One-dimensional time-dependent modeling of conductive heat transfer during the melting of an initially subcooled semi-infinite PCM

L. MANSOURI\textsuperscript{a}, M. BALISTROU\textsuperscript{a}, B. BAUDOIN\textsuperscript{b}

\textsuperscript{a} Laboratory of Energetics \& Mechanics \& Engineering, Faculty of Engineering, M'Hamed BOUGARA University, Boumerdes, Algeria
larbimansouri@yahoo.fr, mouradbalistrou@yahoo.fr

\textsuperscript{b} Laboratory of Industrial Energetic Department, High National Engineering School of Mines, Douai, France
baudoin@ensm-douai.fr

Abstract:

In this study, the melting phenomenon of a phase change material PCM confined in a semi-infinite medium and subcooled beforehand is investigated using the finite volume technique. One presents a numerical model with two phases for the treatment of solid-liquid phase change based on the energy conservation equations. The numerical simulation of the coupled phenomena of melting and purely conductive heat transfer in both solid and liquid phases is performed by using a computer code. The present phase change model is validated by comparing the numerical solution with Neumann analytical solution. The results obtained show a good agreement.

Keywords: Semi-infinite medium, melting, phase change material, analytical solution, numerical model, finite volume technique

1 Introduction

The study of the kinetic of the heat transfers during the phase change, and more particularly solid-liquid phase change, causes much interest in various scientific fields and technology sectors. Among the sectors which have been interested in the phase change problem, one finds in particular the sector of metallurgy, agro-alimentary, electronic systems or that of energy storage by latent heat [1,2]. The challenges posed by this problem are numerous namely: intrinsic non-linearity, abrupt change in the thermophysical properties of the material on both sides of the phase change front, variable temperature during the phase change of an impure material (mixture, alloy, etc) where appears a two-phase zone (a “mushy region”) between the solid and liquid zones [3], mobile borders generally not known beforehand, and others. Consequently, only the simplest cases (simple geometry, constant boundary conditions, constant thermophysical properties in each phase, etc) are favorable to the analytical tool while the complexity of the real problems requires most often the recourse to the numerical methods [4,5].

In this work, attention is focused on the melting problem in a semi-infinite medium filled with a pure material undergoing isothermal phase change where the one-dimensional (1D) conduction in transient state is the only mode of heat transfer in both solid and liquid phases of the PCM.
2 Modeling

2.1 Geometrical configuration

The configuration adopted is shown schematically in figure 1. This is a semi-infinite medium filled with a PCM. This PCM is completely in a solid state at times \( t \leq 0 \) and its temperature \( T_0 \) is uniform and constant which can be different from the melting temperature \( T_{pc} (T_0 \leq T_{pc}) \). At the time \( t > 0 \), the left side \( X = 0 \) of the semi-infinite medium is suddenly subjected to a constant temperature \( T_w \) and maintained at this value which is higher than the threshold value \( T_{pc} \). Consequently, the PCM now receives heat on the level of the exchange surface \( X = 0 \) and the melting phenomenon of the solid PCM starts as soon as the solid-liquid equilibrium temperature \( T_{K∑28}\sqrt{8} \) is reached. As time increases, the liquid phase develops and takes the place of the solid, thus generating the movement of the solid-liquid interface in the semi-infinite medium from the origin \( X = 0 \) to infinity.

![FIG. 1 – Melting of a pure material confined in a semi-infinite medium and heated at the origin X = 0](image)

2.2 Simplifying assumptions

The phase change model proposed above takes into account the following simplifying assumptions [4,6] :

1) The PCM is perfectly pure and the phase change is isothermal. 2) The PCM is homogeneous and isotropic. 3) The interface between the solid and liquid phases of the PCM is fine (surface). 4) The thermophysical properties of the PCM are constant in the solid and liquid phases, but they can be different from one phase to another, except the densities of the two phases which are taken to be equal. 5) The conduction is the only mode of heat transfer in the two phases of solid and liquid which means that the natural convection within the liquid phase is ignored in the analysis of melting process. 6) The conduction in the PCM is 1D transient.

