# NUMERICAL MODELLING OF CONVECTION-DIFFUSION PHASE CHANGE PROBLEMS

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## 1. SUMMARY

A numerical methodology is presented for the modelling of phase change problems. A continuum model of convection-diffusion controlled mushy region phase-change is used to investigate the solidification of a binary mixture. The conservation equations equally apply to the liquid, mushy and solid regions, thus facilitating use of a fixed grid numerical method.

An efficient and accurate non-staggered control volume method is proposed for the solution of model equations. This method is based on quadratic momentum interpolation and a high-order convection differencing scheme. Special attention is given to numerical instability problems resulting from the non-linearities of the model as well as the release of a great amount of latent heat over a narrow temperature range and the strong coupling between the energy and momentum equations. To overcome these difficulties suitable numerical techniques were implemented.

The proposed method is verified by the solution of a conduction controlled phase change problem. Satisfactory agreement with previously published is observed. Finally, the solidification of a binary mixture in a freezing cavity is solved and results are reported.

## 2. INTRODUCTION

Processes related to melting and solidification are widely encountered in many industrial applications [1], such as metal alloy casting, food freezing, ice forming, thermal energy storage, etc. Mathematical modelling of transport phenomena that occur during phase change is becoming an important tool for predicting the state of the final product. Problems related to improper control of the transport mechanisms include void formation, concentration variation of the dissolved component, and cracking due to thermal stresses.

Due to the absorption or release of latent heat and the presence of complex interfacial structures that characterise the phase change of most materials, the exact solution of conservation equations is impossible [2]. The numerical models for solving phase change problems can be conveniently divided into two categories [2, 3]. The first category involves methods that utilise independent conservation equations for each phase. A moving-front practice is followed, where the mesh is continuously updated so that it always coincides with

the phase change front. Such methods are referred to as *multiple region* or *multiple grid* methods and are usually applied on the analysis of pure materials. The second category consist of *single region* models that utilise a system of conservation equations that can be equally applied to both phases [4-8]. The latent heat evolution is accounted for in the energy equation by the enthalpy formulation [9-11]. In this case, no explicit conditions on the interface are required and the numerical solution can be carried out on a *fixed grid*. These methods are well suited for treating the phase change of mixtures where, the latent heat is evolved over a temperature range.

The major advantage of the single region models is that the solution can be achieved by conventional numerical methods. However, the numerical treatment of phase change problems requires special attention. In order to predict the complex interfacial structures, high accurate numerical schemes must be used. Moreover, particular attention must be directed to the handling of the latent heat evolution associated with the phase change.

In this paper, a numerical method for the solution of convection-diffusion controlled phase change problems is presented. The method combines high accuracy and numerical stability and can be used to analyse complex problems with minimal effort.

## 3. PROBLEM DESCRIPTION

The configuration of the test problem considered is depicted in Fig. 1. A binary mixture of initial concentration $C_{init}$ and initial temperature $T_{init} > T_l$ (the liquidus temperature), is located in a rectangular cavity insulated on three sides. At time $t = 0$, the left side is cooled to a temperature $T_{wall} < T_l$ so that freezing occurs. At later times the cavity contains three regions. A solid region near the left side, a liquid region near the right side and a mushy (solid and liquid) region in between. In most materials the mushy region has a dendritic crystalline structure. The system is influenced by diffusion phenomena and natural convection flow which is caused by the temperature and concentration gradients.
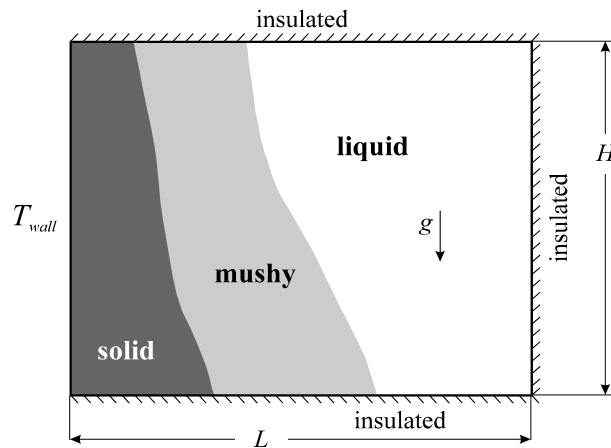


**Fig. 1.** A schematic of solidification in a rectangular cavity.

## 4. MATHEMATICAL FORMULATION

The behaviour of a phase change system can be described by the conservation equations for total mass, momentum, energy and species in the solid, liquid and mushy zones. In addition, appropriate relations are necessary for determining the mass fraction of solid as a function of temperature and concentration and also for representing the variation of mixture properties in the mushy region. The model adopted in this study is similar to that which has been

developed by Bennon and Incropera [4], and can be derived from the mixture theory or through a volume averaged procedure [7].

