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A numerical method for the Rubinstein binary-alloy problem in the presence of an under-cooled liquid

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Abstract

A fixed grid solution for tracking a moving solidification front controlled by coupled heat and mass transport in the presence of an under-cooled liquid is developed. A known closed form similarity solution for the solidification of a binary alloy in a one-dimensional domain is outlined. A previously reported enthalpy based model for this problem is presented and a novel numerical solution devised. Comparisons with the analytical solution show that the proposed numerical solution can produce high-fidelity predictions across a wide range of conditions including cases where the liquid becomes under-cooled.

Keywords: Binary alloy; Enthalpy method; Constitutional under-cooling; Analytical solution

1. Introduction

Solidification problems that exhibit a moving and sharp interface between the solid and liquid phases are computationally challenging. The key difficulty is the requirement to accurately track the solid–liquid interface as it moves over a discrete description of the problem domain. Many popular numerical solutions used to overcome this difficulty are based on the enthalpy formulation [1,2]. Such methods, dating back to the middle of the last century [3,4], are based on a governing equation that conserves the energy (enthalpy). This equation is valid throughout the problem domain (solid + liquid) and can be numerically solved, at each time step, on a fixed space grid. From the calculated nodal enthalpy field an auxiliary variable—the liquid fraction ($f = 1$ in liquid, $f = 0$ in solid)—can be extracted and used to track the movement of the solid–liquid interface [4–6]. Enthalpy methods have been extensively verified against alternative approaches for tracking solidification fronts, e.g., front fixing [7], deforming grids [8], and semi-analytical [9].

The classic solidification problem is the Stefan problem [1]. The problem is set in a one-dimensional semi-infinite domain $x^* \geqslant 0$ containing a single component (pure) liquid, super heated to a temperature T_0^* above the unique solidification temperature T_f^*. A solidified layer is advanced into the liquid by lowering and maintaining the temperature at the surface $x^* = 0$ to $T_{sur}^* < T_f^*$. This is a useful problem because, when the heat transfer is controlled by heat conduction alone, it can admit a closed similarity solution [1]; a solution that can be used to verify numerical solution approaches designed for more general cases.

An explicit time stepping enthalpy solution of the classic Stefan problem will (i) solve for the nodal enthalpy field at the new time level using the nodal temperature field from the previous time step and then (ii) use the updated nodal enthalpy field to calculate an updated nodal temperature field for use in the next time step. A key feature, that enables the updating of the nodal temperature field from the enthalpy, is that node points in the discretization where the phase change is occurring are readily identified. For example, assuming a single constant volumetric specific

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Nomenclature

c^*	volumetric specific heat [J/m^3 K]
c	normalized specific heat
C^+	is solute concentration [wt%]
C_0	initial solute concentration in the liquid [wt%]
C	concentration normalized by C_0
D^*	mass diffusivity [m^2/s]
D	normalized mass diffusivity
f	liquid fraction
H^*	volumetric enthalpy [J/m^3]
H	dimensionless enthalpy
h	dimensionless heat transfer coefficient
k	is the partition coefficient
Le	Lewis number [$=\frac{\alpha_l^*}{D_l^*}$]
l	a length dimension [m]
L^*	volumetric latent heat [J/m^3]
L	dimensionless latent heat
m	slope in phase diagram [K]
q^{H}	dimensionless heat flux
q^{C}	dimensionless solute flux
St	solutal Stefan number [$=-m_l C_0 \frac{c_l^*}{L^*}$]
s	location of the solid–liquid interface
T^*	temperature [K]
T	dimensionless temperature
T_{amb}	dimensionless ambient temperature
T^*_{equ}	equilibrium temperature [K]
T_{equ}	dimensionless equilibrium temperature
T^*_{f}	fusion temperature of solvent [K]
t	time
V	solute potential
x	space dimension

Greek symbols

α^*	thermal diffusivity [m^2/s]
α	normalized thermal diffusivity
λ	similarity variable

Superscripts

f	mixture value
i	solid–liquid interface value
new	new time level
*	quantity with dimension

Subscripts

i	node point counter
i_in	left face of control volume i
i_out	right face of control volume i
l	liquid phase
s	solid phase

heat c^*, a latent heat L^*, and setting the reference temperature for calculating the enthalpy as T^*_{f}, the phase change nodes can be identified by enthalpies falling in the range $c^*T^*_{\mathrm{f}} < H^* < c^*T^*_{\mathrm{f}} + L^*$; in one-dimensional problems there is never more than one node, in a given time step, that will satisfy this condition.

Moving away from the classic Stefan problem a more advanced solidification problem considers the solidification of multi-component alloys, e.g., see recent work by Voller and co-workers [2,10], and Ganguly and Chakraborty [11]. A standard test problem, the so-called "binary-alloy problem", involves the solidification of a binary alloy in the one-dimensional semi-infinite domain $x^* \geqslant 0$. Initially, the alloy is liquid with a uniform solute composition C_0 and temperature above the equilibrium liquidus temperature, i.e., $T^*_0 > T^*_{\mathrm{equ}}$, the liquidus line in the phase diagram (see schematic in Fig. 1). Solidification is nucleated by lowering and fixing the surface temperature to $T^*_{\mathrm{sur}} < T^*_{\mathrm{equ}}$. When the binary liquid solidifies there is a partitioning of the solute between the solid and liquid phases. As a result the movement of the solid–liquid interface is controlled by both heat and mass (solute) transport. As with the case of solidification of a pure liquid, if the heat and mass transport is controlled by diffusion, a closed form similarity solution can be found, Rubinstein [12] (see discussion in Alexiades and Solomon [13]).

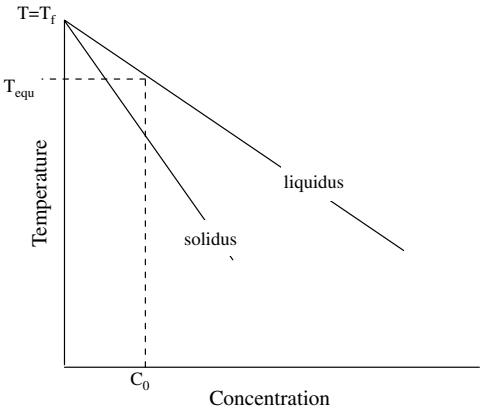

Fig. 1. Schematic of binary phase diagram.

An enthalpy based model and numerical solution of the one-dimensional binary-alloy problem has been presented by Crowley and Ockendon [14]. In this solution the unique node where the solid–liquid interface is located is, assuming a constant specific heat and a reference temperature $T^*_{\mathrm{f}} + mC_0$, identified by the nodal enthalpy falling in the range $c^*T^*_{\mathrm{equ}} < H^* < c^*T^*_{\mathrm{equ}} + L^*$. In contrast to the basic Stefan problem where the phase change temperature T^*_{f} is a fixed constant, the equilibrium temperature T^*_{equ} in this