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# Numerical Modeling of One-Dimensional Binary Solidification with a Mushy Layer Evolution

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**Abstract.** The numerical modeling of a binary solidification with a mushy layer mechanism is considered in this manuscript. The nonlinear coupled system of equations describes the heat and mass diffusions of a one-dimensional spatial variable in the semi-infinite interval. Also formulated is a transformed system in a finite interval. We propose numerical methods for solving the nonlinear system using a threshold strategy based on fixed computation-domain approach. Our calculated results and those from the LeadEx field experiment are well-matched in their tendencies.

**AMS subject classifications**: 35K05, 65-05, 65M06

**Key words**: Direct numerical simulation, Heat and mass transfer, Mushy layer, Solidification, Stefan problem.

## 1. Introduction

Binary solidification of liquids has received considerable attention in the literature due to its wide applicability. If the liquid is an alloy (a mixture of two or more components), its crystallization process completely differs from the solidification process of a pure liquid. In particular, various distributions of impurity in the solid phase lead to different mechanical and physical properties of ingots. This phenomenon arises due to the impurity displacements in the melting process by the moving front of the solidification. If the impurity displacement is rather large, the constitutional supercooling originates ahead of the planar solid-liquid interface [23] and, generally speaking, the two-phase zone (mushy region) appears. Moreover, solid nuclei in the form of newly born crystals may evolve in this zone.

Mathematical descriptions of crystallization processes play a very important role in crystal growth [10, 26], engineering [33], oceanography [22] and metallurgy [12]. The mathematical models allow for the accurate predictions of the many properties of solids

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produced by the melt cooling process. The authors of Ref. [21] developed a full set of thermodynamic equations for a mushy zone, and approximately solved a mush-reduced set of them for the constrained growth of a binary alloy. A more complete solution has since been given in [1] for the steady-state solidification conditions. Nevertheless, solidification with a constant rate is the specific regime.

Generally speaking, the rate of solidification is a function of all operating and physical parameters and also it is a time-dependent function. First of all, the structure of this mushy region depends upon a relation between the kinetics of both the solid-phase formation and the front motion. When the former is much slower than the latter and, thus, the mushy region is almost free from solid elements, the classical Stefan problem provides for a sufficiently acceptable approximation. In the opposite limiting case, the two-phase zone structure is nearly at equilibrium so that its local temperature coincides with the phase transition temperature at a given point. In that situation the solidification is described with the help of Borisov's quasiequilibrium mushy region model [8]. The scenario suggested by Borisov is described by nonlinear heat and mass transfer equations and boundary conditions accounting for moving boundaries [8, 21].

Our previous study [1–5] considerably extended the range of the theoretical application, by solving approximately the Stefan problem in terms of analytical formulae in the special case of simple mushy region for the modeling of moving boundary processes frequently met in geophysics and metallurgy [12, 30, 38]. The solidification problem can be considered as a generalization of the classical two-phase Stefan problem [20]. Nonetheless, much of previous theoretical works have involved substantial approximations to facilitate the derivation of analytical solutions.

There exist various theoretical approaches to the classical Stefan problem in different forms with variable coefficients. The analysis can be based on generailzed functions [29], or Green's function via the method of images [34], or an integral formulation and Schauder's fixed point theorem [25] or contraction mapping theory [16]. The arguments of existence of a solution, in many works, rely on functional iterations by finite differencing in the temporal variable. However, many of these assume that the temperatures are kept at zero on the free boundary and the maximum principle applies. This is not true in a mushy layer model, in which undercooling (or supercooling) is allowed. Furthermore, heat and mass diffusions are coupled. To the author's knowledge, there are no published results in a journal regarding computer simulations of this real-life problem [30]. We refer to [19, 37] for further theoretical references in the classical Stefan problem.

Very recently, the advent of numerical methods such as level set methods [28, 31, 35] and more powerful computers have provided for the opportunity to use DNS ( direct numerical simulation ) of binary solidification. Due to the high nonlinearity shown in the field experiments during the solidification process, we propose in this work numerical procedures to simulate the dynamical evolution of the process based on the mushy layer model [3]. The numerical computation of the Stefan problem has been studied by researchers over decades, e.g., [13, 18, 24] and references therein. Even so, the sheer size of the computational time-step remains the primary difficulty encountered in numerical evolution. As depicted by many researchers, the size of a time-step is around $10^{-5}$ second