A numerical study of PCM melting
heated from a vertical wall of a rectangular enclosure

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ABSTRACT

This paper presents the first research effort of our group to formulate, implement, and validate a numerical method in order to optimize the design of solar passive walls involving phase change materials (PCM). The fusion of ice, gallium, and the commercially available PCM 27 (hydrated salt), engineered by Cristopia and later embedded within an experiment unit, were studied. Comparisons against other prediction methods and experimental data for the fusion of gallium were carried out with good agreement of the solutions. The proposed enthalpy based method is found excellent to predict the fusion, but still fails to reproduce adequately the exact solidification pattern measured for the PCM 27. Further work is then undergoing to improve the model.

Keywords: phase change material, fixed-grid numerical method, enthalpy-porosity formulation, fusion.
NOMENCLATURE

A  Matrix coefficients
B  Porosity function
b  A small constant ($b=0.0003$)
C  Morphological constant in the Carman-Kozeny relation
c  Specific heat (J/kg.K)
f  Liquid fraction
g  Gravity vector (m/s²)
k  Thermal conductivity (W/m.K)
L  Latent heat of fusion (J/kg)
L_x  Length of rectangular enclosure in x direction (m)
L_y  Length of rectangular enclosure in y direction (m)
Pr  Prandtl number
p  Pressure (Pa)
R  Aspect ratio ($L_x/L_y$)
Ra  Rayleigh number
S  Source term
Ste  Stefan number
T  Temperature (K)
T_0  Initial temperature (K)
T_F  Melting point of materials (K)
T_w  Isothermal left wall temperature (K)
t  Time (s)
u  Velocity in the x direction (m/s)
v  Velocity in the y direction (m/s)
ΔV Control volume
x Component of x direction (m)
y Component of y direction (m)

Greek symbols
α Thermal diffusivity (m²/s)
β Expansion coefficient (K⁻¹)
□ Time step (s)
Γ Diffusion coefficient
μ Viscosity (kg/m.s)
ρ Density (kg/m³)
□ Generalized variable
ω Relaxation factor

Subscripts
c Interface position
F Fusion
h Enthalpy equation
l Liquid phase
P Present node
ref Reference temperature value
S Solid phase
W, E, P, N, S Respectively west, east, centre, north and south nodes
0 Initial value

Superscripts
k Iteration level
1. INTRODUCTION

The thermal latent energy storage provides more attractive features than its sensible counterpart. This is mainly due to its high energy storage density and to the isothermal nature of the storage process at the melting temperature of the material. Latent heat thermal energy storage systems find application in space craft, refrigerated cargo transport, solar energy system, greenhouses, and, with respect to this paper, also in heating and cooling of buildings.

The use of phase change material (PCM) for thermal storage in buildings was one of the first applications considered for such materials along with typical sensible heat storage reservoirs and enclosures. The works of Telkes [1975] and Barkman and al. [1975] were among the firsts to be published in the context of buildings heating and cooling. At that time, the petrol crisis alarmed anyone concerned with safe, abundant, and relatively cheap energy supplies. However, the perspective of development changed. In 1986, the work of Farid [1986] concluded that PCM do not offer economic savings for thermal storage at low temperatures, since these systems cost much more than their hot water based counterparts.

Nowadays, the context is changing. In the document entitled World Energy Outlook 2006, the International Energy Agency concludes that: «the world is facing twin energy related treats: that of not having adequate and secure supplies of energy at affordable prices and that of environmental harm caused by consuming too much of it». This statement, combined with ever increasing prices for fossil fuels, makes the economical viability increasingly interesting.

Today, PCM are the subject matter of several review papers: encapsulated materials used in plasterboard or packed beds are reviewed in a paper by Regin, Solanki, and Saini [2008]; PCM in buildings applications are the subject of the syntheses by Tyagi and Buddhi [2007] and Zhang and al. [2007] while general storage applications are reviewed in that of Sharma and al. [2007] and Farid and al. [2004]. Casedy’s book [2000] provides an overview of the applications.
In this context, the overall objective is here to insert PCM in a passive solar component such as the « composite Trombe wall » investigated by Zalewski and al. [2002]. However, optimized performances require parametric studies of relevant properties and dimensions, and therefore an appropriate design tool. This paper here presents the first steps of an effort aimed at formulating, implementing, and validating a numerical method to be used as such.

The objective of the present study is to numerically investigate the fusion process of a PCM brick in two dimensions. The numerical code is first validated by comparing the obtained results with 1D analytical, 2D numerical and experimental melting results available in the literature for two different materials, which are ice and gallium.

2. PHYSICAL PHENOMENON AND RELATED PREDICTION DIFFICULTIES

This section is only an overview of the basic difficulties encountered when a prediction method based on the solution of a mathematical model is required. The topic is exhaustively discussed in an excellent textbook on the subject [Bejan, 1995; Burmeister, 1993]. A specific recent review of mathematical modeling of latent heat thermal energy storage using PCM is provided by Verna and Singhal [2008]. During the early stages of the melting process, conduction is the dominant mode of heat transfer even within the liquid phase. This is followed by a short transition phase for which both conduction and natural convection occur. Then, as the melt volume increases, natural convection becomes dominant [Zhang and Bejan, 1989].

