

## NUMERICAL SIMULATION OF PCM MELTING PROCESS

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### ABSTRACT

This study deals with a numerical investigation on the melting process of a PCM in a rectangular enclosure differentially heated. A FEM-based code is used in order to solve Navier-Stokes and energy equations in the considered system. Adopting the enthalpy formulation, one single equation is used to solve transient conduction and convection heat transfer in both the solid and liquid phase. The liquid flow patterns during the melting process have been captured and the instantaneous marching of the liquid-solid interface is presented. In addition, the temperature distributions in the phase change material are reported. A successfully comparison between obtained numerical results with experimental ones found in literature is presented.

### INTRODUCTION

Melting and solidification phenomena involve in several industrial processes, such as materials processing, metallurgy, purification of metals, growth of pure crystals from melts and solutions, solidification of casting and ingots, welding, electroslag melting, zone melting, thermal energy storage using phase change materials (PCM), and so forth. A complete understanding of the phase change phenomenon involves an analysis of the various processes that accompany it. The most important of these processes, from a macroscopic point of view, is the heat transfer process. This is complicated by the release, or absorption, of the latent heat of fusion at the “moving” solid-liquid interface [1]. The literature on phase change thermal problems, their formulation, solution, models and results is extremely rich [2-3]. Highlighting a key aspect connected to the present study, the research works realized by Sparrow et al. [4] and Kemink and Sparrow [5] clearly indicated the importance of natural convection during the solidification process, resulting in increasing of the solidification time of the PCM. From a modelling point of view, heat transfer in a PCM storage is a transient, non-linear

phenomenon with a moving solid-liquid interface, generally referred to as a “moving boundary” problem. Non-linearity is the source of the difficulties when solving numerically moving boundary problems. In order to ride out this inconvenience, some numerical methods have been proposed [6-8] and applied. Rao and Sastri [9] proposed an efficient numerical method that isolates the non-linearity associated with the moving interface and accurately tracks the interface movement. Voller [10] proposed an alternative discretization scheme for the enthalpy formulation which was based on separating the sensible and latent heat terms. This approach also resulted in a non-linear system of equations but with the non-linearity isolated as a source term of nodal latent heat. Kim and Kaviany [11] developed a highly accurate and efficient finite difference method for phase change problems with multiple moving boundaries of irregular shape by employing a coordinate transformation to immobilize moving boundaries and preserve the conservation form of the basic equations. A stable ADI method for simulating multi-dimensional solidification problems was proposed by Mampaey [12]. He substituted the explicit temperature calculation by an implicit one which was employed on a limited number of adjacent elements. Voller [13] presented a rapid implicit solution technique for the enthalpy formulation of the conduction controlled phase change problems. He examined three implicit schemes and proposed a new enthalpy solution scheme requiring no under or over relaxation. Lee and Tzong [14] proposed an enthalpy formulation for a phase change material having a distinct freezing temperature. Raw and Lee [15] reported a numerical formulation based on the weighting function scheme for convection-conduction phase change problems in which the solid phase is regarded as a liquid having an infinite viscosity. Rabin and Korin [16] presented a simple numerical technique for solving transient multi-dimensional heat transfer problems with melting or solidification processes. Clavier et al. [17] reported a fixed grid method using an updating iterative implicit scheme to solve one-dimensional phase change

problems. More recently, Lamberg [18] proposed an approximate analytical model for two-phase solidification problem in a finned phase-change material storage. Ismail et al. [19] studied the thermal performance of a PCM storage unit. In spite of the copious literature concerning the numerical simulation of the PCM melting process, few numerical contributions take into account the natural convection effect occurring in the liquid phase, that enhances heat transfer at the solid-liquid interface. In order to contribute to this subject, the present study is devoted to the validation of a numerical FEM based model for simulating the melting process of a paraffin. Numerical results, carried-out by a convection-conduction heat transfer model, are compared with experimental ones previously published [20].

