A Numerical Study of Thermosolutal Melting

Thomas J Scanlon[1] and Matthew T Stickland[1]

[1]*Department of Mechanical Engineering, University of Strathclyde, Glasgow, G1 1XJ, Scotland*
* e-mail tscanlon@mecheng.strath.ac.uk

Abstract

This paper describes the numerical investigation into the melting of a pure ice block into an aqueous solution of sodium carbonate (Na_2CO_3). The numerical study is concerned with capturing the evolving solid-fluid interface during phase change while solving sequentially the double-diffusive conditions resulting from the combined effects of thermal and solutal buoyancy in the flow field. The results show that, with a relatively simple phase change model incorporated into a fixed grid, finite volume numerical formulation, reasonable concurrence may be obtained in comparison with published experimental data.

Introduction

The melting of ice in mixtures began as a problem for the melting of glaciers in sea water motivated by oceanographers. The melting of glaciers in sea water has assumed further importance recently because of the apparent increasing temperature in the earth's environment. Therefore, it is important to analyse correctly the characteristics of the melting of ice in mixtures.

Such natural convection phenomena, driven by the twin competing buoyancy forces due to concentration and temperature gradients, have been of interest to many authors during the latest decades. The thermosolutal natural convection is seen to play an important role in controlling the characteristics of solid-liquid phase change in mixtures [1-2]. It has been found that the time evolution of the solid-liquid interface and the local equilibrium conditions existing at the interface are strongly coupled to the interface heat and mass transfer due to thermosolutal convection. In solidification processes, changes in the time evolution of this coupling is one of the principal criteria which governs the front velocity and any micro or macro segregation effects. Such effects are thus considered to impinge directly on the homogeneity of the forming solid [3-8].

A significant number of experimental and numerical studies have been devoted to double-diffusive convection associated with melting or solidification. In the case of solidification, the existence of a mushy zone adjacent to the solid-liquid interface is a specific problem that will not be considered in this paper. In the context of melting, a series of fundamental experimental and theoretical studies have been executed concerning buoyancy-induced flows driven by combined thermal and solute transport near a vertical melting ice surface in saline water [9-12]. Considering melting in a cavity [13-21], an analytical and experimental study has been carried out [13] which focused upon the different modes of double-diffusive convection arising from a horizontal melting interface. Using the same configuration, a quantitative model and scaling analyses of melting or dissolving driven by compositional convection has also been developed [14-16]. When the phase change interface is vertical, multicellular flow structures are seen to arise in the cavity that strongly influence the melting characteristics [17-21].

Numerical Methodology

The aim of the computational is to develop, as far as possible, a reliable model of the thermo-fluid behaviour of a block of pure ice melting into an aqueous solution of sodium carbonate under conditions of natural convection as detailed in figure 1. The computational model would be based on a coupled thermo-fluid system with laminar natural convection heat and mass transfer with phase change occurring. The aim would be to establish the critical modelling parameters encountered in such flows. The computational model is undertaken within the framework existing commercial computational fluid dynamics analysis software FLUENT which
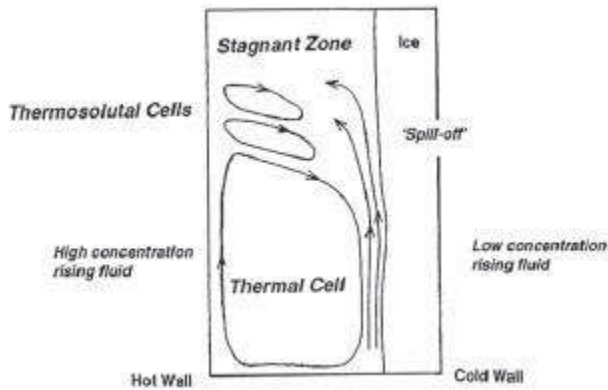
Figure 1 Tyical flow structures involved in thermosolutal melting.

offers current capabilities for coupled thermal and fluid analysis but cannot address the details of the thermo-physical modelling being required here. Such features need to be incorporated using user subroutines. Such work has recently been described by Scanlon and Stickland [22-27].