The first difficulty an analyst has to deal with, is the high nonlinearity of the governing equations which precludes the general use of analytical solutions. Other difficulties pertain to the time-dependence of location, shape, and orientation of the solid-liquid interface as well as that of the presence of a time-dependent « mushy » zone that may involve solid particles surrounded by the liquid phase next to the interface. Moreover, in the case of solidification, problems are even more complex : superfusion phenomena occur [Ehmimed, 2003]. In the experimental counterpart of the
numerical analysis proposed here, the solidification process analysis was found to be impossible to carry out because of the importance of superfusion within the PCM [Younsi and al., 2008].

3. PROPOSED MODEL

In the work presented here, the investigated material (hydrated salts) has a melting point (announced by the manufacturer) equal to 27°C [Cristopia]. The phase change material samples are 210x140x25 mm³ parallelepiped elements. As the bricks of PCM used – hereafter called PCM 27 – have to be installed vertically in a wall, a two-dimensional behavior is assumed. Several approximate analytical solutions have been worked out for problems involving a pure substance [Poots, 1962] or even two substances [Rathjen and al., 1971; Budhia and al., 1973]. But as soon as the geometry or the material is complex, they are no longer amenable to provide solutions.

Hence, numerical solutions of the governing equations are generally proposed. Some of these formulations are temperature-based methods while others base their mathematical model upon enthalpy. The first ones rely on the prediction of the front of fusion/solidification while the other, much easier to implement, does not.

In the mathematical model involved herein, the enthalpy formulation is used, because the following advantages take place: (1) the governing equations are similar to the single phase equations, (2) there is no explicit condition to be satisfied at the solid-liquid interface; (3) the enthalpy formulation involves the solution within a mushy zone, involving both solid and liquid material, between the two standard phases; and (4) the phase change problem becomes much easier to solve.

In this work, as an overall method is sought for the prediction of a complete set-up embedding different brick arrangements and sizes, the enthalpy formulation has been retained. The temperature based methods that follow the progression of the interface position could be too complex to implement in an upcoming three dimensional context.
The enthalpy (or weak) formulation has been the subject matter of several publications [Bénard, Gobin, and Martinez, 1985; Gadgil and Gobin, 1984; Gobin, 1984; Ho and Viskanta, 1984; Lacroix and Voller., 1992; Lacroix and Garon, 1990; Lacroix, 1989; Lacroix, 1992; Okada, 1984; Viswanath and Jaluria.,1993; Webb and Viskanta, 1986]. Independently of the formulation retained, several numerical methods have been used to implement PCM. Here, a finite volume method (FVM) formulated for the solution on Cartesian grids was retained [Patankar, 1980]. As both the weak formulation of the melting problem and the finite volume methods have been the subject of several publications, they will not be repeated here to avoid making this paper overly lengthy. The interested reader should consult the paper by [Voller, 1990] or the text book by [Patankar, 1980] for details.

3.1 GEOMETRY AND GENERAL BOUNDARY CONDITIONS

A validation procedure has been carried out to later simulate the melting of PCM 27 bricks. In this procedure, the following geometry was used for both ice and pure gallium. Figure 1 shows a rectangular two-dimensional cavity (brick) of length $L_x$ and height $L_y$ subject to the following boundary conditions:

- **Heated surface (left surface, $x = 0, y, t$)**
  \[ u=v=0 \quad T=T_v \]

- **Solid / liquid interface ($x = x_c, y = y_c, t$)**
  \[ u=v=0 \quad T=T_f \]

- **Cooling surface (right surface, $x = L_x, y, t$)**
  \[ u=v=0 \quad T=T_0 \]
Top \((x, y=0, t)\) and bottom \((x, y=L_y, t)\) surfaces

\[ u=v=0 \quad \frac{\partial T}{\partial y}=0 \]

where \(T_0>T>T>0\)

[Insert figure 1 about here]

### 3.2 RELEVANT ASSUMPTIONS

To obtain a solution of the governing equations [Voller, 1997; Patankar, 1980], several assumptions are essential to understand the limits of the validity of the selected method:

1. The problem is two-dimensional.
   
   Strictly speaking, edge effects should be taken into account for a single brick of material. But, these bricks will be inserted into a wall into which the heat transfer is nearly one-dimensional. Hence, the two-dimensional behavior is retained to account for natural convection within the bricks.

2. The horizontal walls are adiabatic.
   
   This allows for a one-dimensional comparison with standard solutions for the Neumann problem, and the vertical heat fluxes \((y\text{-direction})\) will indeed be quite negligible compared to those in the horizontal direction \((x\text{-direction})\).

3. Conduction occurs in both phases.
   
   This is strictly true with thermophysical properties that may differ.

4. Natural convection occurs in the liquid phase.
   
   The Neumann one-dimensional solution is only for conduction but the two-dimensional
solutions proposed here will account for natural convection within the liquid phase.

5. Radiative heat transfer is neglected.

The temperature gradients are small and the overall temperatures are low. Consequently, it is assumed that any radiation heat transfer is accounted for in the effective thermal conductivity.

6. The flow in the liquid phase is Newtonian, laminar, incompressible, and the Boussinesq approximation holds.

7. Viscous dissipation is neglected.

The liquid phases of either ice or gallium as well as that of PCM 27 have low viscosities and this assumption holds.

