23rd ABCM International Congress of Mechanical Engineering
December 6-11, 2015, Rio de Janeiro, RJ, Brazil

ERYTHRITOL SOLIDIFICATION IN A SPHERE: A NUMERICAL STUDY

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Abstract. *The aims of this work were develop a mathematical and numerical model capable of reproducing the solidification of a phase change material (PCM) in a sphere, as well as, verify the influence of the system temperature under the PCM solidification. The geometry used in this study is a spherical capsule, made of aluminum and filled by erythritol (PCM) and air, with 40 mm in diameter (D). The problem studied is two-dimensional and governed by the equations of continuity, momentum, energy and volume fraction. All transient numerical simulations of the solidification process were carried out using the commercial software ANSYS FLUENT-14. In order to check whether the mathematical and numerical model, presented in this work, is valid for the numerical study of the solidification process into a sphere, a qualitative validation was performed. The results of the qualitative validation shows a good agreement between the numerical results obtained in the present work and the results reported in the literature. Therefore, the mathematical and numerical model, developed here, is suitable for the numerical study of the solidification process in a sphere. Regarding the influence of the system temperature under the PCM solidification, results show that the system temperature is a predominant factor in the time in which the PCM solidifies.*

Keywords: *erythritol, solidification, phase change materials, thermal energy storage, CFD.*

1. INTRODUCTION

Several studies show the growing global demand for energy, especially in recent decades. Among the main factors that influenced this growth, one can mention the intense global industrialization occurred in the last century, as well as the population's access to household refrigeration systems. Alternative systems of generation or energy savings are being tirelessly studied around the world, such studies in order to slow down this rapid growth. Among the new technologies studied, the thermal energy storage systems, based on the use of phase change materials (PCMs), can be highlighted. Systems based on this technology works in an active manner, in the other words, the energy accumulation/release occur in the latent heat form, and this occurs at constant temperature. It is worth mentioning that the amount of energy stored/released is extremely dependent of the phase change enthalpy of the PCM used. Thus, it is important that the value of this property is high so you can store/release a lot of energy with a minimum of mass. Therefore, the correct choice of PCM used is a crucial stage to the good performance of the built system.

Regarding the PCMs, various types can be found in the market. To facilitate the differentiation of various types of PCM a classification system was adopted. The PCM classification is based on the chemical characteristics of each group. Thus, the phase change materials, currently available, are classified as organic (paraffins and non-paraffins), inorganic (metallic and salt hydrates) and eutectics (mixture of organic and/or inorganic materials) [Rathod and Benerjee, 2013]. Among the organic materials, stand out the paraffins by its wide use for thermal energy storage. According to Rathod and Banerjee (2013), the wide use of these materials (paraffins) is due to some properties, such as: high fusion heat, chemically inert and stable, varied phase change temperatures and a reasonable cost if they are compared with the non-paraffins. However, this type of PCM has a limiting factor for its use. This factor refers to its melting temperature, which is below 100 °C. Therefore, in situations where the temperature ranges is higher than 100 °C, the non-paraffins or the salt hydrates are used as the phase change material.

The use of the thermal energy storage/release systems, based on the use of PCMs, is a viable alternative for the optimization of a wide range of processes in many areas. This great use, in different areas, is given by two factors: storage/release of energy at a constant temperature, as well as, a great storage/release density. Due to the use of these

systems in different areas/applications, the PCMs are subjected to two different operating conditions: cooling of PCM (solidification) and heating of PCM (melting). However, to a better control over the phase change process of the PCM, contained within the system, is necessary to allow the development and optimization of these innovative systems. Thus, in order to obtain a better understanding of the phase change process of a PCM contained within a sphere, the aims of this work are develop a mathematical and numerical model capable of reproducing the solidification of a PCM in a sphere, as well as, verify the influence of the system temperature under the PCM solidification.

