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Research Article

Numerical Analysis of Convection Driven Melting of Metals and Alloys Using Fixed Grid Methods

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Abstract

This paper describes the results of a numerical heat transfer model and CFD based simulation for natural convection during melting of metals and alloys. The influence of natural convection on the evolving melt front and the undergoing transport phenomena in the individual phases were investigated. An enthalpy formulation based fixed grid methodology was developed for the numerical solution of convection-diffusion controlled phase change problems. To understand the basic heat transfer mechanism during melting both 1-D and 2-D problems were solved. The basic feature of the proposed method lies in the representation of the latent heat evolution, and of the flow in the solid-liquid mushy zone, by suitable chosen sources. Results obtained from the numerical study were compared to experimental data available in the literature. The method converged rapidly and was capable of accurately predicting both the position and morphology of the melt front at various times with relatively modest computational requirements.

Keywords: *Numerical heat transfer, Phase change problems, Fixed grid methodology, Enthalpy.*

1. Introduction

The computational modeling of systems with solid and liquid phase has become a highly popular subject due to its promotion to better understand nature as well as in the development of the advanced technologies. The physical properties of the materials are in general dependent upon the direction. As such, numerous studies necessitate the inclusion of the anisotropic thermo-physical properties when modeling the solid-liquid phase changes. In Most practical situations involving a liquid/solid phase change, however convection effects (either forced or free) are important and in fact may totally dominate over conduction. The melting of pure gallium in a rectangular cavity has been numerically investigated using the enthalpy-porosity approach for modeling combined convection-diffusion phase change in the present work. Several works has been carried out in the field of Phase change (melting or solidification) of metals and alloys.

N. Shamsundar and E. M. Sparrow (1975) worked on multidimensional conduction phase change via the enthalpy model. It is shown that enthalpy model developed was equivalent to the conventional conservation equation of the solid and liquid regions and at the solid-liquid interface The solution method was used to obtain results for local and face integrated heat transfer rates, boundary temperature, solidified fraction and interface position, all as function time. At low values of the Biot number, the surface-integrated heat transfer rate was relatively constants during the entire solidification which is a desirable characteristic for phase change thermal energy storage.

V.R.Voller and C. Prakash (1987) worked on convection-diffusion mushy region phase change problems. An enthalpy formulation based fixed grid methodology was developed for the numerical solution of convection-diffusion controlled mushy region phase change problems. The basic feature of the proposed method lies in the representation of the latent heat of evolution and the flow in the solid-liquid mushy zone by suitable chosen sources. In a numerical modeling analysis of mushy region solidification the enthalpy is a sound starting point in that any functional relationship $\Delta H = f(T)$ may be readily incorporated in to the enthalpy function. This method is general and can handle situations where phase change occurs at a distinct temperature or over a temperature range. A. D. Brent, V.R.Voller, and K. J. Reid (1998) worked on convection-diffusion phase change by using the enthalpy-porosity technique for the melting of the pure metal. C. J. Ho and C. H. Chu of Taiwan (1994) worked on phase change problems for multiple moving boundaries during melting inside an enclosure imposed with cyclic wall temperature. The focus of the this study was the numerical simulation of multiple moving solid-liquid interfaces during natural-convection-dominated melting of a pure material contained in a

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vertical square enclosure imposed with time-periodic large-amplitude oscillatory wall temperature. V. R.Voller, P. Felix, and C. R. Swaminathan (1996) worked on cyclic phase change with fluid flow. C. K. Chun and S. O. Park (2000) worked on fixed grid finite difference method for phase change problem. A simple finite method was developed for solid-liquid phase change problems. The method was based on a fixed grid and implicit in time. A fictitious temperature concept was introduced to derive finite difference equations to deal with the nodal points across the solid-liquid interface. The algorithm was applied to a one dimensional Stefan problem for which exact solution were available. The computational results were found an excellent agreement with the exact solutions. The proposed method yielded no oscillations of temperature and phase front which were commonly observed with the typical enthalpy method. Voller et, al, (1990) also worked on fixed grid techniques for phase change problems. They categorize the major fixed grid formulations and solution methods for conduction controlled phase change problems. Using a two phase model of a solid-liquid phase change, the basic enthalpy equation was derived. Many important physical processes, including both solid-liquid transformations and solid state transformations, involve phase change. The emphasis in the numerical modeling of such systems centres on the treatment of the latent heat evolution. This paper presents the characteristics of solid –liquid interface change against time on melting of metals and alloys. The velocity and temperature were tracked in the process.

