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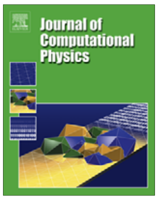

# Simulation of directional solidification, thermochemical convection, and chimney formation in a Hele-Shaw cell

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ABSTRACT

We have developed fully resolved, two-dimensional, finite volume simulations of directional solidification of a binary alloy in a Hele-Shaw cell. Use of Darcy's law and the Enthalpy Method throughout the computational domain allows us to avoid prescribing internal boundary conditions on the interfaces between solid, mushy, and liquid regions. We present a description of the theoretical model, computational approach, two reduced benchmark calculations, and simulations of the full governing equations. In simulations with parameter values that approximate experiments, boundary-layer-mode convection produces corrugations in the mush–liquid interface. Some of these corrugations become chimneys that grow and interact within the mushy layer. We consider two porosity–permeability relations and examine their consequences for chimney spacing and mushy layer height. Our results are broadly similar to experiments on directional solidification of $NH_4Cl$ [S.S.L. Peppin, H.E. Huppert, M.G. Worster, Steady-state solidification of aqueous ammonium chloride, J. Fluid Mech. 599 (2008) 465–476; S.H. Whiteoak, H. Huppert, M.G. Worster, Conditions for defect-free solidification of aqueous ammonium chloride in a quasi 2d directional solidification facility, J. Cryst. Growth (2008)]. We describe other simulations that are tuned to suppress boundary layer mode convection and that, instead, go unstable by the mushy layer mode [M.G. Worster, Instabilities of the liquid and mushy regions during solidification of alloys, J. Fluid Mech. 237 (1992) 649–669]. We investigate the morphological evolution of the mush well beyond the linear instability regime.

## 1. Introduction

Solidification of multi-component melts from a cold boundary generally gives rise to a solid–liquid interface that is unstable to the growth of crystalline dendrites [30]. The ensemble of dendrites forms a porous, permeable mushy layer [49]. In general, crystals have a composition different from their parental melt, so solidification leads to changes in solute concentration of the melt in a narrow region around the crystals. Changes in solute concentration correspond to changes in melt density. In some cases [48], this causes compositional convection to occur within the mushy region. Reactions between moving melt and the dendritic matrix lead to the formation of chimneys of zero-solid-fraction and to focusing of flow into these chimneys. This instability is observed in a wide variety of systems from industrial (e.g. casting [17,24]) to natural (e.g. for-

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mation of sea ice [44]). In the casting of turbine blades, chimneys represent defects that weaken the final product; in sea ice, chimneys allow for enhanced drainage of concentrated brine and hence have important implications for oceanic deep water formation. A thorough understanding of the dynamics of convection in mushy layers is thus of great interest and wide applicability.

Laboratory experiments on the solidification of two-component liquids are a primary tool for investigating mushy layer dynamics. In experiments, the fluid is typically contained in a tank whose top or bottom is cooled to a temperature below the liquidus. Because the cold boundary is stationary, such experiments are termed “fixed chill.” Although solutions of NaCl–water [44], sugar–water [3], and alcohol–water [48], as well as metallic alloys [10], have been used in experiments, aqueous ammonium chloride is most common. This is because $NH_4Cl$ crystallizes over a temperature range easily accessible in the laboratory and forms dendrites that are similar to those formed from metallic alloys. Chimney formation in fixed chill experiments on $NH_4Cl$ has been well studied (e.g. [41,42,13]). Theoretical models of chimney formation, however, have typically been derived under conditions of directional solidification rather than fixed chill.

Directional solidification refers to a system in which a liquid-filled container is moved through a device that chills it, causing a freezing front to propagate through the liquid at the same rate as but in the opposite direction to the motion of the container. An experimental apparatus for directional solidification was recently developed to provide a better correspondence between experiments and mushy layer theory [33]. It consists of a vertical, fluid-filled Hele-Shaw cell that is translated through two sets of fixed-temperature heat exchangers, one set warm, the other cold. The heat exchangers impose a vertical temperature gradient in the fluid. Solidification progresses from the cold end toward the warm end and, eventually, an equilibrium mushy layer height is reached [34,45]. Fig. 1 shows an image of light transmitted through the mushy layer of an experiment that has reached an approximately steady mushy layer height. Darker regions correspond to lower porosity, chimneys appear as lighter, vertical bands.

Profiles of steady-state temperature, porosity and concentration have been predicted theoretically for the case of directional solidification with no fluid motion [21,19]. Worster [47] studied the linear instability of this basic state with simple constitutive equations for permeability. This work demonstrated the existence of two modes of convective instability. At longer wavelengths, convective cells penetrate to the bottom of the mushy layer, while at shorter wavelengths, convection is mainly confined to the liquid region. The long-wavelength mushy layer mode seems the obvious candidate to explain the formation of chimneys, however neither experiments nor stability analysis confirm this conclusively. To model the evolution of convection and the development of chimneys requires an analysis that captures all the nonlinearities in the governing equations.

Past models that incorporate nonlinearities have typically been used to look for steady-state solutions with prescribed chimney locations (e.g. [36,29,16]). While interesting, such models cannot elucidate the path to chimney formation, nor can they investigate the dynamical interactions between chimneys. These goals require a time-dependent solution to the governing equations. Owing to the complexity of the full equations, such a solution can only be obtained numerically. While numerical simulations are more difficult to interpret than analytical solutions, they offer several advantages. Among these

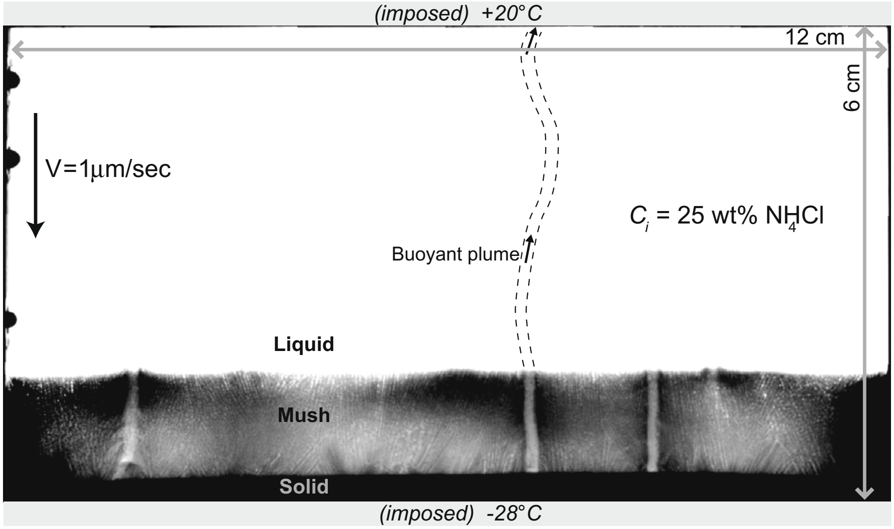

**Fig. 1.** An example of directional solidification of $NH_4Cl$ in the laboratory. This image was acquired when the mushy layer had reached a constant height above the bottom heat exchanger, about 220 min after the start of the experiment. The Hele-Shaw cell is illuminated from behind. The initial concentration is 25 wt% $NH_4Cl$, the translation rate of the cell is 1 μm/s downward, and the temperature at the top and bottom heat exchangers is 20 and −28 °C, respectively. Three chimneys are clearly visible on the near side of the cell and several others are obscured because they are adjacent to the far side. A plume of chemically buoyant fluid rises out of each chimney although, because of the lighting, these are not visible here (see images in [34,45]).