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NUMERICAL FORMULATION FOR THE PREDICTION OF SOLID/LIQUID CHANGE OF A BINARY ALLOY

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FOREWORD

This is the final report on the research project "Binary Metal Phase Change Energy Transport." Special attention was directed to "Numerical Formulation for the Prediction of Solid/Liquid Phase Change of a Binary Alloy." The period of performance on this research was May 16, 1989 through December 31, 1989.

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Summary

A computational model is presented for the prediction of solid/liquid phase-change energy transport including the influence of free convection fluid flow in the liquid phase region. The computational model considers the velocity components of all non-liquid phase change material control volumes to be zero but fully solves the coupled mass-momentum problem within the liquid region. The thermal energy model includes the entire domain and employs an enthalpy-like model and a recently developed method for handling the phase-change interface non-linearity. Convergence studies are performed and comparisons made with experimental data for two different problem specifications. The convergence studies indicate that grid independence has been achieved and the comparison with experimental data indicates excellent quantitative prediction of the melt fraction evolution. Qualitative data is also provided in the form of velocity vector diagrams and isotherm plots for selected times in the evolution of both problems. The computational costs incurred are quite low by comparison with previous efforts on solving these problems.

Nomenclature

A	= finite difference coefficients
b	= right hand side
c	= specific heat
C	= transient coefficient
e	= specific energy
Fo	= Fourier modulus
g	= gravitational acceleration
h	= enthalpy
H	= half-height of domain
k	= thermal conductivity
n	= normal to interface
P	= pressure
Pr	= Prandtl number
Ra	= Rayleigh number
Ste	= Stefan number
T	= temperature
u, v	= Cartesian velocity components
V_i	= interface velocity
W	= width of domain
x, y	= Cartesian coordinates

Greek

α	= thermal diffusivity
β	= isobaric compressibility
δ, Δ	= change in accompanying variable
γ	= nondimensional domain width
Γ	= modified diffusion coefficient
ϵ	= half-fusion temperature range
λ	= latent heat of fusion
ν	= kinematic viscosity
ρ	= density

Superscripts

c	= continuity
e, w, n, s, p	= geographical molecule location
u, v, p, T	= u and v velocity, pressure, temperature
uu, up, vv	= equation of first variable, multiplier
vp, TT	of second variable
$(*)$	= nondimensional

Subscripts

$1, 2, 3$	= solid, melt, or liquid
d	= dynamic
e	= east
f	= fusion
i, j	= discrete location
i	= interfacial or dummy variable
ℓ	= liquid
n	= north
r	= reference
s	= solid, or south
sp	= specified
w	= working variable, or west
x, y	= x or y direction

Chapter 1

Introduction

The Stefan problem, describing energy transport within a single component, phase change material, is intrinsically highly non-linear. This non-linearity is due to the compatibility constraints imposed at the solidification/melt front and involves the energy fluxes and front propagation velocity at the interface location. However, neither the fluxes, the interface propagation velocity, nor the interface location itself are known a priori. As a result of this non-linearity, analytical solutions to the Stefan problem are difficult, at best, and available for only a few relatively simple configurations [1,2,3,4,5]. For more realistic problem specifications, discrete methods are required to effect the solution. Traditionally, finite difference or finite element methods have been used; the suitability and/or methodology of the spectral method has not yet been fully established. the enthalpy method of Shamsundar and Sparrow is widely used [6].

In the application of the enthalpy model to phase change energy transport problems, the solution of the algebraic system of equations consumes a considerable amount of computing time. This is attributable to the fact that complete transient histories are generally required and, more significantly, to the fact that Gauss–Siedel iteration or an equivalent procedure has been used to solve the equation system. The requirement for an iterative solution procedure emerges from the highly non-linear character of the interface compatibility constraint [7]. In the enthalpy method, the interface location is not tracked explicitly and its precise location can be resolved only to within one mesh spacing. The interface non-linearity, then, appears in the enthalpy model in the form of a highly non-linear equation of state relating enthalpy to temperature. In addition, this non-linear behavior is highly concentrated within the immediate vicinity of the phase change interface, and is extremely difficult to accommodate within the context of a simultaneous variable procedure for the equation system [8].

This difficulty is further augmented in problems for which more than one phase change boundary must be accommodated within the domain.

Williams and Curry [9] presented a more implicit procedure for the solution of the algebraic equation system for the case of one–dimensional phase change energy transport. In their paper, they attest to the difficulties involved in solving phase change problems and provide a procedure for implementation to multiple interface problems. They achieve this through an energy distribution technique in the vicinity of phase change interfaces which leads to a very complex solution procedure. In addition, extension of their procedure to more than one space dimension does not appear possible [10]. Since the majority of problems of practical importance involve two or three space dimensions, this is a serious disadvantage of their procedure.

The numerical solution of solid/liquid phase change problems has been considerably simplified and the associated costs dramatically reduced as a result of the method proposed by Schneider and Raw [11] for one–dimensional problems. This procedure has also been employed in a two–dimensional environment by Raw and Schneider [12] with comparable cost reductions to those observed for the one–dimensional situation. Cost reductions are typically two orders of magnitude. All of the above-referenced methods and applications, however, have been restricted to conduction as the mode of energy transport without regard for buoyancy induced free convective motion. In practice, in terrestrial situations, it is frequently this free convective motion itself which is the dominant mechanism for the thermal energy transport. As such, it is crucial that this fluid motion predictive capability be available in a computational scheme in order to predict energy transport with sufficient accuracy so as to be of practical value.

Unlike pure substances, multiconstituent systems do not exhibit a sharp interface between solid and liquid phases. In fact, due to impurities (intentional or otherwise), discrete phase change rarely occurs in practice. The phase change behavior of such systems depends on many factors including the phase change environment, composition, and thermodynamic descriptions of specific phase transformations. Moreover, solidification occurs over extended temperature ranges and solid formation often occurs as a permeable crystalline-like matrix which coexists with the liquid phase.

Since they need not track phase interfaces, single region formulations are well suited for treating the continuous transition between solid and liquid phases, as well as the evolution of latent energy over a finite temperature range. Such formulations are generally developed from volume averaging techniques based on classical mixture theory. Detailed developments of the theory are available in the open literature [13]-[18], as are applications to inert systems such as dispersed oil droplets in

water and fluid saturated granular materials [19]-[21]. The theories have been extended to phase change processes [22]-[24], although treatments have been restricted to one-dimensional, conduction dominated conditions.

While continuum formulations have been shown to provide realistic predictions of transport behavior for conduction phase change problems, inclusion of advective components of momentum, energy and species transfer does not appear to have been considered. Such an extension necessitates consideration of multiphase region morphology, as well as relative phase velocities. While classical theories clearly acknowledge the significance of these factors, the desire to maintain universal generality prohibits description beyond that of symbolic representations. Accordingly, the primary objective of the present work is to develop a consistent set of continuum equations for the conservation of mass, momentum, energy, and species in a binary, solid-liquid phase change system. Emphasis is placed on casting the equations into forms which are amenable to clear physical interpretation, as well as to solution by conventional finite-difference or finite-element methods. Although achieving this objective must come at the expense of a loss of generality, related assumptions and constraints will be clearly identified and justified on the basis of physical considerations.

Chapter 2

Formulation of the Mathematical Model

2.1 Binary Mixture Phase Change Problems

In the solid/liquid phase change of pure materials a discrete interface always separates the two phases. Only solid exists on one side of the interfacial surface and only liquid on the other. In a binary constituent phase change system the interface can take two forms. The interface may behave like that of a pure material as described above. Frequently however, between the region of solid and the region of liquid, there is a finite region with liquid finely interdispersed with solid. This region is often described as being "mushy". Morphologies like this may be caused by supercooled dendritic growth. Dendrites can grow into each other creating a solid matrix having pockets or channels of entrapped liquid throughout.

If a binary system exhibits a behavior like that of a pure material, then conservation of mass and conservation of momentum for the liquid region are described by the familiar two-dimensional equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0, \tag{2.1}$$

$$\frac{\partial (\rho U)}{\partial t} = -\nabla \cdot (\rho U \vec{V}) - \nabla \cdot \vec{\tau}_x - \frac{\partial p}{\partial x} + \rho b_x, \text{ and} \tag{2.2}$$

$$\frac{\partial (\rho v)}{\partial t} = -\nabla \cdot (\rho v \vec{V}) - \nabla \cdot \vec{\tau}_y - \frac{\partial p}{\partial y} + \rho b_y, \tag{2.3}$$

where $\vec{\tau}_x$ and $\vec{\tau}_y$ are the stress vectors defined by

$$\vec{\tau}_x = \tau_{xx}\hat{i} + \tau_{yx}\hat{j} \text{ and } \vec{\tau}_y = \tau_{xy}\hat{i} + \tau_{yy}\hat{j} \tag{2.4}$$

and where b_x and b_y are the per unit volume body force components for the x and y directions respectively. The energy equation for the liquid portion is

$$\frac{\partial(\rho e_l)}{\partial t} = -\nabla \cdot (\rho e_l \vec{V}) + \nabla \cdot (k_l \nabla T) \tag{2.5}$$

where e_l represents the specific internal energy for the liquid and k_l is the thermal conductivity of the liquid. Internal energy generated by viscous dissipation and compression work have been neglected. Conservation of energy for the solid region does not need to include convective terms since the velocity of the solid is assumed zero:

$$\frac{\partial(\rho_s e_s)}{\partial t} = \nabla \cdot (k \nabla T). \tag{2.6}$$

In a binary system which has a region of interdispersed solid and liquid, the above equations are not convenient. It becomes impractical to resolve all of the details of the solid/liquid structure in the mushy region. The mathematical formulation for this phase change situation will be derived assuming solid and liquid phases can coexist in a locally distributed manner within control volumes of differential dimensions.