2. Heat Transfer Modeling

2.1 One-dimensional Phase Change Problem (Melting)

A solid bar as shown in Fig. 1 was considered having a single phase-change temperature (melting temperature) T_m confined to a semi infinite region $0 < x < \infty$. Initially, the solid is at a uniform temperature T_i which is equal to the phase change temperature T_m. At time $t > 0$, the temperature of the boundary surface at $x = 0$ is raised to T_0, which is higher than T_m and maintained at that temperature for times $t > 0$. As a result, melting starts at the surface $x \geq 0$ and the solid- liquid interface moves in the positive x-direction as shown in Fig. 1.

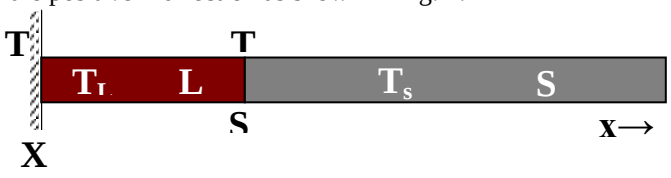


Fig. 1: Semi-infinite bar

Fig. 2 shows the coordinates and the temperature profile. The solid phase being at a constant temperature T_m throughout. The temperature is unknown only in the liquid phase; hence the problem is a 1-D single phase Stefan problem. In the following analysis, the temperature distribution in the liquid phase and the location of the solid-liquid interface are determined as a function of time. The governing equation with associated initial and boundary condition for the above said problem is given as:

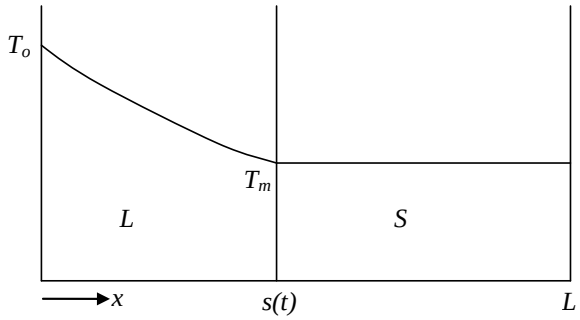


Fig. 2: Schematic of the 1-D problem in the Enthalpy based FG method.

Governing equation

$$K\frac{\partial^2 T_l(x,t)}{\partial x^2} = \rho C\frac{\partial T_l(x,t)}{\partial t} \quad \text{at } t > 0,\ 0<x< s(t) \tag{1}$$

The initial condition is:

$$T(x, t) = T_i \quad \text{for } t = 0,\ T_i = T_m \tag{2}$$

The Boundary conditions are:

$$T_l(x, t) = T_o \quad \text{at } x = 0,\ t > 0,\ T_o > T_m \tag{3}$$

$$T_l(s(t), t) = T_m \quad \text{at } s(t) \leq x < \infty,\ t > 0 \tag{4}$$

The interface condition is:

$$T_l(x, t) = T_m \quad \text{at } x = s(t),\ t > 0 \tag{5}$$

$$-K\frac{\partial T_l}{\partial x} = \rho L\frac{ds(t)}{dt} \quad \text{at } x = s(t),\ t > 0 \tag{6}$$

The exact solution (R) to the Equation (1) and the temperature distribution is:

$$\frac{T_l(x,t) - T_o}{T_m - T_o} = \frac{erf[x/2(\alpha_l t)^{1/2}]}{erf(\lambda)} \tag{7}$$

