NUMERICAL AND EXPERIMENTAL STUDY OF PHASE CHANGE MATERIAL THERMO-ACCUMULATORS

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Abstract. *This paper reports a combined numerical and experimental study of several organic and inorganic phase change materials (PCMs) applied to control the temperature of ambiences subjected to a cyclic thermal source. In this respect, two simulation models were developed. The first one is based on a one-dimensional formulation and linked to an external optimization code that finds the best type and volume of PCM for a certain thermal load condition. The second approach is a three-dimensional model that simulates both the PCM and the heat diffusion through the heated wall. The accuracy of both models was assessed by comparisons with experimental data. As expected, although more accurate, the three-dimensional model possess a much higher computational cost. For this reason, such a model was only adopted to validate the one-dimensional model. From tests carried out in an especially designed experimental setup, it was verified that a great amount of energy can be stored by PCMs. Tests with extreme situations also showed that PCMs are capable of reducing the wall temperature by 40°C.*

Keywords*: phase change material, thermo-accumulators, heat transfer*

1. INTRODUCTION

Thermal energy storage (TES), also commonly called heat and cold storage, allows the storage of heat or cold to be used later (Mehling and Cabeza, 2008). In order to retrieve thermal energy, it is necessary to use a reversible method, by using either a physical or a chemical process. Physical methods can be divided into two categories: sensible heat and latent heat. The most common physical process of heat storage uses sensible heat, in which heat is transferred to the thermo accumulator as its temperature is proportionally increased. On the other hand, latent heat storage thermo accumulators allow a large amount of heat to be absorbed taking advantage of phase change.

Materials which are suitable for storage of heat or cold by changing their phase are called phase change materials (PCMs). Initially, heat is supplied to the material and stored as sensible heat by means of temperature increase. When the material starts to phase change, its phase change temperature is maintained at a constant level. At this point, the heat storage is changed from sensible process to a latent process. If the phase change is completed, further heat transferred to the material will again be stored as sensible heat. Figure 1 shows the temperature variation during sensible and latent heat storage processes. PCMs are ideal to control room temperature and also to store heat or cold that is expected to be used latter. The freezing of water to subsequently keep beverages cold is the most common use of PCMs.

By chemical composition PCMs can be classified as eutectic, salt hydrates and organic materials. Eutectics PCMs are solution of salts in water with a phase change temperature below 0°C. Salt hydrates are specific salts able to incorporate water of crystallization during the freezing process, presenting normally a phase change temperature above 0ºC (PCM Products, 2009). Finally, organic materials are polymers composed primarily of carbon and hydrogen and can be as simple as oil, waxes or fatty acid, with a change phase temperature above 0°C. These three chemical categories present different phase change characteristics, such as latent heat and melting temperature. As shown in Fig. 2, PCMs have a large range of working temperature, which implies a great number of applications, such as buildings, transportation, electronics and clothes. In the present study, some organic and salt hydrates with different phase change temperature were selected to analyze their performance in controlling a certain ambience temperature under a cyclic thermal load.

In order to understand the applicability of PCMs to keep the room temperature colder, by absorbing heat during the heating period and releasing it during the cooling period, an experimental bench was built to test four PCM samples inside an aluminum enclosure subjected to a cyclic thermal load. A sixty minute cycle was adopted, in which the enclosure is heated during thirty minutes and cooled via a fan for the next thirty minutes. The results showed that PCMs are able to store a great amount of heat and, therefore, keep the enclosure walls much colder than is no PCM was employed. The study is complemented with the development of numerical models to simulate the same phenomenon tested in the experiment setup. After the validation of such models, the effects of PCMs in other situations can be investigated in a very straightforward manner.