2.2 Phase Conservation of a General Scalar Quantity

2.2.1 Introduction and Definitions

Mass, momentum, energy and species conservation equations are derived in this section for a single phase within a control volume which may contain more than this one phase. Here phase refers to either solid or liquid while constituent refers to either a chemical element or a compound. In this formulation α constituents within k phases are allowed to occupy any differential volume in space simultaneously.

The control volumes used in the derivations are shown in Figs. 1, 2, and 3 with discrete interfaces separating solid from liquid. The precise location of the phase interfaces will generally not be known but the volume fractions of solid and of liquid will be used to characterize the state of dispersion at any location.

Some nomenclature relating to the distribution of solid and liquid must be defined before proceeding. The mean velocity of the constituents comprising phase k relative to a fixed reference frame is denoted by $\vec{V}_k$. The volume fraction of constituent α in phase k, that is, the volume occupied by constituent α divided by the volume of phase k which contains the volume of constituent α, is

denoted by g_k^α. Similarly the volume fraction of phase k, that is the volume occupied by phase k divided by the volume over which g_k is evaluated which may be partially occupied by other phases, is denoted by g_k. The actual density of constituent α in phase k is denoted by ρ_k^α. This density is the same that would be determined from a sample of constituent α removed from phase k. The actual density of phase k is denoted by ρ_k and describes the mass per unit volume of a volume containing only phase k. It should be noted that the sum over all phases of g_k gives the result

$$\sum_k g_k = 1. \tag{2.7}$$

The partial density of constituent α in phase k, denoted by $\bar{\rho}_k^\alpha$, describes the mass of constituent α contained by a volume occupied only by phase k, divided by that volume. This volume may contain other constituents than just constituent α. A mathematical expression relates partial density to actual density:

$$\bar{\rho}_k^\alpha = g_k^\alpha \rho_k^\alpha. \tag{2.8}$$

The partial density of phase k, denoted by $\bar{\rho}_k$, describes the mass of phase k in a volume which may contain phases other than phase k, divided by that volume. Mathematically $\bar{\rho}_k$ is defined by

$$\bar{\rho}_k = g_k \rho_k. \tag{2.9}$$

In a manner analogous to Dalton's rule of partial pressures, here the sum of all partial densities at a location represents the actual density

$$\rho = \sum_k \bar{\rho}_k \tag{2.10}$$

where ρ denotes the actual density.

The mass fraction of constituent α in phase k, f_k^α, is related to the partial density of constituent α in phase k, $\bar{\rho}_k^\alpha$, by

$$f_k^\alpha = \frac{\bar{\rho}_k^\alpha}{\rho_k}. \tag{2.11}$$

This mass fraction represents the mass of constituent α in a volume entirely occupied by phase k divided by the mass of the entire volume. The mass fraction of phase k, f_k, is defined as

$$f_k = \frac{\bar{\rho}_k}{\sum_k \bar{\rho}_k} \tag{2.12}$$

the mass of phase k in a volume partially occupied by other phases divided by the mass of the total volume.

The conservation of a general quantity ϕ for a single phase k, ϕ_k, is derived here in a Cartesian coordinate framework for a two-dimensional control volume containing a mixture of phases. The

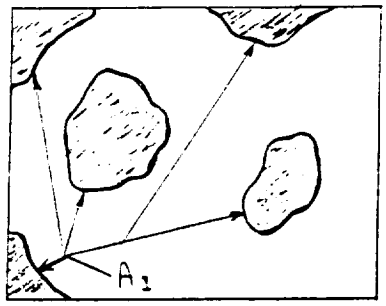


Figure 2.1:

control volume contains two phases with the total interfacial surface between the phases denoted by A_I as shown in Figure 1. For convenience the bottom left corner of the control volume is located at (x_0, y_0). The total volume $\Delta\forall$ includes both solid and liquid portions and is the product of the width Δx and the height Δy since unit depth is considered.

The general conservation principle is given in words by

$$\begin{array}{lcl} \text{Time rate of change of} & & \text{Net flow of } \phi \text{ across} \\ \phi_k \text{ in volume occupied} & = & \text{phase } k \text{ portion of control} \\ \text{by phase } k & & \text{faces} \\ (T1) & & (T2) \end{array} \tag{2.13}$$

$$\begin{array}{lcl} + \text{ Net flow into phase } k & + & \text{Source of} \phi_k \text{ in} \\ \text{across interfacial surface} & & \text{phase } k \text{ volume.} \\ (T3) & & (T4) \end{array}$$

These four terms, the accumulation term $(T1)$, the control face flow term $(T2)$, the interfacial flow term $(T3)$, and the source term $(T4)$ will be treated individually in the subsections that follow. Expressions will be determined for a control volume of differential dimensions and the limiting result per unit volume will be presented as the control volume dimensions are shrunk to zero.

2.2.2 The Accumulation Term

The symbolic representation of the accumulation term ($T1$) is given by

$$T1 = \frac{\partial}{\partial t} \int_{\forall_k} (\rho_k \phi_k) d\forall \tag{2.14}$$

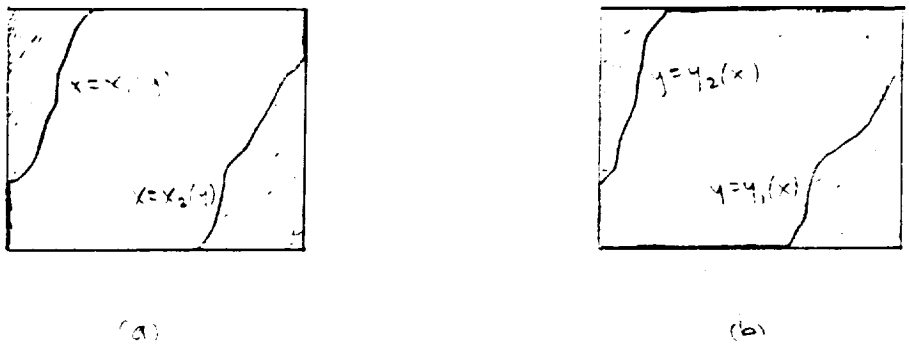


Figure 2.2:

where $\forall_k$ is the portion of the control volume occupied by phase k. In Cartesian coordinates this integration could be viewed as an integration between two curves, say $x_1(y)$ and $x_2(y)$, or $y_1(x)$ and $y_2(x)$, as shown in Figure 2. The integral part of the accumulation term can then be written in the forms

$$\begin{aligned} \int_{\forall_k} (\rho_k \phi_k) d\forall &= \int_{y_0}^{y_0+\Delta y} \int_{x_1(y)}^{x_2(y)} (\rho_k \phi_k) dx dy \\ &= \int_{x_0}^{x_0+\Delta x} \int_{y_1(x)}^{y_2(x)} (\rho_k \phi_k) dy dx \end{aligned} \tag{2.15}$$

Performing a Taylor series expansion of the integrand about (x_0, y_0) gives

$$\begin{aligned} \int_{\forall_k} (\rho_k \phi_k) d\forall = \int_{y_0}^{y_0+\Delta y} \int_{x_1(y)}^{x_2(y)} \Big[&(\rho_k \phi_k)|_0 + \frac{\partial}{\partial x}(\rho_k \phi_k)\,|_0 (x - x_0) \\ &+ \frac{\partial}{\partial y}(\rho_k \phi_k)\Big|_0 (y - y_0) + \ldots \Big] dx dy. \end{aligned} \tag{2.16}$$

By bringing constants out of the integral and adjusting the limits, the above expression may be simplified to

$$\int_{\forall_k} (\rho_k \phi_k) d\forall = (\rho_k \phi_k)|_0 \, \Delta \forall_k + \frac{\partial}{\partial x}(\rho_k \phi_k)\,|_0 \int_{y_0}^{y_0+\Delta y} \int_{x_1(y)}^{x_2(y)} (x - x_0) dx dy + \frac{\partial}{\partial y}(\rho_k \phi_k)\,|_0$$

$$\int_{x_0}^{x_0+\Delta x}\int_{y_1(x)}^{y_2(x)}(y-y_0)dydx+\ldots \tag{2.17}$$

It can be shown that all terms except the first one become zero when Eq. 2.14 is divided by $\Delta\forall = \Delta x\Delta y$ and the limit is taken as Δx, $\Delta y \to 0$. The second term is considered below, although similar treatment applies to the third and all higher order terms.