2. COMPUTATIONAL DOMAIN

As previously mentioned, the phase change materials can be used in several areas, thus the thermal energy storage systems must be designed so that meet the specific characteristics (system geometry and operating conditions) of each area/application. Among the commonly used geometries for such systems, can highlight the spherical geometries. Several studies have reported a large number of potential applications for this type of geometry in different areas, for example: building cited by Schossig et al. (2005) and Tyagi et al. (2011), fluidized beds cited in the work of Brown et al. (1998) and smart textiles cited by Mondal (2008). Thus, considering the importance and the great potential of application of these systems, constituted by spherical capsules filled with PCMs, the geometry studied in this work was defined. The geometry used in this study is a spherical capsule, made of aluminum, with 40 mm in diameter (*D*). This geometry is represented by the computational domain shown in Fig. 1.

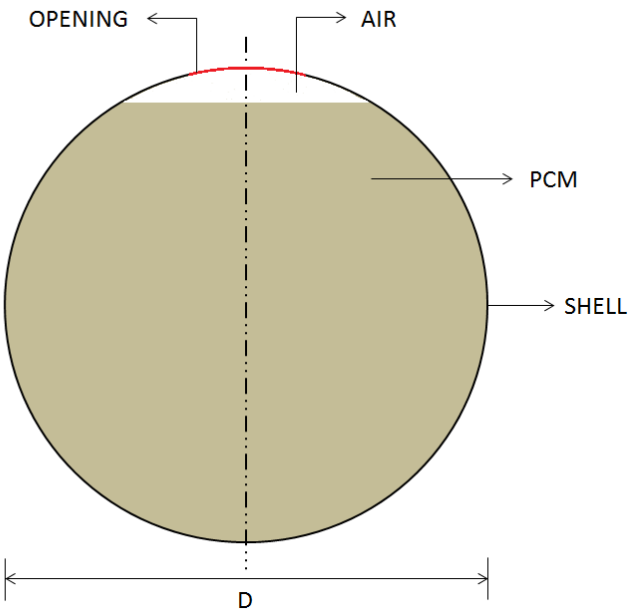

Figure 1. Computacional domain

The computational domain, shown in the Fig.1, consists of a longitudinal cut in the central axis of the spherical capsule studied in this work. Therefore, the thermal energy storage system was considered as a two-dimensional (axisymmetric) problem. The computational domain, previously presented, is filled by two different materials: air and erythritol (PCM). It is important to mention that 98% of the sphere volume is filled by erythritol, while the 2% remaining are filled by air. This ratio (air-erythritol) is not constant during the solidification process, since it is possible to observe a ratio variation due the air that flows into the sphere through the opening. The mass of air entering through the opening has a purpose. The purpose is to fill the voids generated by the PCM contraction during the solidification process.

The erythritol, the PCM used in this work, is a material that is appropriate for systems that operate at high temperatures (above 100 ºC). Thus, it is a material commonly used in industrial thermal storage systems. Regarding its physical properties, they were obtained in the work of Borahel et al. (2014) and all adopted values can be seen in the Tab. 1. Physical properties of the air and aluminum are also necessary. The values adopted for the properties of these two materials were the default values contained in Fluent-14, except the density of the air. This property was described by a polynomial function mentioned in the study of Assis et al. (2007).

Table 1. Physical properties of erythritol.

Property	
Density (kg m^{-3})	1480 (at 389 K); 1300 (at 413 K)
Latent heat capacity (J kg^{-1})	339800
Specific heat (J kg^{-1} K^{-1})	2250 (at 389 K); 2740 (at 413 K)
Solidification temperature (K)	389
Thermal conductivity (W m^{-1} K^{-1})	0.733 (at 389 K); 0.326 (at 413 K)
Thermal expansion coefficient (K^{-1})	0.00552825
Viscosity (kg m^{-1} s^{-1})	0.000027749 T^2 – 0.0231747 T + 4.844