## 4.1 The governing equations

*Conservation of mass*

$$\frac{\partial \rho}{\partial t} + div(\rho \mathbf{u}) = 0 \tag{1}$$

*Conservation of momentum*

$$\frac{\partial}{\partial t}(\rho u) + div(\rho \mathbf{u} u) = div\left(\mu_l \frac{\rho}{\rho_l} grad\, u\right) - \frac{\partial p}{\partial x} - \frac{\mu_l}{K}\frac{\rho}{\rho_l} u \tag{2}$$

$$\frac{\partial}{\partial t}(\rho v) + div(\rho \mathbf{u} v) = div\left(\mu_l \frac{\rho}{\rho_l} grad\, v\right) - \frac{\partial p}{\partial y} + \rho B - \frac{\mu_l}{K}\frac{\rho}{\rho_l} v \tag{3}$$

*Conservation of energy*

$$\frac{\partial}{\partial t}(\rho h) + div(\rho \mathbf{u} h_l) = div(k\, grad\, T) \tag{4}$$

*Conservation of species*

$$\frac{\partial}{\partial t}(\rho C) + div(\rho \mathbf{u} C) = div(\rho D\, grad\, C) + div(-D\, grad(C_l - C)) - div[\rho \mathbf{u}(C_l - C)] \tag{5}$$

In the above equations, the mixture density, velocity, enthalpy, concentration, thermal conductivity and diffusion coefficient are defined as follows:

$$\rho = g_s \rho_s + g_l \rho_l, \qquad \mathbf{u} = f_l \mathbf{u}_l, h = f_s h_s + f_l h_l, \qquad C = f_s C_s + f_l C_l$$

$$k = g_s k_s + g_l k_l \qquad D = f_l D_l \tag{6}$$

The term $\rho B$, in the v-momentum equation, is the buoyancy term used to induce natural convection in the cavity. Assuming the Boussinesq approximation to be valid, this term is replaced by:

$$\rho B_x = \rho_{ref}\, g\left[b_T\left(T - T_{ref}\right) + b_C\left(C_l - C_{ref}\right)\right] \tag{7}$$

where $T_{ref}, C_{ref}$ are the reference values of temperature and concentration (usually coincide with the eutectic values), $\rho_{ref}$ is the density existing at the reference conditions and $b_T, b_C$ are the thermal and solutal expansion coefficients. The last terms of the right hand side of equations (5) and (6) represents the interactions of two phases in the mushy region and are derived on applying the Darcy's law for flows in a porous media. Assuming the permeability $K$ to be isotropic, it is evaluated from Karman-Kozeny equation:

$$K = K_o\left[\frac{g_l^3}{\left(1 - g_l\right)^2}\right] \tag{8}$$

## 4.2 Closure of the system

In the continuum phase change model described above, the phase mass fraction and composition are indirectly determined from the equilibrium phase diagram. On assuming straight liquidus and solidus lines, the solid mass fraction can be expressed as:
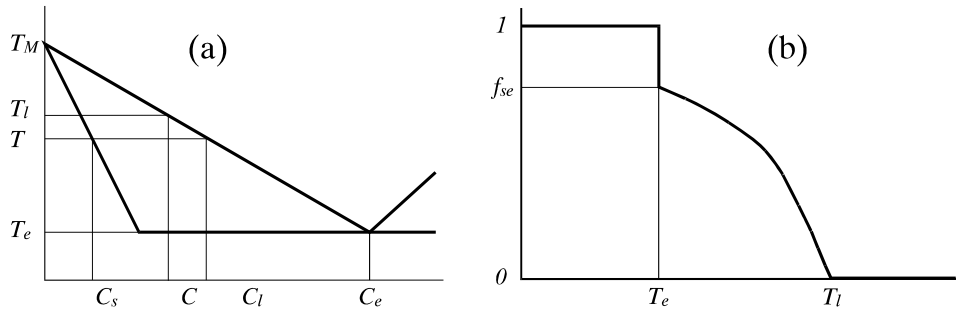
$$f_s = \begin{bmatrix} 1 & T < T_e \\ [f_{se}, 1] & T = T_e \\ \dfrac{1}{1-k}\dfrac{T_l - T}{T_M - T} & T_e < T < T_l \\ 0 & T \geq T_l \end{bmatrix} \tag{9}$$

where $T_l = T_M + \dfrac{T_e - T_M}{C_e}C$ is the liquidus temperature and $f_{se} = \dfrac{1}{1-k}\dfrac{T_l - T_e}{T_M - T_e}$ is the solid mass fraction at the onset of the eutectic reaction.