A new variable representing the local range of x-direction integration is introduced by the definition

$$\delta x(y) = x_2(y) - x_1(y) \tag{2.18}$$

Incorporating this definition we have that

$$\frac{\partial}{\partial x}(\rho_k\phi_k)\mid_0 \int_{y_0}^{y_0+\Delta y}\int_{x_1(y)}^{x_2(y)}(x-x_0)dxdy$$

$$= \frac{\partial}{\partial x}(\rho_k\phi_k)\mid_0 \int_{y_0}^{y_0+\Delta y}\left[\frac{1}{2}\delta x^2(y) + (x_1(y)-x_0)\delta x(y)\right]dy. \tag{2.19}$$

The terms $\delta x(y)$ and $(x_1(y) - x_0)$ are both of the same order of size as Δx and can be expressed as a fraction of the control volume width Δx in the form

$$\delta x(y) = R_1(y)\Delta x \quad \text{and} \quad x_1(y) - x_0 = R_2(y)\Delta x. \tag{2.20}$$

With substitution of these definitions the above equation becomes

$$\frac{\partial}{\partial x}(\rho_k\phi_k)\mid_0 \int_{y_0}^{y_0+\Delta y}\int_{x_1(y)}^{x_2(y)}(x-x_0)dxdy$$

$$= \frac{\partial}{\partial x}(\rho_k\phi_k)\mid_0 \int_{y_0}^{y_0+\Delta y}\left[\frac{1}{2}R_1^2(y)\Delta x^2 + R_1(y)R_2(y)\Delta x^2\right]dy. \tag{2.21}$$

It is convenient to define

$$f(y) \equiv \frac{1}{2}R_1^2(y) + R_1(y)R_2(y) \tag{2.22}$$

such that the integrand is now $\Delta x^2 f(y)$. The mean value theorem for integrals states that if $f(y)$ is continuous in $[y_0,\ y_0 + \Delta y]$, then there exists some point ξ in $(y_0,\ y_0 + \Delta y)$ such that

$$\int_{y_0}^{y_0+\Delta y} f(y)dy = \Delta y f(\xi). \tag{2.23}$$

Using this result we can now write

$$\frac{\partial}{\partial x}(\rho_k\phi_k)\mid_0 \Delta x^2\Delta y\int_{y_0}^{y_0+\Delta y} f(y)dy = \frac{\partial}{\partial x}(\rho_k\phi_k)\mid_0 \Delta x^2\Delta y f(\xi);\quad y_0 \le \xi \le y_0+\Delta y. \tag{2.24}$$

The range of R_1 and R_2 is $0 \leq R_1 \leq 1$ and $0 \leq R_2 \leq 2$. Further, both R_1 and R_2, and hence $f(\xi)$, are independent of Δx and Δy. If this term is now divided by $\Delta\forall = \Delta x \Delta y$ and the limit is taken as $\Delta x,\ \Delta y \rightarrow 0$, the result is

$$\lim_{\substack{\Delta x \rightarrow 0 \\ \Delta y \rightarrow 0}} \frac{\partial}{\partial x}(\rho_k \phi_k) \mid_0 \frac{\Delta x^2 \Delta y}{\Delta x \Delta y} f(\xi) = \frac{\partial}{\partial x}(\rho_k \phi_k) \mid_0 f(\xi) \lim_{\substack{\Delta x \rightarrow 0 \\ \Delta y \rightarrow 0}} \Delta x = 0. \tag{2.25}$$

In a similar manner all terms in the Taylor series except the first reduce to zero when this limit is taken. Thus the only contribution from the accumulation term, $T1$, is

$$T1 = \frac{\partial}{\partial t}(\rho_k \phi_k) \mid_0 \frac{\Delta\forall_k}{\Delta\forall}. \tag{2.26}$$

The volume ratio of the liquid volume to the total volume as defined earlier is $g_k = \frac{\Delta\forall_k}{\Delta\forall}$ so that the accumulation term is finally given on a per unit volume basis by

$$T1 = \frac{\partial}{\partial t}(g_k \rho_k \phi_k) \mid_0. \tag{2.27}$$

2.2.3 The Control Face Flow Term

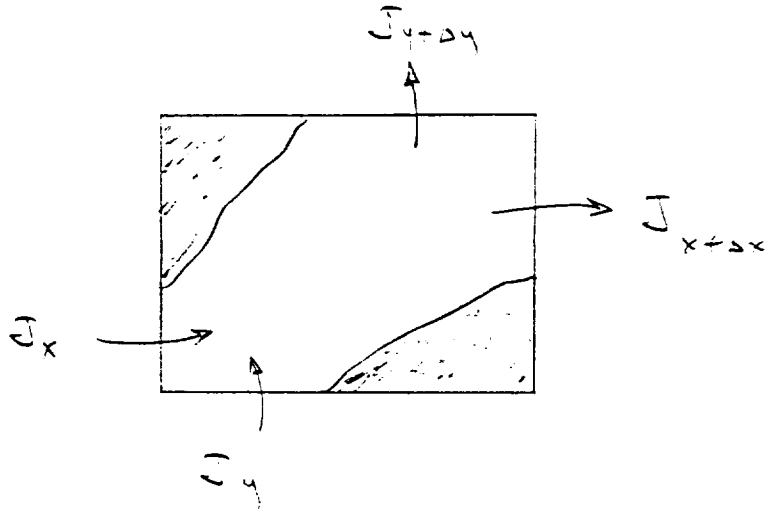


Figure 2.3:

The term representing the flow across the portion of the control face occupied by phase k, $T2$, is shown by Figure 3 to have four contributing components, one at each of the control faces. In symbolic form the net flow of ϕ is given by

$$T2 = J_x - J_{x+\Delta x} + J_y - J_{y+\Delta y} \tag{2.28}$$

Considering the x-component, a Taylor series expansion can be performed about x_0 giving

$$J_x - J_{x+\Delta x} = J_x - \left[J_x + \Delta x \frac{dJ_x}{dx} \mid_{x_0} + \frac{1}{2!}\Delta x^2 \frac{d^2 J_x}{dx^2} \mid_{x_0} + \ldots \right] \tag{2.29}$$

Note that the flows considered here are only those associated with phase k. The effective portion of the control faces for which there is a flow of ϕ_k can be given by the ratio R times the actual area of the respective control faces. For the x-component flux the effective area is then $R_x \cdot 1 \cdot A_y$ so that the flow itself becomes

$$J_x = 1 \cdot \Delta y R_x j_x \tag{2.30}$$

where j_x is the average flux over the actual area of the control volume surface occupied by phase k. The net x-component flux term is then given by

$$J_x - J_{x+\Delta x} = -\Delta x \Delta y \frac{\partial}{\partial x}(R_x j_x) \mid_0 - \frac{1}{2!}\Delta x^2 \Delta y \frac{\partial^2}{\partial x^2}(R_x j_x) \mid_0 + \ldots \tag{2.31}$$

Dividing the x-component flow term by $\Delta \forall = \Delta x \Delta y$, and taking the limit as $\Delta x,\ \Delta y \rightarrow 0$ reduces the term to

$$\lim_{\substack{\Delta x \rightarrow 0 \\ \Delta y \rightarrow 0}} \frac{1}{\forall}(J_x - J_{x+\Delta x}) = \frac{\partial}{\partial x}(R_x j_x) \ . \tag{2.32}$$

The y-component flow term similarly reduces to

$$\lim_{\substack{\Delta x \rightarrow 0 \\ \Delta y \rightarrow 0}} \frac{1}{\forall}(J_y - J_{y+\Delta y}) = \frac{\partial}{\partial y}(R_y j_y) \tag{2.33}$$

The control face flux term ($T2$) for phase k is then

$$T2 = -\frac{\partial}{\partial x}(R_x j_x) \mid_0 - \frac{\partial}{\partial y}(R_y j_y) \mid_0 \tag{2.34}$$

where R_x and R_y are the effective ratios of areas for phase k flows at the control faces, and j_x and j_y are area averaged fluxes of the actual areas occupied by phase k.

2.2.4 The Interfacial Flow Term

The flow of ϕ_k across the phase interface surface is defined by

$$T3 = \int_{A_I} j_{k_i} \cdot \vec{n} \, dA \tag{2.35}$$

where j_{k_i} is a flux across the interface and $\vec{n}$ is the normal to the interface directed into phase k. Beyond this representation, the interfacial flux term will not be specifically evaluated because later in the development this term is cancelled by a similar term associated with another phase. For convenience this term is denoted by

$$T3 = I_i \ . \tag{2.36}$$

2.2.5 The Source Term

The source term is symbolically represented by

$$T4 = \int_{\forall_k} S_k \, d\forall \tag{2.37}$$

where S_k is a per unit volume source variable. The only specific form for S_k that will be considered is the body force in the momentum conservation equation. By a procedure similar to the one used to reduce the control face flow term, the source term may be reduced to

$$T4 = (g_k \, \dot{S}_k) \mid_0 \tag{2.38}$$

2.2.6 Composed Equation for Phase Conservation of a General Scalar Quantity

The terms have been derived for the conservation equation of a general scalar quantity ϕ for a single phase k, ϕ_k, for a control volume of differential size containing a mixture of phases. Substituting these terms ($T1 - T4$) into Eq. 2.13 gives

$$\frac{\partial}{\partial t}(g_k \rho_k \phi_k) \mid_0 = -\frac{\partial}{\partial x}(R_x j_x) \mid_0 - \frac{\partial}{\partial y}(R_y j_y) + I_i \mid_0 + (g_k \dot{S}_k) \mid_0. \tag{2.39}$$



(a) (b)

Figure 2.4:

In order to simplify this equation, an assumption is made about the effective area ratios R_x and R_y. Figure 4 shows two cases in which the volume fraction of phase k, g_k, is equal to the effective area ratios R_x and R_y. The assumption will be made here that

$$R_x = R_y = g_k \tag{2.40}$$

since in some cases it is true and since it is reasonable. Equation 2.39 now simplifies to

$$\frac{\partial}{\partial t}(g_k\rho_k\phi_k)\mid_0 = -\frac{\partial}{\partial x}(g_k j_x)\mid_0 - \frac{\partial}{\partial y}(g_k j_y)\mid_0 + I_i + (g_k\dot{S}_k)\mid_0 . \tag{2.41}$$

Because the control volume has been reduced to differential size and the balance used in its derivation must apply for any choice of $(x_0,\ y_0)$, the above equation can now be written as

$$\frac{\partial}{\partial t}(g_k\rho_k\phi_k) = -\frac{\partial}{\partial x}(g_k j_x) - \frac{\partial}{\partial y}(g_k j_y) + I_i + g_k\dot{S}_k. \tag{2.42}$$

2.3 Phase Conservation Equations for Mass, Momentum, Energy and Species

Equation 2.42 represents the conservation of a general scalar quantity ϕ for a single phase k, ϕ_k, for a control volume containing a mixture of phases. The scalar quantity ϕ_k, and the flux terms j_x and j_y are specified in this section for the conservation equations for mass, momentum, energy and species.