3. MATHEMATICAL AND NUMERICAL MODEL

In the present work, the problem studied is governed by the equations of continuity, momentum, energy and volume fraction. These conservation equations, used to model the PCM-air system, are based on the enthalpy-porosity approach and are presented below (ANSYS FLUENT, 2013):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0 \tag{1}$$

$$\frac{\partial (\rho \vec{V})}{\partial t} + \nabla \cdot (\rho \vec{V} \vec{V}) = -\nabla p + \nabla \cdot (\mu \nabla \vec{V}) + \rho g + \vec{S} \tag{2}$$

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \vec{V} h) = \nabla \cdot (k \nabla T) \tag{3}$$

$$\frac{\partial (\alpha_n)}{\partial t} + \nabla \cdot (\gamma_n \vec{V}) = 0 \tag{4}$$

where ρ is the density, t is the time, V is the velocity vector, p is the pressure, μ is the dynamic viscosity, g is the gravity acceleration, S is the momentum source term, h is the specific enthalpy, k is the thermal conductivity, T is the temperature and γ_n is the nth fluid's volume fraction in the computational cell.

It is important to mention that the Boussinesq approach was used in this study. This approximation treats the density as a constant value in all solved equations, except for the buoyancy term in the momentum equation, where the density takes the following form (ANSYS FLUENT, 2013):

$$\rho = \rho_0 (1 - \beta \Delta T) \tag{5}$$

where ρ_0 is the (constant) density and β is the thermal expansion coefficient.

As the problem studied is a PCM-air system with a moving internal interface, but without interpenetration of the two fluids, the volume-of-fluid (VOF) model had to be used to describe this interface. According to Ye et al. (2012), this model describes three situations: if $\gamma_n = 0$ the cell does not contain the nth fluid, if $\gamma_n = 1$ the cell is full of the nth fluid, and, if $0 < \gamma_n < 1$ the cell contains the interface between the nth fluid and one or more other fluids.

Regarding the enthalpy, this variable was defined as the sum of the sensible enthalpy (h_s) and the variation of latent enthalpy (γL), where h_{ref} is the reference enthalpy at the reference temperature (T_{ref}), c_p is the specific heat, L is the specific enthalpy of melting/solidification (latent heat of the material), and γ is the liquid fraction during the phase change which occurs over a range of temperature $T_{solidus} < T < T_{liquidus}$, defined by the following relation (Shmueli *et al.*, 2010):

$$h_s = h_{ref} + \int_{Tref}^{T} c_p dT \tag{6}$$

$$\gamma = \begin{cases} 0 & if \quad T < T_s \\ 1 & if \quad T > T_l \\ \dfrac{T - T_s}{T_l - T_s} & if \quad T_s < T < T_l \end{cases} \tag{7}$$

It is worth mentioning that the mushy region (partially solidified region) is treated as a porous medium by the technique of enthalpy-porosity. The porosity of each cell is defined as being equal to the fraction of liquid on the cell. In fully solidified regions, the porosity is equal to zero, thereby extinguishing the velocities in these regions. Due to reduced porosity in the mushy zone, the source term in Eq. (2) takes the following form (Assis *et al*., 2007):

$$\vec{S} = -A_{(\gamma)}\vec{V} \tag{8}$$

where $A(\gamma)$ is the "porosity function" defined by Brent et al. (1988) and represented by the following equation:

$$A_{(\gamma)} = \frac{C(1-\gamma)^2}{(\gamma^3 + \varepsilon)} \tag{9}$$

where ε is a small constant (= 0.001) to avoid division by zero and C is the mushy zone constant that depends of the morphology of the mushy zone (Voller and Prakash, 1987). Studied by some researchers [Voller and Prakash (1987), Brent et al. (1988), Shmueli et al. (2010), among others], C is a constant whose value was investigated over a range from 10^5 to 10^{10}. In the present work, it was adopted the value of 10^5 for the constant C. It is important to mention that this value was adopted due to the study conducted by Assis et al. (2009), where the authors conclude that the solidification process in a sphere is well represented when using this value.