## NOMENCLATURE

### Symbol

C	[J/(kg K)]	Specific heat at constant pressure
g	[m/s <sup>2</sup> ]	Acceleration of gravity
H	[J/m <sup>3</sup> ]	Specific enthalpy
k	[W/(m K)]	Thermal conductivity
p	[Pa]	Pressure
<b>U</b>	[m/s]	Velocity vector
t	[s]	Time
T	[K]	Temperature

### Greek symbols

β	[1/K]	Coefficient of thermal expansion
η	[Pa s]	Dynamic viscosity
Γ	[J/(K m <sup>3</sup> )]	Thermal capacity
ρ	[kg/m <sup>3</sup> ]	Density

### Subscripts

L	Liquid
S	Solid
SL	Solid-Liquid

## PROBLEM FORMULATION

Because of natural convection effect in the liquid phase, the governing equations for transient analyses of the PCM melting process include the Navier-Stokes equations, the continuity equation, and the energy equation. Under assumption of laminar and incompressible flow, invoking the Boussinesq approximation in modelling the buoyancy force, the governing equations can be written as follows:

$$\rho_L \frac{\partial \mathbf{U}}{\partial t} + \rho_L (\mathbf{U} \cdot \nabla) \mathbf{U} = \nabla \cdot [-p\mathbf{I} + \eta_L (\nabla \mathbf{U} + (\nabla \mathbf{U})^T)] + \rho_L g \beta (T - T_0) \quad (1)$$

$$\nabla \cdot \mathbf{U} = 0 \quad (2)$$

$$\rho_L C_L \frac{\partial T}{\partial t} + \rho_L C_L \mathbf{U} \cdot \nabla T = k_L \nabla^2 T \quad (3)$$

For the solid phase no convection effect have to be considered, so that heat transfer can be expressed by the following transient conduction equation:

$$\rho_S C_S \frac{\partial T}{\partial t} = k_S \nabla^2 T \quad (4)$$

In the solid-liquid interface the net amount of heat, which achieves the solid-liquid interface in a time unit, moves the distance of the phase change interface, which depends on the latent heat of the material. The energy balance for the solid-liquid interface can be expressed as:

$$k_S \left. \frac{\partial T}{\partial n} \right|_{\Omega} + h \Delta T_n = \rho_S L \frac{d\Omega}{dt} \quad (5)$$

where h is the convection heat transfer coefficient in the solid-liquid interface and  $\Delta T_n$  is the temperature difference between the “moving” solid-liquid interface and the boundary in the normal direction of the solid-liquid interface. One of the most used techniques for formulation and consequent solution of phase change problems is the enthalpy method [7]. In the enthalpy method, one single equation is used to solve both the solid and liquid domains of the problem. The method is based under the assumption that phase change happens with a small temperature variation, therefore  $\Delta T = T_L - T_S$ , where  $T_S$  is the temperature of the solid phase when the fusion process begins, while  $T_L$  is the temperature of the liquid phase once the medium is fully melted. This assumption can be considered as realistic for a large number of media employed for thermal storage. Let consider the specific enthalpy function during a global transformation involving solid state heating, melting process and liquid state superheating:

$$H(T) = \int_{T_1}^{T_S} \rho_S C_S(T) dT + \int_{T_S}^{T_L} \rho_{SL} \left[ C_{SL}(T) + \frac{dL}{dT} \right] dT + \int_{T_L}^{T_2} \rho_L C_L(T) dT \quad (6)$$

By defining the thermal capacity as:

$$\Gamma = \frac{\partial H}{\partial T} \quad (7)$$

From Eq. (6) and (7), we can write:

$$\begin{aligned} \Gamma &= \rho_S C_S && \Leftrightarrow && (T < T_S) \\ \Gamma &= \rho_{SL} \left( C_{SL} + \frac{L}{T_L - T_S} \right) && \Leftrightarrow && (T_S \leq T \leq T_L) \\ \Gamma &= \rho_L C_L && \Leftrightarrow && (T > T_L) \end{aligned} \quad (8)$$

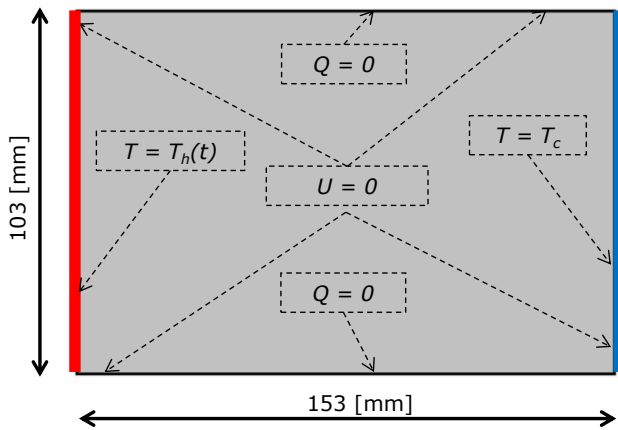
Being  $\rho_{SL}$  and  $C_{SL}$  evaluated as the average value of density and specific heat respectively between the solid and the liquid phase. Hence, one single equation can be used for solving temperature field both in solid and liquid phase, that reads as follows:

$$\Gamma \left( \frac{\partial T}{\partial t} + \mathbf{U} \cdot \nabla T \right) = k_{SL} \nabla^2 T \quad (9)$$

Where the thermal conductivity  $k_{SL}$  is the average solid-liquid value computed as defined above. From this formulation, it appears that Eq. (4) does not need to be solved for monitoring solid-liquid interface, that is just located in correspondence of the isothermal line defining the phase change temperature  $T_m = (T_L + T_S)/2$ .