8. Thermophysical properties are constant.

Although different in the liquid and the solid phases, densities, heat capacities, and thermal conductivities are assumed to remain constant with time and to be independent of temperature. Properties for PCM 27 are determined experimentally while standard properties are taken from the literature for water and gallium. In the liquid phase, an effective thermal conductivity is obtained and this eases the comparison with the standard one-dimensional Neumann solutions.

9. The PCM material is pure, homogeneous, and isotropic.

This is certainly not the case for a hydrated salt as shown in figure 2 for the crystallization of PCM 27, but once again the main idea is to propose a design tool and the assumption is not too bad as the fusion process displays much less discontinuities than its solidification
counterpart.

10. The effect of thermal expansion is neglected.

Indeed, the brick involves an air space within its polyolefin envelope that will act as a buffer to take the solidification related expansion. Accounting for expansion does not modify the overall thermophysical properties observed here.

During the fusion process, three different states coexist, the fully liquid state, the solid state, and the “mushy” region, involving a mixture of solid particles surrounded by liquid.

[Insert figure 2 about here]

3.3 MATHEMATICAL MODEL

Based on the above assumptions, the governing equations for the heat transfer melting process are as follows:

Solid region:

\[
\frac{\partial T}{\partial t} = \alpha_s \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right]
\]  

Liquid region:

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0
\]  

\[
\rho_l \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = -\frac{\partial p}{\partial x} + \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + Bu
\]  

\[
\rho_l \left( \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = -\frac{\partial p}{\partial y} + \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + \rho g \beta (T - T_{ref}) + Bv
\]  

\[
\left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = \alpha_s \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) - \frac{L}{c_l} \frac{\partial f}{\partial t}
\]
In the enthalpy-porosity approach, the condition that sets the velocities in the solid regions is provided by appropriately defining a parameter $B$ in the momentum equations [Brent, 1988]. The basic principle is to reduce gradually the velocities from a finite value in the liquid to zero in the solid, over the computational cell that undergoes phase change. This can be achieved by assuming that such cells behave like a porous media with a porosity equal to the liquid fraction. In order to achieve this behavior, an appropriate definition of $B$ is:

$$B = -\frac{C(1 - f)^2}{(f^3 + b)}$$

which is the Carman-Kozeny relation. In this model, $f=1$ in the liquid region while $f=0$ in the solid region while it takes a value between 0 and 1 in the mushy zone. The constant $C$ has a large value to suppress the velocity as the cell becomes solid and $b$ is a small constant used to avoid a division by zero when a cell is fully located in the solid region, namely $f = 0$. The choice of the constants is arbitrary. However, the constants should ensure sufficient suppression of the velocity in the solid region and should not influence the numerical results significantly. In this work, $C = 1 \times 10^9 \text{ kg/m}^3 \text{ s}$ and $b = 0.0003$ are used [Viswanath and Jaluria, 1993].

The relevant dimensionless parameters are then:

$$Ra = \frac{\rho c_i g \beta_i \beta_f}{\mu k_i} \left( T_w - T_f \right)$$

$$Ste = \frac{c_i \left( T_w - T_f \right)}{L}$$

$$Pr = \frac{c_i \mu}{k_i}$$

which are respectively, the Rayleigh, Stefan, and Prandtl numbers. The overall formulation is nondimensionalized to enable comparisons with several test cases found in the literature. This dimensionless model is provided in Appendix 1.
As recommended by Patankar [1980], a single algorithm can be used where all the equations can be casted into a general form. Here, equations (1-5) can be formulated such that:

$$\frac{\partial (\rho \phi)}{\partial t} + \nabla \cdot (\rho V \phi) = \nabla \cdot (\Gamma \nabla \phi) + S$$  \hspace{1cm} (11)

where the appropriate variables for this problem are specified in Table 1:

[Insert Table 1 about here]

The phase change was handled using a single-domain with an enthalpy porosity technique [Brent, 1988]. In this method, the absorption of latent heat during melting is included as a source term $S_h$ in the energy equation (Table 1). Latent heat content of each control volume in the PCM is evaluated after each energy equation iteration cycle. Based on the latent heat content, a liquid fraction for each control volume is determined. For control volumes containing a liquid phase of PCM, $f$ is set to 1, and for control volumes containing solid phase, $f$ is set to 0. The control volumes with values of $f$ between 0 and 1 are treated as mushy. Even though the phase change is assumed to be isothermal, the idea of mushy zone is introduced to gradually switch off the velocities from liquid to solid at the interface. The switching off is controlled by the source terms $S_u, S_v$ in the momentum equations (Table 1).

3.4 NUMERICAL PROCEDURE

The conservation equations are discretized by a finite-volume method on a uniform Cartesian grid. The coupled energy-liquid fraction, resulting from the use of an enthalpy formulation, is handled by the procedure suggested by Brent and al. [1988]. The SIMPLER algorithm is used to solve the coupled continuity and momentum equations. This code is fully implicit in time, for transient computations, and the convection-diffusion terms are treated by the hybrid scheme [Patankar, 1980]. A line by line solver based on the TDMA (tri-diagonal matrix algorithm) is used to solve
The general form of the discretized equation for any variable $\varphi$ is given by

$$ A_p \varphi_p = \sum_{i=W,E,N} A_i \varphi_i + S $$

(12)

For each iteration, the solid-liquid interface has to be determined. In this work, it is based on the value of the liquid fraction. The liquid fraction is updated using the equation:

$$ f_p^{k+1} = f_p^k + \omega \frac{\Delta t A_p h_p}{\rho L \Delta V} $$

(13)

where $\omega$ is an appropriate under-relaxation factor.