The enthalpies of two phases and the composition of the liquid phase are given by:

$$h_s = c_s T, \qquad h_l = c_l T + h_f, \qquad C_l = \frac{T - T_M}{T_e - T_M}C_e \tag{10}$$

where $h_f$ is the latent heat of phase change.



**Fig. 2.** (a) A typical equilibrium phase change diagram and (b) the solid mass fraction - temperature relationship.

## 5. NUMERICAL METHOD

Each of the governing equations, except the energy one, can be recast in the form:

$$\frac{\partial}{\partial t}(\rho\varphi) + div(\rho\mathbf{u}\varphi) = div(\Gamma \, grad\,\varphi) + S_\varphi \tag{11}$$

by properly defining the quantities $\varphi$, $\Gamma$ and $S_\varphi$. The numerical method used is based on a control volume formulation and the SIMPLEC algorithm is applied to resolve the pressure-velocity coupling. The second order QUICK scheme, as presented in Ref.[12] is used for the discretization of the convective terms. A non-staggered grid is adopted and the cell-face velocities are evaluated with the quadratic momentum interpolation practice, ensuring high accurate results. Full details of the numerical method have been recently reported [13].

Properly handling the right hand side of the energy equation, it can be recast in the form of Eq. (11) with dependent variable the temperature of the system. However, in this way the

determination of the solid mass fraction in the mushy region becomes impossible, because of the discontinuity of the $f_s(T)$ curve at the eutectic point (Fig. 2(b)). Also, the abrupt increment of solid mass fraction and the release of the latent heat causes numerical instabilities, since the system oscillates between liquid and solid phase. A usual practice to overcome this problem is the introduction of a small artificial temperature range $\left[T_e - \varepsilon, T_e + \varepsilon\right]$ at the jump, where the solid mass fraction depends linearly on temperature. This practice even though settles the singularity of mass fraction, does not improve the numerical instabilities while introduces modifications to the physical problem.

In the present study a general predictor-corrector method proposed in [9] is followed. This methodis based on the direct discrete analog of equation (4):

$$a_P\, T_P = \sum_M a_M\, T_M + \frac{(\rho V)_P}{c_l \Delta t}\left(h_p^o - h_p\right) + b \tag{12}$$

In the predictor step the enthalpy is linearized using a Taylor expansion:

$$h_p^{m+1} = h_p^m + \frac{dh}{dT}^m \left(T_P^{m+1} - T_P^m\right) \tag{13}$$

Using this expression, (12) can be written as:

$$\left(a_P - S_P\right) T_P^{m+1} = \sum_M a_M\, T_M^{m+1} + b + S_U \tag{14}$$

where $S_P = -\dfrac{(\rho V)_P}{c_l \Delta t}\dfrac{dh}{dT}^m$ and $S_U = \dfrac{(\rho V)_P}{c_l \Delta t}\left(h_P^o - h_P^m + \dfrac{dh}{dT}^m T_P^m\right).$

Equation (14) is solved for the current temperature field $T_P^{m+1}$.

In the corrector step the enthalpy field is updated via Eq. (14) from the current temperature field. Following this step, the values of temperature at nodes that are changing phase is corrected to be consistent with the corrected values of enthalpy.

According to the definition of mixture enthalpy, the slope $dh^m/dT$ is calculated by

$$\frac{dh}{dT}^m = \left(f_s^m c_{ps} + f_l^m c_{pl}\right) + \left(\left(c_{ps} - c_{pl}\right) T - h_F\right)\frac{df_s^m}{dT} \tag{15}$$

where the slope of solid mass fraction is analytically derived from Eq. (9). At the discontinuity of the $f_s(T)$ curve, the slope is approximated by an arbitrarily large value (e.g. $10^{10}$).

It is well known that the control volume methods show poor convergence properties at large Rayleigh and Prantl numbers, due to the strong bi-directional coupling between the energy and momentum equations. In order to decrease this coupling a progressively smaller under-relaxation factor is used in the momentum equations as follows.

$$\omega = \omega_{init}\, e^{-rn} \tag{16}$$

where $\omega_{init}$ is the initial under-relaxation factor, $n$ is the iteration number and $r$ determines the rate of decrease. A rate value of 0.5 is used.