The liquid fraction (γ) for different instants is obtained using the Eq. 10. This equation was adapted from an equation presented in the work of Shmueli et al. (2010).

$$\gamma_{(t)} = \frac{\forall_{(t)}}{\forall_{(t=0)}} \tag{10}$$

where $\forall$ is the volume occupied by the PCM in the liquid phase.

3.1 Initial and boundary conditions

Initial and boundary conditions of the problem studied are necessary to perform a numerical simulation for CFD (Computational Fluid Dynamics). Such conditions are inserted in the software used for the problem modeling, in other words, the software used to define the physical conditions of the problem. Thus, due to the high complexity of the problem studied a large number of initial and boundary conditions were used. In this work two initial conditions were used. The initial conditions are the initial temperatures of the air and PCM, both temperatures are equal to 393 K. Different boundary conditions were prescribed for the shell of the sphere, opening and the central axis of the computational domain. The shell of the sphere was considered as a solid wall, therefore, the no-slip condition was specified. It is worth mentioning that three different temperatures were prescribed in the shell of the sphere. Thus, the numerical simulations were carried out for three differences (ΔT) between T_{shell} and the solidification temperature of the PCM: 10, 15 and 20 K. Regarding the opening, pressure-outlet condition was used with gauge pressure equal to 0 Pa and backflow temperature equal to 393 K. The symmetry condition also was used in this work. This condition was used in the remaining part (central axis of the computational domain).

3.2 Simulation control

The numerical simulations of the solidification process were carried out using the commercial software ANSYS FLUENT-14. The effects of the mesh size and time step were investigated in this work. Thus, three grid meshes, with different number of elements, were created and tested in the computational domain. All grid meshes tested are structured, hexahedral and refined near the solid wall (shell of the sphere). Preliminary results showed no significant

differences between medium (4100 elements) and most refined (6200 elements) grids. Therefore, the results presented in this paper were obtained with the medium value of spatial grid (4100 elements). This grid mesh, composed of 4100 elements and refined near the solid wall, is shown in the next figure (Fig. 2):