This numerical methodology proposes that the governing equations are solved in a manner such that if the temperature falls below the freezing isotherm then the convection terms in the equations of motion are effectively disengaged. Variations in the specific heat of the material are incorporated in order to account for the phase change according to the graph shown in figure 2, where Δh_{fus} is the latent heat of fusion of ice, ΔT is the finite temperature bandwidth over which phase change is assumed to occur and *PCZ* is an acronym for the phase change zone.
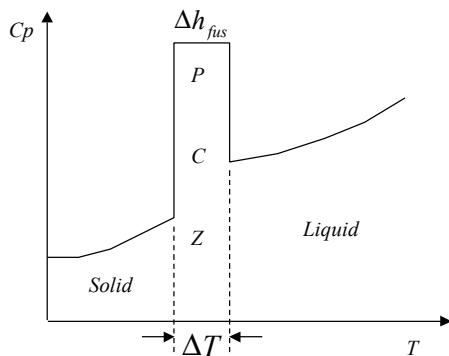

Figure 2 Variation in specific heat with temperature

The model of Scanlon and Stickland [22-27] has been shown to be a stable, computationally efficient, uncomplicated numerical technique that provides reasonable solutions to complex problems involving natural convection with phase change, as shown in figures 3 and 4.

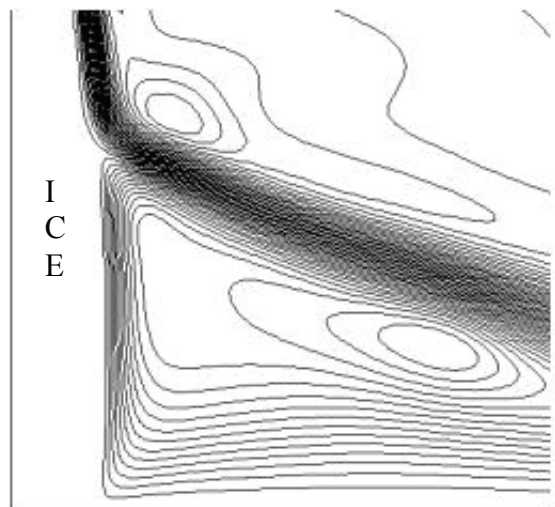Figure 3 Experimental results (particle tracers) for the freezing of pure water on a vertical wall [24].

Figure 4 Numerical prediction (streamlines) for the freezing of pure water o a vertical wall [24].

The experimental work of Bénard *et al* [20], to which the numerical solution will be compared, is detailed in figure 5
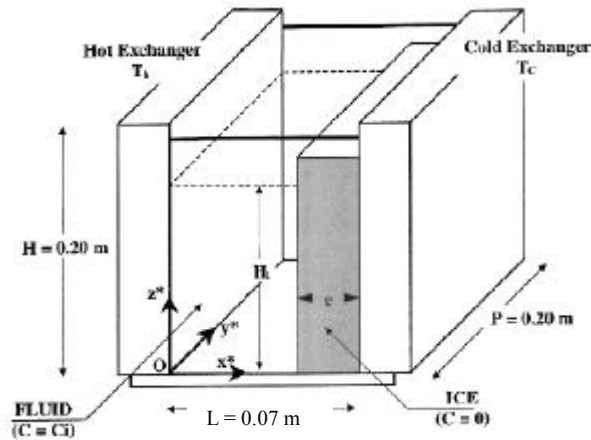

Figure 5 Experimental set up of Bénard *et al* [20].

The experimental cell consists of a rectangular cavity (height $H = 20$ cm, width $L = 7$ cm and depth $P = 20$ cm) designed to generate a two-dimensional flow. The two opposing walls are heat exchangers which are differentially heated at constant and uniform temperatures controlled by two independent thermal loops where a water-glycol mixture is circulated.

For the experimental conditions considered in this paper, pure water (concentration C = 0) is contained within distance *e*. the rest of the cell contains a still solution of Na_2CO_3 of concentration $C_i = 2$ % by mass. This aqueous solution is separated from the pure water by a thin metal plate. Initially, the whole experimental system is maintained a few tenths of a degree under 0 °C after which a rectangular block of pure ice will have formed and is attached to the cold wall.

The initial dimensions of the ice block are 3 cm thickness (distance *e*) and height $H_i = 14$ cm. This implies an initial length for the aqueous solute of 4 cm. For an initial solute concentration of 2 % (by mass), the corresponding equilibrium liquidus temperature is –0.66 °C, so the solute mixture remains in its liquid phase. At time $t = 0$ the metal barrier is removed very slowly such that the fluid is not disturbed and the hot exchanger is raised quickly to a temperature of $T_h = 10$ °C which is maintained throughout the experiment. The cold exchanger temperature is kept at Tc = 0 °C. For the numerical solution the bottom wall is considered to be adiabatic while at the top surface symmetric solutions are assumed.