To prevent the calculation of unrealistic values for $f$, variations of $f_p$ from one iteration to the next are limited by use of:

$$ f_p^{k+1} = \begin{cases} 1 & \text{if } f_p^{k+1} > 1 \\ 0 & \text{if } f_p^{k+1} < 0 \end{cases} $$

(14)

Hence, despite the particular additions to the momentum and energy equations with respect to a standard mathematical description, the procedure proposed by Patankar [1980] can readily be used to obtain discretized algebraic equations, to incorporate boundary conditions, to solve, and to provide relevant dependent variables via an adequate post-processing. Suffice it to say that for a given time step, when a converged solution is obtained for the discretized algebraic equations, the dimensionless liquid fraction is updated until no further change is detected in the solution for this particular time step. Then, the procedure proceeds with the next time step until $t_{\text{max}}$ is reached.

4. SPECIFIC TEST PROBLEMS

4.1 MELTING OF ICE

Problem specification

The first test problem used to assess the correct implementation and set-up of the numerical analysis tool is that of ice melting for which several numerical [De Groh III and Lindstrom, 1994] and
experimental [Kowalewski and Rebow, 1997] solutions can be found. The following thermal characteristics were used for water and ice: \( k_l = 0.606 \text{ W/m.K} \), \( k_s = 1.92 \text{ W/m.K} \), \( c_l = 4181 \text{ J/kg.K} \), \( c_s = 1960 \text{ J/kg.K} \), \( \rho_l = 1000 \text{ kg/m}^3 \), \( \rho_s = 917 \text{ kg/m}^3 \). The latent heat of fusion, which occurs at \( T_F = 273.15 \text{ K (0°C)} \), is \( L = 333.4 \text{ kJ/kg} \) and the characteristic length of the enclosure, \( L_c \) is 0.2 m. The heating is provided by a temperature difference of 25\(^\circ\)C. Initially, the ice is considered to be at \( T_0 = 268.15 \text{ K} \) and suddenly, the left wall temperature is set at \( T_w = 293.15 \text{ K} \).

The relevant dimensionless parameters are \( Pr = 0.69; Ste = 0.251, c_s/c_l = 0.469, \) and \( k_s/k_l = 3.168 \). The Rayleigh number for aspect ratios \( R = 0.5; 1; 4 \) is \( 2.25 \times 10^{10}; 2.82 \times 10^9; \) and \( 4.4 \times 10^7 \), respectively.

**Numerical details**

One-dimensional and two-dimensional numerical analyses have been carried out. The one-dimensional solution was validated by comparing the numerical predictions with the analytical solution for the classical Stefan problem. These results are not presented here to avoid making this paper overly lengthy.

For the two-dimensional test, several grids were used in conjunction with different time steps until an optimal set of domain discretization parameter was obtained. The aspect ratio involved in the first problem is \( R = 1 \). Figure 4 shows the calculated melting interface location with different time steps (\( \Delta t = 1s, \Delta t = 5s \) and \( \Delta t = 10s \)). The interface is shown for three different times (\( t = 10000s, t = 20000s \) and \( t = 30000s \)) from the onset of melting.

The effects of grid density and of the under-relaxation factor on the liquid fraction formation are shown respectively in figure 5 and figure 6. The convergence criteria were to reduce the maximum residual in all the dependent variables, namely temperature and the velocities to be less than \( 10^{-7} \).

An increase in the grid size from \( 80 \times 80 \) cells to \( 100 \times 100 \) cells produced a maximum difference in the numerical results for liquid fraction of 5%. Based on the results, a \( 90 \times 90 \) uniform square grid
was employed for the final computations. The maximal discrepancy for the under-relaxation factors from $\omega_h=0.1$, $\omega_u=\omega_v=0.3$ to $\omega_h=\omega_u=\omega_v=0.3$ is found to be 4%.

Hence, the simulations are carried out with the following numerical parameter values: under-relaxation factors $\omega_h=0.1$, $\omega_u=\omega_v=0.3$, time step $\Delta t=5s$ and grid data $(90 \times 90)$.

**Results**

Figure 7 shows the curve of the liquid fraction for different aspect ratios $R$ (Table 3) to compare with that obtained into one-dimensional simulations. It is noticed initially that the convection heat transfer accelerates the process of ice fusion. At the beginning of fusion, the thermal transfer is governed by conduction, both in one-dimension and two-dimensions. Then, it is the convection which dominates the thermal transfer into two-dimensional problems.

An indication of the natural convection phenomenon appears in figure 7. The liquid formation is different when simulations are performed in 1D and in 2D, in the phase where convection occurs. 2D results for the three different aspect ratios are very similar, especially in the final stages of the liquid formation. When natural convection begins to dominate the heat transfer, the shape of the liquid fraction curve is slightly changing when increasing the aspect ratio, before reaching a quasi steady state. Thanks to these curves, the fusion rates can be estimated in 1D and in 2D. This rate is always larger when convection occurs than in the pure conduction case, especially when the aspect ratio is important, meaning that convection dominates in the top of the cavity, shrinking the progression of the solid-liquid interface at the bottom.