2.3 Mathematical formulation

The 1D transient heat transfer coupled with the isothermal melting of a pure material confined in a semi-infinite medium is described by one of the most classical mathematical formulations of the phase
change process which is that applied to the «Stefan problem». The temperature variations for the liquid and solid phases are governed by the following energy conservation equations [6,7]

\[ \frac{\partial T_l}{\partial t} = \frac{\partial}{\partial X} \left( \alpha_l \frac{\partial T_l}{\partial X} \right), \quad 0 < X < X_f, \quad t > 0 \quad \text{liquid phase} \] (1)

\[ \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial X} \left( \alpha_s \frac{\partial T_s}{\partial X} \right), \quad X > X_f, \quad t > 0 \quad \text{solid phase} \] (2)

where \( \alpha = k/(\rho C_p) \) is the PCM thermal diffusivity. Also, the subscripts \( l \) and \( s \) refer to liquid and solid phases, respectively.

At the solid-liquid interface, there is the continuity of the temperature on one hand:

\[ T_l(X_f, t) = T_s(X_f, t), \quad X = X_f, \quad t > 0 \] (3)

and on the other hand a discontinuity of the heat flux because of the phase change. In a global manner, one can say that the algebraic sum of fluxes incoming and outgoing is equal to energy necessary to the melting which represents the instantaneous energy absorbed in the form of enthalpy of state change by the progression of the front. This results in the following Stefan condition:

\[ k_s \frac{\partial T_s}{\partial X}(X_f, t) - k_l \frac{\partial T_l}{\partial X}(X_f, t) = \rho_l L \frac{\partial X_f}{\partial t}, \quad X = X_f(t), \quad t > 0 \] (4)

where \( k \) represents the PCM thermal conductivity, \( L \) is the latent heat of the phase change and \( X_f \) is the melting front position.

Initial conditions at \( t = 0 \):

\[ T_s(X, 0) = T_0 \quad \text{pour} \quad 0 \leq X \leq \infty, \quad X_f(0) = 0 \] (5)

Boundary conditions at \( t > 0 \):

\[ T_l(X = 0, t) = T_w, \quad T_l(X = X_f, t) = T_s(X = X_f, t) = T_{pc}, \quad T_s(X \to \infty, t) = T_0 \] (6)

The thermophysical properties used in calculation (not necessary realistic) as well as the determining parameters for the PCM melting are summarized as follows [6]: \( T_{pc} = 0°C, \) \( k_l = k_s = 1 \text{ W/mK}, \) \( \rho C_p_l = \rho C_p_s = 10^6 \text{ J/m}^3\text{K} \) and \( \rho L = 10^8 \text{ J/m}^3. \) The PCM is initially \( t \leq 0 \) at \( T_0 = -10°C \) whereas, at the time \( t > 0 \), the left side temperature is suddenly raised and maintained at \( T_w = 10°C. \)

### 3 Analytical solution of Neumann

This melting problem admits in this form a similarity solution, commonly known as the Neumann solution, one of the solutions available of the Stefan problem. By introducing the similarity variable \( \eta = X/(2\sqrt{\alpha_l t}) \) and seeking a solution in the form of \( T(X, t) = F(\eta) \), one finds the final analytical Neumann’s solution which can be written as follows [7,8]

\[ \frac{T_l(X, t) - T_w}{T_{pc} - T_w} = \frac{\text{erf} \left( \frac{X}{2\sqrt{\alpha_l t}} \right)}{\text{erf}(\xi)}, \quad 0 < X < X_f, \quad t > 0 \quad \text{liquid phase} \] (7)
The temporal evolution of the melting front position in the semi-infinite medium is given by:

\[ X_f(t) = 2\xi\sqrt{\bar{a}_1 t} \]  

(9)

The parameter \( \xi \) appearing in the three last equations is a constant implicitly given by the transcendental equation:

\[ \frac{St_i}{e^{\xi^2} \text{erf}(\xi)} - \frac{St_s}{ve^{v^2\xi^2} \text{erfc}(v\xi)} = \xi\sqrt{\pi} \]  

(10)

where \( \text{erf} \) and \( \text{erfc} \) are respectively the well-known error function and complementary error function and \( v = \sqrt{a_1/\bar{a}_s} \). \( St_i = \rho C_p (T_w - T_p) / \rho L \) and \( St_s = \rho C_p (T_p - T_0) / \rho L \) are the dimensionless numbers of Stefan for the liquid and solid phases respectively.

