



**Introduction**

Several methods have been proposed for treating phase change problems, ranging from interface-tracking methods to fixed-domain methods. The latter, also known as enthalpy methods, are the most popular due to the fact that they need not track the solid-liquid interface, and that they may be applied to complex multi-dimensional phase change problems.

Enthalpy methods may be derived from a continuum model or from a volume averaging model. The former is based on the mixture theory, and the microscopic interactions between phases are overlooked. The latter rests on the averaging of the microscopic equations over a representative elementary volume (REV). This model brings further insights on the different terms involved in the resulting macroscopic equations while it eliminates the need for specifying the microscopic configurations of the interphase boundaries. Their effects appear at the macroscopic level in the expressions for the macroscopic constants.

These models are, in fact, not new. Bowen (1967) and Muller (1968) developed continuum models for transport phenomena in mixtures. Bennon and Incropera (1987) have developed a continuum model for the solidification process of mixtures. The volume averaging model was considered by Whitaker (1977) for the prediction of drying processes. Bashmat and Beer (1980) introduced the concept of a representative elementary volume as opposed to an arbitrarily elementary volume, and re-established in different forms the averaging rules involved in the model. In an accompanying paper, Beer and Bashmat (1980) applied their theory to the transport of mass, energy and momentum in a porous medium. Lately, Beckermann and Viskanta (1988) and Ni and Beckermann (1991) have employed this model for predicting solidification processes of mixtures.

In all the aforementioned papers, there is no explicit mathematical determination of the effective thermal conductivity of a porous medium. The effective thermal conductivity of a porous medium has been determined, however, on a practical/statistical basis. Veinberg (1967) developed a relation for the effective thermal conductivity of a packed bed filled randomly with spherical inclusions. He claims that his relation is universal for this type of inclusions. Tien and Vafai (1979) established statistical bounds of the effective thermal conductivity for microspheres and fibrous insulation media. They state that the pertinent parameters for determining the effective thermal conductivity are the conductivities of the constituent phases, their volume fractions and a constant that is a function of the cell geometry.

Enthalpy methods as applied to phase change problems have two major deficiencies. First, they do not accurately estimate the thermal conductivity of a control volume containing the two phases. As a consequence, poor accuracy will be produced in the results, in particular when the phases exhibit large thermal conductivity differences. Second, they produce oscillatory behavior in the thermal field and in predicting the interface, due to the assumption of thermal equilibrium of phases involved in the aforementioned models. To

eliminate these oscillations, Tacke (1985) employed an explicit scheme to solve a one-dimensional solidification problem. Tacke calculated first the liquid fraction by equating the calculated total enthalpy to the average enthalpy of a control volume, and then he determined the nodal temperature using a linear profile near the interface. Lee and Tzong (1991) proposed a modified weighting scheme for discretizing the energy equation using a source-term based formulation. They calculated first, the interface position using a linear interpolation between nodes adjacent to the interface, and next the local liquid fraction. Recently, Voller and Swaminathan (1993) have proposed a rigorous method for treating discontinuities in the thermal conductivity at the interface. Their method is based on the Kirchhoff transformation. According to the authors, however, oscillations in the thermal field are dampened but may still prevail.

The objectives of this paper are:

- To develop a general expression for the effective thermal conductivity of a two-phase composite medium.
- To develop a numerical method for removing the unrealistic oscillations in the thermal field.

The methodology involves averaging the microscopic conservation equations of a two-phase composite medium over a representative elementary volume (REV) in order to obtain macroscopic equations expressed in terms of the averaged physical quantities of the medium. The model assumes that the phases may coexist at a temperature different from that of fusion.

### Macroscopic averaged equations

In the present development, heat conduction with no internal heat sources is considered in a two-phase composite medium. The general microscopic balance equation for an intensive physical quantity such as the enthalpy may be written as follows:

$$\frac{\partial H_k}{\partial t} + \nabla \cdot \mathbf{q}_k = 0 \quad (k = 1, 2) \quad (1)$$

and the jump condition at the interface is given by:

$$\mathbf{q}_1 \cdot \mathbf{n}_1 = \mathbf{q}_2 \cdot \mathbf{n}_1 + [H_1 - H_2] \cdot \mathbf{w} \cdot \mathbf{n}_1 \quad (2)$$

The variables in equations (1) and (2) are defined in the nomenclature. The idea here is to average equation (1) over a representative elementary volume (REV) that contains portions of each phase. To achieve this goal, intensive quantities continuous over the entire domain are defined. Let  $\psi_k$  stand for a physical quantity defined in the phase  $k$ , i.e. it has non zero values in the phase  $k$  and

zero values elsewhere. The averaged value of  $\psi_k$  over the REV is expressed in two forms:

*Phase average:*

$$\langle \psi_k \rangle = \frac{1}{\Omega} \int_{\Omega} \psi_k d\omega = \frac{1}{\Omega} \int_{\Omega_k} \psi_k d\omega \quad (3)$$

*Intrinsic phase average:*

$$\bar{\psi}_k = \frac{1}{\Omega_k} \int_{\Omega_k} \psi_k d\omega = \frac{1}{\Omega_k} \int_{\Omega} \psi_k d\omega \quad (4)$$

Obviously,  $\langle \psi_k \rangle = \varepsilon_k \bar{\psi}_k$ , where  $\varepsilon_k = \Omega_k/\Omega$  is the phase volume fraction. The quantities  $\langle \psi_k \rangle$  and  $\bar{\psi}_k$  are defined over the entire REV, and may take non-zero values in the phase  $j$  ( $j \neq k$ ). Implicitly, the phase volume fraction  $\varepsilon_k$  is also continuous over the entire domain. Taking the average of equation (1) over the REV, and applying the following averaging rules (Bashmat and Beer, 1980; Gray, 1975; Whitaker, 1977):

$$\left\langle \frac{\partial H_k}{\partial t} \right\rangle = \frac{\partial}{\partial t} \langle H_k \rangle - \frac{1}{\Omega} \int_{A_i} H_k \mathbf{w} \cdot \mathbf{n}_k dA \quad (5)$$

$$\langle \nabla \mathbf{q}_k \rangle = \nabla \langle \mathbf{q}_k \rangle + \frac{1}{\Omega} \int_{A_i} \mathbf{q}_k \mathbf{n}_k dA \quad (6)$$

$$\langle \mathbf{q}_k \rangle = \langle -k_k \nabla T_k \rangle = -k_k \varepsilon_k \nabla \bar{T}_k - \frac{k_k}{\Omega} \int_{A_i} [T_k - \bar{T}_k] \mathbf{n}_k dA \quad (7)$$

the averaged form of equation (1) becomes:

$$\frac{\partial}{\partial t} \langle H_k \rangle = \nabla \cdot \left\{ k_k \varepsilon_k \nabla \bar{T}_k + \frac{k_k}{\Omega} \int_{A_i} [T_k - \bar{T}_k] \mathbf{n}_k dA \right\} + \frac{1}{\Omega} \int_{A_i} [H_k \mathbf{w} \cdot \mathbf{n}_k - \mathbf{q}_k \cdot \mathbf{n}_k] dA \quad (8)$$