## NUMERICAL MODEL

Equations (1), (2) and (9) are numerically solved by using the FEM based software Comsol Multiphysics v3.5a [21]. Because of the main goal of the present work consists in validating the adopted numerical approach, the considered physical system corresponds to that used by Wang et al. [20] in their experimental research. As a consequence, a rectangular enclosure with dimensions of 153 mm in width and 103 mm in height is considered filled by polyethylene glycol 900 (PEG900), whose geometry and applied boundary conditions are shown in Figure 1 and physical properties are reported in Table 1, both for solid and liquid phase.



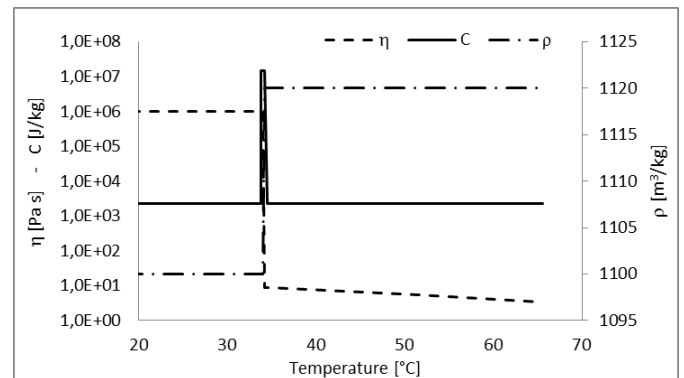
**Figure 1** Outline of geometry for physical system and indication of applied boundary conditions.

	Solid	Liquid
Density [ $\text{kg m}^{-3}$ ]	1100	1120
Specific heat at constant pressure [ $\text{J kg}^{-1} \text{K}^{-1}$ ]	2260	2260
Thermal conductivity [ $\text{W m}^{-1} \text{K}^{-1}$ ]	0.188	0.188
Coefficient of thermal expansion [ $\text{K}^{-1}$ ]	-	7.6E-4

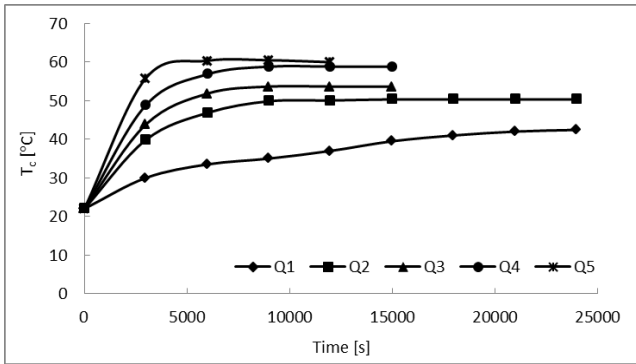
**Table I** Physical properties for PCM.

Momentum equations are solved overall the computational domain by adopting a smoothed Heaviside step function to locally define the viscosity value: for temperature higher than the melting temperature (liquid phase), the step function assumes values characterizing the real physical viscosity for the liquid; otherwise (solid phase), it assumes a chosen very high value ( $1\text{E}+6$ ), determining motion impossibility for the medium