Where λ is a parameter which can be determined from the given relation:

$$\lambda e^{\lambda^2} erf(\lambda) = C_p(T_o - T_m)/L\sqrt{\pi} \tag{8}$$

The position of the solid –liquid interface at any instant‘t’ can be found using the following relation:

$$S(t) = 2\lambda(\alpha_l t)^{1/2} \tag{9}$$

2.2 Two-dimensional Phase Change Problem (Melting of Pure Gallium in a rectangular Cavity)

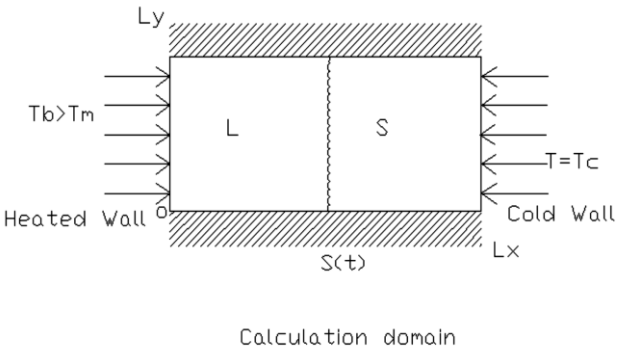


Fig. 3: Solid gallium in a rectangular cavity

To verify the applicability of the enthalpy porosity approach to metallurgical systems, the modelling of an isothermal phase change was under taken for which reliable experimental data exists in the literature. The study examined the two dimensional melting of pure gallium in a rectangular cavity with one heated wall and two sides are insulated, as shown in Fig. 3.

Melting and solidification in a 2-D rectangular gallium cavity is taken into account to study the influence of melting temperature on the phase front evolution. The proposed model accounted for the natural convection effect in the melt zone. The assumptions considered are:

- The thermal properties of the material are assumed to be constant.
- Boussinesq approximation is used for treating the buoyancy term in the momentum equation.

Two types of boundary conditions are analysed in this problem i.e., Constant temperature and constant heat flux.

The governing equations are:

Continuity equation:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0 \text{ at t > 0, } 0 \le x \le s\ (t),\ 0 \le y \le L_y \quad (10)$$

X- Momentum equation:

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=-\frac{\partial P}{\partial x}+\upsilon\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right) \text{ at t > 0, } 0 \le x \le s(t),\ 0 \le y \le L_y. \quad (11)$$

Y- Momentum equation:

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}=-\frac{\partial P}{\partial y}+\upsilon\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right)+g\beta(T-T_m), \text{ at t > 0, } 0 \le x \le s\ (t),\ 0 \le y \le L_y. \quad (12)$$

Energy equation:

For liquid zone:

$$\rho C\left(\frac{\partial T_l}{\partial t}+u\frac{\partial T_l}{\partial x}+v\frac{\partial T_l}{\partial y}\right)=K\left(\frac{\partial^2 T_l}{\partial x^2}+\frac{\partial^2 T_l}{\partial y^2}\right) \text{ at t > 0, } 0 \le x \le s\ (t),\ 0 \le y \le L_y. \quad (13)$$

For solid zone:

$$\rho C\frac{\partial T_s}{\partial t}=K\left(\frac{\partial^2 T_s}{\partial x^2}+\frac{\partial^2 T_s}{\partial y^2}\right) \text{ at t > 0, } s(t) \le x \le L_x,\ 0 \le y \le L_y. \quad (14)$$

Initial conditions:

$$T = T_m \quad \text{at t > 0, } 0 \le x \le L_x,\ 0 \le y \le L_y. \quad (15)$$

Boundary conditions (for t > 0)

$$T = T_b, \quad x = 0,\ 0 \le y \le L_y. \quad (16)$$

$$\frac{\partial T}{\partial y}=0, \quad y = 0,\ 0 \le x \le L_x \text{ and } y = L_y,\ 0 \le x \le L_x. \quad (17)$$

$$T = T_c, \quad x = L_x,\ 0 \le y \le L_y. \quad (18)$$

Interface condition:

$$K_s\frac{\partial T_s}{\partial n}-K_l\frac{\partial T_l}{\partial n}=\rho L v_n, \quad x = s\ (t) \quad (19)$$