Equation (8) is written in terms of averaged variables, and it is valid over the entire domain. Unfortunately, it contains interface terms that cannot be easily handled. To eliminate these terms, equation (8) is rewritten in terms of the averaged variables of the medium. Adding equations (8) for  $k = 1$  and  $2$ , taking into account the jump condition (equation 2) and the temperature continuity ( $T_1 = T_2 = T$ ) at the interface, and assuming that the phases are in thermodynamic equilibrium ( $\bar{T}_1 = \bar{T}_2 = \bar{T}$ ), one obtains:

$$\frac{\partial H_m}{\partial t} = \nabla (k_m \nabla \bar{T}) + \nabla \left\{ \frac{k_1 - k_2}{\Omega} \int_{A_i} [T - \bar{T}] n_1 dA \right\} \quad (9)$$

where  $H_m = \varepsilon_1 H_1 + \varepsilon_2 H_2$  and  $k_m = \varepsilon_1 k_1 + \varepsilon_2 k_2$ . Equation (9) still contains an interface term which is difficult to determine since the interface is unknown a priori. The goal here is to express equation (9) in a conventional form. A Taylor series expansion for the temperature in the REV yields:

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$$T = \bar{T} + \mathbf{dx} \cdot \nabla T + \frac{1}{2} [\mathbf{dx} \cdot \nabla T]^2 + \dots \quad (10)$$

where  $\mathbf{dx} = \mathbf{x} - \mathbf{X}$ .  $\mathbf{x}$  is the position vector of a microscopic point and  $\mathbf{X}$  is the position vector of the point (macroscopic) associated with the REV (e.g. its geometrical center). Furthermore, one can pose  $\nabla T = \mathbf{D} \cdot \nabla \bar{T}$ , where  $\mathbf{D}$  is a coefficient (tensor), which may be a function of space and time. If the first two terms on the right hand side of equation (10) are retained, the interface term in equation (9) takes the following form:

$$\frac{1}{\Omega} \int_{A_i} [T - \bar{T}] n_1 dA = \frac{1}{\Omega} \int_{A_i} [\mathbf{dx} \cdot (\mathbf{D} \cdot \nabla \bar{T})] n_1 dA = \mathbf{G} \cdot \nabla \bar{T} \quad (11)$$

where  $\mathbf{G}$  is a tensor given by:

$$\mathbf{G} = \frac{1}{\Omega} \int_{A_i} [(\mathbf{n}_1 \cdot \mathbf{dx}) \cdot \mathbf{D}] dA \quad (12)$$

It is now possible to define a tensorial thermal conductivity associated with the interface:

$$k_i = (k_1 - k_2) \mathbf{G} \quad (13)$$

Thus, the effective thermal conductivity of a composite medium is defined as:

$$k_{eff} = k_m + k_i \quad (14)$$

and, as a result, equation (9) becomes:

$$\frac{\partial H_m}{\partial t} = \nabla (k_{eff} \nabla \bar{T}) \quad (15)$$

It is interesting to note that equation (15), developed using a volume averaging technique, is similar in form to that developed using the continuum model

approach (Bennon and Incropera, 1987). According to the foregoing derivation, the presence of the interface and of the temperature gradients in the REV may have significant effects on the averaged physical properties of the medium. These effects, however, are overlooked in the continuum model.

### Determination of the effective thermal conductivity

According to the previous demonstration, the presence of an interface in a composite medium introduces a thermal conductivity tensor which depends on its morphology and, thus, renders the medium anisotropic. Owing to this a priori-unknown morphology, one can assume, as a first approximation, that the conductivity tensor  $\mathbf{G}$  is isotropic, and that  $\mathbf{G}$  is a function of space and time, of the phase volume fractions, of the physical properties of each phase, and of any pertinent parameters. The conductivity  $k_i$  may then be written as follows:

$$k_i = (k_1 - k_2) \mathbf{G} = A \cdot |k_1 - k_2| \cdot \Phi(X, t, \epsilon_1, \epsilon_2, k_1, k_2, \dots) \quad (16)$$

where  $A$  is a constant and  $\Phi$  a function, which has to satisfy the following criterion:

$$\Phi|_{\epsilon_1=0} = \Phi|_{\epsilon_1=1} = 0 \quad (17)$$

Two types of composite media are distinguished according to the nature of the interface (fixed or moving). In the case of a fixed interface medium, the heat flux across the interphase boundaries is continuous (see equation (2)). The thermal conductivity is lowerly bound by the harmonic mean (when the phases are connected in series) and upperly bound by the arithmetic mean (when the phases are connected in parallel):

$$\frac{k_1 k_2}{k_1 \epsilon_2 + k_2 \epsilon_1} \leq k_{eff} \leq k_1 \epsilon_1 + k_2 \epsilon_2 \quad (18)$$

which yields:

$$-|k_1 - k_2| / k_{max} \leq A \leq 0 \quad (19)$$

where  $k_{max}$  is the maximum of  $k_1$  and  $k_2$ . However, in the case of a moving interface medium, the heat flux is discontinuous at the interphase boundaries. The outward heat flux ( $q_2$ ) depends basically on the physical properties of phase two while it is independent of the inward heat flux ( $q_1$ ). As a consequence, the harmonic mean, which assumes a continuous heat flux at the interface, is no longer valid while the arithmetic mean holds. Consider, for instance, a one-dimensional slab as shown in Figure 1. The heat flux that crosses the interface situated between points one and two may be defined as:

$$q_{1-2} = \frac{k_{eff}}{\Delta x} [T_1 - T_2] \quad (20)$$

The subscripts <sub>1</sub> and <sub>2</sub> refer to the phases left and right of the interface, respectively. The interface may move from left to right. Writing similar expressions for  $q_1$  and for  $q_2$ , one obtains:

$$k_{eff} = \frac{q_{1-2}}{q_1 \epsilon_1 / k_1 + q_2 \epsilon_2 / k_2} \quad (21)$$

The heat flux  $q_{1-2}$  may be expressed as follows:

$$q_{1-2} = \frac{1}{\Delta x} \int q dx = q_1 \epsilon_1 + q_2 \epsilon_2 \quad (22)$$