Thermosolutal convection is characterized by five dimensionless parameters; the Prandtl number *Pr*, the Lewis number *Le*, the thermal Rayleigh number Ra_T, the buoyancy ratio *N* and the aspect ratio *A* (*A = Hi/e* in Figure 5). This leads to the conditions outlined in Table 1 which are considered in this study. Such a range of parameters may be varied through the initial concentration of the liquid and the temperature difference

Table 1 Parameters considered in the numerical study

Pr	11
Le	190
Ra_T	3.8×10^8
N	-8
A	4.667

between the heat exchangers. The buoyancy ratio *N* represents the effects of solutal buoyancy to thermal buoyancy where *N* is defined as:

$$N = \frac{\beta_S C_i}{\beta_T \Delta T} \tag{1}$$

For an initial concentration $C_i = 2$ % by mass, a temperature difference $?T = 10$ K and a thermal expansion coefficient $\beta_T = 3.275 \times 10^{-4}$ K^{-1} this produces a solutal expansion coefficient $\beta_S = -1.31002$ wt percent^{-1}. The experimental conditions are such that the initial solute mass fraction ranges between 2 % and 5 %. Under such conditions, the density is observed to be a linear function of temperature and concentration such that the standard linear Boussinesq approximation can be applied and the density inversion effects found in pure water are negated. In this manner the density may be considered as a linear function of temperature and concentration according to [20]:

$$\rho = \rho_0 \left(1 - \beta_T \delta T - \beta_S C\right) \tag{2}$$

where $?_0 = 999.8$ kg/m^3 is the density of pure water at $T = 0.01$ °C. In order to incorporate mass transfer an additional transport equation is required for the solute transport with appropriate initial and boundary conditions. For the initial solute conditions a concentration is applied to the ice (C = 0) and solute ($C_i = 0.02$) regions respectively. As the numerical solution progresses, it is only when melting of an initially solid cell in the ice zone occurs that the nascent fluid cell will allow the solute to be advected into the melt flow.

For the numerical solution a computational mesh of 180000 rectangular cells was employed and a time step of 4 s was adopted. For the pressure-velocity coupling the conventional SIMPLE scheme was used. Temporal discretisation was based on an implicit method and for convective discretisation the QUICK scheme was employed. This led to total computational times of approximately 30 hours on a Pentium4 3GHz PC with 512 Mb RAM.

Results and Discussion

The following results show the comparison between the numerical work (contours of solute concentration) and the experimental results of Bénard *et al* [20] (observations by fluorescence – lighter regions = lower concentration):
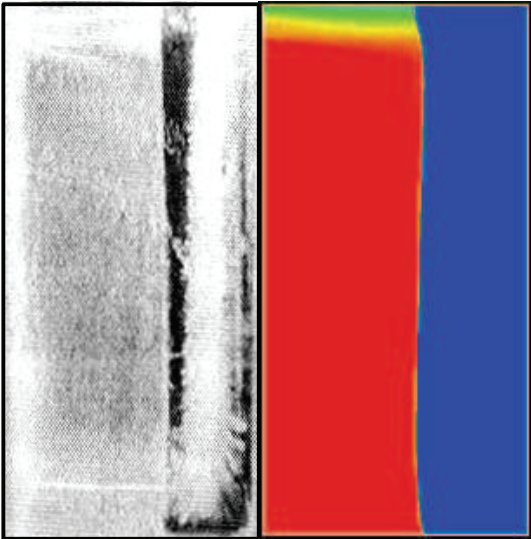
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Fig. 6 Experiment (left), Numerical (right), *t* = 7 min
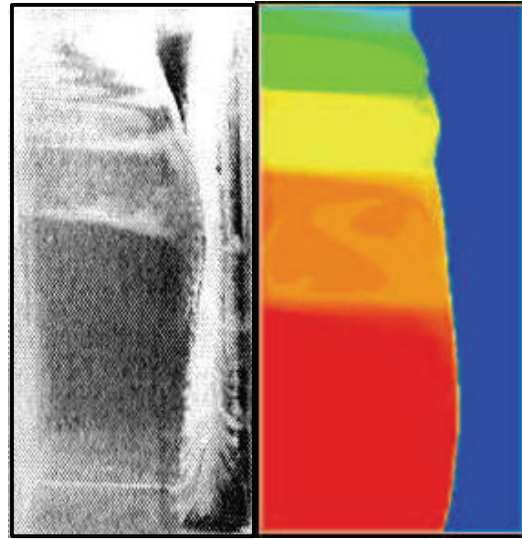

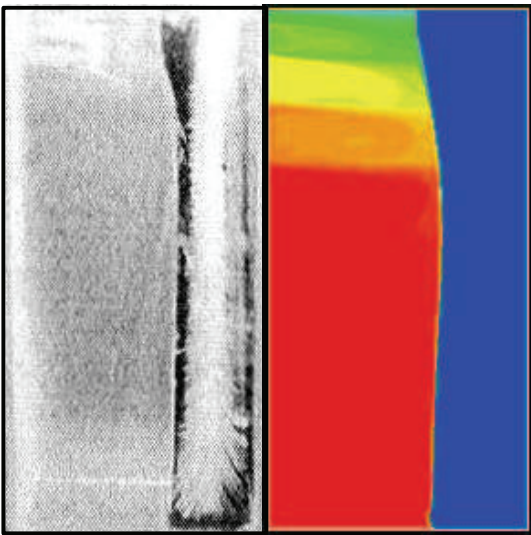Fig. 9 Experiment (left), Numerical (right), *t* = 25 min