In order to be able to represent graphically this exact Neumann’s solution, an interpolation by polynomial collocation of the error function and complementary error function is made by adjusting at best the representative polynomial curve on the tabulated values which are available in the literature [9]. The resulting polynomial is of order 5 and is then written in the form:

\[ \text{erf}(X) = a_0 + a_1 X + a_2 X^2 + a_3 X^3 + a_4 X^4 + a_5 X^5 \]

where the coefficients \( a_i \) are the following: \( a_0 = -0.00401 \), \( a_1 = 1.18669 \), \( a_2 = -0.14559 \), \( a_3 = -0.33443 \), \( a_4 = 0.16069 \) and \( a_5 = -0.02155 \). The same polynomial has been used for the complementary error function \( \text{erfc}(X) \) but this time the coefficients \( a_i \) take the values:

\( a_0 = 1.00401 \), \( a_1 = -1.18669 \), \( a_2 = 0.14559 \), \( a_3 = 0.33445 \), \( a_4 = -0.1607 \) and \( a_5 = 0.02155 \). The relation \( \text{erfc}(X) = 1 - \text{erf}(X) \) is thus checked. Also, the root \( \xi \) of the nonlinear equation (10) is, first of all, located in the interval \([A−B] = [0.01−3.0]\) then obtained using the iterative dichotomy (bisection) algorithm. In spite of its convergence speed which is relatively weak, this algorithm has nevertheless the advantage of being convergent. By adopting, for this melting problem, the various parameters enumerated at the end of the previous paragraph (§2.3), the iterative process of calculation of the solution \( \xi \) converges toward the value \( \xi = 0.1879537 \) once the length of the starting interval \([0.01−3.0]\) is reduced to a precision of \( B − A ≤ 10^{-7} \).

### 4 Method of numerical resolution

The melting problem is governed by the Fourier’s conduction equation in each phase of the PCM (equations 1 and 2) coupled with the Stefan condition at the phase change interface (equation 4) on one side and with the initial conditions (5) and boundary conditions (6) on the other side. Its numerical modeling involves finite volume method. The numerical resolution of this 1D transient problem is ensured by a simulation code treating of 2D cases where the power law approximation scheme is considered, while fixing an infinitely small length in the 2\text{nd} direction. The linearization of the governing differential equations with partial derivative (1) and (2) gives the following system of algebraic equations for the variable \( T \) at the node \( P : a_P T_P = \sum a_{nb} T_{nb} + b \). These last algebraic equations are solved iteratively by using the line by line method with which the algorithm TDMA is associated. A fixed and uniform grid of 300 nodes in the axial direction is used over a finite length of \( XL = 30\text{cm} \) of the calculation domain with a constant step size of \( \Delta X = 0.30/(300 − 2) = 1.01\text{mm} \). The employed time step is fixed at \( \Delta t = 0.34\text{s} \). Note that these space and time steps as well as the
numbers of nodes and iterations are thoroughly selected so that the numerical model suggested can provide a solution as accurate as possible to the melting problem. As for the equation (4) of the thermal balance at the solid-liquid interface, it can be written after discretization as:

\[ X_{I}^{1} = X_{I}^{0} + \frac{\Delta t}{\Delta X} \left[ \frac{k_{s}}{\rho_{l} L} \left( -T_{I}^{1+2} + 4T_{I}^{1+1} - 3T_{I}^{1} \right) - \frac{k_{l}}{\rho_{l} L} \left( 3T_{I}^{1} - 4T_{I-1}^{1} + T_{I-2}^{1} \right) \right] \] (11)

In this last linear equation, a fully implicit scheme for the discretization in time and a combination of the forward (on the right) and backward (on the left) finite differences with second order accuracy at the node changing phase for the discretization in space have been used. Let’s remind here that the superscripts \( ^{1} \) et \( ^{0} \) denote respectively the current and previous iterations in a given time step.

5 Results and discussion

The numerical work has been implemented to simulate the heat transfer coupled with the phase change in the case of a semi-infinite medium filled with a pure phase change material (phase change point: \( T_{pc} = 0 ^{\circ}C \)) at the solid state beforehand. At times \( t \leq 0 \), a constant temperature \( T_{0} \leq T_{pc} \) is imposed on the PCM while in \( t > 0 \), the left side \( X = 0 \) of the semi-infinite medium is suddenly heated and maintained at a constant temperature also \( T_{w} \) higher than the melting temperature of the PCM chosen. This last thus undergoes an isothermal melting. By simulating this melting phenomenon, in fact one seeks a solution which consists of determining during times the temperature field in the solid and liquid phases as well as the position of the melting front from the exchange surface.