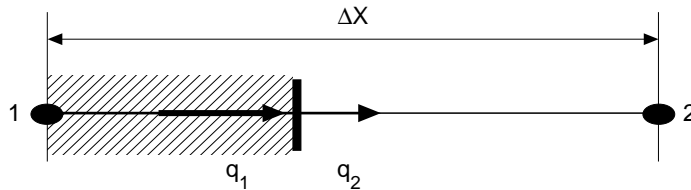
Comparing equation (21) with equation (14), one obtains:

$$A = \text{sign}(k_1 - k_2) \cdot (k_2 - \sigma k_1) / k_{max} \quad (23)$$

$$\Phi = \frac{\epsilon_1 \epsilon_2}{(k_2 / k_{max}) \epsilon_1 + \sigma (k_1 / k_{max}) \epsilon_2} \quad (24)$$

where  $\sigma = q_2 / q_1$ . Three limiting cases are possible:

- $\sigma = 1$ : This case corresponds to a series connection for a fixed interface medium, or asymptotically to  $k_1 \ll k_2$  for a slowly moving interface medium. Equation (21) yields the harmonic mean.
- $\sigma = k_2 / k_1$ : This case corresponds to a parallel connection for both fixed or moving interface media. Equation (21) yields the arithmetic mean.
- $\sigma = 0$ : This case corresponds to  $q_2 = 0$  (when phase two is saturated), or asymptotically to  $k_1 \gg k_2$  for a moving interface medium. Equation (21) is reduced to  $k_{eff} = k_1$  while the harmonic mean would yield  $k_2 / \epsilon_2$ .



**Figure 1.**  
Composite slab

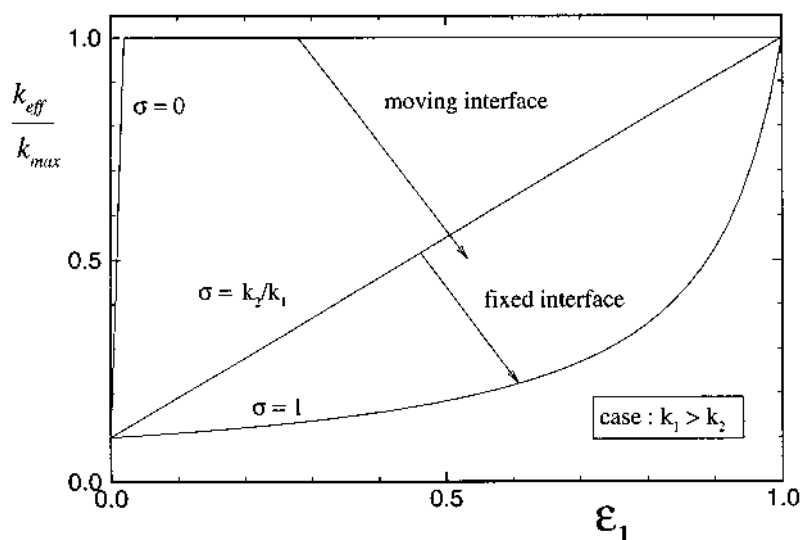
Equations (23) and (24) are then valid for any phase connection (series, parallel or mixed) for both fixed or moving interface media. Accordingly, the effective thermal conductivity of a composite medium is dependent on the thermal conductivities of its constituents, on their volume fractions and on a constant which determines the geometric structure of the medium and the nature of the interface. This constant should be determined experimentally for a fixed interface medium, or by knowing the heat flux ratio at the interface for a moving interface medium. In the case of a fixed interface medium, the parameter  $\sigma$  varies in the range  $[k_2/k_1, 1]$  while for the case of a moving interface medium it varies in the range  $[0, 1]$ . Figures 2 and 3 exemplify the zones of the effective thermal conductivity corresponding to fixed and moving interface media as delimited by the limiting values of the parameter  $\sigma$ .

As an example, two available relations for  $k_{eff}$  for fixed interface media are considered for comparison purposes. The first relation, proposed by Veinberg (1967), is for a packed bed randomly filled with spherical inclusions. The relation is given by the following:

$$k_{eff} = k_2 + \epsilon_1 \left[ k_{eff} / k_1 \right]^{1/3} \cdot (k_1 - k_2) \quad (25)$$

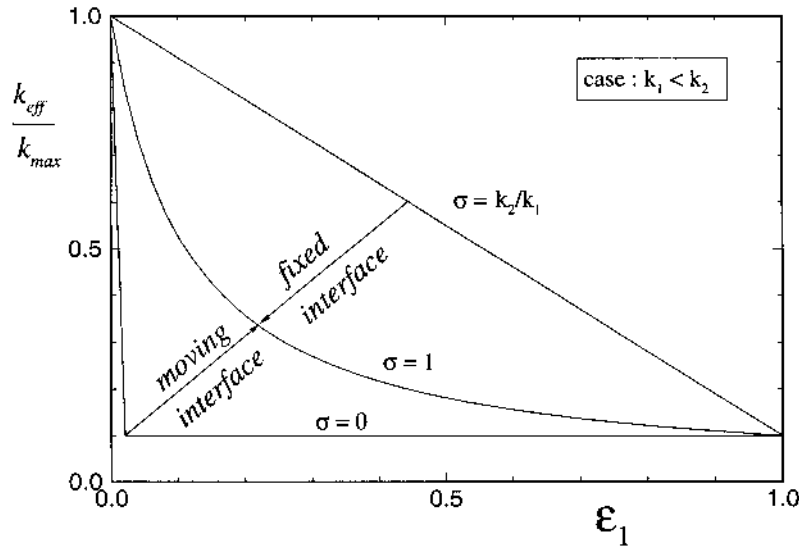
Veinberg (1967) claims that this relation is universal for this type of inclusion.

The second relation is given in *Chemical Engineering Guide* (1986), p. 242. It was developed for an amorphous medium:



**Figure 2.**  
Zones of the effective  
thermal conductivity for  
fixed and moving  
interface media:  
case  $k_1 > k_2$





**Figure 3.**  
Zones of the effective  
thermal conductivity for  
fixed and moving  
interface media:  
case  $k_1 > k_2$

$$\frac{k_{eff}}{k_2} = \frac{k_2 + \epsilon_1^{2/3} (k_1 - k_2)}{k_2 + (k_1 - k_2) (\epsilon_1^{2/3} - \epsilon_1)} \quad (26)$$

These two relations along with the proposed one are represented in Figure 4. The proposed relation gives close results to the aforementioned relations, equations (25) and (26), with the parameter  $\sigma = 0.16$  and  $0.325$ , respectively.

