

A Generalized Formulation for Evaluation of Latent Heat Functions in Enthalpy-Based Macroscopic Models for Convection-Diffusion Phase Change Processes

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A standard approach for the numerical modeling of macroscopic phase change processes in the convection-diffusion problem is the so-called “fixed-grid enthalpy-based” method.^[1] In this method, the enthalpy is related to the liquid volume fraction of fluid in a control volume, which, in turn, determines a porous-medium-like resistance toward fluid flow in the phase changing domain.^[2] For accurate prediction of the same, the latent heat content of each computational cell needs to be updated according to the temperature and/or species concentration values predicted by the macroscopic conservation equations, during each iteration within a time-step. In a physical sense, such an updating attempts to neutralize the difference in the nodal temperature predicted from the energy equation and that dictated by the phase-change considerations. Thus, the enthalpy updating scheme plays a pivotal role in successful implementation of most of the enthalpy-based solution methods.

A reliable method for updating of latent heat of each computational cell has been developed by Brent *et al.*^[2] This method avoids oscillations in the iterative procedure that could result in an instability to achieve a converged solution. Voller and Prakash^[3] applied this formulation for modeling mushy zone phase-change problems, where a linear variation of temperature within the mushy zone was assumed. However, the authors clearly indicated that the latent heat function would actually depend on the nature of solute redistribution and the associated phase diagram, a detailed assessment of which was beyond the scope of their work. It may be noted here that in the subsequent literature of phase-change modeling, the development of a systematic procedure for formulation of latent heat functions consistent with the microscopic considerations is not found. On the other hand, advanced numerical models have recently been established that are capable of addressing various microscopic issues regarding nonequilibrium phase-change situations.^[4,5,6] It is, therefore, desirable to develop a systematic procedure for mathematical formulation of appropriate latent heat functions, consistent with the phase-change morphology. Accordingly, we outline a procedure to formulate the latent heat function for any metallurgical phase change situation. The aim is to prepare a guideline so that metallurgically inconsistent results from a macroscopic model can be avoided. For this purpose, we subsequently outline an algorithm illustrated by suitable examples addressing a wide variety of phase-changing situations.

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As described in Brent *et al.*,^[2] a general form of the enthalpy updating expression can be written as

$$[\Delta H_p]_{n+1} = [\Delta H_p]_n + \frac{\alpha_p}{\alpha_p^0} \lambda \{h_p\}_n - cF^{-1}\{\Delta H_p\}_n \quad [1]$$

where ΔH_p is the latent heat content of the computational cell surrounding the grid point P , h is the sensible enthalpy, c is the specific heat, λ is a relaxation factor, n is the iteration level, α_p and α_p^0 are the coefficients of finite volume discretization equation,^[7] and F^{-1} is the inverse of the latent heat function. The physical interpretation of the terms in Eq. [1] is described in detail in Brent *et al.*^[2]

As a starting point, we consider the metallurgical phase diagram in a general functional form of $T = T(T_L, T_m, C_0/C_l)$, where T_L , T_m , C_0 , and C_l are the liquidus temperature, melting temperature (of a pure component), nominal alloy concentration, and liquid composition, respectively. As a specific example, this function may take the form

$$T = T_L \frac{C_l}{C_0} - T_m \left(\frac{C_l}{C_0} - 1 \right) \quad [2]$$

for the case of a linearized phase diagram, which is a common assumption in many of the macroscopic models quoted in the literature.^[4] The next step is to substitute the proper metallurgical relation for C_0/C_l as a function of liquid fraction (depending upon the metallurgical model under consideration), appropriately representing the microscopic solute balance. For the case of a nonequilibrium solidification situation,^[4] the preceding may be described by Scheil's model^[8] as

$$(C_l - C_s)df_s = (1 - f_s)dC_l \quad [3]$$

where f_s is the mass fraction of the solid and C_s is the solid phase composition. On integrating Eq. [3], we obtain

$$f_L = \exp \left\{ - \int_{C_0}^{C_l} \frac{dC_l}{C_l(1 - k_p)} \right\} \quad [4]$$

where f_L is the mass fraction of the liquid and k_p is the partition coefficient. Equation [4], in principle, can be integrated when the variation of k_p with C_l is known. For the specific case of a constant partition coefficient (or, a partition coefficient independent of composition), integration of Eq. [4] gives

$$C_l = C_0 f_L^{k_p-1} \quad [5]$$

It can be noted that k_p in Eq. [5] can be corrected on account of solutal undercooling, in which case it can be expressed as a function of solutal diffusion boundary layer thickness, interface speed, and species diffusion coefficient in the liquid.^[5] Thus, more general cases of nonequilibrium solidification may effectively be addressed. Now, substituting Eq. [5] in Eq. [2], and using $f_L = \Delta H/L$, we obtain

$$\frac{h - cT_L}{h - cT_m} = 1 - \left(\frac{\Delta H}{L} \right)^{(1 - k_p)} \quad [6]$$