This simple problem of phase change has been resolved by finite volumes. At the time of the numerical simulation of the model presented, the accuracy obtained has been checked by comparing the numerical results with the exact analytical Neumann’s solution as shown in figures 2, 3, 4, 5 and 6. It appears that constant spatial and temporal steps of \( \Delta X = 1,01 \text{mm} \) and \( \Delta t = 0,34 \text{s} \), respectively, give a satisfactory accuracy. Indeed, taking into account the errors made on calculations of the melting front position as well as of the temperature which are noted on these figures, one can conclude that the agreement is even very good.

Figures 2 and 3 present the evolution of the melting front position as a function of time for two different values of the initial temperature of the PCM considered namely \( T_{0} = 0 ^{\circ}C = T_{pc} \) (one-phase model) and \( T_{0} = -10 ^{\circ}C < T_{pc} \) (two-phase model) [8] and two different values of the thermal conductivity of the same PCM in the case where \( k_{l} = k_{s} = k \) namely \( k = 1 \text{W/mK} \) and \( k = 2 \text{W/mK} \). The position of the solid-liquid interface in the semi-infinite medium is determined by expressing in this interface that the heat flux yielded by the liquid material minus the heat flux transmitted by conduction within the solid material is equal to the latent heat flux of melting involved in the phase change. Because of the heat flux received at the exchange surface, one notes close to this one since the first ten minutes, the appearance of a melting front in the semi-infinite medium which progresses in it from \( X = 0 \) to infinity. It is clear that the propagation velocity of the melting front in the PCM is more important for \( T_{0} = T_{pc} \) than in the case \( T_{0} = -10 ^{\circ}C < T_{pc} \) (figure 2). The same tendency is noted from figure 3 by varying the thermal conductivity. Indeed, the increase of this latter conductivity causes an increase of the displacement velocity of the solid-liquid interface within the PCM. Nevertheless, these two figures permit to note that the displacement velocity of the melting front as well as the rate of production of the liquid are rather very sensitive to the thermal conductivity \( k \) but a little less sensitive to the initial temperature \( T_{0} \).
The evolution of the PCM temperature is illustrated in figures 4, 5, 6 and 7 for various axial positions, at various time instants and for two different values of the thermal conductivity of the material considered. Figures 4 and 5 show that as the solid-liquid interface moves away from the exchange surface X = 0, during phase change, the stage corresponding to the process of thermal transfer within the fondant material is more important. Also, the zone of the semi-infinite medium located near to the surface X = 0 is heated, whereas the one located at infinity remains quite cold and consequently the PCM temperature stays equal to its initial temperature $T_0 = -10^\circ C$, according to figure 6. One notices that the melting front moves from the position $X_f = 0.693cm$ at $t = 5.66min$ toward the internal layers of the semi-infinite medium to reach the position $X_f = 2.685cm$ at $t = 85min$, that is to say an advancement of 1.992cm for a duration of phase change process relatively high of 79.34min. Therefore, the numerical simulation must be carried out for a more important length of the calculation domain ($X_L \gg 30cm$) with a higher melting duration close to five hours so that the temperature curves of the liquid phase can take a form which clearly resembles the one of the solid phase. In addition,
figure 7 shows that more time is required for the temperature of the material to reach the temperature imposed at the exchange surface as the thermal conductivity of this latter material decreases.

FIG. 6 – Evolution of the PCM temperature in the semi-infinite medium at various times for \( k = 1 \text{ W/mK} \) and \( T_0 = -10^\circ\text{C} \)

FIG. 7 – Evolution of the PCM temperature during the time for various axial positions and two different values of the thermal conductivity with \( T_0 = -10^\circ\text{C} \)

6 Conclusions and future outlook

The validation results obtained show that the numerical model presented, treating the solid-liquid phase change in conductive mode within a semi-infinite medium, permit to predict satisfactorily the temporal evolution of the melting front position as well as of the temperature in the solid and liquid phases. In spite of its simplicity, this model of phase change can constitute an important and reliable tool of validation of the computer codes for the researchers. The simplified model will be adapted in a future work to study these phenomena of solid-liquid phase change but in convective mode (natural convection) in more complex configurations.

References