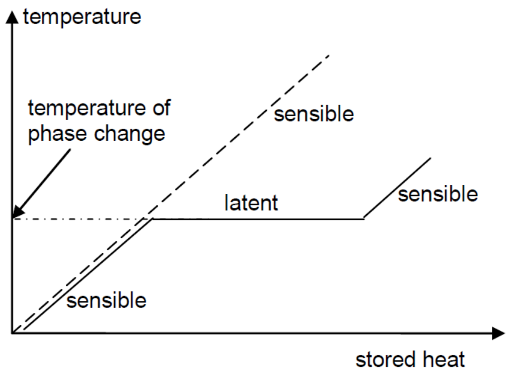


Figure 1. Temperature change as heat is supplied to a PCM.

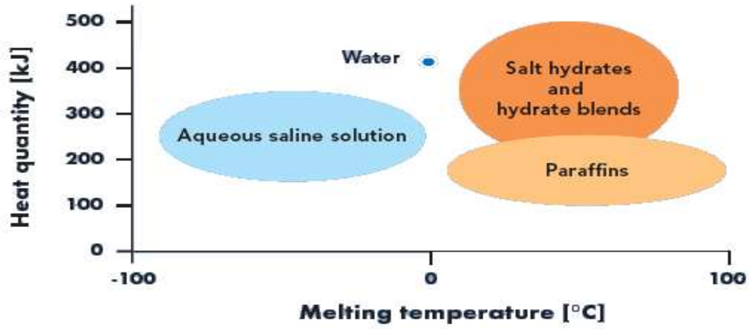


Figure 2. Melting temperature and latent heat for different types of PCMs.

2. EXPERIMENTAL SETUP

The objective of the experimental investigation is to study the effect of PCM thermo-accumulators in ambiences with a cyclic thermal source, such as buildings in regions where temperatures vary significantly along a day/night period. The experiment is used to verify the difference of temperature in an aluminum enclosure with and without the use of PCMs to store heat, as illustrated in Fig. 3. The temperature at the wall is the most important parameter to be controlled, since it determinates the comfort inside a room.

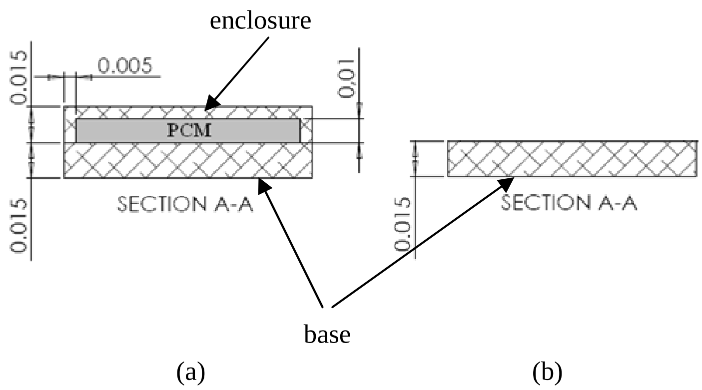


Figure 3. Aluminum sample sketches, with PCM (a), without PCM (b)

An experimental facility was developed to analyze the resulting temperature in each sample, being capable to test four samples at the same time, as shown in Fig 4. This test bench is equipped with a heating system composed of a pair of resistances and a cooling system compose of a 80mm diameter fan cooler for each sample. The temperature is monitored at three strategic points in each sample at the coordinates (x, y, z): T1 (0.0525, 0.0525, 0.010), T2 (0.0525, 0.0525, 0.020) and T3 (0.0525, 0.0525, 0.020), as illustrated in Fig. 5. Thermocouples type T were selected for temperature measurements and an acquisition system connected to a computer, via a LabView algorithm interface, obtain the required data collected in an excel file for post-processing.

The experiment consists of 24 cycles of sixty minutes each, with thirty minutes for heating and thirty minutes for cooling. A heat rate of 35W, or 3174.6 W/m^2, was supplied by a electrical heater and the cooling was made possible by using a 80mm diameter fan with a air flow rate of 0.02 m^3/s, resulting a convective heat transfer coefficient of approximately 60 W/(m^{2}K). The room temperature was controlled by an air conditioning system set to 23°C.