From Eq. [6], we get

$$F^{-1}(\Delta H) = T_m - (T_m - T_L) \left(\frac{\Delta H}{L} \right)^{(k_p-1)} \quad [7]$$

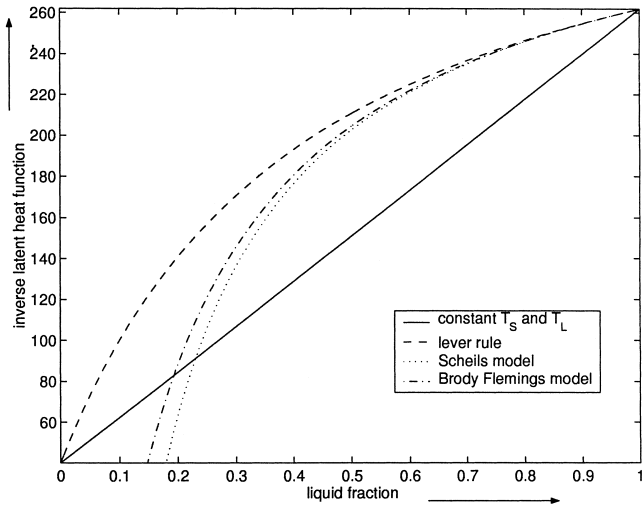


Fig. 1—Variation of inverse of latent heat function, corresponding to various models (for numerical calculation, the constant α_p is taken as 0.1 in the Brody–Flemings model).

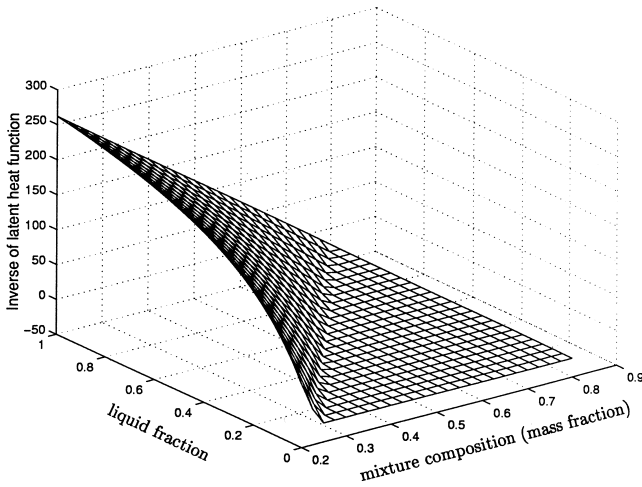


Fig. 2—Variation of inverse of latent heat function with liquid fraction and mixture composition corresponding to lever rule model.

Equation [7] is an expression for the inverse of the latent heat function corresponding to the case of nonequilibrium solidification described by Scheil’s model. It has to be noted that T_L in the preceding equations is not a constant, but a natural variable occurring during the phase-change process, which can be determined from the current value (during iteration) of the nominal alloy composition using the phase-diagram information.

As a second illustration, we consider the equilibrium model governed by the “lever rule,”^[8] where C_0 is given by

$$C_0 = (1 - f_L)k_p C_l + f_L C_l \quad [8]$$

Substituting Eq. [8] in Eq. [2], we obtain

$$\frac{h - cT_L}{h - cT_m} = \left(1 - \frac{\Delta H}{L}\right)(1 - k_p) \quad [9]$$

Solving the preceding, we obtain

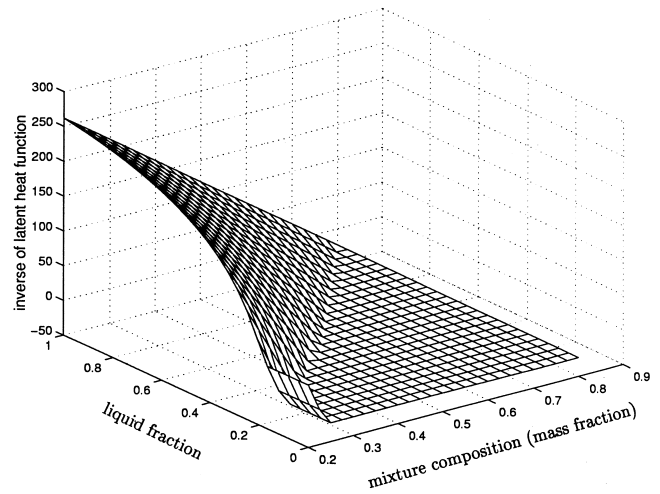


Fig. 3—Variation of inverse of latent heat function with liquid fraction and mixture composition corresponding to Scheil’s model.

$$F^{-1}(\Delta H) = \frac{T_L - T_m \left(1 - \frac{\Delta H}{L}\right)(1 - k_p)}{1 - \left(1 - \frac{\Delta H}{L}\right)(1 - k_p)} \quad [10]$$

