

Numerical modeling of convection-diffusion phase change problems

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Abstract A numerical methodology is presented for the modeling of convection-diffusion controlled mushy region change problems. An efficient and accurate non-staggered control volume method, based on the momentum interpolation practice and on a high-order convection differencing scheme, is proposed for the solution of the continuum model equation. Suitable numerical techniques are implemented to overcome the numerical instability problems resulting from the strong coupling between the equations of the model. Special attention is given on the efficient treatment of the latent heat evolution in the energy equation. A new numerical technique is developed which accounts for the dependence of the latent heat on the variation of temperature and concentration fields. The proposed method is applied on two phase change problems. Satisfactory agreement with previously published results is observed.

1 Introduction

Processes related to melting and solidification are widely encountered in many industrial applications (Flemings 1974), such as metal alloy casting, food freezing, ice forming, thermal energy storage, etc. Mathematical modeling 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 involve 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 characterize the phase change of most materials, the exact solution of conservation equation is impossible (Zerroukat and Chatwin 1994). The numerical models for solving phase change problems can be conveniently divided into two categories (Samarkii et al. 1993). The first category involves methods that utilize independent conservation equations for each phase. A moving-front practice is fol-

lowed, 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 consists of single region models that utilize a system of conservation equations than can be equally applied to both phases (Benon and Incropera 1987; Voller et al. 1989). The latent heat evolution is accounted for in the energy equation by the enthalpy formulation (Swaminathan and Voller 1992, 1993; Yang and Ebadian 1994), while no explicit conditions on the interface are required and the numerical solution can be carried out on a fixed grid. Single region models are well suited for treating the phase change of mixtures where, the latent heat is evolved over a temperature range (Raghavarao and Sanyasiraju 1996).

The major advantage of the single region models is that their 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.

The purpose of this paper is to develop an efficient and accurate numerical methodology to deal with binary solid-liquid phase change problems. A control volume numerical method based on non-staggered grids and a high-order convection differencing scheme will be used. The focus in this paper is on the numerical treatment of the energy equation, in particular on the efficient handling of the coupling effects of the temperature and concentration on the evolution of the latent heat. The performance of the present method will be examined through the solution of two test problems. The first problem concerns the isothermal solidification of a liquid driven by conduction and the second problem concerns the solidification of an aqueous NH_4Cl solution.

2 Mathematical formulation

2.1 Problem description

Consider a binary mixture (e.g. a binary alloy) of initial concentration C_{init} and initial temperature $T_{\text{init}} > T_l$ (the liquidus temperature), in a rectangular cavity insulated on three sides as illustrated in Fig. 1. At time $t = 0$, the left side is cooled to a temperature $T_{\text{wall}} < T_l$ so that freezing

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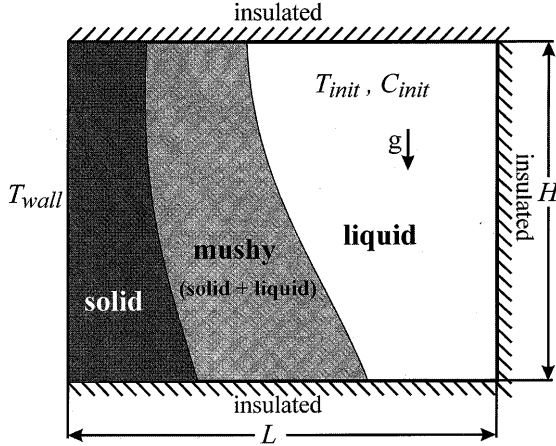


Fig. 1. A schematic of solidification in a rectangular cavity

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 (Flemings 1974). The system is influenced by diffusion phenomena and natural convection flow, which is caused by the temperature and concentration gradients.