In figure 8, the melting position interface is shown at different times, for the three different aspect ratios studied. Simulations have been performed in 1D and in 2D. Comparing the 1D and 2D effects, the interface always moves faster in the 2D simulations than in the 1D case. When the thickness of liquid fraction increases with time, the interface develops a curved shape. Similar
results have been found by several authors (Yanxia 2007, Hamdan 1996).

It can be noticed from this figure that the rate at which the interface progresses at the top of the brick is always larger than at the bottom, where natural convection has a smaller effect. Once again, this figure shows the large difference for this interface when natural convection is not taken into account.

For an aspect ratio $R=1$, convection dominates the heat transfer and at $t=40000$ s, the solid-liquid interface has reached the upper part of the cold wall, whereas this interface is located at mid position in the bottom of the enclosure. On the other hand, for a bigger aspect ratio $R=4$, the interface is almost vertical, meaning that the conduction plays an important role in the heat transfer.

**Discussion**

Results presented here first indicate that the 1D solution that neglects convection falls short from predicting the thermal behavior of ice as it melts. And this is of course worst as the melting front propagates within the domain thus increasing the liquid phase ratio.

**4.2 MELTING OF GALLIUM**

**Problem specification**

As a second benchmark problem, the melting of gallium was considered. Several numerical solutions involving temperature and enthalpy based methods can be found in the literature [Lacroix, 1990; Viswanath and Jaluria, 1993; Dessai and Vafai, 1993], as well as experimental results (Gau and Viskanta, 1986; Gong, 1996). The relevant thermophysical and physical properties for the problem are provided in Table 4.

[Insert Table 4 about here]

As a result, the following dimensionless parameters were obtained and shown in Table 5.
Numerical details

As for the previous problem for ice, several cells of different sizes or proportions, as well as time intervals are used to ascertain that the solutions are independent of the discretization. The relevant grid size, time step, and under-relaxation factors for the momentum and energy equation are for the 2D simulations: $50 \times 50$, $\Delta t = 1s$, $\omega_h = 0.6$ and $\omega_u = \omega_v = 0.8$.

A closer look at past published works about gallium and melting problems shows that most authors specify that their solution is grid independent. Viswanath and Viskanta [1993] obtained a change of 3% in their results when the grid was refined from $30 \times 20$ to $50 \times 40$ and concluded that this change is acceptable.

Results

Figure 9 presents several results: those obtained with the proposed genuine 2D FVM code, those obtained by means of an one-dimensional conduction analysis, those proposed by Lacroix for the same problem ($R=2$) but with a temperature based model, and finally the experimental results given by Gau and Viskanta [1986] and Gong [1996].

In this figure, it can be noticed that the FVM model is in agreement with the results of the references mentioned above. For the prediction of the position of fusion front obtained from the FVM code and from the experiments of Gau and Viskanta [1986], one records a small variation which is due to two possible reasons. Initially, it is necessary to take account of the subcooling of the solid phase. Indeed, the experiment of Gau and Viskanta [1986] revealed that the block of gallium was initially at a temperature of 2°C under its melting point (29.78°C). This subcooling of metal has determined consequences on the course of the experiment, because on the one hand, the heated wall is only at 8°C above the melting point, and on the other hand, the thermal conductivity
of the material ($k=32 \text{ W/m.K}$) is high. Moreover, the temperature of the cold wall was not constant during their experiment. The second reason is that it is difficult to heat impulsively a vertical wall at a desired temperature (discussed in Kim and al., 2001). Concerning the difference between the FVM model and that of Lacroix, it is due to the difference of the numerical methods employed. Lacroix used a method involving a mobile grid, while this FVM model employs the enthalpic method with a fixed grid to model the effects of change phase. At 5 min, the two numerical methods provide results close to the two experimental sets of data concerning the bottom of the enclosure. At the top of the brick, the present FVM results seem to be in good agreement with the temperature-based method used by Lacroix. At 8 min, the discrepancy between all the results is not too large, especially between the FVM results and the experimental ones of Gong. On the other hand, at 12 min, there is a great concordance between the FVM results and the experimental ones of Gau and Viskanta, except for the bottom region. It should be noticed that, at this time, the temperature based method provides numerical results closer to the experimental results of Gong, and there is a large discrepancy between the two numerical methods. However, at the top end of the rectangular enclosure, all the results tend to converge.

[Insert figure 9 about here]

In Figure 10, the numerical predictions code is verified by comparison with the experimental results of Gau and Viskanta [1986], with the transformed-grid results by Viswanath and Jaluria [1993], and, finally, the finite element solutions obtained by Dessai and Vafai [1993] for the melting of a pure metal (gallium) inside a two-dimensional rectangular cavity ($R=1.4$). Figure 10 shows the solution for the displacement of the solid-liquid interface obtained by the proposed numerical FVM formulation and those by the studies mentioned above. The transformed-grid method gives good agreement with the experimental data at 5 min and at 10 min. However, at 19 min, these results of Viswanath and Jaluria present much more discrepancies with the experimental data of Gau and Viskanta. The finite element method used by Dessai and Vafai seems to provide better results at 19
than the finite volume method. One can notice that all the numerical results at 19 min present more discrepancies with the experimental data than those obtained at 5 min and 10 min. Hence, a somewhat good agreement is observed between the present method and the experiments of Gau and Viskanta, particularly at 5 and at 10 minutes. However, the simulations appear to be slightly offset at 19 minutes as the melting front is behind that proposed by other solutions at the top of the cavity while it is in front at the bottom. Nevertheless, remembering the relative simplicity of the numerical formulation (enthalpy based), accounting for the assumptions formulated to solve the problem, and considering the uncertainty of the experimental results, the numerical predictions are satisfactory.