with respect to the load conditions. The same strategy of implementation is adopted in order to define density and thermal capacity as functions of the temperature. For thermal capacity definition, a two-steps function is applied in order to take into account the contribution of the latent heat of fusion, exchanged throughout the solid-liquid interface, spatially identified by the local thermal conditions ( $T_S < T < T_L$  with  $T_L - T_S = 0.01 \text{ }^\circ\text{C}$ ). The continuous and derivable Heaviside functions used for simulations are graphically reported in Figure 2. As for the experimental apparatus used by Wang et al. [20], the cavity is differentially heated: the right vertical wall is kept at the constant temperature of  $22^\circ\text{C}$ , while heating is imposed at the hot left wall, applying a time-dependent temperature function. Horizontal walls are considered adiabatic. Five boundary heating conditions are simulated, using different time evolutions of temperature on the hot wall, as graphically reported in Figure 3. The melting temperature for the considered PCM is  $34 \text{ }^\circ\text{C}$  and the latent heat of fusion is  $150.5 \text{ kJ/kg}$ . From fluid-dynamical point of view, adherence conditions are applied at all boundaries. For all test-cases analysed (Q1, ..., Q5), at the initial conditions the system is at the rest and kept in solid state at the temperature of  $22 \text{ }^\circ\text{C}$ . Continuous equations are discretized by a finite elements method on a no-structured and no-uniform computational mesh made of triangular Lagrange elements of order 2. Influence of spatial discretization has been preliminary checked, in order to assure mesh-independent results. Finally, a computational grid made of about 30,000 elements has been retained for computations. Time-marching is performed by adopting an Implicit Differential-Algebraic (IDA) solver [22], based on a variable-order and variable-step-size Backward Differentiation Formulas (BDF). Because the time-marching scheme is implicit, a nonlinear system of equations is solved each time step by applying a modified Newton algorithm. Algebraic systems of equations coming from differential operators discretization have been solved by a PARDISO package, a direct solver particularly efficient in order to solve unsymmetrical sparse matrixes by a LU decomposition technique.



**Figure 2** Smoothed Heaviside step functions used for define viscosity (dashed line), thermal capacity (continuous line) and density (dashed-dotted line) as a function of the local temperature.