2.2

Model equations

The behavior 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 developed by Bennon and Incropera (1987), and can be derived from the mixture theory or through a volume averaged procedure (Ni and Beckermann 1991). Under the assumptions of Newtonian laminar flow, constant densities except for the buoyancy terms, negligibly shrinkage-caused flow, local thermodynamic equilibrium and negligible species diffusion in solid, the governing equations may be written as follows:

Conservation of mass

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

Conservation of momentum

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

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

Conservation of energy

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

Conservation of species

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

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

$$\rho = g_s \rho_s + g_l \rho_l \quad (6)$$

$$\mathbf{u} = f_l \mathbf{u}_l \quad (7)$$

$$h = f_s h_s + f_l h_l \quad (8)$$

$$C = f_s C_s + f_l C_l \quad (9)$$

$$k = g_s k_s + g_l k_l \quad (10)$$

$$D = f_l D_l \quad (11)$$

where f_s, f_l are the mass fraction of the solid and liquid phase respectively and are related to the volume fractions g_s, g_l through:

$$\rho f_s = \rho_s g_s \quad \text{and} \quad \rho f_l = \rho_l g_l \quad (12)$$

The term ρB , 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:

$$\rho B_x = \rho_{\text{ref}} g [b_T (T - T_{\text{ref}}) + b_C (C_l - C_{\text{ref}})] \quad (13)$$

where $T_{\text{ref}}, C_{\text{ref}}$ are the reference values of temperature and concentration (usually coincide with the eutectic values), ρ_{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 Eqs. (5) and (6) represent 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, this term is given from the Karman-Kozeny equation:

$$K = K_0 \left[\frac{g_l^3}{(1 - g_l)^2} \right] \quad (14)$$

where the permeability coefficient K_0 depends on the morphology of the porous media. In the pure liquid region ($g_l = 1$) and in the pure solid region ($g_l = 0$), Eq. (14) reduces to $K = \infty$ and $K = 0$, respectively.

2.3

Closure of the system

Closure of the system of governing equations requires additional relationships for the phase mass fractions f_s, f_l and the liquid phase composition C_l . In the continuum phase change model described above these quantities are indirectly determined from the equilibrium phase diagram (Fig. 2). On assuming straight liquidus and solidus lines, the solid mass fraction can be expressed as:

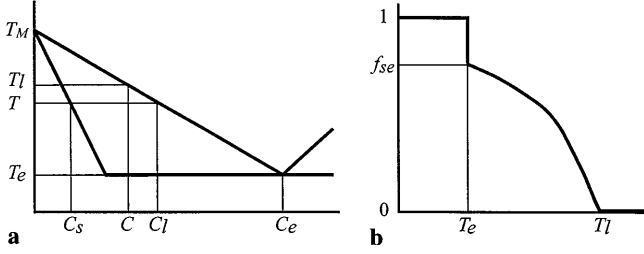


Fig. 2 a A typical equilibrium phase change diagram and (b) the solid mass fraction – temperature relationship

$$f_s = \begin{cases} 1 & T < T_e \\ [f_{se}, 1] & T = T_e \\ \frac{1}{1-k_p} \frac{T_l - T}{T_M - T} & T_e < T < T_l \\ 0 & T \geq T_l \end{cases}, \quad (15)$$

where T_e is the eutectic temperature. T_M is the melting point of the pure material (as $C \rightarrow 0$), T_l is the liquidus temperature give be:

$$T_l = T_M + \frac{T_e - T_M}{C_e} C. \quad (16)$$

k_p is the equilibrium partition ratio ($k_p = C_l/C_s$) and f_{se} is the solid mass fraction at the onset of the eutectic reaction:

$$f_{se} = \frac{1}{1 - k_p} \frac{T_l - T_e}{T_M - T_e}. \quad (17)$$

The liquid phase species concentration is given by:

$$C_l = \frac{T - T_M}{T_e - T_M} C_e. \quad (18)$$

Finally, assuming constant specific heats of the two phases (c_{ps}, c_{pl}), though not necessarily equal, the phase enthalpies can be expressed as:

$$h_s = c_{ps}T, \quad h_l = c_{pl}T + h_f \quad (19)$$

where h_f is the latent heat of phase change.

3 Numerical methodology

3.1 Control volume method

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

$$\frac{\partial}{\partial t}(\rho\phi) + \text{div}(\rho\mathbf{u}\phi) = \text{div}(\Gamma \text{grad } \phi) + S_\phi \quad (20)$$

by properly defining the quantities ϕ , Γ and S_ϕ . The system of equations, subjected to the required boundary conditions, was solved by an implicit control volume based method. The main characteristics of the method are:

- The adoption of a non-staggered grid arrangement using the momentum interpolation method (Rhie and Chow 1983) as modified by Majumdar (1988), to avoid the non-physical “checkerboard” oscillations in the pressure field.
- The application of the segregated SIMPLEC algorithm to resolve the pressure velocity coupling.