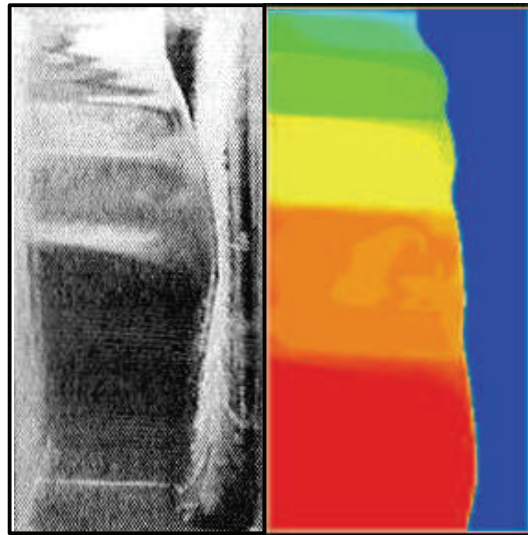Fig. 7 Experiment (left), Numerical (right), *t* = 15 min

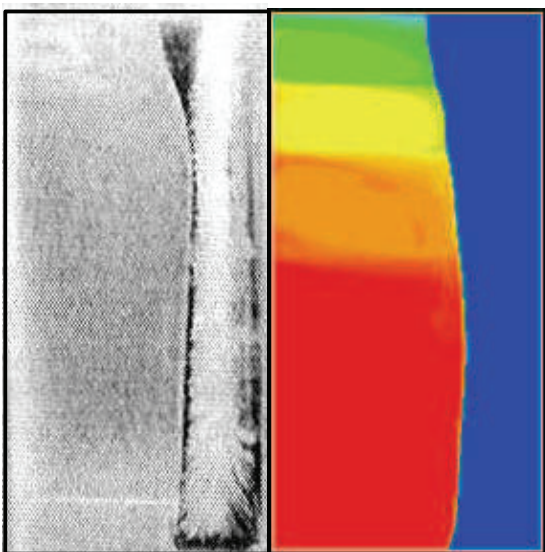Fig. 10 Experiment (left), Numerical (right), *t* = 30 min

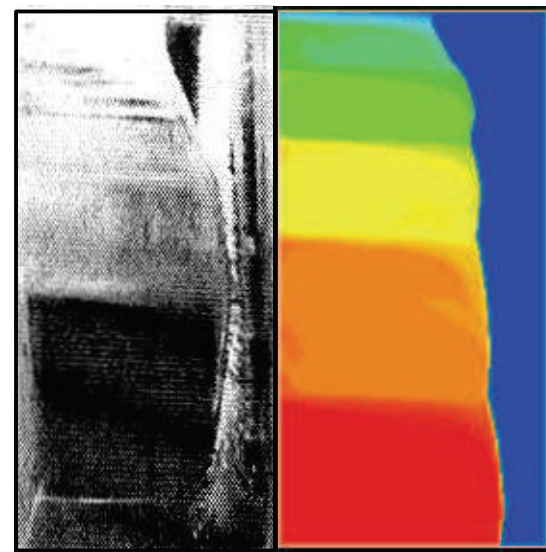Fig. 8 Experiment (left), Numerical (right), *t* = 20 min

Fig. 11 Experiment (left), Numerical (right), *t* = 35 min

In figures 6-11 we can observe the temporal evolution of the thermosolutal melting process over a period of 35 minutes. It is evident that the competing effects of thermal and solutal buoyancy in the melt flow result in the non-linear solid-fluid interface profiles observed. The general form of this interface is of a progressive 'waisting' effect around the central core of ice with thicker upper and lower solid regions.

From the numerical study it was observed that horizontal fingers of warmer fluid existed which traversed the fluid region and effectively 'bit' into the ice via the melting process. Such multicellular regions of varying concentration appear to have been captured qualitatively by the numerical techniques employed in this study.

Conclusions

A numerical study of thermosolutal melting has been carried out. The numerical techniques employed have attempted to capture the time-evolving interface of pure ice melting into an aqueous solution of Sodium Carbonate and the resulting double-diffusive flow with its competing influences due to thermal and solutal buoyancy.

The numerical results show a reasonable qualitative concurrence with published experimental work with the general trends of solid-fluid interface evolution and thermosolutal melt flow characteristics being captured.

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