Numerical study of Kim and al [2001] shows that the delayed heat-up affects the melting process and causes the discrepancy between the numerical and experimental results. Their numerical method with delayed heat-up provides better agreement with the results of Gau and Viskanta, especially at 19 min.

The difference between the two configurations is the aspect ratio, in the first case the value of the aspect ratio is 2 and in second case 1.4 (figure 11). When the Rayleigh number increases, the difference between 1D and 2D solutions is larger showing the inadequacy of the Stefan solution.

4.3 MELTING OF PCM 27

Problem specification

PCM 27 was considered for simulation using the proposed FVM method. The thermophysical properties of relevant parameters used here were measured and reported in Table 6.
As a result, the following dimensionless parameters were obtained in Table 7.

[Insert Table 7 about here]

**Numerical details**

Several domain discretizations were studied in 2D. Mesh deployment has been used to refine the discretization along the hot wall \( (x=0) \). A \( 80 \times 100 \) grid was found to be satisfactory to obtain converged solutions, with \( \omega_h=\omega_u=\omega_v=0.1 \). The appropriate time step used was found to be problem dependent: different temperature scales (differences between the hot and the cold surfaces) were found to require different time steps. The ensure independence, \( \Delta t = 1s \), was used for all calculations. Calculations were carried out for conditions used in the experiments.

**Results**

Figure 12 shows and compares the curves for the liquid fraction obtained in one-dimensional (Stefan solution) and two dimensional simulations. Results indicate that the fusion rate is dominated by conduction as the liquid fraction evolves much faster for the 1D than for the 2D simulations. For the later, convection takes place in the upper part of the cavity while the liquid fraction remains much less important at the bottom. The 1D solution cannot predict convection and, here again, although very easy to implement, it should not be used as a suitable prediction method.

[Insert figure 12 about here]

Figure 13 shows the calculated melting interface location for five different times \( (t=1000s, t=10000s, t=20000s, t=30000s, \) and \( t=40000s \) ) from the onset of melting. At the time \( t=1000s \), the solid-liquid interface is almost vertical, suggesting the dominance of the conduction regime. As the process continues, the fusion is influenced by convection. As time increases, buoyancy induces the motion of the fluid due to the temperature gradient, and then causes the liquid volume at the top to move at a faster rate compared to the fluid at the bottom. This becomes more obvious for the melt
interfaces at times $t=10000-40000$ s, which are curved due to the effect of the natural convection, thus augmenting the overall melting process.

Figure 13 also shows the corresponding melting front location for one-dimensional simulations. These results confirm those shown in figure 12 for which the overall liquid fraction is always more important for the 1D simulations than for its 2D counterpart.

5. CONCLUSION

In this paper, a preliminary numerical work is conducted to study the thermal behavior of a PCM to be used as a latent heat reservoir in a specific building application. The proposed parallelepipedic-shaped brick of such PCM is heated from the side: this simulates the solar irradiation impinging on a vertical wall.

An enthalpy-based mathematical model is proposed to analyze PCM behavior. The solution is obtained by use of a control volume-based finite difference method. The proper formulation and implementation of the method has been verified by applications to two materials for which solutions are well documented in the literature: namely, ice and gallium.

The proposed solutions are found to be in good agreement with both existing experimental results and numerical predictions.

One dimensional predictions, based upon the well known Stefan solution, were found to be in poor agreement with those accounting for natural convection in the liquid phase.

The model has then been applied to predict the thermal behavior of PCM 27, a material designed to melt at 27°C. Here again, natural convection played an important role after the first stages of melting that were dominated by conduction. The hydrated salts behave like the former materials (ice and gallium) that is buoyancy effects become more and more important at later stages of the fusion process.

Globally, the proposed enthalpy based method was found satisfactory to predict the melting of the
Current efforts are aimed at predicting the thermal behavior of the MCP by use of the Fluent commercial code. The validation will be carried out with both FDM predictions for selected cases and experimental measurements. Another current activity deals with the thermal characterization of solid walls involving several bricks of MCP arranged along different patterns and thicknesses.


Gong Z-X.,“ Time-Dependent Melting and Freezing Heat Transfer in Multiple Phase Change Materials“, Thèse de Doctorat, Department of Chemical Engineering, McGill University, Canada, 1996.


Tyagi, V.V., Buddhi, D., PCM thermal storage in buildings: A state of art, Renewable and Sustainable Energy Reviews, Vol. 11, No. 6, 1146-1166, 2007


APPENDIX 1: DIMENSIONLESS FORMULATION

To allow a direct comparison between our two test cases (ice and gallium) and the proposed hydrated salt (PCM27) used in the experiments, the dimensionless governing equations [Voller, 1997; Patankar, 1980] are undimensionalized with respect to the following variables:

\[ X = \frac{x}{L_y}, \quad Y = \frac{y}{L_y}, \quad U = \frac{uL_y}{a_L}, \quad V = \frac{vL_y}{a_L}, \quad \theta = \frac{(T - T_F)}{T_w - T_F} \]

\[ P = \frac{pL_y^2}{\rho a_L^2}, \quad \alpha = \frac{a_s}{a_L}, \quad F_0 = \frac{t a_L}{L_y}, \quad B = \frac{B L_y}{\rho a_L}, \quad B = \frac{C(1 - f)^2}{(f^3 + b)} \]

Here, parameter B* arises from the Darcy [Viswanath et al., 1993] model used to set velocities at zero at the solid-liquid interface.