- The use of the second order QUICK differencing scheme, as presented in Arampatzis et al. (1994), for the discretization of convective terms, to ensure the accuracy of the results.
- The solution of the set of the algebraic equations, resulting from the discretization of the model equations, by the strongly implicit procedure (SIP) (Stone 1968), aided by a block-correction procedure.

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.

$$\omega = \omega_{\text{init}}e^{-rm} \quad (21)$$

where ω_{init} is the initial under-relaxation factor, m is the iteration number and r determines the rate of decrease. A rate value of 0.05 was used.

3.2 The treatment of the energy equation

The finite volume discretization of the energy equation (4) cannot be directly accomplished, because it contains as unknowns both the temperature and the mixture enthalpy. However, properly handling the terms of this equation, it can be recast in the form of Eq. (20) with dependent variable the temperature (T -based methods) (Zeng and Faghri 1994) or the enthalpy (h -based methods) (Bennon and Incropera 1987). The major problem with the numerical solution of the energy equation is the treatment of the latent heat evolution. In T -based methods, the latent heat is accounted for by defining an effective heat capacity or through a heat source term while in the h -based methods it is included in the definition of the mixture enthalpy (Eqs. (8), (9)). Special attention should be given to the treatment of the latent heat evolution when modeling binary phase change systems, because this term is a function of the temperature as well as of the mixture concentration. This fact produces a strong coupling between the energy and species concentration equations and causes numerical instability problems.

In the present study, an extended version of the predictor-corrector method proposed by Swaminathan and Voller (1993) has been developed. The focus was be on the efficient handling of the coupling effects of temperature and concentration on the evolution of the latent heat. The key steps in this approach are:

- In a given time step, the energy equation (4) is written if the following discretized form:
$$a_P T_P^{m+1} = \sum_M a_M T_M^{m+1} + \frac{(\rho V)_P}{c_1 \Delta t} (h_P^0 - h_P^{m+1}) + b \quad (22)$$

where the superscript m indicates the iteration level.

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

$$h_p^{m+1} = h_p^m + \frac{\partial h^m}{\partial T} (T_P^{m+1} - T_P^m) + \frac{\partial h^m}{\partial C} (C_P^{m+1} - C_P^m) \quad (23)$$

c) Using this expression, Eq. (22) can be written as:

$$(a_p - S_p)T_P^{m+1} = \sum_M a_M T_I^{m+1} + b + S_U \quad (24)$$

where

$$S_p = -\frac{(\rho V)_p \partial h^m}{c_l \Delta t \partial T} \quad (25)$$

$$S_U = \frac{(\rho V)_p}{c_l \Delta t} \times \left(h_p^0 - h_p^m + \frac{\partial h^m}{\partial T} T_P^m + \frac{\partial h^m}{\partial C} (C_P^m - C_P^{m+1}) \right) \quad (26)$$

- d) Equation (24) is solved for the current temperature field T_P^{m+1} .
e) In the corrector step the enthalpy field is updated via Eq. (23). Then, the temperature at nodes where phase change occurs is corrected to be consistent with the new values of the enthalpy.

The partial derivatives of the enthalpy with respect to temperature and concentration can be evaluated from the definition of the mixture enthalpy (Eqs. (8), (19)) as:

$$\frac{\partial h}{\partial T} = (f_s c_{ps} + f_l c_{pl}) + ((c_{ps} - c_{pl})T - h_F) \frac{\partial f_s}{\partial T} \quad (27)$$

$$\frac{\partial h}{\partial C} = ((c_{ps} - c_{pl})T - h_F) \frac{\partial f_s}{\partial C} \quad (28)$$

where the derivatives of the solid mass fraction can be analytically derived from Eq. (15) and the lever rule. At the discontinuity of the $f_s(T)$ curve, the slope is approximated by an arbitrarily large value (e.g. 10^{10}).

The corrector step (e) is similar to the post-iterative correction scheme (Comini et al. 1990) and will take into account of cases where a nodal temperature falls from above the liquidus to below the solidus temperature in one time step.