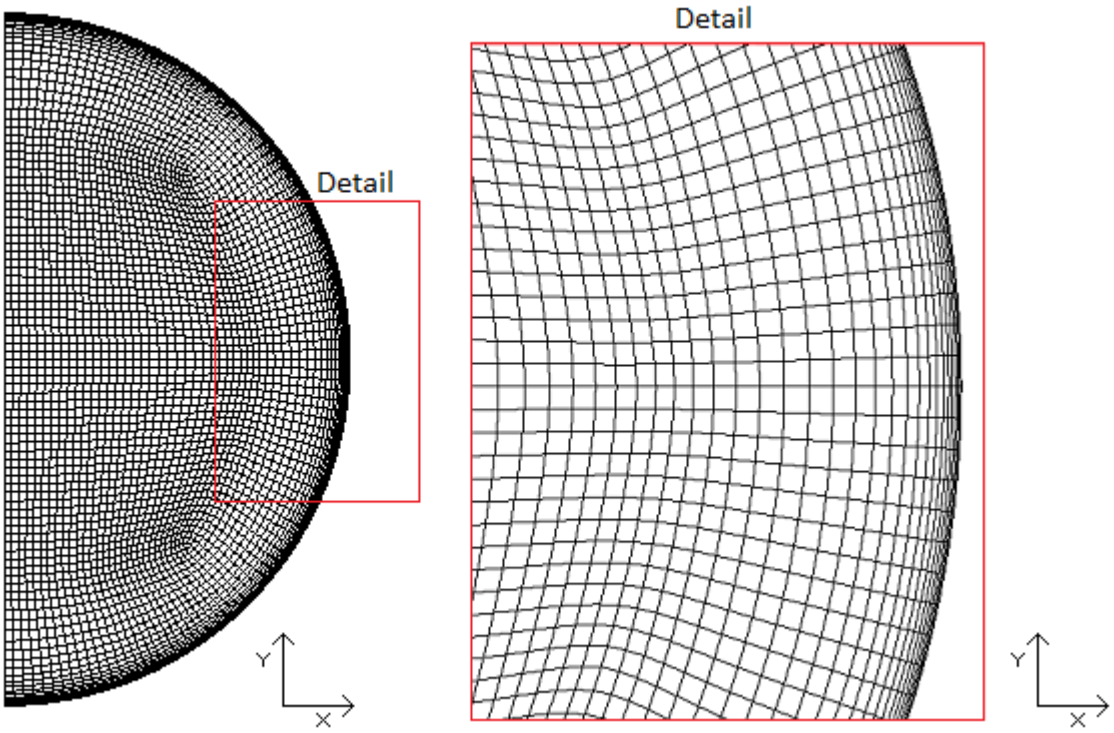

Figure 2. Grid mesh used in this work.

Regarding the time step, a value of 0.01s with a maximum of 1000 iterations per time step was used. The value used was chosen after a careful examination of the results obtained with other values tested: 0.001, 0.002 and 0.005s. These tests did not show any difference between the results obtained with the value used and the values tested. It is noteworthy that the Eqs. (1-9) were solved for each point at the computational domain. PRESTO scheme was used for the pressure correction equation, SIMPLE for pressure–velocity coupling and Second Order Upwind to solve the momentum and energy equations. Different convergence criteria were adopted for all simulations performed. A convergence criterion of 10^{-8} was used for energy and a criterion of 10^{-5} was used for the continuity and velocity components.

4. RESULTS AND DISCUSSIONS

Initially, the mathematical and numerical model, shown above, was used to reproduce the study conducted by Assis et al. (2009). Thus, the results obtained in this work, compared to those presented by Assis et al. (2009), were used to validate the model implemented. The problem studied by Assis et al. (2009), reproduced here for validation purposes, consists in the solidification process of the RT27 (PCM used) in a plastic sphere. It is important to mention that the plastic sphere has the same dimensions of the sphere studied in this work, 40 mm in diameter (D).

In order to check whether the mathematical and numerical model, previously presented, is valid for the numerical study of the solidification process into a sphere, a qualitative validation was performed. The qualitative validation is a visual comparison of the liquid fraction fields at different instants. The results for the qualitative validation are shown in the Fig. 3 through the liquid fraction fields, after 5, 10, 15, 20 and 25 minutes of cooling. It is noteworthy that this figure shows the experimental and numerical results presented by Assis et al. (2009), as well as, the numerical results obtained in the present work. The results of the qualitative validation show a good agreement between the numerical results obtained here and the results (experimental and numerical) presented by Assis et al. (2009) in the initial stages (5 e 10 minutes). After 10 minutes, perceptible differences between the numerical results obtained in this study and the numerical results presented by Assis et al. (2009) are observed. It is worth noting that while the numerical results of Assis et al. (2009) distance themselves from the experimental results, the numerical results, obtained here, remain similar to the experimental results. Therefore, the mathematical and numerical model, developed here, is suitable for the numerical study of the solidification process in a sphere.