The conventional approach for solving the phase change problem is moving grid (MG) method. The derivation of interface condition from the modified governing equation is given below.

$$(K\frac{\partial T}{\partial n*})_s-(K\frac{\partial T}{\partial n*})_l-\rho\lambda v_n^*=0 \quad (20)$$

2.3 Updatation of ΔH

Isothermal phase change:

$$\Delta H_P^{n+1}=\Delta H_P^n+\frac{\alpha\Delta t}{\rho\Delta V_P}(T_P^n-T_m) \quad (21)$$

Non-isothermal phase change:

Taking a linear variation $\Rightarrow T_m=\frac{2\varepsilon\Delta H}{L_f}+T_{PC}-\varepsilon$

$$\therefore \Delta H_P^{n+1}=\Delta H_p^n+\frac{\alpha a_P\Delta t}{\rho\Delta V_P}(T_P^n-T_m) \quad (22)$$

$$=\Delta H_P^n+\frac{\alpha a_P\Delta t}{\rho\Delta V_P}(T_P^n-T_{PC})-\frac{\alpha a_P\Delta t\varepsilon}{\rho\Delta V_P L_f}(2\Delta H_P^n-L_f)$$ If $\varepsilon = 0$, the above equation reduces to the conventional isothermal phase change process.

3. Numerical Solution

Phase change processes are basically referred to as a transient diffusion problem which is mathematically classified as Stefan problem where the moving boundary is priory an unknown.

3.1The Tri-diagonal Matrix Algorithm (TDMA) Method

The Tri Diagonal Matrix Algorithm (TDMA) also known as Thomas algorithm was used to solve the system of linear algebraic equations. The solution procedure using TDMA to solve one-dimensional and two-dimensional problems are briefly described below.

One-Dimensional Case

For one-dimensional problems, the discretized algebraic equations have a simple structure. A typical one-dimensional node point distribution is shown in Fig. 4. The linear algebraic equation is applied to each node points and a system of algebraic equations will result comprises of all nodal points. The coefficient matrix is a tri-diagonal matrix, in which the non-zero terms exist only on its main diagonal and the diagonals immediately above and below it. The algebraic equation for a one-dimensional problem can be written as

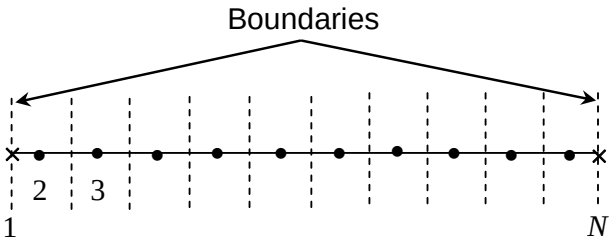


Fig. 4: The control volume node points in one-dimensional problem. (Note: • points where the variable values are calculated; × known boundary values).

$$a_i\phi_i=b_i\phi_{i+1}+c_i\phi_{i-1}+d_i;\ i=2,3,\ldots N-1 \quad (23)$$

ϕ_1 and ϕ_N are the boundary conditions (as shown in Fig. 4). The forward elimination and backward substitution can be used to solve this algebraic equation.

In the forward elimination ϕ_{i-1} is substituted by ϕ_i

$$\phi_{i-1} = P_{i-1}\phi_i + Q_{i-1} \quad (24)$$

Substituting Eq. (24) into Eq. (23) gives

$$\phi_i = \frac{b_i}{a_i - c_i P_{i-1}}\phi_{i+1} + \frac{c_i Q_{i-1} + d_i}{a_i - c_i P_{i-1}} \quad (25)$$