Several tests were carried out with five different PCM types, with three of them being organics and the other two composed of salt hydrates. The behavior of both salt hydrates was quite unstable because there was a trend for the salt to accumulate on the bottom of the container when the PCM was in liquid phase. Therefore, when the salt is solidified, its properties do not correspond to that in the previous cycles (PCM Products, 2009).

The three organic PCMs analyzed were A42 and A53 (PCM Products, 2009) and RT65 from Rubitherm Inc (2009). From these three samples, RT65 was the only one to present the required characteristics for the experiment, represented by a high latent heat (152kJ/kg) and a melting temperature around 60°C.

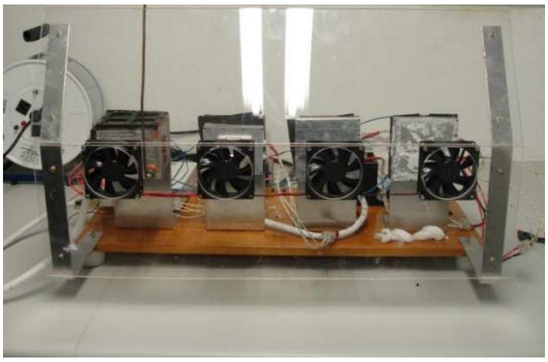


Figure 4. Experimental bench

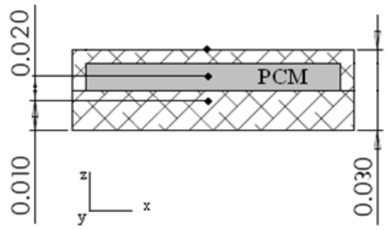


Figure 5. Position of the thermocouples in a sample; dimensions in m.

4. NUMERICAL MODEL

Numerical simulations were employed to complement the analysis. This numerical models purpose is to predict the behavior of the PCM subjected to conditions that differ from those tested in the experimented setup. For example, validated numerical models allow the study of the phenomenon for different values of ambience temperature, heat flux and cycle period, without the need of further experiments. As a consequence, there is a reduction of time and cost for investigating several alternatives.

A three-dimensional simulation model was developed by using the commercial software Fluent v, 6.3.26 (ANSYS, 2006), which is applicable for problems with phase change. Moreover, the code ICEM 12.0.1 (ANSYS, 2009) was adopted to generate the geometry and mesh required for the simulation.

As shown in Fig. 10, the geometry of the problem consists of a base, where heat is supplied, the encapsulated PCM and the PCM container, which is separated from the base by a thin layer of silicone. The silicone layer was modeled as a thin layer in order to avoid the requirement of mesh discretization. This thin layer represents a considerable thermal contact resistance that directs the heat flux to the encapsulated PCM.

The Cartesian mesh generated for this geometry consists of 395,455 hexahedral elements, all of them verified for a good quality level. The problem is numerically solved following an unsteady three-dimensional formulation, via a first-order accurate pressure-based implicit solver, in which gradients are calculated by the Green-Gauss Node Based method. The physical properties of each material (aluminum, silicone layer and PCM) are given in Tab. 1.

A number of simplifying hypotheses were adopted to simplify the problem, but keeping it as realistic as possible. Initially, heat transfer by conduction was assumed isotropic and mass transfer was neglected. This is very reasonable for pure materials, small enclosures and moderate temperature gradients. Moreover, the phase-change temperature was fixed according to the data made available by the supplier. A liquid-solid phase change with no supercooling was considered in the analysis. Finally, density was assumed to remain constant during the phase change process, which is probably the most questionable hypothesis.

