



Semi-implicit method for thermodynamically linked equations in phase change problems (SIMTLE)

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ABSTRACT

Thermodynamic coupling of temperature and composition fields in phase-change problems has been a challenge for decades. A compromise has been always desired between numerical efficiency and detailed physical consideration, toward a general scheme. In the present work, a macro–micro numerical method is proposed to link the conservation equations of energy and species with the thermodynamics of the solidification problems. Firstly, the basic structure of the method, simplified with a local equilibrium assumption, is presented. The method is then extended to a multi-phase model, demonstrating a three-phase approach to the solidification of a eutectic binary alloy. Relaxing the limitations imposed by the equilibrium assumption, non-equilibrium and microscale considerations was also included subsequently by a suggested modification to the macroscopic mathematical model. Advantages gained through the general algorithm proposed are concerned with two features of the method; (a) consistency with the energy and species equations. (b) No need of a predefined solidification path; that allows for the usage of raw phase diagram curves and offers simplicity and generality for extension through complex problems (i.e. microscopic, multi-phase or non-equilibrium). A benchmark problem was employed to test the performance of the proposed method in two cases of local equilibrium and Scheil-like solidification. The obtained results were validated in comparison with available semi-analytical solution.

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1. Introduction

Phase change problems, like solidification processes, are basically described by a set of highly coupled Partial Differential Equations of macroscopic transport phenomena. However, an important part of the highly coupled models is closure which links the energy and species conservation equations. The closure equations are derived from the thermodynamics of the phases to calculate phase fractions (as a simple key example see [1]). Although this part of the model is mathematically simpler than the conservation equations, it makes the model a tough problem itself, for two reasons; (1) those closure equations are strict relations just when all the variables are in the equilibrium state. Even if the equilibrium is considered, the conservative and iterative variables do not satisfy the equilibrium state numerically, while they are being solved from a rough primary guess. Forcing these numbers into the strict equilibrium relations may cause divergence, numerical instability and/or inconsistency. In such a case, much care must be taken for the primary guess, under-relaxation or time-relaxation. (2) Those closure equations, derived for an assumed simple state, become inapplicable when the problem involves a few degree of

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Nomenclature

Letters

a	coefficients of discretized equations
\mathbf{B}	body force vector
C	composition [†]
\bar{C}_S	volume-averaged solid composition
c	heat capacity [†]
D	coefficient of diffusion [†]
D	diffusion-like source term
F	convection-like source term
f	mass fraction
f	correction for mass fraction
\mathbf{f}	function of equilibrium curve on phase diagram
h	enthalpy [†]
h^{ref}	reference enthalpy [†]
k	thermal conductivity [†]
l	characteristic interfacial diffusion length
\mathbf{M}	interfacial drag force vector
p	pressure
S_V^i	interfacial area concentration
T	temperature
T^{eq}	phase implicit equilibrium temperature (PIET)
t	time
x	distance in the coordinate
\mathbf{v}	velocity vector [†]
$†$	variables without a phase index refer to the mixture.

Greek Letters

α	thermal diffusivity = $k/\rho c$, relaxation factor
ε	volume fraction
δ_S^i	interfacial diffusion factor
Γ	interfacial mass transfer rate
μ	viscosity [†]
ρ	density [†]
ζ	similarity variable = $x/2\sqrt{\alpha t}$

Superscripts

*	primary guess
i	interfacial
new	updated value
ϕ	general dependent variable
eq	equilibrium

Subscripts

α	α -phase
β	β -phase
ij	phase index
L	liquid
e	eutectic
nb	neighbors of node P
o	initial condition
P	node P
S	solid

complexity in the thermodynamics of the phase change microscopic phenomena. Thereafter, simplicity, generality and efficiency of such a model are not saved and specific solution methodologies will be necessary. On the other hand, equilibrium phase changes are of rare physical evolutions and researchers are usually interested in non-equilibrium phase transformation with micro-scale considerations.

The problem of coupling solute and thermal fields has been extensively studied in the literature, from which several studies can be addressed giving effective schemes to overcome a couple of matters mentioned above. Regarding the problem of

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