## 6. RESULTS AND DISCUSSION

### 6.1 Verification of the model

In order to check the model and code, simulations of previous published results for a diffusion controlled phase change problem is undertaken. The problem concerns the isothermal solidification of a liquid in a impermeable and rigid box. The box has an initial temperature of $T_{init} = 1535\,°C$ and at time zero, the temperature at walls was set to $T_{wall} = 1150\,°C$ which is lower then the melting temperature $T_s = 1500\,°C$. The thermophysical properties of the liquid and solid are assumed to be equal and constant, $\rho = 7200\,kg/m^3$, $c = 750\,J/kg\,K$, $k = 30\,W/m\,K$ and $k = 262.5\,kJ/kg\,K$. Due to symmetry of the problem, only one quarter of the box is considered. A uniform grid of 40x40 nodes was used and a time step of 250 s. Plotted in Fig. 3 are the temperature history at the center of the domain and the variation of solid fraction in the box. The predicted results are compared with those presented by Swaminathan and Voller [10]. The overall agreement between results, verifies the accuracy of the model and the numerical code.
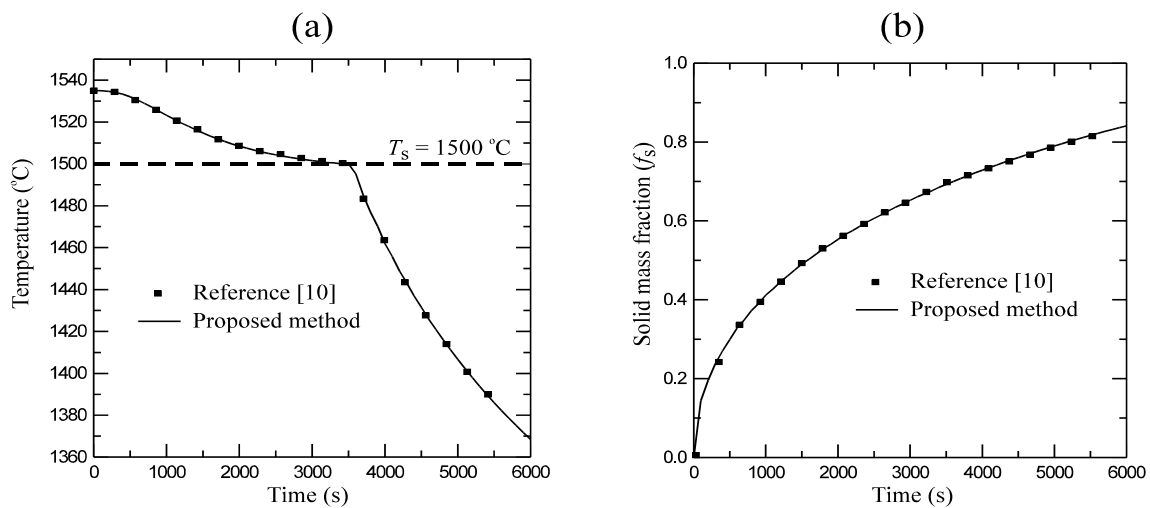
(a) (b)



**Fig. 3.** (a) Temperature history and (b) progress of solidification.

### 6.2 Implementation

In order to show the capabilities of the proposed model, results from the solution of the test problem described in section 2 are presented. The problem domain and the boundary conditions are shown in Fig. 1. The geometric data and the thermophysical properties (approximating an aqueous ammonium chloride solution) are given in Table 1. A 40x40 space grid, properly refined near the walls, and a fixed time step of 1 s were used. Iterations for each time step were terminated when the sum of absolute residuals in mass, momentum, energy and solute equations dropped below $1 \times 10^{-4}$.

The progress of solidification and thermo-solutal driven flow with time are shown in Figs. 4(a)-(c) in which streamlines and contours of solid mass fraction are plotted. Once cooling is initiated at the left wall, a strong counter-clockwise flow field is established in the liquid. This field is driven by the high thermal gradients. The formation of three distinct regions (solid, mushy and liquid) is also indicated. Due to the presence of dendrites, the natural convection inside the mushy zone is very weak. As solid forms, the solute phase is rejected from the solid in the adjoining liquid, making it less dense than the bulk liquid. Due to thermal natural convection, this cold, solute-rich fluid, accumulates at the top of the cavity.