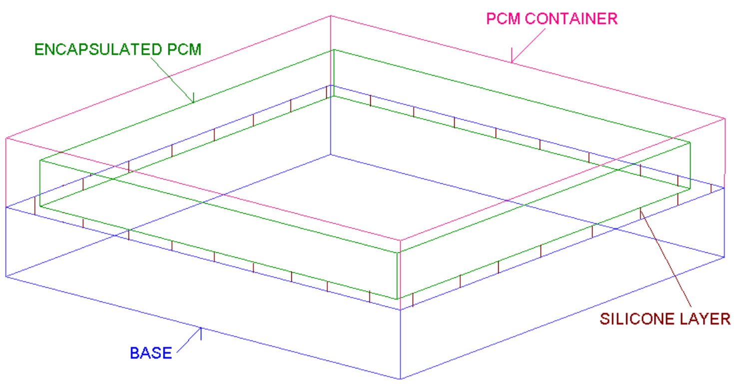


Figure 6. Problem geometry and solution domain.

The energy equation is solved based on the assumption that natural convection inside the container is negligible, since the temperature gradients are small. This is very convenient reducing significantly the associated computational cost. For solidification/melting problems, the energy equation is written based on the enthalpy, Eq. (1):

$$\frac{\partial}{\partial t}(\rho H) + \nabla \cdot (\rho \vec{v} H) = \nabla \cdot (k \nabla T) + S \qquad (1)$$

where

$$H = h + L * f_L \qquad (2)$$

Table 1. Material physical properties.

Material	Density [kg/m³]	Specific Heat [J/(kg.K)]	Thermal Conductivity [W/(m.K)]	Latent Heat [kJ/kg]	Phase Change Temperature [K]
Silicone(1)	970	65.68	0.20	---	---
Aluminum(2)	2719	871	202.4	---	---
Rubitherm RT65(3)	880	1500	0.20	152	338

(1): Data from SAC BRASCOVED; (2): Data from Fluent 6.3.26 database; (3): Data from Rubitherm data sheet

The initial and boundary conditions are based on experimental data acquired in the test bench. Two boundary conditions were adopted: one during the first half of the cycle in which the heater is on and a second for the second half when the heater is off and the fan is activated. Heat is supplied at the bottom surface of the sample, while all other surfaces are exposed to natural and forced convection during the first and second cycles, respectively. The convective heat transfer coefficient for the first period is obtained from natural convection correlation on vertical surfaces, Eq. (4). The Rayleigh number is defined through Eq. (3) and is equal to approximately 10^8 in the present problem. When Rayleigh number is moderately large, the second term on the right-hand side of Eq. (4) dominates, being then in excellent quantitative agreement with the analytical solution (Incropera *et al*, sixth edition). Concerning the upper surface, correlations for horizontal hot plate are considered, Eqs. (5)-(6). Finally the heat transfer coefficient , h, is calculated via Eq. (7).

$$Ra_L = \frac{g.\beta.(T_S - T_\infty).L^3}{\alpha.\nu} \qquad (3)$$

$$\overline{Nu_L} = 0,68 + \frac{0,670 Ra_L^{1/4}}{\left[1 + \left(0,492/Pr\right)^{9/16}\right]^{4/9}} \qquad Ra_L \leq 10^9 \qquad (4)$$

$$\overline{Nu_L} = 0,54 Ra_L^{1/4} \qquad 10^4 \leq Ra_L \leq 10^7 \qquad (5)$$

$$\overline{Nu_L} = 0,15 Ra_L^{1/3} \qquad 10^7 \leq Ra_L \leq 10^{11} \qquad (6)$$

$$h = \frac{Nu.k_{ar}}{L} \qquad (7)$$

For the period in which the heater is off, q'' is zero and a forced convection is estimated from an impinging jet condition. Based on the fan characteristics a value of approximately 60 W/(m²K) was estimated. These aforementioned equations were implemented via the user-defined function (UDF) available in the Fluent code (ANSYS, 2006). Figure 7 shows a scheme with the different boundary conditions used.