The last term in Eq (26) includes the effects of the concentration variation on the latent heat evolution and effectively handles the coupling of energy and species conservation equations. However, the solution of species conservation differences ($C_P^m - C_P^{m+1}$) must be stored in order to be used in the source term of the energy equation.

4 Results and discussion

4.1 Model verification

In order to check the model and code, simulations of previous published results for diffusion controlled phase change problem were undertaken. The problem concerns the isothermal solidification of a liquid in a impermeable and rigid box. The box has an initial temperature of $T_{init} = 1535^\circ\text{C}$ and at time zero, the temperature at walls

was set to $T_{wall} = 1150^\circ\text{C}$ which is lower than the melting temperature $T_s = 1500^\circ\text{C}$. The thermophysical properties of the liquid and solid are assumed to be equal and constant, $\rho = 7200 \text{ kg/m}^3$, $c = 750 \text{ J/kgK}$, $k = 30 \text{ W/mK}$ and $k = 262.5 \text{ kJ/kg K}$. Due to the symmetry of the problem, only one quarter of the box is considered. A uniform grid of 40×40 nodes and a time step of 250 s were used. In Fig. 3 the temperature history at the center of the domain and the variation of solid fraction in the box are portrayed. The predicted results are compared with those presented by Swaminathan and Voller (1992). The overall agreement between results, verifies the accuracy of the model and the numerical code.

4.2 Implementation to test problem

In order to show the capabilities of the proposed model, results from the solution of the test problem described in Sect. 2.1 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

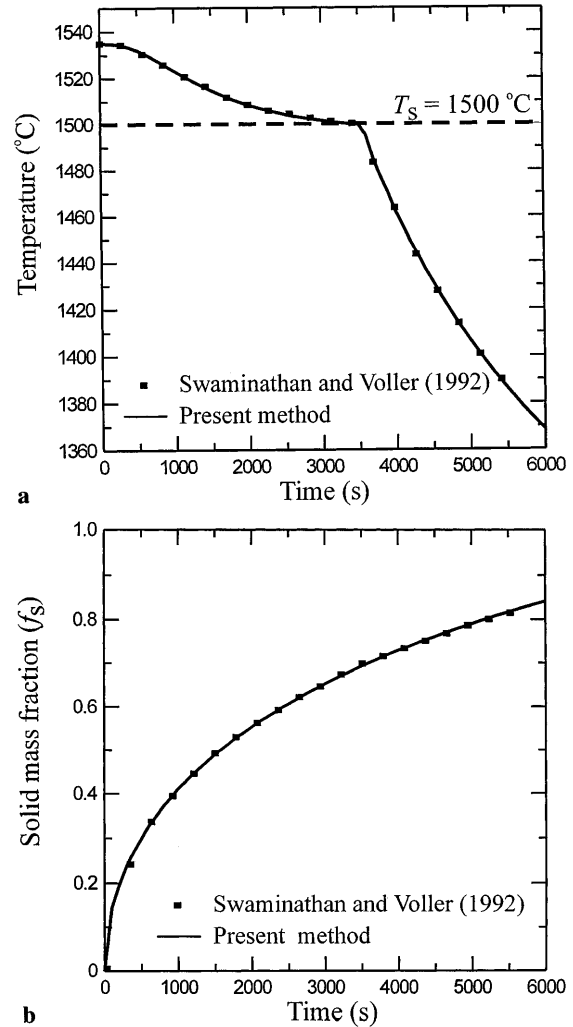


Fig. 3a,b. Isothermal solidification in a box. (a) Temperature history and (b) progress of solidification

Table 1 Solidification of a binary mixture in a freezing cavity. Test problem data and thermophysical properties