The backward substitution equation is

$$\phi_i = P_i\phi_{i+1} + Q_i \quad (26)$$

Where,

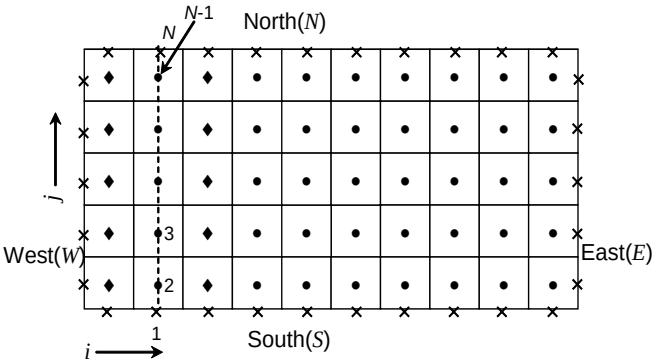
$$P_i = \frac{b_i}{a_i - c_i P_{i-1}}, \quad Q_i = \frac{c_i Q_{i-1} + d_i}{a_i - c_i P_{i-1}} \quad (27)$$

$$P_1 = \frac{b_1}{a_1} = 0, \quad Q_1 = \frac{d_1}{a_1} = \phi_1 \quad (28)$$

In every inner iterative step, the coefficients are constant. The outer iteration refers to the solution of the nonlinear problem. The coefficients and source terms must be updated after every outer iterative step.

Two-Dimensional Case

The two-dimensional grid system shown in Fig. 5 was considered. The standard two-dimensional discretized transport equation is given as:



Property	Value
Specific heat capacity (C)	409.58 J/kg-K
Thermal expansion coefficient (β)	1.3054×10^{-4} K^{-1}
Thermal diffusivity (α)	1.4145×10^{-5} m^2/s
Latent heat (L)	80160 J/kg
Phase change temperature (T_m)	0 K
Kinematic viscosity (ν)	2.97×10^{-7} m^2/s

Fig. 5: Line-by-line application of the TDMA in two-dimensional geometry. (Note: • calculated; ♦ temporarily known values; × known boundary values).

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + a_N\phi_N + a_S\phi_S + b \quad (29)$$

Equation (29) is re-arranged in the form

$$-a_S\phi_S + a_P\phi_P - a_N\phi_N = a_W\phi_W + a_E\phi_E + b \quad (30)$$

To solve the system, TDMA is applied along chosen, for example north-south (*N*-*S*) lines as shown in Fig. 5.

Table1: Properties of Gallium

The right hand side of Eq (30) is assumed to be temporarily known. The system of equations can be solved along the *N*- *S* direction of the chosen line for values j = 2, 3, 4, …, N-1 as shown in Fig. 5. Subsequently the calculation is moved to the next *N*- *S* line. The sequence in which lines are chosen is known as the sweep direction. If sweep from west (*W*) to east (*E*) the values of ϕ_W to the west of point *P* are known from the calculations on the previous line. Values of ϕ_E to its east, however, are unknown so the solution process must be iterative. At each iteration cycle ϕ_E is taken to have its value at the end of the previous iteration or a given initial value at the first iteration. The line-by-line calculation procedure is repeated several times until a converged solution is obtained.

3.2 Convergence Criteria

The solution is deemed converged with the difference in the values of a given variable between two successive iterations is less than a prescribed tolerance. For the phase change problem considered here, the variables which were calculated at each iteration are the temperature (T) and the latent heat content (ΔH). The tolerance value was set to 10^{-11} for both T and ΔH.

4. Results and Discussion

4.1 Isothermal Phase Change

For one dimensional case of phase change problem, melting of pure Gallium in a semi-infinite domain is chosen. This 1-D problem is the class of a one phase Stefan problem. The domain length is taken as L = 0.1 m for maximum melting time of 1 minute. This domain length is equivalent to semi-infinite domain as it is much higher than the diffusion length ($2\sqrt{\alpha t}$) which is found to be 0.058 m. The thermal properties of pure Gallium are listed in Table 1. Three control volume sizes, namely 40, 80 and 160 (in terms of number of control volumes) are chosen to carry out this test. This is evident from Fig. 6. that beyond the control volume size of 1.25×10^{-3} m (which corresponds to number of control volume as 80), there is no significant change in the melt front variation with respect to time.