2.3.1 Mass

The conservation of mass equation can be obtained from 2.42 with $\phi = 1$, $j_x = \rho_k u_k$, $j_y = \rho_k v_k$ and $I_i = \dot{M}_k$ giving

$$\frac{\partial}{\partial t}(g_k\rho_k) = -\frac{\partial}{\partial x}(g_k\rho_k u_k) - \frac{\partial}{\partial y}(g_k\rho_k v_k) + \dot{M}_k \tag{2.43}$$

where $\dot{M}_k$ represents the contributions of mass flow into the phase k portion of the control volume across the phase interface A_I.

2.3.2 Momentum

The statement of x-momentum conservation can be obtained from Eq. 2.42 with $\phi_k = u_k$, $j_x = \rho_k u_k^2 - \tau_{kxx} + p$, $j_y = \rho_k u_k v_k - \tau_{kyx}$, $I_i = G_{kx}$ and $\dot{S}_k = \rho_k g_x$. That is

$$\frac{\partial}{\partial t}(g_k\rho_k u_k) = -\frac{\partial}{\partial x}[g_k(\rho_k u_k^2 - \tau_{kxx} + p_k)] - \frac{\partial}{\partial y}[g_k(\rho_k u_k v_k - \tau_{kyx})] + \dot{G}_{kx} + g_k\rho_k g_x \tag{2.44}$$

where $\dot{G}_{kx}$ represents the production of momentum due to movement of the phase interface, g_x is the x-component of the gravity vector, and p_k is the pressure associated with phase k.

The classical Newtonian constitutive equations need to be modified here due to spatial variations in the phase volume fraction. Bennon and Incropera [25] define the dilation rate of phase k as

$\nabla \cdot (g_k V_k)$ on a per unit volume of mixture basis. This was done to maintain consistency with the conservation of mass equation, Eq. 2.43. In their definition of dilation rate these authors use $g_k V_k$ for the velocity terms as they arise in the mass conservation equation. Following Bennon and Incropera, any occurence of a velocity component will be replaced by g_k times the velocity component. With this requirement the constitutive equations for phase k are then given by

$$g_k \tau_{kxx} = 2\mu_k \left[-\frac{1}{3} \nabla \cdot (g_k \vec{V}_k) + \frac{\partial}{\partial x}(g_k u_k) \right], \quad \text{and}$$

$$g_k \tau_{kyx} = \mu_k [\frac{\partial (g_k v_k)}{\partial x} + \frac{\partial (g_k u_k)}{\partial y}]. \tag{2.45}$$

The statement of y-momentum conservation follows directly from Eqs. 2.44 and 2.45 with the x and y subscripts, and the velocity components permuted. The y-momentum conservation equations are given by

$$\frac{\partial}{\partial t}(g_k \rho_k v_k) = -\frac{\partial}{\partial x}[g_k(\rho_k v_k u_k - \tau_{kxy})] - \frac{\partial}{\partial y}[g_k(\rho_k v_k^2 - \tau_{kyy} + p_k)] + \dot{G}_{ky} + g_k \rho_k g_y, \tag{2.46}$$

$$g_k \tau_{kxy} = g_k \tau_{kyx} = \mu_k \left[\frac{\partial (g_k v_k)}{\partial x} + \frac{\partial (g_k u_k)}{\partial y} \right], \quad \text{and}$$

$$g_k \tau_{kyy} = 2\mu_k \left[-\frac{1}{3} \nabla \cdot (g_k \vec{V}_k) + \frac{\partial}{\partial y}(g_k v_k) \right] . \tag{2.47}$$

2.3.3 Energy

The conservation requirement for energy can be obtained from Eq. 2.42 with $\phi_k = e_k$, $j_x = \rho_k u_k e_k - k_k \frac{\partial T}{\partial x}$, $j_y = \rho_k v_k e_k - k_k \frac{\partial T}{\partial y}$ and $I_i = \dot{E}_k$ yielding

$$\frac{\partial}{\partial t}(g_k \rho_k e_k) = -\frac{\partial}{\partial x}\left[g_k \left(\rho_k u_k e_k - k_k \frac{\partial T}{\partial x} \right) \right] - \frac{\partial}{\partial y}\left[g_k \left(\rho_k v_k e_k - k_k \frac{\partial T}{\partial y} \right) \right] + \dot{E}_k \tag{2.48}$$

Here e_k is the specific internal energy of phase k, that is the internal energy of a volume containing only phase k divided by the mass of that volume. Also k_k is the thermal conductivity associated with phase k and $\dot{E}_k$ represents the energy flow into phase k across the phase boundary, which is partially due to movement of the phase interface.

2.3.4 Species

The conservation of species equation can be obtained from Eq. 2.42 with $\phi_k = f_k^\alpha$, $j_x = \rho_k u_k f_k^\alpha - \rho_k D_k^\alpha \frac{\partial f_k^\alpha}{\partial x}$, $j_y = \rho_k v_k f_k^\alpha - \rho_k D_k^\alpha \frac{\partial f_k^\alpha}{\partial y}$, and $I_i = \dot{M}_k^\alpha$. Hence

$$\frac{\partial}{\partial t}(g_k \rho_k f_k^\alpha) = \; - \; \frac{\partial}{\partial x}\left(g_k \rho_k u_k f_k^\alpha - g_k \rho_k D_k^\alpha \frac{\partial f_k^\alpha}{\partial x} \right)$$

$$- \frac{\partial}{\partial y}\left(g_k \rho_k v_k f_k^\alpha - g_k \rho_k D_k^\alpha \frac{\partial f_k^\alpha}{\partial y}\right) \qquad (2.49)$$
$$+ \dot{M}_k^\alpha$$

where D_k^α is the Fickian mass diffusion coefficient associated with the diffusion of constituent α in phase k across the phase boundary due to the movement of the phase interface.

2.3.5 Summary

Mass, momentum, energy and species conservation equations for a single phase k in a mixture of phases, Eqs. 2.43, 2.44, 2.48 and 2.49, are conveniently summarized in Table 1. The individual conservation equations are formed by substituting the terms in the body of the table for the corresponding term in Eq. 2.42 indicated by the appropriate column heading.

Table 2.1: Summary of Conservation Equations for a Single Phase

	ϕ_k	j_k	j_y	I_i	$\dot{S}_k$
Mass	1	$\rho_k u_k$	$\rho_k v_k$	$\dot{M}_k$	—
x-Momentum	u_k	$\rho_k u_k^2 + \tau_{kxx} + p_k$	$\rho_k u_k v_k + \tau_{kyx}$	$\dot{G}_{kx}$	$\rho_k g_x$
y-Momentum	v_k	$\rho_k u_k v_k + \tau_{kxy}$	$\rho_k v_k^2 - \tau_{kyy} + p_k$	$\dot{G}_{ky}$	$\rho_k g_y$
Energy	e_k	$\rho_k u_k e_k - k_k \frac{\partial T}{\partial x}$	$\rho_k v_k e_k - k_k \frac{\partial T}{\partial y}$	$\dot{E}_k$	—
Species	f_k^α	$\rho_k u_k f_k^\alpha - \rho_k D_k^\alpha \frac{\partial f_k^\alpha}{\partial x}$	$\rho_k v_k f_k^\alpha - \rho_k D_k^\alpha \frac{\partial f_k^\alpha}{\partial y}$	$\dot{M}_k^\alpha$	—

2.4 Continuum Conservation Equations

Closure of the system of conservation equations for a binary mixture solid/liquid phase change problem requires fewer equations than the number of solid and liquid phase equations implied in

Section 2.3. By adding like solid and liquid phase conservation equations together, the number of equations to be solved is reduced. The system of conservation equations is closed by relationships for phase mass fraction f_k and composition f_k^α which are discussed in Section 2.4.2, Material Properties. The continuum equations formed by summing over the phases are simplified in this section by invoking the definitions of fractional quantities, Eqs. 2.8 - 2.12, and by introducing physically realistic assumptions for a solid/liquid phase change system.

2.4.1 Mass

Summing the mass conservation equations for a phase k, Eq. 2.43, over all phases results in

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}(\rho u) - \frac{\partial}{\partial y}(\rho v) \tag{2.50}$$

where ρ, u and v are the mass averaged quantities of density, u-velocity, v-velocity as defined by Eq. 2.10 and by

$$\vec{V} = \frac{1}{\rho} \sum_k \bar{\rho}_k \vec{V}_k \tag{2.51}$$

where $\vec{V}$ is the mass averaged velocity vector. The sum of the terms representing the flows of mass across the phase boundaries is zero ($\sum_k \dot{M}_k = 0$), since continuity requires that these flows, being internal to the control volume, occur at each other's expense.