Density	$\rho_s = \rho_l = 1077 \text{ kg/m}^3$
Cavity dimensions	$H = L = 0.025 \text{ m}$
Initial conditions	$T_{\text{init}} = 600 \text{ K}, C_{\text{init}} = 0.1$
Wall temperature	$T_{\text{wall}} = 200 \text{ K}$
Specific heat	$c_{ps} = 1870, c_{pl} = 3249 \text{ J/kg} \cdot \text{K}$
Thermal conductivity	$k_s = 0.393, k_l = 0.468 \text{ W/m} \cdot \text{K}$
Viscosity	$\mu_l = 0.001 \text{ kg/m} \cdot \text{s}$
Diffusion coefficient	$D_l = 4.8 \times 10^{-9} \text{ m}^2/\text{s}$
Latent heat	$h_f = 3.138 \times 10^5 \text{ J/kg}$
Expansion coefficients	$b_T = 3.83 \times 10^{-4} \text{ K}^{-1},$ $b_C = 0.257$
Eutectic temperature	$T_e = 257.75 \text{ K}$
Melting point of pure material	$T_M = 633.6 \text{ K}$
Eutectic concentration	$C_e = 0.8$
Equilibrium partition ratio	$k_p = 0.3$
Permeability coefficient	$K_0 = 5.56 \times 10^{-11}$

Table 1. A 40×40 space grid, property 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, solute and energy equations dropped below 1×10^{-6} . Calculations were performed on an Intel 133 MHz Pentium processor and required approximately 20 s of CPU time for each second of simulation time.

The progress of solidification and the thermo-solutal driven flow with time are shown in Figs. 4a–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 is formed, 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. At time $t = 6$ min, 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 the underlining fluid.

Figures 5a–d show velocity vectors of the flow field and the temperature field as lines of constant temperatures at four different times. The velocity vectors clearly show the development of the thermal and solutal driven flow field. The isotherms indicate that the temperature gradients are concentrated in the solid and mushy regions, where the energy transport is driven by conduction.

The extend of macro-segregation is shown in Fig. 6, in which the contours of solute concentration at time $t = 6$ min are plotted clearly showing the accumulation of solute-rich fluid at the top of the cavity.

5

Conclusions

A stable and accurate numerical method for the solution of phase change problems has been presented. An extension of a predictor corrector scheme has been developed which

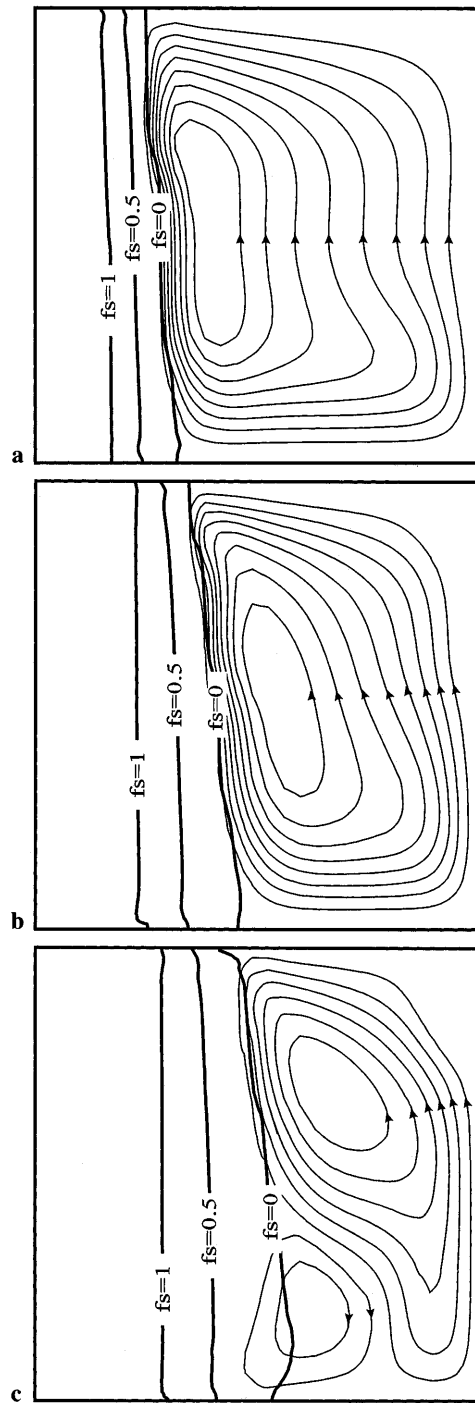


Fig. 4a–c. Solidification of a binary mixture in a freezing cavity. Streamlines and solid mass fraction contours at (a) $t = 2$ min, (b) $t = 4$ min and (c) $t = 6$ min

handles the coupling effects of the temperature and concentration on the evolution of the latent heat. The method applied 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 used to analyze various phase change processes.