As a third illustration, we consider a model using Brody–Flemings’ equation,^[9] in which some solid diffusion is also assumed along with the other assumptions in Scheil’s equation, and hence, it represents nonequilibrium solidification situations in a more general sense than Scheil’s model does. The corresponding metallurgical governing equation is given by^[9]

$$\frac{C_l}{C_0} = \left[1 - f_s(1 - 2\alpha_p k_p)\right]^{\frac{k_p - 1}{1 - 2\alpha_p k_p}} \quad [11]$$

where $\alpha_p = D_{stf}/X^2 = D_{st}/(f_s X)^2$, with X being the solidification length and t being the time under consideration. Equation [11] can be substituted into Eq. [2] and solved to obtain the inverse latent heat function as

$$F^{-1}(\Delta H) = T_m - (T_m - T_L) \left(\frac{\Delta H}{L}(1 - 2\alpha_p k_p) + 2\alpha_p k_p\right)^{\frac{k_p - 1}{1 - 2\alpha_p k_p}} \quad [12]$$

From the preceding illustrations, we can outline the summary of the basic steps to obtain metallurgically consistent latent heat functions for numerical simulation of any solidification process. It can be noted that an essential prerequisite is first to identify the governing metallurgical relation for solidification, physically consistent with the model under consideration (namely, lever rule, Scheil’s equation, Brody–Flemings’ equation, *etc.*). Then, for each iteration, the following steps are to be sequentially followed.

Step 1: Obtain the temperature-concentration coupling from the phase diagram in a functional form.

Step 2: Calculate T_L and T_S corresponding to the current iteration value of the nominal alloy composition, using step 1.

Step 3: Substitute the metallurgical governing relation

Table I. Table of Inverse of Latent Heat Functions

Model Description	F^{-1}
Pure metal phase change	T_m
Constant T_S and T_L	$\frac{E}{L}(2\Delta H - L) + T_{pc}$, where $E = \frac{T_L - T_S}{2}$, $T_{pc} = \frac{T_L + T_S}{2}$
Lever rule	$\frac{T_L - T_m \left(1 - \frac{\Delta H}{L}\right) (1 - k_p)}{1 - \left(1 - \frac{\Delta H}{L}\right) (1 - k_p)}$
Scheil's model	$T_m - (T_m - T_L) \left(\frac{\Delta H}{L}\right)^{k_p - 1}$
Brody-Flemings' model	$T_m - (T_m - T_L) \left(\frac{\Delta H}{L} (1 - 2\alpha_p k_p) + 2\alpha_p k_p\right)^{\frac{k_p - 1}{1 - 2\alpha_p k_p}}$

for concentration in terms of liquid fraction (for example, Scheil's equation), in the functional form of step 1.

Step 4: Write f_L as $\Delta H/L$ and T as h/c in the algebraic form obtained from step 1.

Step 5: Solve from step 4, to find an expression for F^{-1} explicitly.

Step 6: Constrain the F^{-1} thus formed in meaningful limits, *i.e.*,

$$\text{if } F^{-1} > T_L, F^{-1} = T_L; \text{ if } F^{-1} < T_S, F^{-1} = T_S.$$

It can be noted that the preceding outline is perfectly general and can be applied to any metallurgical model governing the phase-change behavior. In fact, the case of pure metal melting solidification can be obtained as a special case of the generalized model if we substitute $T_L = T_m$ into Eq. [7]. In that case, F^{-1} becomes T_m . Similarly, the case of an alloy with constant T_L and T_S and the linear variation of latent heat content between T_L and T_S can also be effectively obtained under the same framework.

For a ready reference, a number of useful forms of F^{-1} (appropriate to several metallurgical phase-change situations) is tabulated in Table I, assuming a linearized form of the phase diagram. Figure 1 compares the variation of F^{-1} as a function of liquid fraction, corresponding to several cases of modeling assumptions. It is seen from Figure 1 that the behavior of the F^{-1} function differs significantly from one model to another in its variation with liquid fraction in the mushy region, corresponding to alloy solidification occurring between two temperature limits. However, since the liquidus and solidus temperatures are themselves functions of the nominal composition of the alloy, the situation

is actually more complex than revealed by the preceding figure. Taking that into account, a combined variation of $f_L - C_0 - F^{-1}$ can be plotted, which can be visualized as a three-dimensional surface, as shown in Figures 2 and 3, for the cases of two most popular microscopic models, namely, the lever rule model and Scheil's model, respectively. The preceding figures are plotted corresponding to the thermo-physical properties^[4] of a solidifying $\text{NH}_4\text{Cl-H}_2\text{O}$ system with an initial composition of 0.2 mass fraction of water.

The algorithm developed previously, in general, can be applied for latent heat updating in enthalpy-based methods for more accurate macroscopic phase-change models to follow in future studies.

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