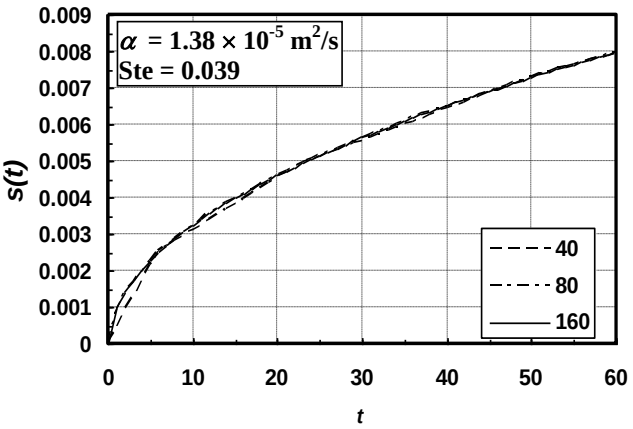


Fig. 6: Grid independent test for one-phase Stefan problem in a semi-infinite domain.

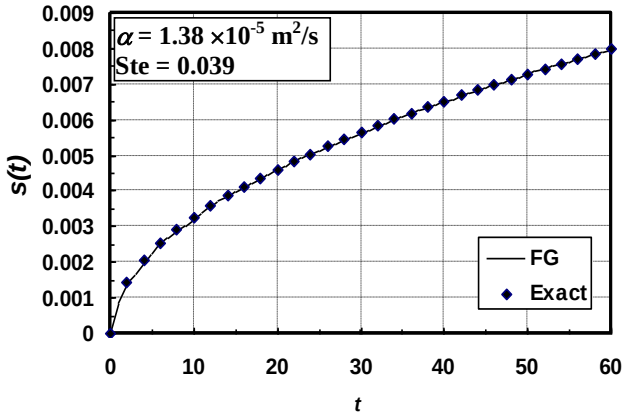


Fig. 7: Comparison of melt front position with the exact solution.

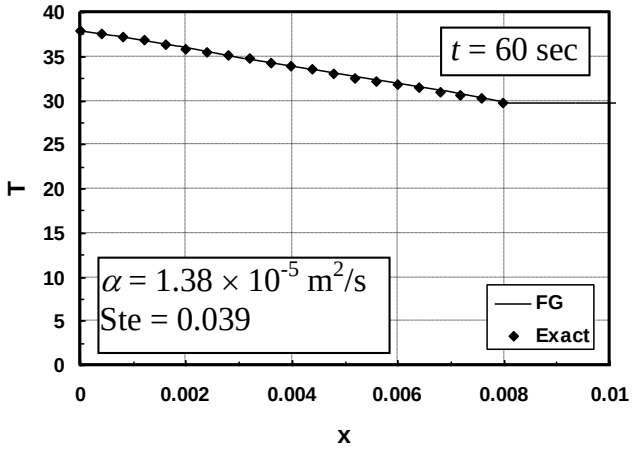


Fig. 8: Comparison of temperature distribution in the melt region with the exact solution.

So, this above control volume size is chosen for further presentation of results in this problem. To validate the proposed method, results were compared with the exact solution for our 1-D problem case.

A comparison for the temporal variation of melt front position is shown in Fig. 7. An excellent agreement was found between the proposed method and the exact solution. The temperature distribution in the melt region at t = 60 sec is also found to be in very good agreement with the exact solution which is shown in Fig. 8.

For each of the 3 set of the grid size a time independent test was being conducted and it was found that beyond a time step size of $\Delta t = 0.01$, there is no significant change in the front evolution. So $\Delta t = 0.01$ was used for presentation of results.

In case of two-dimensional isothermal phase change problem, the melt front is virtually planer after 1 min as the natural convection field is just about to start as shown in Fig. 9.