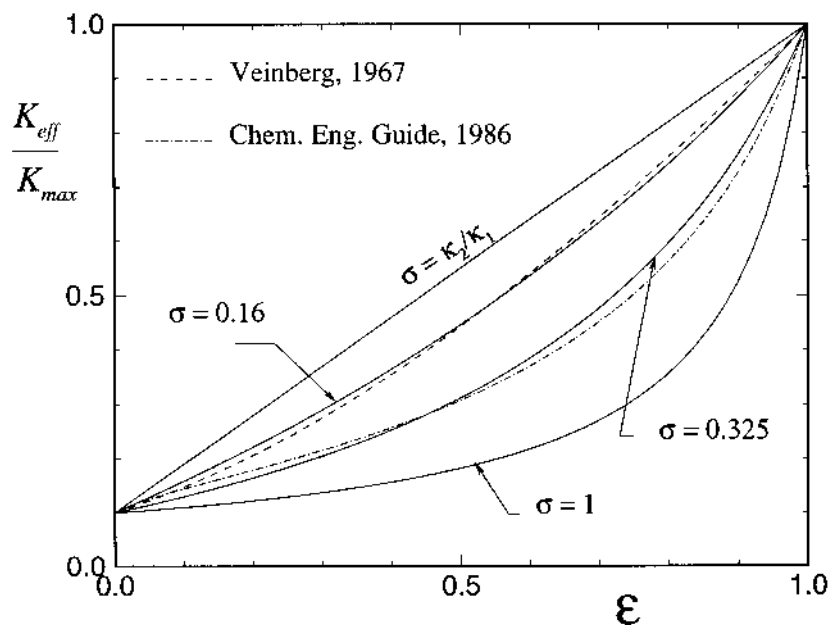
### Source term formulation

It should be noted that equation (15) contains explicitly two physical variables,  $H_m$  and  $T$ , and implicitly the volume fractions of each phase. This makes the equation for the conservation of energy highly nonlinear. Thus, as suggested by Voller (1990), it is preferable to cast equation (15) in terms of one unknown variable with a variable source term in order to implement a numerical procedure for the solution. For a two-phase medium (solid-liquid), the enthalpy of each constituent may be written as:

$$H_s = \rho_s \int_{T_r}^T c_s d\theta \quad \text{and} \quad H_l = \rho_l \int_{T_r}^T c_l d\theta + \delta H \quad (27)$$

where  $c$  is the specific heat,  $\rho$  the density,  $\delta H$  the reference enthalpy for the liquid, and  $T_r$  the reference temperature. The mixture enthalpy becomes:

**Figure 4.**  
Effective thermal  
conductivity of porous  
media: comparison



$$H_m = (\rho\epsilon)_l \int_{T_r}^T c_l d\theta + (\rho\epsilon)_s \int_{T_r}^T c_s d\theta + \delta H \epsilon_l = h + \delta H \epsilon_l \quad (28)$$

The mixture enthalpy is split into two terms: a sensible heat term ( $h$ ) and a latent heat term ( $\delta H \epsilon_l$ ). Using the sensible enthalpy ( $h$ ), equation (15) may be rewritten as:

$$\frac{\partial h}{\partial t} = \nabla (\alpha_{eff} \nabla h) - \delta H \frac{\partial \epsilon_l}{\partial t} - \nabla \left\{ \alpha_{eff} \left[ \rho_l \int_{T_r}^T c_l d\theta - \rho_s \int_{T_r}^T c_s d\theta \right] \cdot \nabla \epsilon_l \right\} \quad (29)$$

where  $\alpha_{eff} = k_{eff}/C_m$ ,  $C_m$  is the thermal capacity of the mixture which is defined as  $(\epsilon\rho c)_s + (\epsilon\rho c)_l$ . Couched in terms of temperature, equation (15) becomes:

$$C_m \frac{\partial T}{\partial t} = \nabla k_{eff} \nabla T - \delta H' \frac{\partial \epsilon_l}{\partial t} \quad (30)$$

with

$$\delta H' = \delta H + \rho_l \int_{T_r}^T c_l d\theta - \rho_s \int_{T_r}^T c_s d\theta \quad (31)$$

Equations (29) and (30) are compatible with Fourier's heat conduction equation with a source term and, thus, they may be solved using a standard finite-difference method. Equations (29) and (30) may be used either for isothermal or non-isothermal phase change problems. Equation (30) is recommended for tackling phase change problems occurring over a temperature range since the liquid fraction is, in general, given in terms of temperature. Each of these problems requires a separate treatment.

#### *Isothermal phase change*

Equations (29) or (30) may be used indifferently. Let  $T_f$  be the fusion temperature. The latent heat of fusion ( $L$ ) is defined as:  $\rho_l L = H_l(T_f) - H_s(T_f)$ . Thus, the reference enthalpy for the liquid ( $\delta H$ ) becomes:

$$\delta H = \rho_l L - \rho_l \int_{T_r}^{T_f} c_l d\theta + \rho_s \int_{T_r}^{T_f} c_s d\theta \quad (32)$$

Equations (29) or (30) contain two unknown variables,  $h$  or  $T$  and  $\epsilon_l$ . A relation between them is therefore necessary. According to the assumption of thermal equilibrium between phases, one can consider the following relation:

$$\begin{cases} \epsilon_l = 0 & : & T < T_f \\ 0 < \epsilon_l < 1 & : & T = T_f \\ \epsilon_l = 1 & : & T > T_f \end{cases} \quad (33)$$

This relation was used by many authors (Voller, 1990). However, from a numerical point of view, a control volume that contains the two phases may be at a temperature different from that of fusion, and, thus, the phases are presumed to coexist in a "numerical" temperature range. This assumption violates the phase thermal equilibrium. However, if a control volume is nearly solid (or liquid), the phases will be at different temperatures, particularly if there is a large thermal conductivity jump at the interface. It should be pointed out that this assumption was also considered by Beckermann and Viskanta (1988) and by Hashemi and Sliepcevich (1973).

The task is now to determine the temperature variation in this "numerical" temperature range. One may assume that the temperature or the sensible enthalpy is a function of the liquid fraction. Thus, performing a Taylor series expansion of the general variable  $\phi$ , that stands for  $T$  or  $h$ , around  $\epsilon_l = 1/2$ , one obtains:

$$\phi = \phi(T_f) + (\epsilon_l - 1/2) \left\{ \frac{\partial \phi}{\partial \epsilon_l} + \frac{1}{2} \frac{\partial^2 \phi}{\partial \epsilon_l^2} (\epsilon_l - 1/2) + \dots \right\} = \phi(T_f) + B(\epsilon_l - 1/2) \quad (34)$$

where it is assumed that for  $\epsilon_l = 1/2$ ,  $\phi = \phi(T_f)$  (e.g. one-dimensional case). Estimation of the extent of the “numerical” temperature range of the phase change, that is of the coefficient  $B$ , will be discussed later. A similar relation was also employed by Beckermann and Viskanta (1988) and by Hashemi and Slepcevich (1973). These authors specified a temperature range  $\Delta T$  and, thus, the coefficient  $B$  was considered constant. However, the coefficient  $B$  in equation (34) may vary with space and time. The authors believe that the liquid zone is strictly dependent on this coefficient, and the oscillations of the solid-liquid interface produced by previous enthalpy methods may be eliminated.