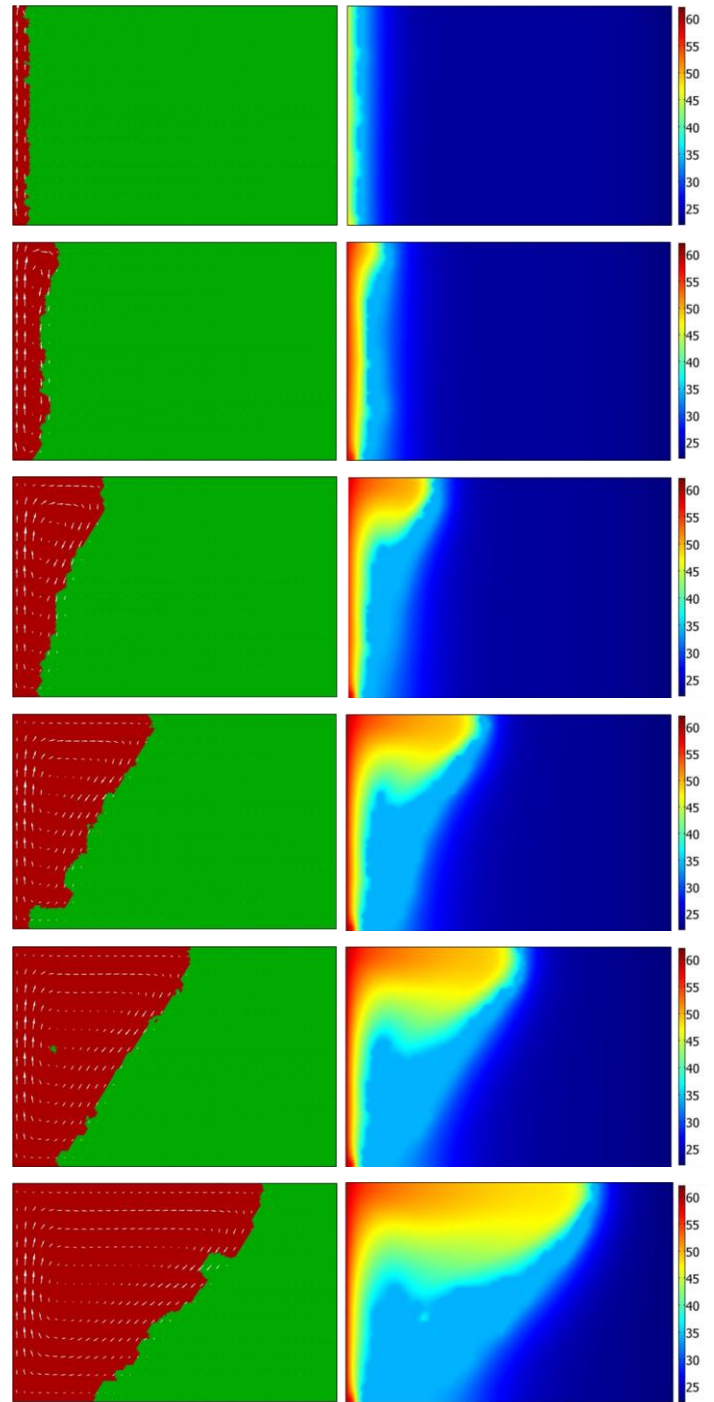


**Figure 3** Time-dependent boundary condition applied at the hot left wall for test-run labelled as Q1, Q2, Q3, Q4, Q5.

## RESULTS

As claimed by Wang et al. [20], in a rectangular enclosure with one of its vertical walls suddenly elevated to a higher temperature, a thin melt layer forms adjacent to the heated surface at the initial stage, indicating that conduction is the dominant mode of heat transfer. As time progresses, the buoyancy induces a flow due to temperature gradient causing the melt volume at the top to recede at a faster rate compared to the bottom of the enclosure. The onset of natural convection causes the liquid-solid interface to curve, thus augmenting the melting process. What above discussed finds good comparison in simulations' results obtained in the present study, as illustrated in Figures 4. For several time instants, Figures 3 report the portion of the volume occupied by the liquid and solid phase respectively, the velocity vectors and the temperature distribution inside the cavity. Results refer to the Q5 heating conditions. A post-processing logical function, labelled as B (if  $T < T_m$  then  $B=0$  else  $B=1$ ) is expressed in order to visualize the portion of the cavity where the PCM is at liquid or solid state respectively. Maps of B function values stand on the left side of Figures 4, highlighting by a red/green filling the liquid/solid phase. In these maps the white arrows identify vectors of the velocity field. As time is increased, fluid is propelled up by the thermal buoyancy, determining the onset of a convection roll in the left portion of the cavity. The convective structure grows with time and involves the solid-liquid interface to deform from its original almost vertical lying. The thermal transport induced by fluid motion is well appreciable from reported temperature fields in the right side of Figures 4. At the beginning of the process, isotherms appear almost vertical, indicating the conduction as the predominant mechanism in heat transfer. While melting progresses, the liquid motion induces a strong isotherms deformation, that assume a global shape similar to the well-known one characterizing natural convection of a single phase fluid in a rectangular enclosure. The motion field enhances heat transfer in top left region of the cavity, that induces an oblique lying of the moving solid-liquid interface. By exploiting the results presented by Wang et al. in their paper [20], we also quantitatively compared our numerical results with experimental ones gathered by the reference, in terms of temperature distribution along chosen horizontal planes for a

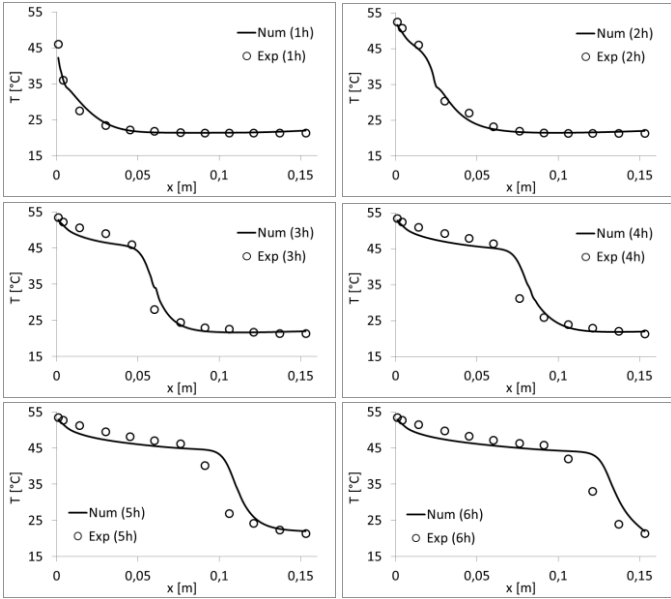
chosen time instant and referring to the different time-wise heating imposed (Q1-Q5).