From Fig. 10, it is evident that after 3 min the shape of the melt front is governed primarily by convection effects, with conduction exerting very little influence. Although the upper section of the melt front advances rapidly due to the impingement of warm fluid, the lower section moves considerably slower, there by resulting in the irregular morphology.

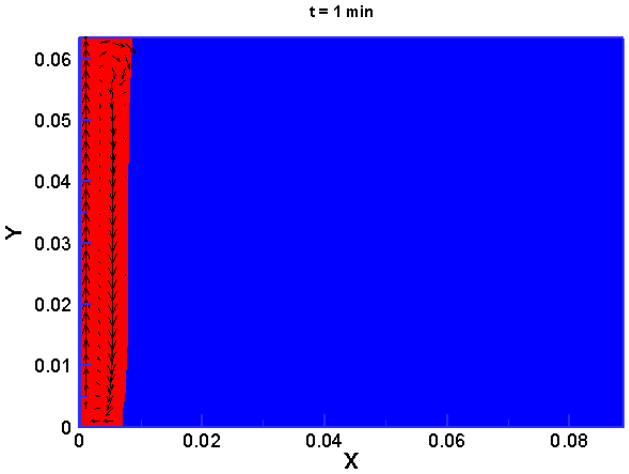


Fig. 9: Velocity vector plot and melting front position at time (t) = 1 min. for melting of pure gallium under isothermal phase change condition.

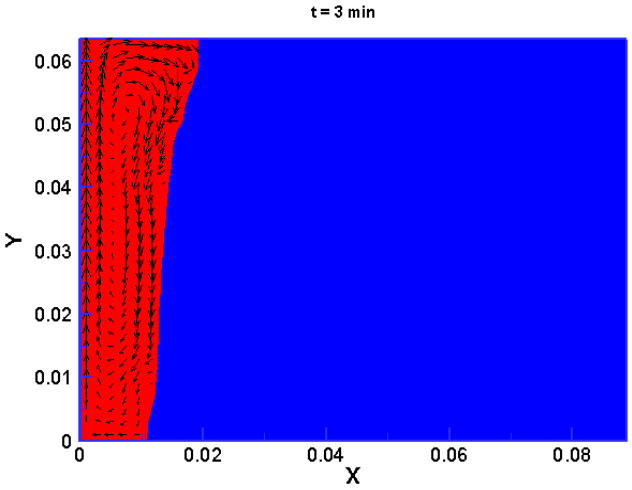


Fig. 10: Velocity vector plot and melting front position at time (t) = 3 mins for melting of pure gallium under isothermal phase change condition.

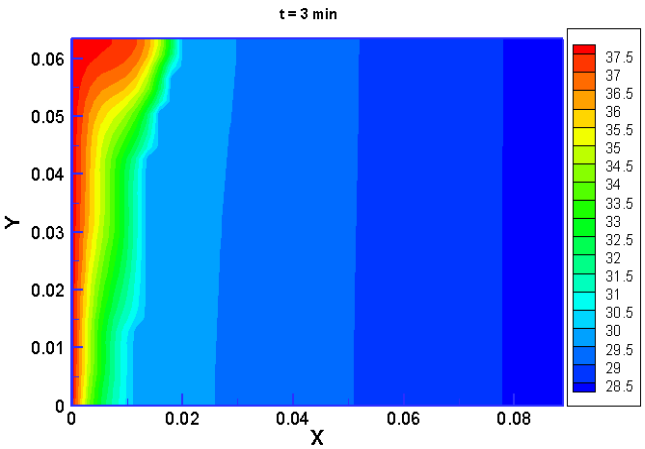


Fig. 11: Isotherm plot and melting front position at time (t) = 3 mins for melting of pure gallium under isothermal phase change condition.

The region of maximum heat flux may be identified by examining the isotherm plot given in Fig. 11. The steepest temperature gradients are presents in two areas, viz., at the upper section of the melt face where warm fluid impinges on the solid, and at the lower section of the heated wall where cool fluid returning from the melt front impinges on the heated wall.