*Phase change over a temperature range*

In this case, equation (30) is adopted. Assume that the phase change occurs in the range  $\Delta T = T_h - T_l$ . The heat of fusion is defined as:  $\rho_l L = H_l(T_h) - H_s(T_l)$ . Thus, equation (31) becomes:

$$\delta H' = \rho_l L + \rho_l \int_{T_h}^T c_l d\theta - \rho_s \int_{T_l}^T c_s d\theta \quad (35)$$

The liquid fraction is given by:

$$\begin{cases} T \leq T_l & : & \epsilon_l = 0 \\ T_l < T < T_h & : & \epsilon_l = [T - T_l] / \Delta T \\ T \geq T_h & : & \epsilon_l = 1 \end{cases} \quad (36)$$

Equation (36) represents the simplest form that the liquid fraction may take. If the liquid fraction exhibits a non linear profile in terms of temperature, equation (36) may be viewed as a linearization of the liquid fraction-temperature relation.

### Numerical procedure

Equations (29) and (30) are first rewritten in a standard form:

$$\lambda_\phi \frac{\partial \phi}{\partial t} = \nabla \Gamma_\phi \nabla \phi - \beta_\phi \frac{\partial \epsilon_l}{\partial t} - S_\phi \quad (37)$$

Also, equations (34) and (36) take the following form:

$$\phi = b_0 + b_1 \epsilon_l \quad (38)$$

The variables and parameters in equations (37) and (38) are given in Table I. Using the control volume approach of Patankar (1980) and the implicit scheme, the discretized form of equation (37) is:

$$a_p \phi_p = \sum a_{nb} \phi_{nb} - \beta_\phi \frac{\Delta V}{\Delta t} \epsilon_{l_p} + b \quad (39)$$

with

$$a_{nb} = s_{nb} \frac{(\Gamma_\phi)_{nb}}{|\Delta x_{nb}|} ; \quad b = \frac{\Delta V}{\Delta t} \left\{ \lambda_\phi \phi_p^0 + \beta_\phi \epsilon_i^0 - S_\phi \right\} \quad (40)$$

and

$$a_p = \frac{\Delta V}{\Delta t} \lambda_\phi + \sum a_{nb} \quad (41)$$

The symbols in equations (39)-(41) are defined in the nomenclature. The diffusion coefficient at the control volume interfaces  $(\Gamma_\phi)_{nb}$  is evaluated using the harmonic mean.

#### Estimation of the constant B

*One-dimensional problems.* Consider a control volume of a node P containing the two phases and having neighbouring points W and E. The interface is located somewhere between the points W and P or between the points P and E. Let the subscripts 1 and 2 stand for the phases left and right of the interface, respectively. Considering a linear profile of  $\phi$  near the interface,

$$\phi_p = \phi(T_f) - \frac{\partial \phi}{\partial x} (x_i - x_p) = \phi(T_f) - \frac{\Delta x}{\Delta x_{nb}} (\Delta \phi_{nb}) (\epsilon_i - 1/2) \quad (42)$$

Variable/ parameter	Isothermal phase change		Non-isothermal phase change
	Equation (29)	Equation (30)	Equation (30)
$\phi$	h	T	T
$\lambda_\phi$	1	$C_m$	$C_m$
$\Gamma_\phi$	$\alpha_{\text{eff}}$	$k_{\text{eff}}$	$k_{\text{eff}}$
$\beta_\phi$	$\delta H$ , equation (32)	$\delta H'$ , equation (31)	$\delta H'$ , equation (35)
$S_\phi$	$\nabla \{ \alpha_{\text{eff}} [\rho_l \int_{T_r}^T c_l d\theta - \rho_s \int_{T_r}^T c_s d\theta] \cdot \nabla \epsilon_p \}$	0	0
$b_0$	$h(T_f) - B/2$	$T_f - B/2$	$T_1$
$b_1$	B	B	$\nabla T$

**Table I.**  
Definition of variables  
and parameters involved  
in equations (37) and (38)

which yields:

$$\phi_p = \frac{\Delta x_e / \Delta x \phi(T_f) - (\epsilon_l - 1/2) \phi_E}{\Delta x_e / \Delta x - \epsilon_l + 1/2} ; \quad \text{for } \epsilon_l \leq 1/2 \quad (43)$$

$$\phi_p = \frac{\Delta x_w / \Delta x \phi(T_f) + (\epsilon_l - 1/2) \phi_W}{\Delta x_w / \Delta x + \epsilon_l - 1/2} ; \quad \text{for } \epsilon_l > 1/2 \quad (44)$$

$\Delta x$  is the width of the control volume.  $\Delta x_w$  and  $\Delta x_e$  are the distances between nodes P and W and between nodes E and P, respectively. Comparing equations (43) or (44) with equation (34), one finally obtains for a melting process ( $\epsilon_l = \epsilon_f$ ):

$$B = \begin{cases} \frac{-\phi_E + \phi(T_f)}{\Delta x_e / \Delta x - \epsilon_l + 1/2} ; & \epsilon_l \leq 1/2 \\ \frac{\phi_W - \phi(T_f)}{\Delta x_w / \Delta x + \epsilon_l - 1/2} ; & \epsilon_l > 1/2 \end{cases} \quad (45)$$

The above expression may be generalized for multi-dimensional problems. Performing a Taylor series expansion for the dependent variable  $\phi$  around the interface, one obtains:

$$\phi_p = \phi(T_f) - \frac{\partial \phi}{\partial x}(x_i - x_p) - \frac{\partial \phi}{\partial y}(y_i - y_p) - \frac{\partial \phi}{\partial z}(z_i - z_p) - \dots \quad (46)$$

Assuming that the phase surface fractions in the x, y and z directions are all equal to the phase volume fraction (Bashmat and Beer, 1980), then,

$$x_i - x_p = \Delta x(\epsilon_l - 1/2) ; \quad y_i - y_p = \Delta y(\epsilon_l - 1/2) ; \quad z_i - z_p = \Delta z(\epsilon_l - 1/2) \quad (47)$$

If the liquid and solid phases are continuous (connex), the derivatives in equation (46) are estimated in a manner similar to that for equation (42), and the coefficient  $B$  becomes for a multi-dimensional phase change problem:

$$B = \frac{-\sum [\phi_{nb} - \phi(T_f)] \Delta x / \Delta x_{nb}}{1 - (\epsilon_l - 1/2) \sum \Delta x / \Delta x_{nb}} \quad (48)$$

where  $\Delta x_{nb} = x_{nb} - x_p$  and  $\phi_{nb}$  take the values of the neighbouring points (East, North, Top) if  $\epsilon_l < 1/2$  and the values of the points (West, South, Bottom) if  $\epsilon_l > 1/2$ .