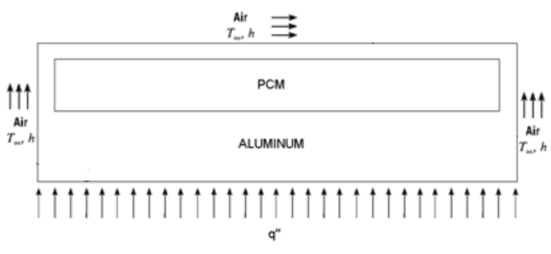


Figure 7. Boundary conditions.

During the simulation several variables were monitored for post-processing, such as the temperatures at the thermocouple locations and at the bottom and upper surfaces. In addition to that, the mean temperatures of the PCM and aluminum, heat flux leaving the sample due to convection, as well as and liquid fraction of PCM, were also evaluated. Such predictions are compared with the experimental data to validate the numerical model. The temperature of the bottom and top surfaces are shown in Fig. 8.

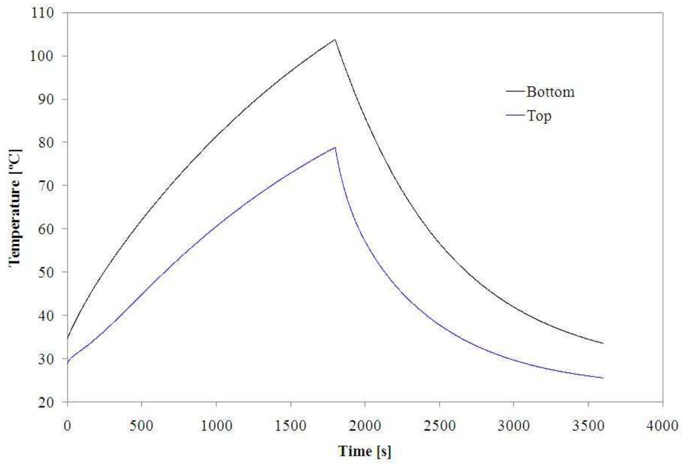


Figure 8. Temperature on the bottom and upper surfaces.

5. RESULTS

Figure 9 shows the temperature variation along the 12th cycle for the experiment with RT65. It is possible to see that the variation rate indicated by the thermocouple T1 slows down after 65ºC, which is the exact moment the PCM starts to melt. The temperature variation rate at T1 increases again when the temperature at T3 reaches 65ºC, an indication that all the material RT65 has been melted and heat begins to be absorbed in the form of sensible heat.

The temperature at T2 is seen to change before the thermocouple T3 reaches 65ºC. This phenomenon is explained by motion of PCM inside the enclosure and, therefore, T2 captures hot PCM moving from the upper region the bottom region inside the enclosure next to surface of PCM. Then, the melting front moves forward and the thermocouple T2 is now placed in the middle of the flow far from the wall region, displaying the previous variation rate of temperature.

Due to limitations of equipment, it was not possible to measure the temperature during a complete cycle of the sample without PCM, because its temperature exceeded 150°C, which is the limit temperature for SCB used to collect the data from the thermocouples. In Fig. 7 was seen that the maximum temperature on the base is 110°C, it proves that the PCM can stabilize the sample temperature with a ΔT of 40°C against a sample without PCM.

Based on the experimental data for temperature, the energy distribution in the sample was evaluated by applying an integral energy balance of enthalpy in region of the sample, as follows:

$$E = \rho . V . \left[C_p(\Delta T) + f . L \right] \tag{9}$$

Figure 10 shows measurements of energy distribution in the sample along the 10th experimental cycle, obtained with Δt = 300s. It shows that most of the energy is stored in the PCM and in the base, with 41.1% and 46.7%, respectively, of the total energy transferred to the sample. This shows the great potential of PCMs as thermo accumulators. Temperature and energy distribution for the first 30 minutes of the 10th cycle are represented in Fig. 11. From the figure, it is clear that the PCM strongly affects the temperature of the base, accumulating a considerable amount of energy during the period in which the heater is on.