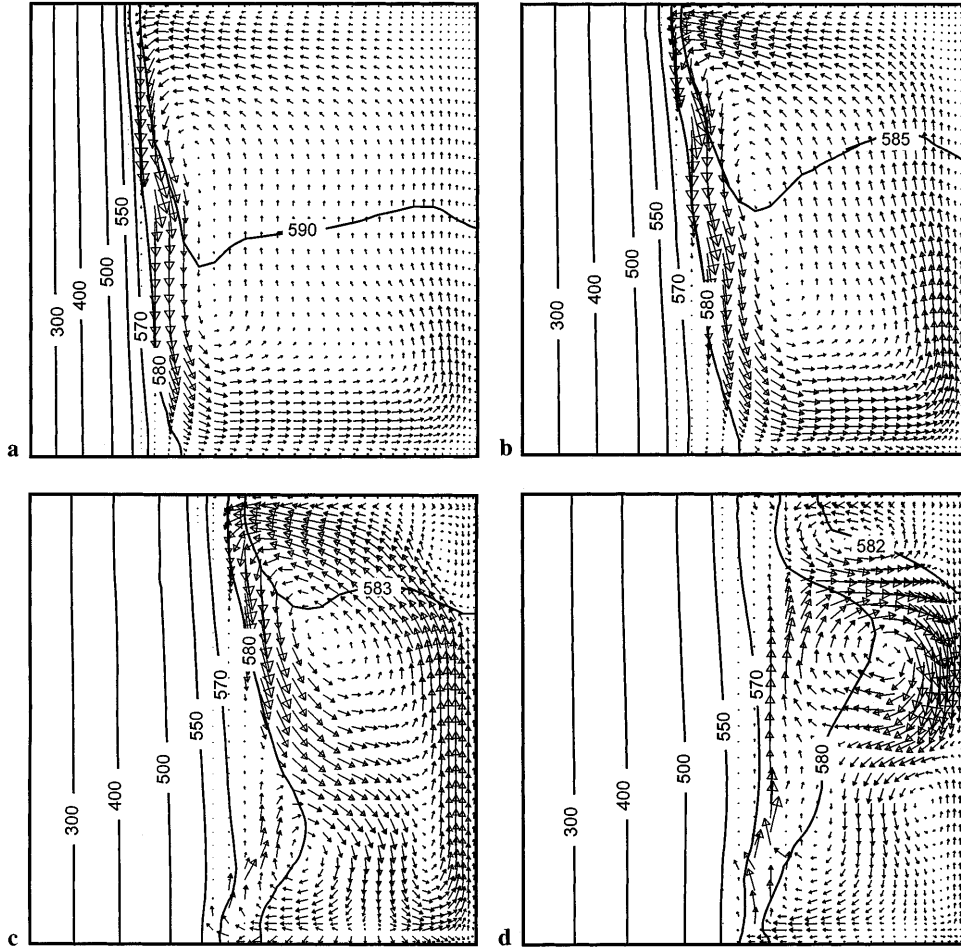


Fig. 5a–d. Solidification of a binary mixture in a freezing cavity. Velocity vectors and isotherms at (a) $t = 2$ min, (b) $t = 4$ min, (c) $t = 6$ min and (d) $t = 8$ min

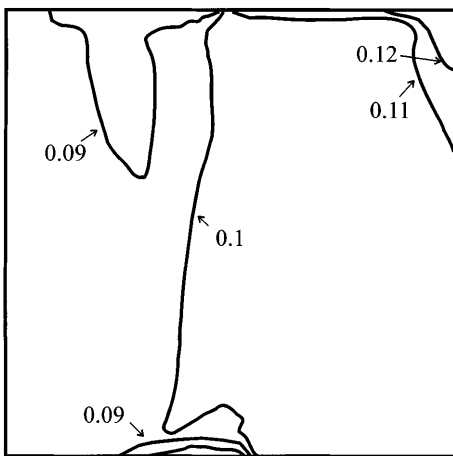


Fig. 6. Solidification of a binary mixture in a freezing cavity. Isocomposition lines at $t = 6$ min

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