*Liquid fraction update procedure*

Equation (37) contains two unknown variables  $\phi$  and  $\epsilon_l$ . An iterative procedure is thus necessary to determine their values. The iterative procedure begins by initializing the liquid fraction field, and then solving for the variable  $\phi$ . The calculated values for  $\phi$  will not, in general, be consistent with the liquid fraction and, thus, updating the latter is necessary to correct the field of  $\phi$ . The proposed procedure reads as follows:

- (1) Initialize  $\epsilon_l$ .
- (2) Solve equation (39) for  $\phi$ .
- (3) Update the liquid fraction.
- (4) Return to step (2) until convergence. Convergence is declared when the maximum residual of equation (39) is less than a specified tolerance (TOL).

The updated values of the liquid fraction at the new iteration  $k+1$ ,  $\epsilon_l^{k+1}$ , for nodes experiencing phase change will result in  $\phi^{k+1} = b_0 + b_1 \epsilon_l^{k+1}$ . Subtracting the corresponding discretized equation (39) at the  $k+1$ th and  $k$ th iterations, respectively, one obtains:

$$a_p [(\phi_p)^{k+1} - (\phi_p)^k] = \sum a_{nb} [(\phi_{nb})^{k+1} - (\phi_{nb})^k] + \beta_\phi [(\epsilon_p)^k - (\epsilon_l)_p^{k+1}] \Delta V / \Delta t \quad (49)$$

Assuming a linear profile between each two nodes for the  $k$ th iteration and retaining its slope for the  $k+1$ th iteration, the neighbouring nodal values of  $\phi$  at the  $k+1$ th iteration may be expressed as:

$$(\phi_{nb})^{k+1} = (\phi_p)^{k+1} + (\phi_{nb})^k - (\phi_p)^k \quad (50)$$

Substituting equation (50) in equation (49), and taking into account equation (41), one obtains:

$$(\epsilon_l)_p^{k+1} = \left[ \frac{\beta_\phi / \lambda_\phi}{\beta_\phi / \lambda_\phi + b_1} \right] (\epsilon_l)_p^k + \left[ \frac{(\phi_p)^k - b_0}{\beta_\phi / \lambda_\phi + b_1} \right] \quad (51)$$

Equation (51) is applied at each node with the following over/undershoot correction:

$$\begin{cases} \epsilon_l = 0 & \text{if } \epsilon_l < 0 \\ \epsilon_l = 1 & \text{if } \epsilon_l > 1 \end{cases} \quad (52)$$

Equation (51) is rather general, i.e. it is valid for isothermal phase change as well as for phase change over a temperature range. It converges in a stable manner for large slopes ( $b_1 \gg 1$ ) as well as for small slopes ( $b_1 < 1$ ). Moreover, equation (51) does not involve a relaxation parameter nor the coefficient  $a_p$ . In some cases, however, a relaxation parameter may be employed for accelerating convergence. It should be added that equation (51) does converge even for  $B = 0$  or  $\Delta T = 0$ . This means that the phase change range has no effect on the convergence while it significantly affects the molten fraction.

Recently, Voller (1990) has proposed a fast procedure for isothermal phase change in which the liquid fraction is updated using the following relation (for  $T_f = 0$ ):

$$(\epsilon_{l,p})^{k+1} = (\epsilon_{l,p})^k + \frac{a_p}{\rho_l L} \phi_p^k \quad (53)$$

where the coefficient  $a_p$  is set equal to a large value (e.g.  $10^{15}$ ) for nodes experiencing phase change ( $0 < \epsilon_l < 1$ ). This procedure cannot be applied for non-isothermal phase change (Voller, 1990), or if the nodal temperature is different from that of fusion. This procedure is used in this study for comparison purposes.

### Model validation

The foregoing computational methodology was validated for phase change materials (PCMs) having a large thermal conductivity jump at the solid-liquid interface. A one-dimensional as well as a two-dimensional conduction-dominated phase change problem will be examined here.

#### *Fusion/solidification in a semi-infinite slab*

Consider a semi-infinite slab of a phase change material (PCM) initially at a uniform temperature  $T_0$ , which may be different from its fusion temperature  $T_f$ . At time  $t > 0$ , the surface at  $x = 0$  is maintained at a uniform temperature  $T_w$  different from  $T_f$ . The solid and the liquid phases have different constant thermophysical properties. A practical example of a PCM that has a large conductivity jump at the solid-liquid interface is the water-ice system. Its physical properties are taken from Voller (1990) and they are:  $T_f = 0^\circ\text{C}$ ,  $k_l = 0.556 \text{ W/mK}$ ,  $k_s = 2.22 \text{ W/mK}$ ,  $\rho_l c_l = 4.226 \times 10^6 \text{ J/m}^3\text{K}$ ,  $\rho_s c_s = 1.762 \times 10^6 \text{ J/m}^3\text{K}$  and  $\rho_l L = 3.38 \times 10^8 \text{ J/m}^3$ . This problem admits an exact solution (Alexiades and Solomon, 1993). The interface position is given by:

$$x_i = 2 \gamma \sqrt{\alpha_1 t} \quad (54)$$

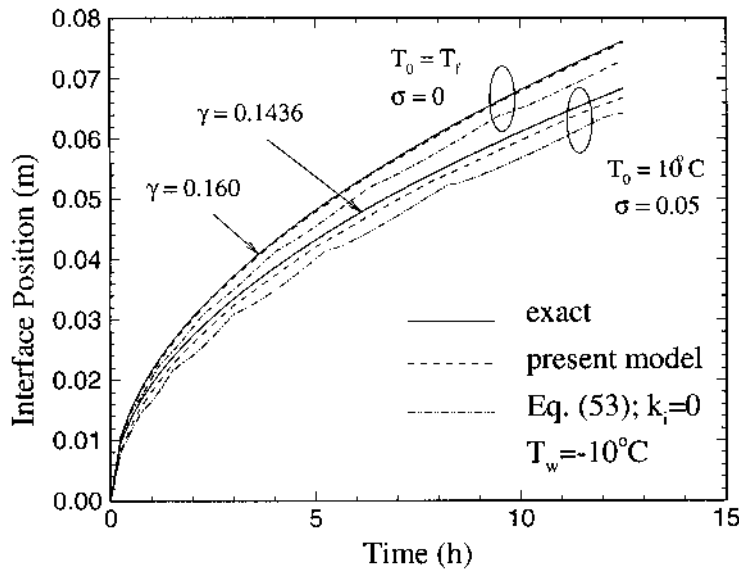


where  $\gamma$  is the root of the transcendental equation:

$$\frac{St_1}{e^{\gamma^2} \operatorname{erf}(\gamma)} - \frac{St_2}{v e^{v^2 \gamma^2} \operatorname{erfc}(v \gamma)} = \gamma \sqrt{\pi} \quad (55)$$