Momentum

The statement of x-momentum conservation for a mixture is obtained by summing the x-momentum conservation equation, Eq. 2.44, over each phase. This gives

$$\begin{aligned} \frac{\partial}{\partial t}\left(\sum_k g_k \rho_k u_k\right) = & - \frac{\partial}{\partial x}\left(\sum_k g_k \rho_k u_k^2\right) - \frac{\partial}{\partial x}\left(\sum_k g_k \tau_{kxx}\right) \\ & - \frac{\partial}{\partial x}\left(\sum_k g_k p_k\right) - \frac{\partial}{\partial x}\left(\sum_k g_k \rho_k u_k v_k\right) \\ & - \frac{\partial}{\partial x}\left(\sum_k g_k \tau_{kyx}\right) \\ & + \sum_k \dot{G}_{kx} + \sum_k g_k \rho_k g_x \end{aligned} \tag{2.52}$$

This equation may be simplified by using the definitions for average fluid quantities and by introducing new variables. By the definition of mass-averaged velocity, Eq. 2.51, the term on the left side of Eq. 2.52 becomes $\frac{\partial}{\partial t}(\rho u)$. The advective fluxes on the right side of the equation can be

decomposed into mean and relative components for each phase. The bracketed quantity of the first term on the right side may be decomposed to give

$$\sum_k g_k \rho_k u_k^2 = \rho u^2 + \sum_k g_k \rho_k (u_k - u)^2 \tag{2.53}$$

by using the definition for mixture density, ρ, and mass-averaged velocity, $\vec{V}$. The fourth term on the right side may be similarly decomposed giving

$$\sum_k g_k \rho_k u_k v_k = \rho u v + \sum_k g_k \rho_k (u_k - u)(v_k - v) \; . \tag{2.54}$$

Often the relative components in Eqs. 2.53 and 2.54 may be neglected depending on the characteristics of the problem. The pressure term may be simplified by defining

$$p \equiv \sum_k g_k p_k \tag{2.55}$$

By using the definition of mixture density ρ, the gravity term in Eq. 2.52 becomes

$$\sum_g g_k \rho_k g_x = \rho g_x \tag{2.56}$$

By incorporating Eqs. 2.53, 2.54, 2.55 and 2.56, and the constitutive equation for stress Eqs. 2.45, Eq. 2.52 becomes

$$\begin{aligned} \frac{\partial}{\partial t}(\rho u) = & - \frac{\partial}{\partial x}(\rho u^2) - \frac{\partial}{\partial x}\left[\sum_k \left(2\mu_k \left(-\frac{1}{3}\nabla \cdot \left(g_k \vec{V}_k\right) + \frac{\partial g_k u_k}{\partial x}\right)\right)\right] - \frac{\partial p}{\partial x} \\ & - \frac{\partial}{\partial y}(\rho u v) - \frac{\partial}{\partial x}\left[\sum_k \left(\mu_k \left(\frac{\partial g_k v_k}{\partial x} + \frac{\partial g_k u_k}{\partial y}\right)\right)\right] \\ & - \frac{\partial}{\partial x}\left[\sum_k g_k \rho_k (u_k - u)^2\right] - \frac{\partial}{\partial y}\left[\sum_k g_k \rho_k (u_k - u)(v_k - v)\right] \\ & + \sum_k \dot{G}_{kx} + \rho g_x . \end{aligned} \tag{2.57}$$

At this point, physically realistic assumptions for a solid/liquid phase change system will be made so that Eq. 2.57 may be simplified. The convective terms Eqs. 2.53 and 2.54 will be addressed first. Two new variables representing the u- and v-velocity components of the liquid relative to the solid, are introduced here by the definitions

$$u_r \equiv u_l - u_s \quad \text{and} \quad v_r \equiv v_l - v_s \tag{2.58}$$

By algebraic manipulation and by use of the above definitions Eqs. 2.53 and 2.54 simplify to

$$- \frac{\partial}{\partial x}\left[g_l \rho_l (u_l - u)^2 + g_s \rho_s (u_s - u)^2\right] = - \frac{\partial}{\partial x}\left(\rho f_s f_l u_r^2\right) \tag{2.59}$$

$$-\frac{\partial}{\partial y}\left[g_l\rho_l(u_l-u)(v_l-v)+g_s\rho_s(u_s-u)(v_s-v)\right]=-\frac{\partial}{\partial y}\left(\rho f_s f_l u_r v_r\right) \tag{2.60}$$

The stress terms may also be simplified for a solid/liquid system. It is assumed that the solid does not contribute to x-momentum through internal stresses. This requires

$$\nabla(g_s u_s)=\nabla(g_s v_s)=0 \tag{2.61}$$

With this assumption the stress terms in Eq. 2.57 become

$$\frac{\partial}{\partial x}\left[\sum_k\left(2u_k\left(-\frac{1}{3}\nabla\cdot(g_k\vec{V}_k+\frac{\partial g_k u_k}{\partial x}\right)\right)\right]=\frac{\partial}{\partial x}\left[2\mu_l\left(-\frac{1}{3}\nabla\cdot\left(g_l\vec{V}_l\right)+\frac{\partial g_l u_l}{\partial x}\right)\right] \tag{2.62}$$

$$\frac{\partial}{\partial x}\left[\sum_k\left(u_k\left(\frac{\partial g_k v_k}{\partial x}+\frac{\partial g_k u_k}{\partial y}\right)\right)\right]=\frac{\partial}{\partial x}\left(g_l\tau_{lxx}\right)=\frac{\partial}{\partial y}\left[\mu_l\left(\frac{\partial g_l v_l}{\partial x}+\frac{\partial g_l u_l}{\partial y}\right)\right] \tag{2.63}$$

It is further assumed that the local density gradients are negligible, that is

$$\nabla\left(\frac{\rho_k}{\rho}\right)=0 \tag{2.64}$$

The divergence of velocity, can be simplified using the assumption in Eq. 2.64 so that

$$\nabla\cdot\vec{V}=\nabla\cdot\left(\sum_k\frac{g_k\rho_k V_k}{\rho}\right)=\sum_k\left(\frac{\rho_k}{\rho}\nabla\cdot(g_k V_k)\right)\,. \tag{2.65}$$

Using the assumption stated in Eq. 2.61, this expression becomes

$$\nabla\cdot\vec{V}=\frac{\rho_l}{\rho}\nabla\cdot(g_l\vec{V})\,. \tag{2.66}$$

Similarly the partial derivatives become

$$\frac{\partial g_l u_l}{\partial x}=\frac{\rho_l}{\rho}\frac{\partial u}{\partial x} \tag{2.67}$$

$$\frac{\partial g_l v_l}{\partial y}=\frac{\rho_l}{\rho}\frac{\partial v}{\partial y} \tag{2.68}$$

$$\frac{\partial g_l u_l}{\partial y}=\frac{\rho_l}{\rho}\frac{\partial u}{\partial y} \tag{2.69}$$

Substituting Eqs. 2.67 - 2.69, the stress terms, Eqs. 2.62 and 2.63 become

$$\frac{\partial}{\partial x}\left[2\mu_l\left(-\frac{1}{3}\nabla\cdot(g_l\vec{V}_l)+\frac{\partial g_l u_l}{\partial x}\right)\right]=\frac{\partial}{\partial x}\left[2\mu_l\left(-\frac{1}{3}\frac{\rho}{\rho_l}\nabla\cdot\vec{V}+\frac{\rho}{\rho_l}\frac{\partial u}{\partial x}\right)\right] \tag{2.70}$$

$$\frac{\partial}{\partial y}\left[\mu_l\left(\frac{\partial g_l v_l}{\partial x}+\frac{\partial g_l u_l}{\partial y}\right)\right]=\frac{\partial}{\partial y}\left[\mu_l\frac{\rho}{\rho_l}\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)\right] \tag{2.71}$$

By assuming constant viscosity, the above equations sum to

$$\frac{\partial}{\partial y}\left[2\mu_l\left(-\frac{1}{3}\frac{\rho}{\rho_l}\nabla\cdot\vec{V}+\frac{\rho}{\rho_l}\frac{\partial u}{\partial x}\right)\right]+\frac{\partial}{\partial y}\left[\mu_l\frac{\rho}{\rho_l}\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)\right]=\mu_l\frac{\rho}{\rho_l}\left[\frac{4}{3}\frac{\partial^2 u}{\partial x^2}+\frac{1}{3}\frac{\partial^2 v}{\partial x\partial y}+\frac{\partial^2 u}{\partial y^2}\right]\,. \tag{2.72}$$

Substituting Eqs. 2.59, 2.60, 2.66 and 2.72 in Eq. 2.57 gives

$$\begin{aligned}\frac{\partial \rho u}{\partial t} = & - \frac{\partial \rho u^2}{\partial x} - \frac{\partial \rho u v}{\partial y} + \mu_l \frac{\rho}{\rho_l}\left[\frac{4}{3}\frac{\partial^2 u}{\partial x^2} + \frac{1}{3}\frac{\partial^2 v}{\partial x \partial y} + \frac{\partial^2 u}{\partial y^2}\right] \\ & - \frac{\partial \rho}{\partial x} - \frac{\partial}{\partial x}\left(\rho f_s f_l u_r^2\right) - \frac{\partial}{\partial y}\left(\rho f_s f_l u_r v_r\right) \\ & + \rho g_x + \sum_k \dot{G}_{kx} \, . \end{aligned} \tag{2.73}$$

The fifth and sixth term on the right side of Eq. 2.73 are non-zero only in multiphase regions, where relative phase velocities are very small. Consequently these terms often may be neglected.