Hence, the mathematical description of the problem can be written as:

**Solid region:**
\[ \frac{\partial \theta}{\partial F_0} = \frac{\alpha_i}{\alpha} \left( \frac{\partial^2 \theta}{\partial X^2} + \frac{\partial^2 \theta}{\partial Y^2} \right) \] (11)

**Liquid region:**

\[ \frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} = 0 \] (12)

\[ \frac{\partial U}{\partial F_0} + U \frac{\partial U}{\partial X} + V \frac{\partial U}{\partial Y} = -\frac{\partial P}{\partial X} + \text{Pr} \left( \frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2} \right) + BU \] (13)

\[ \frac{\partial V}{\partial F_0} + U \frac{\partial V}{\partial X} + V \frac{\partial V}{\partial Y} = -\frac{\partial P}{\partial Y} + \text{Pr} \left( \frac{\partial^2 V}{\partial X^2} + \frac{\partial^2 V}{\partial Y^2} \right) + RaPr\theta + BV \] (14)

\[ \frac{\partial \theta}{\partial F_0} + U \frac{\partial \theta}{\partial X} + V \frac{\partial \theta}{\partial Y} = \left( \frac{\partial^2 \theta}{\partial X^2} + \frac{\partial^2 \theta}{\partial Y^2} \right) - \frac{1}{\text{Ste} dF_0} \frac{\partial f}{\partial \theta} \] (15)

Equations (11) and (15) may be written as:

\[ \frac{\partial \theta}{\partial F_0} + U \frac{\partial \theta}{\partial X} + V \frac{\partial \theta}{\partial Y} = \alpha \left( \frac{\partial^2 \theta}{\partial X^2} + \frac{\partial^2 \theta}{\partial Y^2} \right) - \frac{1}{\text{Ste} dF_0} \frac{\partial f}{\partial \theta} \] (16)

where

\[ \alpha = f + (1-f) \frac{\alpha_i}{\alpha} \] (17)

In this way, in the liquid zone \( \theta > 0, f = 1 \), \( \alpha = 1 \), and in the solid zone \( \theta < 0, f = 0 \), \( \alpha = \frac{\alpha_i}{\alpha} \).

The term \( S_h = -\frac{1}{\text{Ste} dF_0} \frac{\partial f}{\partial \theta} \) takes into account the latent heat due to phase change.

Using the variables (7), undimensionalized boundary conditions are:

**Heated surface:**

\[ \theta_{i,j} = 1 \]

**Cooling surface:**

\[ \theta_{i,j} = \frac{T_0 - T_F}{T_w - T_F} \]
Top wall: \( \theta_{i,1} = \theta_{i,2} \)

Bottom wall: \( \theta_{i,N} = \theta_{i,N-1} \)
Figure 1: Schematic of the problem.

Figure 2: PCM 27 in a state of recrystallization.
Discretization of the dimensionless calculation domain

Discretization of the governing dimensionless equations

Incorporation of initial and boundary conditions

Updating

Solution for and

Pressure correction

Solution for and

Convergence?

\[ t \geq t_{\text{max}}? \]

No

Yes

Updating of the dimensionless liquid fraction

Increment in time

Post-processing

END

Figure 3: Solution algorithm.
Figure 4: Effect of time step on front fusion at three different times.
Figure 5: Effect of grid density on liquid fraction

Figure 6: Effect of under-relaxation factor on liquid fraction
Figure 7: Comparison with numerical results for the effect of aspect ratio on liquid formation for ice melting.
Figure 8: Comparison with numerical results for the effect of aspect ratio on liquid formation for melting of ice
Figure 9: Comparison of melt interface with experimental results for melting of gallium (R=2)

Figure 10: Comparison of melt interface with experimental result for melting of gallium (R=1.4)
Figure 11: Comparison with numerical results for the effect of aspect ratio on liquid formation for melting of gallium.

Figure 12: Comparison of numerical 1D and 2D results for the predicted evolution liquid fraction of PCM 27 with time.
Figure 13: Comparison with numerical results at different times for melting of PCM 27.

<table>
<thead>
<tr>
<th>Equation</th>
<th>$\phi$</th>
<th>$u$</th>
<th>$r$</th>
<th>$s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$T$</td>
<td>0</td>
<td>$[k/c_p]_s$</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>$u$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>$u$</td>
<td>$u$</td>
<td>$S_u = -\frac{\partial P}{\partial x} + Bu$</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$\nu$</td>
<td>$u$</td>
<td>$S_v = -\frac{\partial P}{\partial y} + Bv + \rho g \beta (T - Tr)$</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>$T$</td>
<td>$u$</td>
<td>$[k/c_p]_l$</td>
<td>$S_h = -L \frac{\nu}{c_i} \frac{\partial f}{\partial t}$</td>
</tr>
</tbody>
</table>