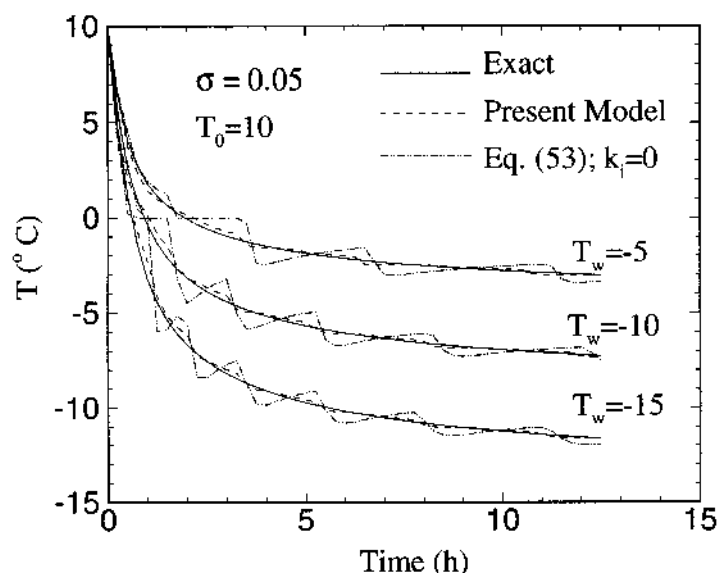
with  $v = (\alpha_1/\alpha_2)^{0.5}$  and  $St_1$  and  $St_2$  are the Stefan numbers given in the nomenclature. Numerical simulations were conducted with a non-uniform grid of  $N = 50$  cells in a  $l = 1m$  slab. The grid is distributed according to  $x_j/l = \{(j-1)/N\}^{1.5}$ . Finer grid is located near the singularity point ( $x = 0$ ). The time increment was fixed at  $\Delta t = 15$  min and the convergence tolerance at  $TOL = 10^{-2}$ .

Figures 5 and 6 illustrate the time histories of the interface position and the temperature recorded at  $x = 0.019m$  during solidification of water (case  $k_1 > k_2$ ), respectively. The value of  $\sigma$  was fixed at 0.05 throughout the calculations for the superheated liquid ( $T_0 \neq T_f$ ). This value was estimated to produce accurate values of the nodal temperature and the interface position. In fact, the parameter  $\sigma$  depends mainly on the thermal conductivities of the phases and also on the specified temperatures. The effect of the latter are not significant for the range considered. Values close to  $\sigma = 0.05$  may also be used without altering the performance of the algorithm. For the saturated liquid ( $T_0 = T_f$ ;  $q_2 = 0$ ), the exact value  $\sigma = 0$  was taken. The exact solution and the results obtained using Voller's procedure (Voller, 1990), equation (53), with the arithmetic mean conductivity ( $k_i = 0$ ) are also presented in these figures for



**Figure 5.**  
Interface position in a  
semi-infinite slab:  
solidification of water

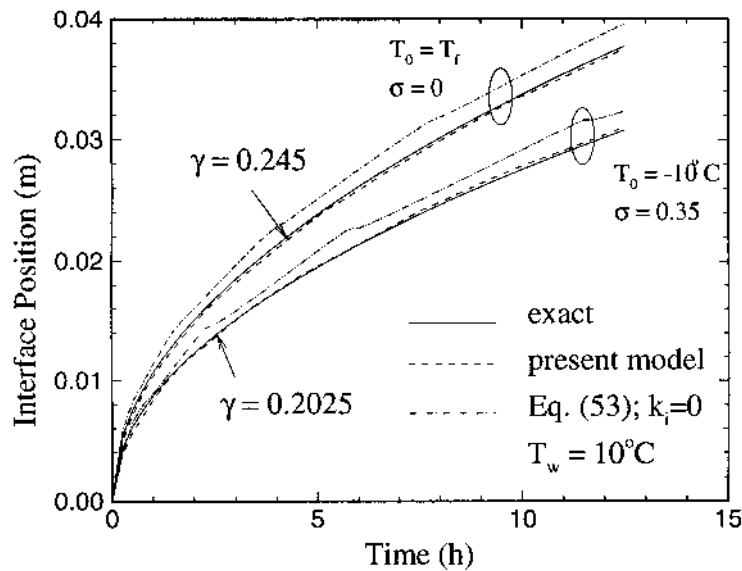
**Figure 6.**  
Predicted temperature  
at  $x = 0.019\text{m}$ :  
solidification of water



comparison purposes. These figures show that the source-based enthalpy method which employs the arithmetic mean conductivity and equation (53) results in poor accuracy and produces oscillations in the thermal field and in the interface position with a period equal to the mesh size. In this regard, fixed-grid (or enthalpy) methods which employ the arithmetic mean conductivity and assume thermal equilibrium have two major drawbacks:

- (1) They underestimate the nodal conductivities and so are the heat fluxes at the interface. Consequently, the interface position is underpredicted.
- (2) The liquid fraction update procedure produces inaccurate results at the boundary of the nodal liquid fraction ( $\epsilon_l \rightarrow 0$  or 1) unless the mesh size is made very small, since it assumes  $T = T_f$  at these nodes. As a result, oscillations are produced in the thermal field and in the prediction of the interface position. However, the proposed method eliminates the aforementioned drawbacks by adequately estimating the nodal conductivities and assuming the solid and liquid phases may coexist at a temperature different from that of fusion. It yields more accurate results and reduces significantly the oscillations in the phase front and temperature.

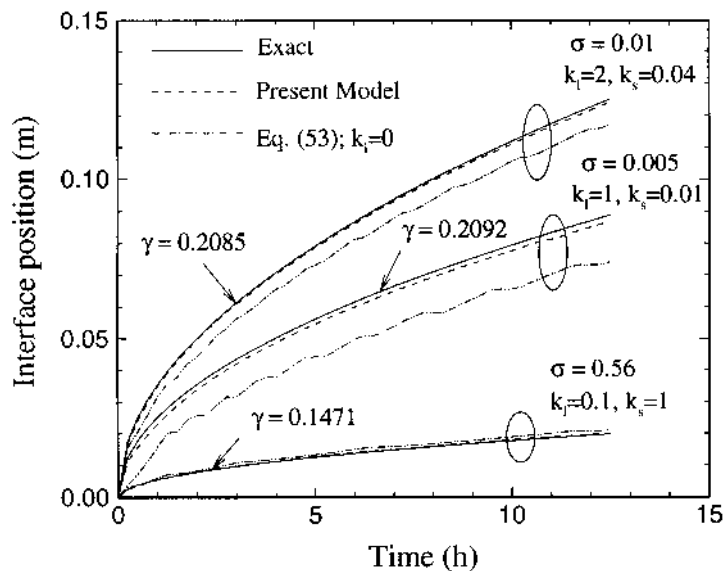
Figure 7 shows the timewise variation of the interface position during the melting of ice (case  $k_1 < k_2$ ). The value of  $\sigma$  was estimated to 0.35. Again, values close to  $\sigma = 0.35$  may also be used without altering the numerical performance of the algorithm. This figure reveals that the source-based enthalpy method which employs the arithmetic mean conductivity and equation (53) overpredicts the interface position due to the fact that the nodal



**Figure 7.**  
Interface position in a  
semi-infinite slab:  
melting of ice

conductivities are overestimated and so are the heat fluxes at the interface. The proposed method, on the other hand, yields stable and accurate results.