The last term on the right side of Eq. 2.73, $\sum_k \dot{G}_{kx}$, represents the production of x-momentum due to movement of the interface and shear stress at the phase interface. The former effect may be neglected for most physically realistic problems. Bennon and Incropera [1] proposed that Darcy's law could be used to approximate the latter effect. Darcy's law models the force on a liquid flowing through a solid porous media such that

$$F_x = \frac{\mu_l}{K_x}\left(g_l u_r\right) \tag{2.74}$$

where K_x denotes the permeability in the x-direction. Knowledge of the morphology of the solid/liquid interface is necessary to determine the suitability of this model as well as the coefficient K_x

The equation for y-momentum conservation can be obtained from equation 2.73 by permuting the subscripts and exchanging v for u. This equation then becomes

$$\begin{aligned}\frac{\partial \rho v}{\partial t} = & - \frac{\partial}{\partial x}\left(\rho v u\right) - \frac{\partial}{\partial y}\left(\rho u^2\right) + \mu_l \frac{\rho}{\rho_l}\left[\frac{4}{3}\frac{\partial^2 v}{\partial y^2} + \frac{1}{3}\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial x^2}\right] \\ & - \frac{\partial \rho}{\partial y} - \frac{\partial}{\partial x}\left(\rho f_s f_l v_r u_r\right) - \frac{\partial}{\partial y}\left(\partial f_s f_l v_r^2\right) \\ & + \rho g_y + \sum_k \dot{G}_{ky} \, . \end{aligned} \tag{2.75}$$

Energy

The statement of energy conservation for a mixture is obtained by summing the energy conservation equation for phase k, Eq. 2.48, over all phases, giving

$$\begin{aligned}\frac{\partial}{\partial t}\left[\sum_k \left(g_k \rho_k e_k\right)\right] = & - \frac{\partial}{\partial x}\left[\sum_k \left(g_k \rho_k u_k e_k\right) - k_k \frac{\partial T}{\partial x}\right] \\ & - \frac{\partial}{\partial y}\left[\sum_k \left(g_k \rho_k v_k e_k\right) - k_k \frac{\partial T}{\partial y}\right] \end{aligned} \tag{2.76}$$

where the mixture conductivity is defined by

$$k \equiv \sum_k g_k k_k \, . \tag{2.77}$$

The sum of the terms representing energy flow into a phase due to interface movement, $\sum_k \dot{E}_k$, is zero since the exchange of energy represented by this sum is internal to the control volume. The advective contribution can be decomposed in a manner similar to that for the x-momentum equation giving

$$\frac{\partial}{\partial x}\left[\sum_k (g_k\rho_k u_k h_k)\right] = \frac{\partial}{\partial x}(\rho u h) + \frac{\partial}{\partial x}\left[\sum_k g_k\rho_k(u_k-u)(h_k-h)\right] \tag{2.78}$$

$$\frac{\partial}{\partial y}\left[\sum_k (g_k\rho_k v_k h_k)\right] = \frac{\partial}{\partial y}(\rho v h) + \frac{\partial}{\partial y}\left[\sum_k g_k\rho_k(v_k-v)(h_k-h)\right] , \tag{2.79}$$

where the mixture enthalpy is defined by

$$h \equiv \frac{1}{\rho}\sum_k g_k\rho_k h_k . \tag{2.80}$$

In the above equations, specific enthalpy h is assumed to be a suitable approximation of specific internal energy e. Substituting Eqs. 2.78, 2.79 and 2.80 into Eq. 2.76 yields

$$\begin{aligned}\frac{\partial}{\partial t}(\rho h) = &- \frac{\partial}{\partial x}(\rho u h) - \frac{\partial}{\partial y}(\rho v h) + \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial y}\right)\\ &- \frac{\partial}{\partial x}\left[\sum_k g_k\rho_k(u_k-u)(h_k-h)\right]\\ &- \frac{\partial}{\partial y}\left[\sum_k g_k\rho_k(v_k-v)(h_k-h)\right] .\end{aligned} \tag{2.81}$$

The temperature T can be eliminated from this expression by using the relation between temperature and enthalpy

$$h_k = \int_0^T c_k dT + h_k^0 , \tag{2.82}$$

and the identity

$$\nabla T = \frac{1}{c_k}\nabla h_k = \frac{1}{c_k}\nabla h + \frac{1}{c_k}\nabla(h_k - h) . \tag{2.83}$$

Here c_k represents the specific heat of phase k. Equation 2.81 then becomes

$$\begin{aligned}\frac{\partial}{\partial t}(\rho h) = &- \frac{\partial}{\partial x}(\rho u h) - \frac{\partial}{\partial y}(\rho v h) + \frac{\partial}{\partial x}\left(\frac{k}{c_k}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{k}{c_k}\frac{\partial h}{\partial y}\right)\\ &+ \frac{\partial}{\partial x}\left[\frac{k}{c_k}\frac{\partial}{\partial x}(h_k-h)\right] + \frac{\partial}{\partial y}\left[\frac{k}{c_k}\frac{\partial}{\partial y}(h_k-h)\right]\\ &- \frac{\partial}{\partial x}\left[\sum_k g_k\rho_k(u_k-u)(h_k-h)\right]\\ &- \frac{\partial}{\partial y}\left[\sum_k g_k\rho_k(v_k-v)(h_k-h)\right]\end{aligned} \tag{2.84}$$

Equation 2.84 may be rewritten specifically for a solid/liquid system. The last two terms can be reduced by using the definitions for mass-averaged velocity, $\vec{V}$, mixture density, ρ, and mixture enthalpy, h. This equation becomes

$$\begin{aligned}\frac{\partial}{\partial t}(\rho h) = &- \frac{\partial}{\partial x}(\rho u h) - \frac{\partial}{\partial y}(\rho v h) + \frac{\partial}{\partial x}\left(\frac{k}{c_s}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{k}{c_s}\frac{\partial h}{\partial y}\right) \\ &+ \frac{\partial}{\partial x}\left[\frac{k}{c_s}\frac{\partial}{\partial x}(h_s - h)\right] + \frac{\partial}{\partial y}\left[\frac{k}{c_s}\frac{\partial}{\partial y}(h_s - h)\right] \\ &- \frac{\partial}{\partial x}\left[\rho f_s u_s h_s + \rho f_l u_l h_l - \rho u h\right] \\ &- \frac{\partial}{\partial y}\left[\rho f_s v_s h_s + \rho f_l v_l h_l - \rho v h\right] . \end{aligned} \tag{2.85}$$

The last two terms of Eq. 2.85 are non-zero only in the multi-phase region.

Species

The species conservation equation for a mixture is obtained from Eq. 2.48 by summing over each phase. Hence

$$\begin{aligned}\frac{\partial}{\partial t}\left[\sum_k (g_k \rho_k f_k^\alpha)\right] = &- \frac{\partial}{\partial x}\left[\sum_k \left(g_k \rho_k u_k f_k^\alpha - g_k \rho_k D_k^\alpha \frac{\partial f_k^\alpha}{\partial x}\right)\right] \\ &- \frac{\partial}{\partial y}\left[\sum_k \left(g_k \rho_k v_k f_k^\alpha - g_k \rho_k D_k^\alpha \frac{\partial f_k^\alpha}{\partial y}\right)\right] \end{aligned} \tag{2.86}$$

The term in Eq. 2.48 representing transport of species α into phase k across the phase boundary, $\dot{M}_k$, does not appear here because this transport, being internal to the control volume, is zero due to mass continuity. The advective contribution may be decomposed such that

$$\sum_k g_k \rho_k u_k f_k^\alpha = \rho u f^\alpha + \sum_k g_k \rho_k (u_k - u)(f_k^\alpha - f^\alpha) \tag{2.87}$$

$$\sum_k g_k \rho_k v_k f_k^\alpha = \rho v f^\alpha + \sum_k g_k \rho_k (v_k - v)(f_k^\alpha - f^\alpha) \tag{2.88}$$

Where the mixture concentration of species α is defined by

$$f^\alpha = \frac{1}{\rho}\sum_k g_k \rho_k f_k^\alpha . \tag{2.89}$$

Equation 2.86 is reduced by substitution of Eqs. 2.87 2.88 and 2.89 giving

$$\begin{aligned}\frac{\partial}{\partial t}(\rho f^\alpha) = &- \frac{\partial}{\partial x}(\rho u f^\alpha) - \frac{\partial}{\partial y}(\rho v f^\alpha) - \frac{\partial}{\partial x}\left[\sum_k g_k \rho_k D_k^\alpha \frac{\partial}{\partial x}(f_k^\alpha)\right] \\ &- \frac{\partial}{\partial y}\left[\sum_k g_k \rho_k D_k^\alpha \frac{\partial f_k^\alpha}{\partial y}\right] - \frac{\partial}{\partial x}\left[\sum_k g_k \rho_k (u_k - u)(f_k^\alpha - f^\alpha)\right] \\ &- \frac{\partial}{\partial y}\left[\sum_k g_k \rho_k (v_k - v)(f_k^\alpha - f^\alpha)\right] . \end{aligned} \tag{2.90}$$

When Eq. 2.90 is applied to a solid/liquid system the assumption can be made that diffusion in the solid is negligible ($D_s^\alpha = 0$). The gradient of f_k^α may be decomposed into mean and relative components leading to

$$\frac{\partial}{\partial x}\left(f_l^\alpha\right) = \frac{\partial}{\partial x}\left(f^\alpha\right) + \frac{\partial}{\partial x}\left(f_l^\alpha - f^\alpha\right), \text{ and}$$
$$\frac{\partial}{\partial y}\left(f_l^\alpha\right) = \frac{\partial}{\partial y}\left(f^\alpha\right) + \frac{\partial}{\partial y}\left(f_l^\alpha - f^\alpha\right). \tag{2.91}$$