As described in this section, the experimental bench is limited to cycle the PCM with a room temperature of 23°C, which constrains the analysis to a specific range of applications. In order to circumvent this limitation, a simulation model was developed to estimate the applications of PCMs in other applications, including the analysis of different PCM, enclosure geometries, etc.

Figure 12 shows a comparison between experimental and numerical results of temperature at the upper and bottom surfaces for a stabilized cycle. As can be seen, the numerical model can successfully predict the variation of temperature in the PCM. On the upper surface, the maximum deviation between the numerical results and the experimental data is 3°C, while on the bottom surface a difference of 12°C is observed at the beginning of the second half of the cycle. In fact, the agreement for the second part of the cycle could be improved if a non-constant heat transfer coefficient was utilized instead. In spite of that, the level of agreement is considered to be acceptable and further applications of PCM can be analyzed numerically.

Another interesting aspect worthwhile mentioning is the temperature levels that are reached in aluminum sample with and without the adoption of PCM (Fig.13). When the PCM is employed, the temperature on the bottom surface is decreased by approximately 40°C, which proves the effectiveness of PCMs as cooling devices. The results in Fig. 13 show that PCMs can be used to maintain the temperature at low levels, by initially storing a great amount of energy and release it afterwards.

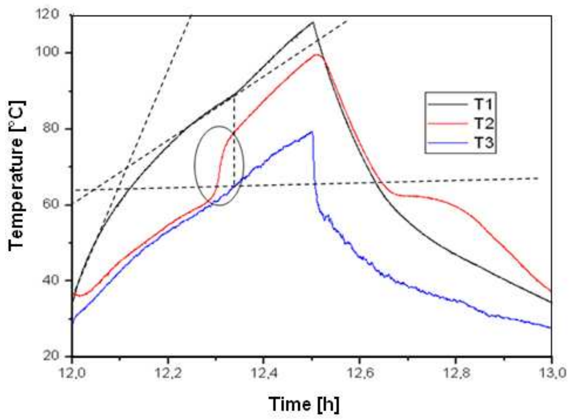


Figure 9. Temperature profile of a sample with PCM RT65

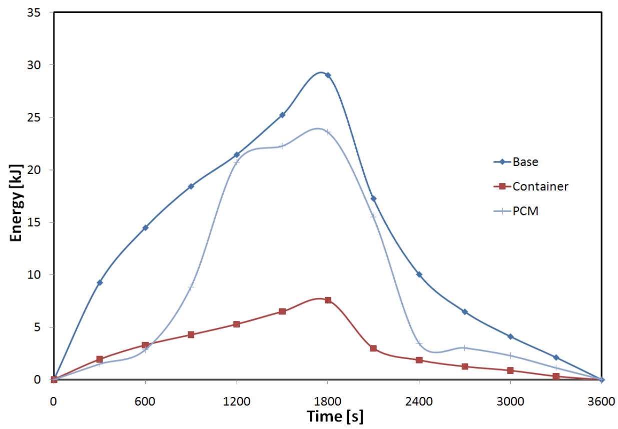
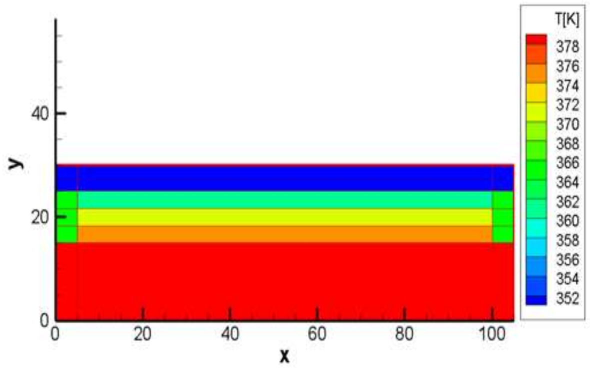
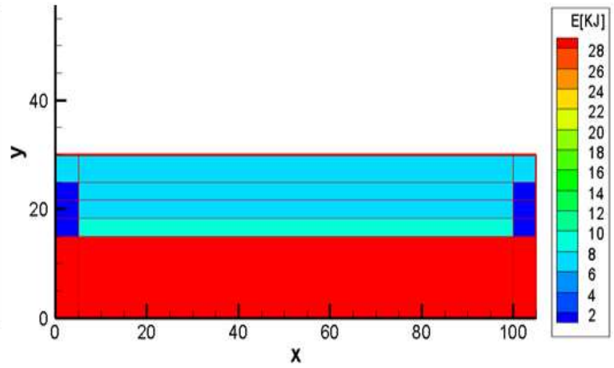