The foregoing results were for a relatively high conductivity jump at the interface ( $k_s/k_l = 4$ ). Results for larger thermal conductivity jumps are shown in Figure 8 for melting of a hypothetical PCM having the following properties:  $T_f = 0^\circ\text{C}$ ,  $\rho_l c_l = \rho_s c_s = 10^6 \text{ J/m}^3\text{K}$ , and  $\rho_l L = 10^8 \text{ J/m}^3$ . Three values of the thermal

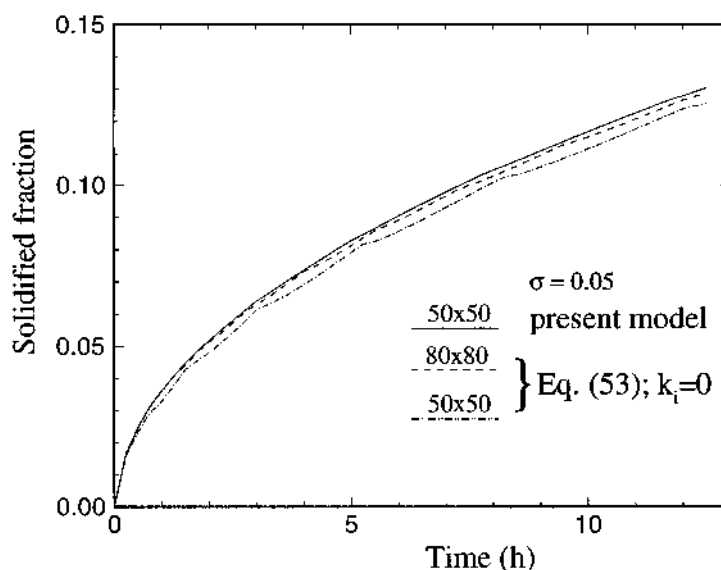


**Figure 8.**  
Interface position  
during melting of a  
semi-infinite slab: effect  
of conductivity ratio

conductivity ratio were considered:  $k_l/k_s = 100, 50$  and  $0.1$ . The wall and initial temperatures were fixed at  $T_w = 10^\circ\text{C}$  and  $T_0 = -10^\circ\text{C}$ , respectively. The results were obtained using a non-uniform grid with 80 cells distributed according to the previously mentioned relation in a 1m slab. The time step was fixed at  $\Delta t = 15$  min and the convergence tolerance at  $\text{TOL} = 10^{-2}$ . This figure clearly shows that the present model is rather accurate and reduces substantially the oscillations normally seen using equation (53) and the arithmetic mean conductivity. It should be noted that the use of the latter makes things worse as the thermal conductivity jump increases in size.

*Solidification in a corner*

Consider a corner long enough, filled with water initially at a temperature  $T_0 = 10^\circ\text{C}$ . At time  $t > 0$ , the two sides of the corner,  $x = 0$  and  $y = 0$ , are maintained at a uniform temperature  $T_w = -10^\circ\text{C}$  while the other sides remain adiabatic. The predicted solidified volume fraction for a  $1\text{m} \times 1\text{m}$  block is depicted in Figure 9. A grid of  $50 \times 50$  non-uniformly distributed cells was employed. Time step was fixed at  $\Delta t = 15$  min. For comparison purposes, the solutions obtained using the arithmetic mean conductivity and equation (53) with the same grid size ( $50 \times 50$  cells) and with a finer grid ( $80 \times 80$  cells) are also presented. It is seen that the predictions of the present model are comparable to that obtained using equation (53) and the arithmetic mean conductivity with a finer grid. Moreover, the solution for the solidified volume fraction does not exhibit oscillations.



**Figure 9.**  
Timewise variation of  
the solidified fraction of  
water in a corner

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## Conclusion

The main contributions of this paper to the basic fixed-grid (or enthalpy) method have been the development of:

- (1) a two-phase physical model for dealing with discontinuous thermal conductivity in composite media with fixed or moving interfaces; and
- (2) a rigorous numerical method for removing oscillations in phase change problems.

The methodology is based on the volume averaging technique with the assumption that the phases present in a control volume may coexist at a temperature different from that of fusion.

The following points must be highlighted:

- The effective thermal conductivity of the composite medium has been mathematically quantified involving only one constitutive constant ( $\sigma$ ). This constant is independent of the phase volume fractions. It depends, however, on the geometric structure of the medium, on the nature of the interface (fixed or moving), on the physical properties of the constituents and on any other pertinent parameters. For fixed interface media, this constant should be determined experimentally whereas for moving interface media, it is determined by knowing the heat flux ratio at the interface. Since this ratio is usually unknown, a value may be estimated based on the limiting cases where the exact values are known. In other words, if  $k_1 \gg k_2$ , a value close to zero may be used while if  $k_1 \ll k_2$ , a value close to one may be used. For  $k_1 \approx k_2$ , the results are insensitive to the values of  $\sigma$ . Note that for saturated PCMs, often considered in practice, the value of  $\sigma$  is exactly determined. The performance of the algorithm is not sensitive to the values of this constant, since the conductivity jump location occurs at only one node. A more rigorous validation would be to test the model for phase change in porous media (e.g. solidification of mixtures) where the conductivity jump locations is present throughout the domain.
- The present model has proved that the nature of the temperature oscillations produced by previous enthalpy methods is due to the fact that the nodal temperature of a control volume undergoing phase change is assumed equal to the fusion temperature. These oscillations are, in fact, independent of the phase conductivity differences. However, the amplitude of the oscillations is dependent on the conductivity ratio while their period is equal to the mesh size.
- The main feature of the present model is that it can be employed for fixed interface media as well as for moving interface media (PCMs). For the latter, both isothermal or non-isothermal phase change can be handled.

Furthermore, the model may be readily implemented in commercial codes where the user supplies only the nodal conductivities.

- The analysis presented in this paper may be applied to other similar diffusion problems (e.g. mass and momentum diffusion). One example is to determine the effective viscosity of a porous medium, or of the mushy zone in solidification of mixtures. Moreover, the analysis may be extended to multi-phase media. In this case, the effective conductivity involves many constants characterizing the interaction of each pair of constituents. For a three-phase medium, three constants are to be determined.

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Treatment of  
phase change  
problems