Table 1: Coefficients for the general equations
<table>
<thead>
<tr>
<th>Variables</th>
<th>Ice</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$ (W/m.K)</td>
<td>1.92</td>
<td>0.606</td>
</tr>
<tr>
<td>$c_p$ (J/kg.K)</td>
<td>1960</td>
<td>4181</td>
</tr>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>917</td>
<td>1000</td>
</tr>
<tr>
<td>$\alpha$ (m$^2$/s)</td>
<td>$1.07\times10^{-6}$</td>
<td>$1.45\times10^{-7}$</td>
</tr>
<tr>
<td>$L$ (kJ/kg)</td>
<td>333.4</td>
<td></td>
</tr>
<tr>
<td>$L$(m)</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>$T_0$ (K)</td>
<td>268.15</td>
<td></td>
</tr>
<tr>
<td>$T_F$ (K)</td>
<td>273.15</td>
<td></td>
</tr>
<tr>
<td>$T_w$ (K)</td>
<td>293.15</td>
<td></td>
</tr>
</tbody>
</table>

Table 2: Data specifications for the melting of ice.

<table>
<thead>
<tr>
<th>$R$</th>
<th>$R_a$</th>
<th>$P_r$</th>
<th>$S_t$</th>
<th>$c_s/c_l$</th>
<th>$k_s/k_l$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>$2.25\times10^{10}$</td>
<td>6.90</td>
<td>0.251</td>
<td>0.469</td>
<td>3.168</td>
</tr>
<tr>
<td>1</td>
<td>$2.82\times10^{9}$</td>
<td>6.90</td>
<td>0.251</td>
<td>0.469</td>
<td>3.168</td>
</tr>
<tr>
<td>4</td>
<td>$4.4\times10^{7}$</td>
<td>6.90</td>
<td>0.251</td>
<td>0.469</td>
<td>3.168</td>
</tr>
</tbody>
</table>

Table 3: Dimensionless parameters for the melting of ice.
<table>
<thead>
<tr>
<th>variable</th>
<th>Solid</th>
<th>liquid</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$ (W/m.K)</td>
<td>32</td>
<td>32</td>
</tr>
<tr>
<td>$c_p$ (J/kg.K)</td>
<td>381,5</td>
<td>381,5</td>
</tr>
<tr>
<td>$\rho$ (kg/m³)</td>
<td>6093</td>
<td>6093</td>
</tr>
<tr>
<td>$\alpha$ (m²/s)</td>
<td>$1,38 \times 10^{-5}$</td>
<td>$1,38 \times 10^{-5}$</td>
</tr>
<tr>
<td>$L$ (kJ/kg)</td>
<td>80,16</td>
<td></td>
</tr>
<tr>
<td>$T_0$ (K)</td>
<td>301,45</td>
<td></td>
</tr>
<tr>
<td>$T_f$ (K)</td>
<td>302,93</td>
<td></td>
</tr>
<tr>
<td>$T_w$ (K)</td>
<td>311,15</td>
<td></td>
</tr>
</tbody>
</table>

Table 4: Data specifications for the melting of gallium.

<table>
<thead>
<tr>
<th>$R$</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$(L_x=0,089m;L_y=0,0445m)$</td>
</tr>
<tr>
<td>$Ra$</td>
<td>$2,1 \times 10^5$</td>
</tr>
<tr>
<td>$Pr$</td>
<td>0,0216</td>
</tr>
<tr>
<td>$Ste$</td>
<td>0,0391</td>
</tr>
<tr>
<td>$c_i/c_o$</td>
<td>1</td>
</tr>
<tr>
<td>$k_i/k_o$</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 5: Dimensionless parameters for the melting of gallium.
### Table 6: Data specifications for the melting PCM 27.

<table>
<thead>
<tr>
<th>variable</th>
<th>Solid</th>
<th>liquid</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k ) (W/m.K)</td>
<td>0,577</td>
<td>0,813</td>
</tr>
<tr>
<td>( c_p ) (J/kg.K)</td>
<td>1751,5</td>
<td>2225</td>
</tr>
<tr>
<td>( \alpha ) (m(^2)/s)</td>
<td>1,93×10(^{-7})</td>
<td>2,39×10(^{-7})</td>
</tr>
<tr>
<td>( \rho ) (kg/m(^3))</td>
<td>1710</td>
<td>1530</td>
</tr>
<tr>
<td>( L ) (kJ/kg)</td>
<td>172,42</td>
<td></td>
</tr>
<tr>
<td>( T_F ) (K)</td>
<td>300,15</td>
<td></td>
</tr>
<tr>
<td>( T_0 ) (K)</td>
<td>288,15</td>
<td></td>
</tr>
<tr>
<td>( T_w ) (K)</td>
<td>323,15</td>
<td></td>
</tr>
</tbody>
</table>

### Table 7: Dimensionless parameters for the melting of PCM 27.

<table>
<thead>
<tr>
<th>( R )</th>
<th>0,12</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Ra )</td>
<td>1,34×10(^{8})</td>
</tr>
<tr>
<td>( Pr )</td>
<td>273,85</td>
</tr>
<tr>
<td>( Ste )</td>
<td>0,2968</td>
</tr>
<tr>
<td>( c_p/c_l )</td>
<td>0,79</td>
</tr>
<tr>
<td>( k_s/k_l )</td>
<td>0,71</td>
</tr>
</tbody>
</table>

Experimental values