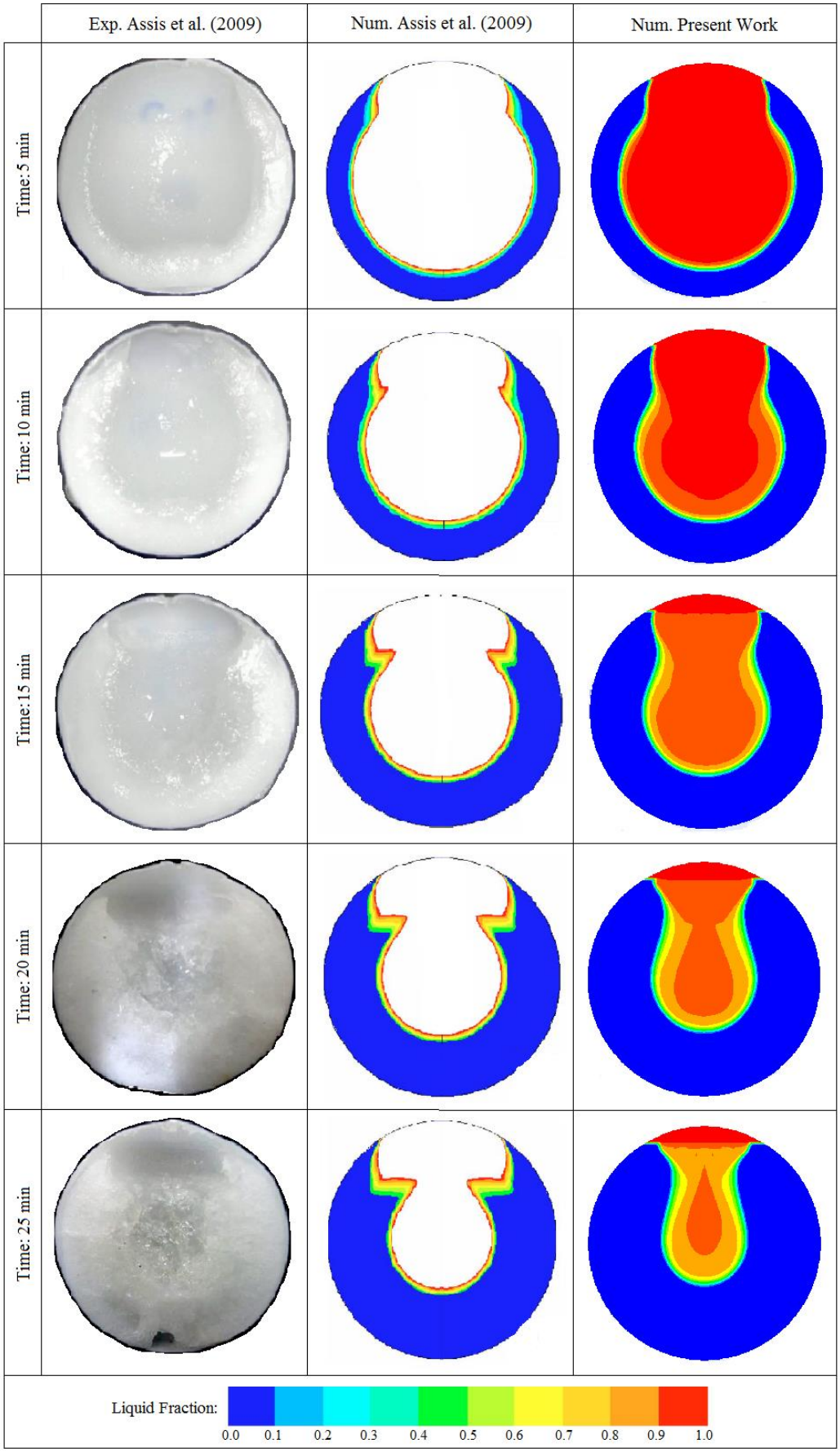

Figure 3. Liquid fraction field at different instants.

Regarding the sphere filled by erythritol and air, computational domain previously presented, a careful evaluation of the influence of system temperature under the solidification process was carried out. In order to obtain a better understanding of the influence of system temperature under the erythritol solidification, the Eq. 10 was used to calculate the liquid fraction contained within the sphere at different instants. The results of liquid fraction as a function of time, for three ΔT (10, 15 and 20 K), are illustrated in Fig. 4. In this figure, it is observed that the higher the ΔT, the faster the PCM solidifies. It is worth noting that such behavior is consistent with other results reported in the literature, since the higher the ΔT greater will be the heat rate loss by PCM.

