D}{k} = AR\alpha^B = A \left(\frac{g\beta(T(r_2, t=0) - T_{bath}) D^3}{\nu\alpha} \right)^B \quad (4)$$

Where A and B are two constants that has been estimated to fit the experimental data A=0.32, B=0.25).

In the case of solidification when the PCM is placed in the cold bath, it is subjected to a fluid motion due the refrigerated circulator that lead to assume the boundary condition for the model as a forced convection. Also in this case, the Nusselt number can be related with some simple empirical correlations, for a cylindrical geometry, with the Reynolds and the Prandtl as[8]:

$$Nu_{forced} = \frac{h_{forced} D}{k} = MRe^N = M \left(\frac{VD}{\nu} \right)^N Pr^{1/3} \quad (5)$$

Where M and N are two constants which depends on the value of the Reynolds number (for $4000 < Re < 40000$ $M=0.193$, $N=0.618$). Since, it is difficult to estimate the velocity (V) of the flow in the cold bath, different assumptions of the Nusselt number has been made in order to find an appropriate value that better represent the phenomena.

In eq. (4-5), the properties have to be calculated for the external fluid at the film temperature $((T(r_2, t=0) - T_{bath})/2)$. The properties of the external fluid are reported in Table 2. When all the boundary conditions are defined, the energy based equation (eq.1) described above has been discretized using a finite difference method with a fully implicit scheme solved by MATLAB software [9].

Table 3. Film temperature warm and cold bath properties used for the heat transfer convection coefficient calculation.

Properties [5]	Warm Bath (water at 7°C)	Cold Bath (ethanol at 7°C)
k (W/m-K)	0.57	0.169
ν (cm ² /s)	0.0151	0.0194
α (m ² /s)	$0.136 \cdot 10^{-6}$	-
Pr	-	21.65
$\beta(1/K)$ [ref]	0.000045	-

Results

Fig.2 reports the experimental results of the melting and the solidification process and the numerical simulation obtained with the 1-D model. A free convection coefficient of 290 (W/m²K) has been estimated from eq. (4) The melting process (Fig. 2a) shows that the part of the experimental curve involving the sensible heat (1m-2m;3m-4m) and the phase change (2m-3m) has a similar trend comparing the numerical results (blue curve) with a good match in the final time of discharge (3m).

Regarding the solidification process, Fig.2b shows the experimental results with different numerical simulations where different flow velocities are considered. From the experimental curve (dotted red), it is observed that pure water supercools (2s) before the start of the phase change from liquid to solid state, that is not replicated by the 1-D model. The numerical results show that assuming a flow velocity of 2,5m/s for the calculation of the heat transfer convection coefficient, it is possible to obtain a good match with the experimental results (blue curve of Fig.2b) regarding the first part involving sensible heat (1s-3s excluding the supercooling effect) and the second part involving the phase change (3s-4s). The difference between experimental and numerical results is relevant in the last part of solidification (4s-5s)

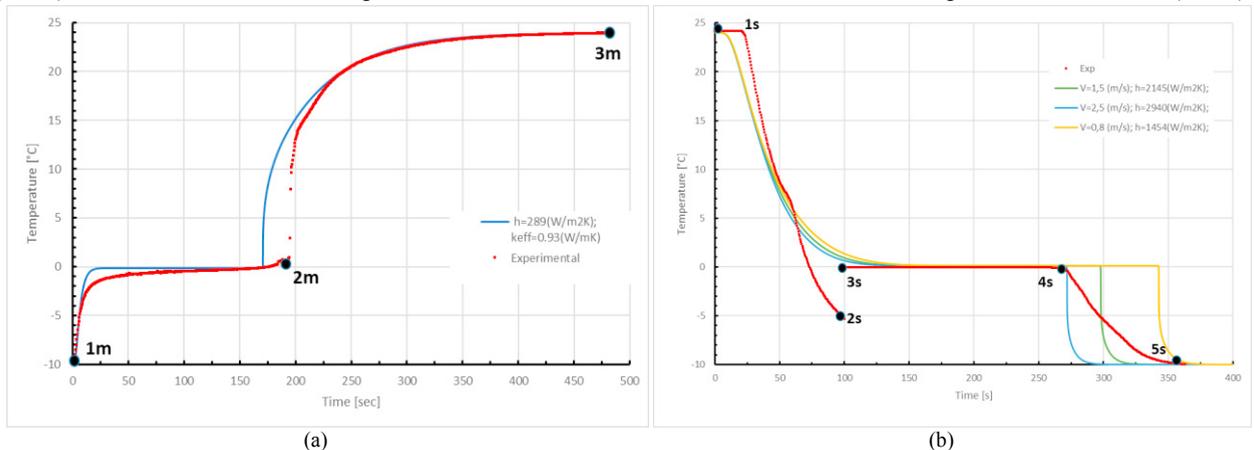


Fig.2 Experimental and numerical results of melting (a) and solidification (b) of the PCM (pure water)

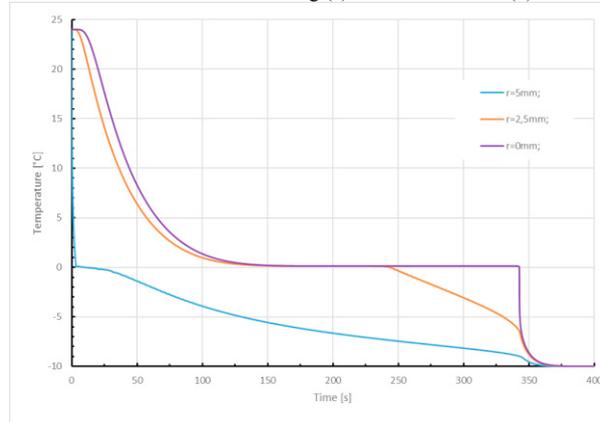


Fig.3 Numerical simulations of the PCM (pure water) at different radius (0mm, 2.5mm, 5mm)

leading to an underestimation of the time where the PCM reaches the bath temperature (time of charge). Indeed, assuming in the numerical model a flow velocity of 0,8 m/s (yellow line), the time of charge better matches the one showed by the experimental results. In this case, the longer phase change duration estimated by the numerical model, can be attributed to the narrow phase change temperature range selected (Table 1). A further reason, attributed to the sudden change of temperature in the final part of solidification (4s-5s), has also been discussed by Bourdillon [11], and can be noticed in Fig.3 where the numerical results at the wall ($r=5\text{mm}$), in the middle radius ($r=2.5\text{mm}$) and at the centre ($r=0\text{mm}$) of the container are showed. Fig.3 shows that when the central part (blue line) is under phase change, the temperature of the other points (orange and purple line) are decreasing inducing at end of phase change a sudden temperature fall in the centre of the container. This model could be more accurate if takes in account the real behaviour of the thermal properties, that are not considered in this part of the work.

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Conclusion

In this work an experimental rig has been presented to characterize the thermal behaviour of the solidification and the melting process of low temperature phase change materials. A PCM container has been designed to replicate a one-dimensional heat transfer. Using water as the PCM, the experimental values are used to validate a simple 1-D numerical model. The results show a general good agreement with the experimental results and the sensibility of the model parameters involves that a correct assumption of the boundary conditions which is fundamental to obtain a good prediction of the thermal behaviour of the material. Future work can extend this methodology to investigate other PCMs and integrate it as part of the design of cold thermal energy storage.

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