The insulating nature of the melt front in the cavity was also evident from the isotherm plots. Almost the entire temperature drop across the cavity occurred in the molten region, left the temperatures of the residual solid essentially uniform near the initial temperature. The reason for this might be that, all the energy entering the cavity at the heated wall was absorbed by the phase change at the melt front, allowing only a small fraction to penetrate the slightly super-cooled solid. As the major temperature gradients occurred in the liquid phase, it was the thermal conductivity of the liquid rather than the solid that controls the heat transfer, and hence the problems associated with the theoretical treatment of anisotropic solid conductivity did not arise.

The melt front evolution at different time levels were compared with the experimental results reported by Gao, C., and Viskanta, R., (1984, 1986) and a good agreement has been found as shown in Fig. 12.

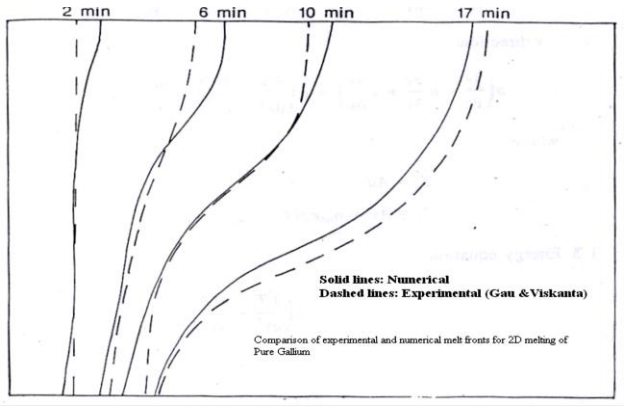


Fig. 12: Comparison and validation with experiment for melting of pure gallium [Ref].

Conclusions

The applicability of the enthalpy-porosity technique or total enthalpy method for modelling an isothermal phase change in a metallurgical system has been verified by examining the two dimensional and one dimensional melting of pure gallium under the influence of natural convection in a rectangular cavity. Results obtained from the numerical study were compared to experimental data available in the literature. The method converges rapidly and is capable of accurately predicting both the position and morphology of the melt front at various times with relatively modest computational requirements. The results of this work may be taken to be a sound validation of the enthalpy- porosity technique for simulating isothermal phase changes in metallurgical systems. Also in this work a generalized methodology for the modelling of mushy-region phase change is developed.

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References

Shamsunder, N., and Sparrow, E.M. (1975), Analysis of Multidimensional Conduction phase change via the enthalpy model, *Int. ASME Journal of heat transfer* January 26, Paper no.75.

Voller, V. R. and Prakash, C. (1987), A fixed grid numerical modelling methodology for convection- diffusion mushy region phase change problems, *Int. J. Heat Mass transfer*, 30, 8.

Brent, A. D., Voller, V. R., and Reid, K. J. (1998), Enthalpy-porosity technique for modelling convection-diffusion phase change: Application to the melting of a pure metal, *Int. J. of Numerical heat transfer*, 13, 297- 318.

Ho C.J., and Chu, C.H. (1994), A simulation for multiple moving boundaries during melting inside an enclosure imposed with cyclic wall temperature, *Int. J. of Heat Mass transfer*, 37, No.16, 2505- 2516.

Voller, V. R., Felix, P., and Swaminathan, R. (1996), Cyclic phase change with fluid flow, *Int. Num. Meth, Heat Fluid Flow*, 6, No.4, 57- 64.

Chun C.K., and Park, S. O. (2000), A fixed grid finite-difference method for phase change problems, *Numerical heat transfer, Part B*, 38:59-73.

Voller, V. R., Swaminathan, C.R., and Thomas, B.G. (1990), Fixed grid techniques for phase change problems: A Review, *Int. Journal for numerical methods in engineering*, 30, 875-898.

Gau, C., and Viskanta, R., (1984), Melting and solidification of a metal system in a rectangular cavity, *Int. J. Heat Transfer*, 27, 113-123.

Gau, C., and Viskanta, R., (1986), Melting and solidification of a pure metal on a vertical wall, *J. Heat Transfer*, 108, 174-181.