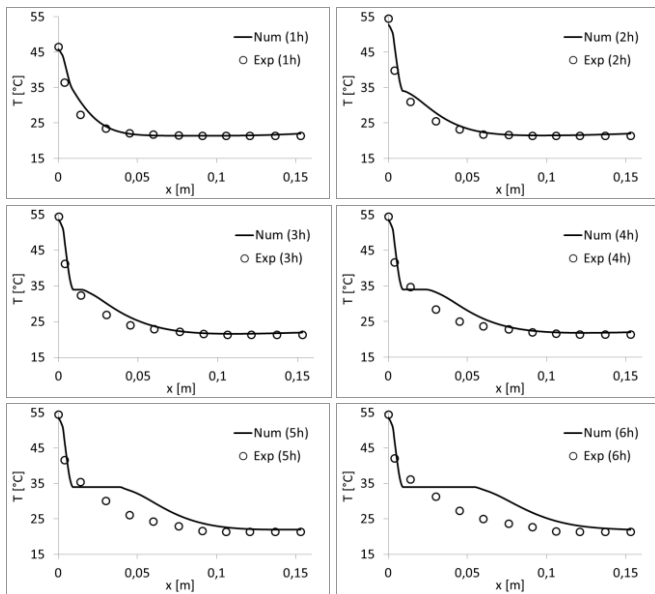
**Figure 4** Melting process for Q5 at several time instants (1800; 3600; 5400; 7200; 9000; 12000 [s]). On the left side: solid (green) and liquid (red) phase, velocity vectors (in white). On the right side: Thermal map on coloured scale.

Figures 5 and 6 report an extract of these comparisons: for instance, they refer to the Q3 test and report temperature values recorded each hour (the heating time was six hours) along the top (Figure 5) and the bottom (Figure 6) wall of the

cavity. Diagrams globally show a good agreement of simulated temperature values with experimental ones. It appears that curves referring to the top wall better fit with reference results than those describing thermal levels in correspondence of the bottom boundary. The numerical model highlights a large almost isothermal portion of the volume at the melting temperature.



**Figure 5** Comparison between present study results (Num) and reference [20] results (Exp): Temperature distribution along the top wall at several time steps.

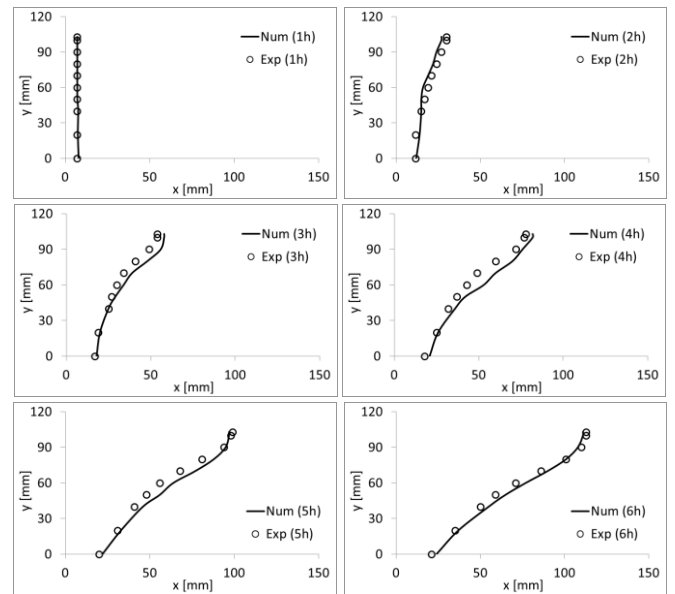


**Figure 6** Comparison between present study results (Num) and reference [20] results (Exp): Temperature distribution along the bottom wall at several time steps.

As a consequence, temperature distribution along the horizontal line lying on the bottom wall present evident discontinuities that have not been recorded by experimental acquisitions performed by Wang et al.. However, shaped curves comparable with ours are presented by Pal and Yoshi [23] in their work concerning an experimental and numerical analysis of the melting process in a side heated tall enclosure. Solid-liquid interface locations referring to test Q5 are also presented for different time and compared with Wang et al. results in Figure 7. The numerical curve refers to the 34 °C isothermal line. Comparison globally shows a good agreement.

## CONCLUSION

The melting process of a paraffin in a differentially heated rectangular enclosure is numerically simulated in this study. The enthalpy method is adopted for modelling heat transfer and the solid phase is regarded as a liquid having an almost infinite viscosity. The solid-liquid interface location and the thermal maps obtained for several transient heating conditions well highlight the natural convection effect, enhancing heat transfer in the top portion of the cavity. The results carried-out by simulations are successfully compared with experimental data previously published in literature and concerning an analogue system. The shapes of the melt front obtained at various times from computations well fit with experiments. Also, quantitative comparison between numerical and experimental results show good agreement. From comparisons, the proposed numerical approach appears validated and suitable for use in the pre-design of PCM storage systems.



**Figure 7** Comparison between present study results (Num) and reference [20] results (Exp): Solid-liquid interface location at several time steps..

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