**Table 1**. Test problem data.

| | |
|---|---|
| Cavity dimensions | $H=L=0.025$ m |
| Initial conditions | $T_{init}=600$ K , $C_{init}=0.1$ kg/m$^3$ |
| Wall temperature | $T_{wall}=200$ K |
| Specific heat | $c_s=1870$, $c_l=3200$ J/kg K |
| Thermal conductivity | $k_s=0.4$, $k_l=0.45$ W/m K |
| Viscosity | $\mu_l=0.001$ kg/m s |
| Diffusion coefficient | $D_l=4.8\times10^{-9}$ m$^2$/s |
| Latent heat | $h_f=3.0\times10^5$ J/kg |
| Expansion coefficients | $\beta_T=4.0\times10^{-5}$ K$^{-1}$ , $\beta_C=0.025$ |
| Eutectic temperature | $T_e=250$ K |
| Melting point of pure material | $T_M=630$ K |
| Eutectic concentration | $C_e=0.1$ kg/kg$_m$ |
| Equilibrium partition ratio | $\kappa=0.3$ |

At time $t=300$ s, a small clockwise circulating region appears at the bottom of the cavity, driven by the solute concentration gradients. Hence, a double-diffusive interface is formed, separating the solute-rich fluid from underlining fluid. The extend of macro-segregation is shown in Fig. 4(d), in which the contours of solute concentration at time $t=100$ s are plotted. This figure clearly shows the accumulation of solute-rich fluid at the top of the cavity.
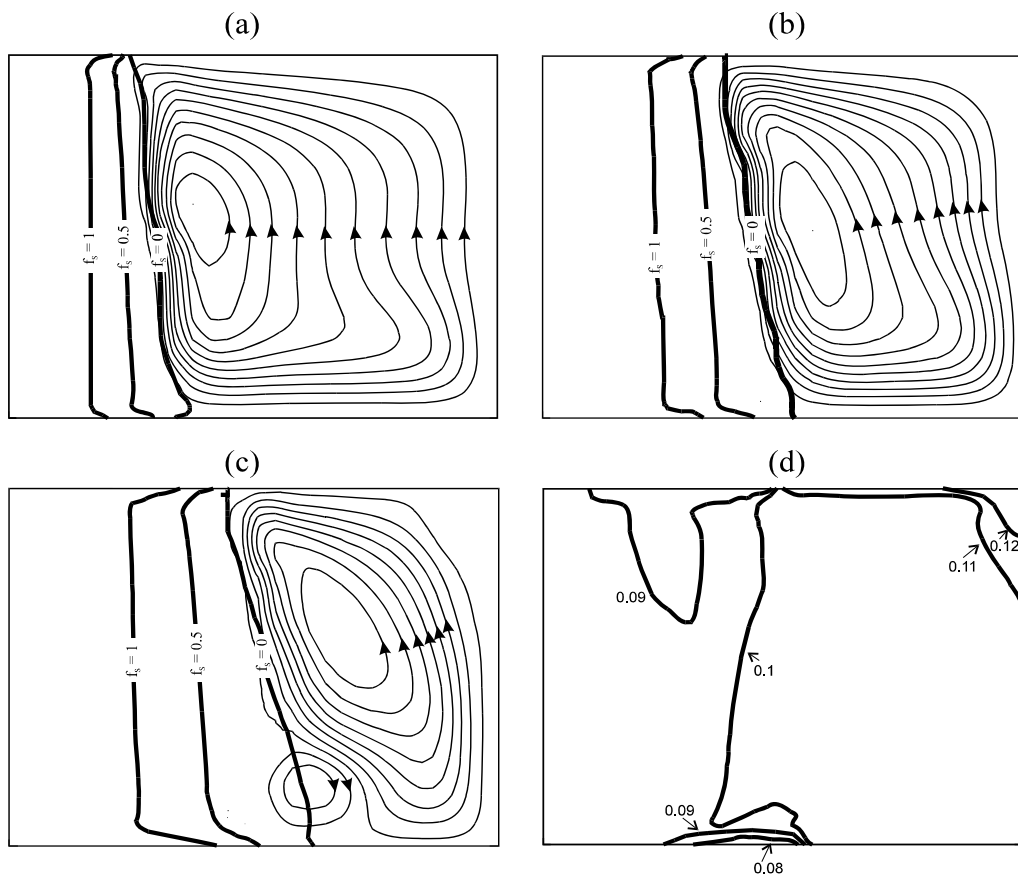


**Fig. 4.** (a), (b), (c) Streamlines and solid mass fraction contours at $t=100$ s, $t=200$ s, $t=300$ s, (d) contours of solute concentration at time $t=100$ s.

## 7. CONCLUSIONS

A stable and accurate numerical method for the solution of phase change problems has been presented. The method applied to a to the solidification of a mixture in a freezing cavity. The proposed method successfully predicts the phenomena observed in experiments such as the growth of the mushy region, the solute macro-segregation, and the double-diffusive flow patterns. From these results, it can be concluded that the proposed method can be applied to analyse various phase change processes.

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