Equation 2.90 then reduced to

$$\begin{aligned}\frac{\partial}{\partial t}(\rho f^\alpha) = & - \frac{\partial}{\partial x}\left(\rho u f^\alpha\right) - \frac{\partial}{\partial y}\left(\rho v f^\alpha\right) \\ & - \frac{\partial}{\partial x}\left[\rho D^\alpha \frac{\partial}{\partial x}\left(f^\alpha\right)\right] - \frac{\partial}{\partial y}\left[\rho D^\alpha \frac{\partial}{\partial y}\left(f^\alpha\right)\right] \\ & - \frac{\partial}{\partial x}\left[\rho D^\alpha \frac{\partial}{\partial x}\left(f_l^\alpha - f^\alpha\right)\right] - \frac{\partial}{\partial y}\left[\rho D^\alpha \frac{\partial}{\partial y}\left(f_l^\alpha - f^\alpha\right)\right] \\ & - \frac{\partial}{\partial x}\left[\sum_k g_k \rho_k (u_k - u)(f_k^\alpha - f^\alpha)\right] \\ & - \frac{\partial}{\partial y}\left[\sum_k g_k \rho_k (v_k - v)(f_k^\alpha - f^\alpha)\right]\end{aligned} \tag{2.92}$$

where the mixture mass diffusion coefficient is defined as

$$D = F_l D_l^\alpha \tag{2.93}$$

since $D_s^\alpha = 0$. The last two terms of Eq. 2.92 may be simplified by using the definition of mass-averaged velocity, $\vec{V}$, mixture density, ρ, and the mass fraction of α, f^α, such that

$$\begin{aligned}\frac{\partial}{\partial t}\left(\rho f^\alpha\right) = & - \frac{\partial}{\partial x}\left(\rho u f^\alpha\right) - \frac{\partial}{\partial y}\left(\rho v f^\alpha\right) \\ & - \frac{\partial}{\partial x}\left[(\rho D \frac{\partial}{\partial x}\left(f^\alpha\right)\right] - \frac{\partial}{\partial y}\left[(\rho D \frac{\partial}{\partial y}\left(f^\alpha\right)\right] \\ & - \frac{\partial}{\partial x}\left[(\rho D^\alpha \frac{\partial}{\partial x}\left(f_l^\alpha - f^\alpha\right)\right] - \frac{\partial}{\partial y}\left[(\rho D^\alpha \frac{\partial}{\partial y}\left(f_l^\alpha - f^\alpha\right)\right] \\ & - \frac{\partial}{\partial x}\left[\rho f_s u_s f_s^\alpha - \rho f_l u_l f_l^\alpha - \rho u f^\alpha\right] \\ & - \frac{\partial}{\partial y}\left[\rho f_s v_s f_s^\alpha - \rho f_l v_l f_l^\alpha - \rho v f^\alpha\right].\end{aligned} \tag{2.94}$$

The last two terms in Eq. 2.94 are non-zero only in the multi-phase region.

For a mixture containing many phases, Eq. 2.94 must be solved for all but one of the constituents, since one of the concentrations f^α may be solved for using species conservation (i.e. $\sum_\alpha f^\alpha = 1$). For a binary mixture then, Eq. 2.94 only needs to be solved for one constituent.

2.4.2 Material Properties

Closure of the system of mixture conservation equations requires relationships for phase mass fraction f_k, phase concentration f_k^α, phase enthalpy h_k and temperature T. These relationships are obtained from material behavior described by the phase diagram, and from thermodynamic relationships for enthalpy. The required expressions are derived assuming constant specific heats, c_s and c_l, and constant latent heat, h_f. Further, a linearized phase diagram is assumed.

A eutectic binary system is first considered. Application of the proposed material relationships for a simpler isomorphous (non-eutectic) binary system follows. Figure 5 shows the linearized binary eutectic phase diagram. Several variables characterize the diagram. The slopes of the liquidus and solidus lines are denoted by m_l and m_s respectively. The equilibrium partition ration k_p is defined as the ratio of these slopes:

$$k_p \equiv \frac{m_l}{m_s} \tag{2.95}$$

The eutectic temperature is denoted by T_e and the fusion temperature as $f^\alpha \rightarrow 0$ is denoted by T_m

From the definition of mixture concentration ($f^\alpha = f_s f_s^\alpha + f_l f_l^\alpha$) and the definitions of the variables that characterize the linearized phase diagram, expressions for the phase mass fraction f_k and phase concentration f_k^α may be derived. The mass fraction of solid f_s for $T \geq T_e$ may be calculated from

$$f_s = \frac{1}{1-k_p}\left[\frac{T - T_{\text{liq}}}{T - T_m}\right] \tag{2.96}$$

At $T = T_e$ the solid mass fraction f_s is described by

$$f_s = 1 - \frac{h - h_{\text{sol}}}{h_f} \tag{2.97}$$

The expressions for phase concentrations are given by

$$f_s^\alpha = \left[\frac{k_p}{f_s(k_p - 1) + 1}\right] f^\alpha \tag{2.98}$$

$$f_l^\alpha = \left[\frac{1}{f_s(k_p - 1) + 1}\right] f^\alpha \tag{2.99}$$

Calculating phase mass fraction and phase concentrations using Eqs. 2.96, 2.98 and 2.99 requires knowing the temperature T of the mixture. Calculations for phase enthalpy h_k also require knowing temperature. Relationships between mixture enthalpy and temperature meet this requirement. The enthalpy for the solid phase is described by one expression for Regions i and ii in Fig. 5:

$$h_s = c_s\, T \tag{2.100}$$

where it is presumed that $h_s = 0$ and $T = 0$. This equation holds on the solidus as well so that

$$h_{\text{sol}} = c_s \, T_{\text{sol}} \tag{2.101}$$

where T_{sol} is the temperature on the solidus.

The enthalpies of the liquid phase and the mixture must be calculated according to the region in Fig. 5 in which the mixture belongs. The liquid phase and the mixture enthalpies for Region ii are discussed here. The temperature remains constant at the eutectic temperature, T_e, until the enthalpy reaches the value

$$h_e = h_{\text{sol}} + \left[1 - \frac{1}{1 - k_p} \left(\frac{T_{\text{sol}} - T_{\text{liq}}}{T_{\text{sol}} - T_m}\right)\right] h_f \tag{2.102}$$

Between this temperature and the liquidus, the enthalpy temperature expression involves solving for the roots of an expression derived in Appendix A. This expression is based on the definition of mixture enthalpy between the solidus and the liquidus namely

$$h = f_s \, h_{\text{sol}} + f_l \, h_{\text{liq}} \tag{2.103}$$

Above the liquidus the mixture enthalpy becomes that of the liquid phase:

$$h_l = c_l T + [(c_s - c_l)T_e + h_f] \tag{2.104}$$

On the liquidus the above expression becomes

$$h_{\text{liq}} = c_l \, T_{\text{liq}} + [(c_s - c_l)T_e + h_f] \tag{2.105}$$

Table 2 summarizes the enthalpy/temperature relationships for Region ii of Fig. 5. In the table, h_o is defined by

$$h_o \equiv (c_s - c_l)T_e = h_f \tag{2.106}$$

For an isomorphous (non-eutectic) binary system or for Region i of Fig. 5 for eutectic system, the enthalpy/temperature expression must be modified. For low concentrations the non-eutectic system has a phase diagram, Fig. 6, similar to Region i of Fig. 5 for a eutectic system. The enthalpy in the solid phase is described by Eq. 2.100 for any system. The liquid enthalpy for the two cases addressed here is obtained from Eq. 2.104 by replacing T_e by T_{sol} giving

$$h_l = c_l \, T + [(c_s - c_l)T_{\text{sol}} \, h_f] \tag{2.107}$$

For these cases, Table 2 reduces since there is no such enthalpy range, $h_{\text{sol}} \leq h \leq h_l$, since h_l may be effectively replaced by h_{sol}. This substitution must also be done for h_o in Table 2 so that

$$h_o = (c_s - c_l)T_{\text{sol}} + h_f \tag{2.108}$$

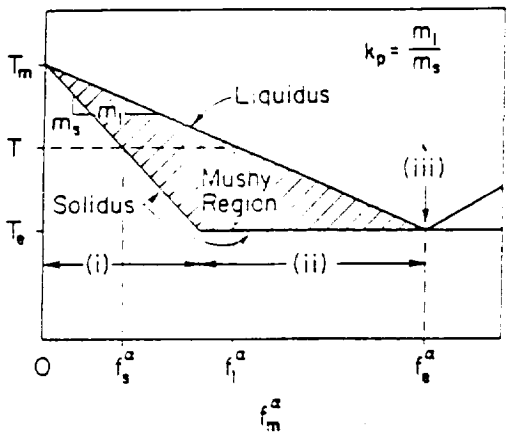


Figure 2.5:

Table 2.2: Enthalpy/Temperature Relationships for Region ii of a Binary Eutectic System

Mixture Enthalpy h	Temperature T
$h \leq h_{\text{sol}}$	$\frac{h}{c_s}$
$h_{\text{sol}} < h \leq h_e$	T_e
$h_e < h < h_{\text{liq}}$	root of $AT^2 + BT + C = 0$ where $A = c_l - \frac{c_l - c_s}{1-k_p}$ $B = \frac{c_l - c_s}{1-k_p} T_{\text{liq}} - \frac{k_p h_o}{1-k_p} - c_l T_m - h$ $C = (h_m - h_o)T_m + \frac{h_o T_{\text{liq}}}{1-k_p}$
$h \geq h_{\text{liq}}$	$\frac{h-h^o}{c_l}$

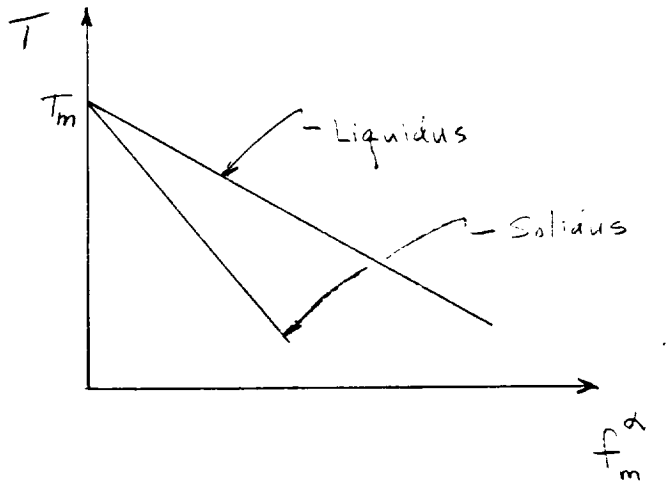


Figure 2.6:

2.4.3 Interfacial Compatability Constraint

The development at this point has not required that the solid/liquid interface be resolved. In some problems it may be desirable to explicitly resolve the interface. When the solid/liquid interface is resolved, the temperature and concentration distributions in the phase change material must satisfy interfacial mass, energy and concentration combatability constraints along the solid/liquid interface.