Figure 10. Energy distribution in the sample over time.



(a)



(b)

Figure 11. Temperature (a) and energy (b) distribution on the sample for the time 30 minutes of the 10th cycle

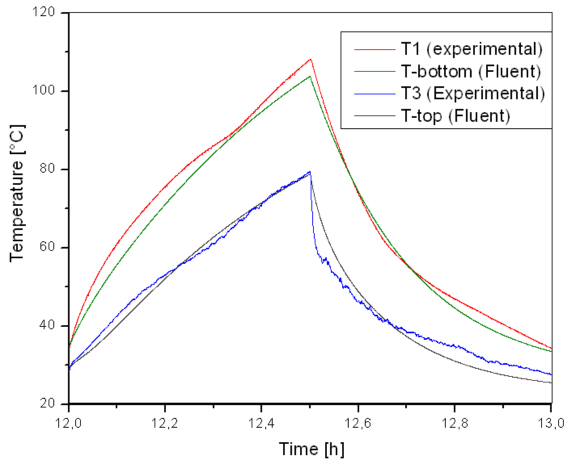


Figure 12. Temperature comparison between experimental and numerical model

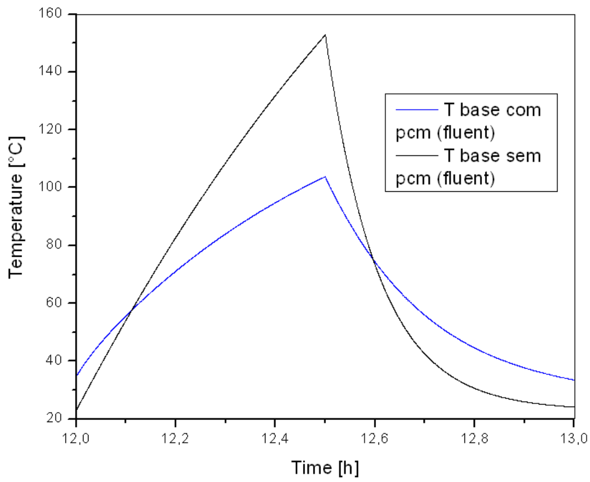


Figure 13. Temperature on bottom surface.

6. CONCLUSION

This paper presented a combined numerical and experimental study of several organic and inorganic phase change materials (PCMs) applied to control the temperature of ambiences subjected to a cyclic thermal source. A numerical model was developed and validated through comparisons between predictions and experimental data. Such a model can be adopted to conveniently predict the behavior of different applications for PCMs. It has been verified that PCMs possesses a great potential for heat and cold storage. In the tests carried out in an especially designed experimental setup, showed that PCMs are capable of reducing the wall temperature by a very significant amount.

7. ACKNOWLEDGEMENTS

The study reported herein was funded by CNPq under National Grant No. 573581/2008-8 (National Institute of Science and Technology in Refrigeration and Thermophysics). The authors would like to express their thanks to Mr. Eduardo L. Silva and Mr. Renato S. Feitoza for their assistance in preparing the experimental setup.

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