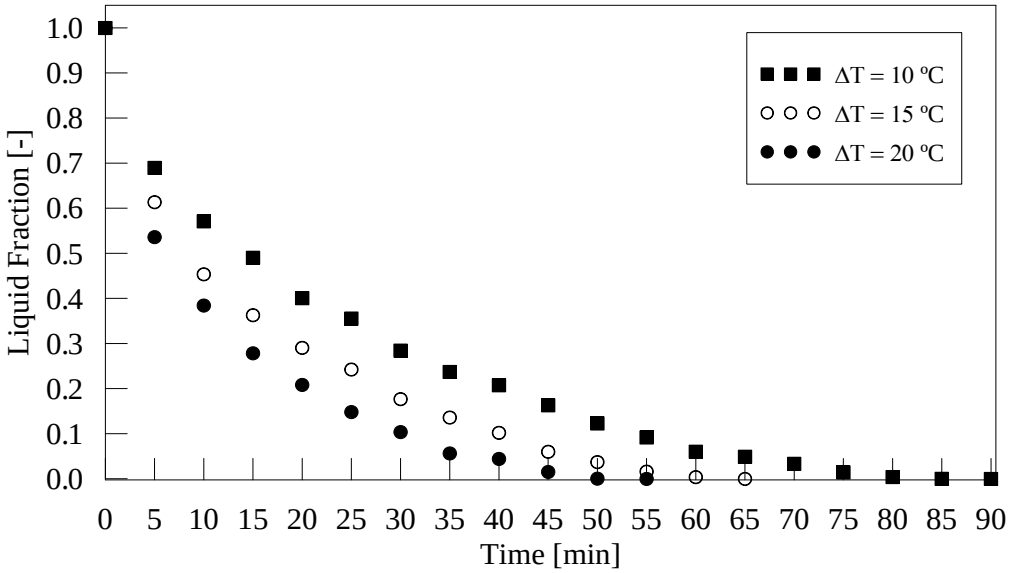

Figure 4. Liquid fraction as a function of time.

5. CONCLUSIONS

The aims of this work were develop a mathematical and numerical model capable of reproducing the solidification of a PCM in a sphere, as well as, verify the influence of the system temperature under the PCM solidification. The geometry used in this study is a spherical capsule, made of aluminum and filled by erythritol (PCM) and air, with 40 mm in diameter (D). The problem studied is two-dimensional and governed by the equations of continuity, momentum, energy and volume fraction. All transient numerical simulations of the solidification process were carried out using the commercial software ANSYS FLUENT-14. It is important to mention that the effects of the mesh size and time step were investigated in this work. Therefore, the grid mesh and time step adopted were chosen after a careful examination of the preliminary results obtained with other grid meshes and values of time step tested. In order to check whether the mathematical and numerical model, previously presented, is valid for the numerical study of the solidification process into a sphere, a qualitative validation was performed. The results of the qualitative validation showed a good agreement between the numerical results obtained in the present work and the results (experimental and numerical) presented by Assis et al. (2009) in the initial stages (5 and 10 minutes). After 5 minutes, perceptible differences between the numerical results obtained in this study and the numerical results presented by Assis et al. (2009) was observed. It is worth noting that while the numerical results of Assis et al. (2009) distanced themselves from the experimental results, the numerical results, obtained here, remained similar to the experimental results. Therefore, it can be concluded that the implemented model is suitable for the numerical study of the solidification process in a sphere. In other words, the mathematical and numerical model, presented here, is appropriate for other studies that addressing the same theme (solidification in a capsule spherical). Regarding the sphere filled by erythritol and air, computational domain previously presented, a careful evaluation of the influence of system temperature under the solidification process was carried out. Results of liquid fraction as a function of time showed that the higher the ΔT, the faster the PCM solidifies. It is worth noting that such behavior is consistent with other results reported in the literature, since the higher the ΔT greater will be the heat rate loss by PCM. Thus, it can be concluded that the system temperature is a predominant factor in the time of the PCM solidification.

6. ACKNOWLEDGEMENTS

The authors acknowledge the financial support of CNPq - Conselho Nacional de Desenvolvimento Científico e Tecnológico do Brasil (National Counsel of Technological and Scientific Development of Brazil), FAPERGS – Fundação de Amparo à Pesquisa do Estado do Rio Grande do Sul (Foundation for Research Support of the State of Rio Grande do Sul) and Universidade do Vale do Rio dos Sinos (University of Vale do Rio dos Sinos).

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