The equilibrium temperature and concentration of the phase change material is determined according to the mixture phase diagram. The concentration of the liquid phase is given by the intersection of the temperature and liquidus lines. The concentration of the solid is specified by the intersection of the same temperature line and the solidus line.

Energy and species balances applied at the interface lead to further compatability constraints. The first of these constraints is developed by applying an energy balance on a control volume element as illustrated in Fig. 7. The heat flow into the interface over time dt from the liquid phase consists of an advective and a convective component:

$$q_l = -\, k_l\, dA\, \left.\frac{\partial T}{\partial n}\right|_l dt \;+\; V_l e_l \rho_l dA dt \tag{2.109}$$

where n is the normal to the interface in the direction of the solid and V_l is a liquid velocity normal to the interface which may partly result from density differences due to the change in phase occurring at the interface. Similarly the heat flow leaving the interface and entering the solid is given by:

$$q_s = -\, k_s dA\, \left.\frac{\partial T}{\partial n}\right|_s dt \;+\; V_s e_s \rho_s dA dt \tag{2.110}$$

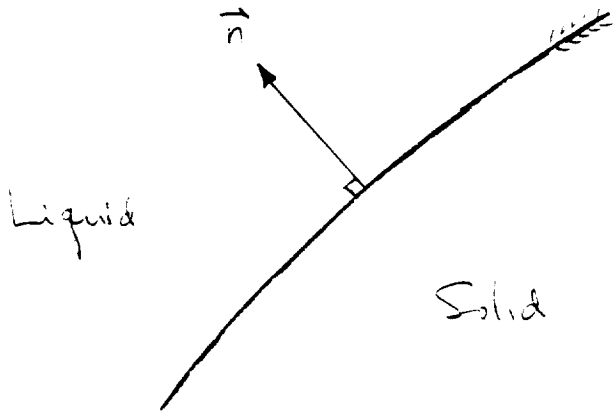


Figure 2.7:

The difference in energy flows entering and leaving the interface results in a change of energy at the interface given by

$$dE = \rho_l e_l dA dn \; - \; \rho_s e_s dA dn \tag{2.111}$$

where dn represents the displacement of the interface occurring over time dt. Applying an energy balance at the interface results in

$$q_l - q_s = dE \tag{2.112}$$

Substituting Eqs. 2.109- 2.111 in Eq. 2.112 gives

$$\begin{aligned} - k_l \left.\frac{\partial T}{\partial n}\right|_l \; + \; V_l e_l \rho_l \; + \; k_s \left.\frac{\partial T}{\partial n}\right|_s \; - \; V_s e_s \rho_s \\ = \; (\rho_l e_l \; - \; \rho_s e_s) \frac{\partial n}{\partial t} \end{aligned} \tag{2.113}$$

The development of the species interfacial compatability constraints is analogous to the above and results in

$$\begin{aligned} - \rho_l \, D_l \left.\frac{\partial f_l^\alpha}{\partial n}\right|_l \; + \; V_l f_l^\alpha \rho_l \; + \; \rho_s \, D_s \left.\frac{\partial f_s^\alpha}{\partial n}\right|_s \; - \; V_s f_s^\alpha \rho_s \\ = \; (\rho_l f_l^\alpha \; - \; \rho_s f_s^\alpha) \frac{\partial n}{\partial t} \end{aligned} \tag{2.114}$$

Conservation of mass leads to the relation

$$\rho_l V_l - \rho_s V_s = (\rho_l - \rho_s) \frac{\partial n}{\partial t} \; . \tag{2.115}$$

Substituting this equation into Eq. 2.113 gives

$$- k_l \left.\frac{\partial T}{\partial n}\right|_l + k_s \left.\frac{\partial T}{\partial n}\right|_s = V_s \rho_s (-e_{ls}) + \rho_s e_{ls} V_i \tag{2.116}$$

where $e_{ls} = e_l - e_s$ and $V_i = \frac{\partial n}{\partial t}$, the speed of the interface. Similarly, substituting the mass equation, Eq. 2.115, into Eq. 2.114 results in

$$- \rho_l D_l \left.\frac{\partial f_l^\alpha}{\partial n}\right|_l + \rho_s D_s \left.\frac{\partial f_s^\alpha}{\partial n}\right|_s = V_s \rho_s (-f_{ls}^\alpha) + \rho_s f_{ls}^\alpha V_i \tag{2.117}$$

where $f_{ls}^\alpha = f_l^\alpha - f_s^\alpha$.

In Eq. 2.116, e_{ls} may be approximated by the latent heat of fusion, h_f. The interfacial compatability constraints for mass, momentum and energy are then

$$\rho_l V_l - \rho_s V_s = (\rho_l - \rho_s) \frac{\partial n}{\partial t} \tag{2.115}$$

$$- k_l \left.\frac{\partial T}{\partial n}\right|_l + k_s \left.\frac{\partial T}{\partial n}\right|_s = - V_s \rho_s h_f + \rho_s h_f V_i \tag{2.118}$$

$$- \rho_l D_l \left.\frac{\partial f_l^\alpha}{\partial n}\right|_l + \rho_s D_s \left.\frac{\partial f_s^\alpha}{\partial n}\right|_s = - V_s \rho_s f_{ls}^\alpha + \rho_s f_{ls}^\alpha V_i \tag{2.117}$$

Since V_s is often very small or zero, the first term on the right side of Eq. 2.118 and the first term on the right side of Eq. 2.117 may be neglected for many problems.

2.4.4 Boundary Conditions

Boundary conditions in this formulation are applied as a general convective-like boundary condition for any general dependent variable, ϕ. The form is then given by the equation

$$k_\phi \frac{\partial \phi}{\partial n} = - h_\phi + C \tag{2.119}$$

where n is the outward normal to the boundary, k_ϕ is the conductivity of ϕ, and h_ϕ is the convective coefficient for the quantity ϕ. The variable ϕ could be any of the dependent variables such as T, u, v, or f_k^α. It is easily shown that through appropriate choice of the constants h_ϕ and C, Eq. 2.119 may be used to represent Dirichlet and Neumann conditions as well as the more general case as specified.

Appendix A

In this appendix the relationship for mixture enthalpy is derived for a binary eutectic system in Region ii shown by Fig. 5, for enthalpies in the range $h_e < h \leq h_{\text{liq}}$. The definition of mixture enthalpy states

$$h = f_s h_s + f_l h_l \,. \tag{A1}$$

For a mixture whose temperature and concentration lie between the liquidus and the solidus, the mixture enthalpy becomes

$$h = f_s\, h_{\text{sol}} + f_l\, h_{\text{liq}} \,. \tag{A2}$$

To proceed, we must first define each of the quantities on the right side of the above equation. The solid mass fraction f_s is given in terms of the phase diagram variables by Eq. 2.96,

$$f_s = \frac{1}{1-k_p}\left[\frac{T-T_{\text{liq}}}{T-T_m}\right] \tag{2.96}$$

Further, the liquid mass fraction f_l can be calculated from Eq. 2.96 since $f_l = 1 - f_s$:

$$f_l = 1 - f_s = \frac{-1}{1-k_p}\left[\frac{T_m - T_{\text{liq}}}{T-T_m} + k_p\right] . \tag{A3}$$

The enthalpy of the solid on the solidus is given by Eq. 2.101

$$h_{\text{sol}} = c_s\, T_{\text{sol}} \tag{2.101}$$

The enthalpy of the liquid on the liquidus is given by Eq. 2.105 which can be rewritten as

$$h_{\text{liq}} = c_l\, T_{\text{liq}} + h_o \tag{A4}$$

where $h_o = (c_s - c_l)T_e + h_f$. Substituting Eqs. 2.96, 2.4.4, 2.101 and A4 into Eq. A7 and rearranging gives

$$\left[c_l - \frac{c_e - c_s}{1-k_p}\right] T^2 + \left[\frac{(c_l - c_s)T_{\text{liq}}}{1-k_p} - \frac{k_p h_o}{1-h_p} - c_l\, T_m - h\right] T$$

$$+ (h - h_o)T_m + \frac{h_o\, T_{\text{liq}}}{1-k_p} = 0 \tag{A5}$$

The root of Eq. 2.4.4 which is physically realistic gives temperature T, as a function of mixture enthalpy h for a mixture between the liquidus and solidus in Region ii shown in Fig. 5. This corresponds to the entry in Table 2 for $h_e < h < h_{\text{liq}}$.

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A computational model is presented for the prediction of solid/liquid phase-change energy transport including the influence of free convection fluid flow in the liquid phase region. The computational model considers the velocity components of all non-liquid phase-change material control volumes to be zero but fully solves the coupled mass-momentum problem within the liquid region. The thermal energy model includes the entire domain and employs an enthalpy-like model and a recently developed method for handling the phase-change interface non-linearity. Convergence studies are performed and comparisons made with experimental data for two different problem specifications. The convergence studies indicate that grid independence has been achieved and the comparison with experimental data indicates excellent quantitative prediction of the melt fraction evolution. Qualitative data is also provided in the form of velocity vector diagrams and isotherm plots for selected times in the evolution of both problems. The computational costs incurred are quite low by comparison with previous efforts on solving these problems.

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