## Abstract

Multi-phase systems with solidification and melting processes are ubiquitous in natural and engineering systems. The current numerical work is divided into two parts: I. study of solidification system II. study of various melting systems. Both parts deal with low Prandtl number material and, the phase-change is modelled using the enthalpyporosity approach for obtaining the thermal fields. In the first part, parametric multiscale, multiphysics grain structure simulations were performed to develop the relationship between process-parameters and grain structure for the casting process over a wide range of process parameters for Al-7 wt. % Si alloy. The effect of interfacial heat transfer coefficient, superheat, and nucleation site density on the grain structure is studied using a coupled finite-volume-method-cellular-automaton (FVM-CA) multi-scale, multiphysics solidification model. The criteria based on the macroscopic thermal field are proposed to predict the occurrence of columnar-to-equiaxed transition (CET) and equiaxed-to-columnar transition (ECT) based on the novel averaging strategy at the solidification front.

The second part of this thesis reports numerical studies on three isothermal melting problems (a), (b) and (c). The problems (a) and (b) deal with the phase-change Rayleigh–Bénard (RB) convection system. Direct Numerical Simulations (DNS) are performed to simulate the transient melting regime (problem-a) and quasi-steady-state oscillatory solidification-melting regime (problem-b) to systematically characterise the effect of the dynamic solid-liquid interface on the onset of buoyancy-driven convection and quasi-steady-state RB convection at Pr= 0.0216. The phase-change RB system comprises of a solid-phase substance which experiences melting in the direction opposite to gravity direction inside the two-dimensional square box.

In problem (a), the buoyancy-driven instability is studied for a wide range of Stefan number  $(1.1445 \times 10^{-2} \le \text{Ste} \le 1.1445 \times 10^2)$ , and global Rayleigh number Ra  $(2.1 \times 10^4 \le \text{Ra} \le 2.1 \times 10^7)$ . Here, criteria are reported to characterise the onset of buoyancy-driven convection for the moderate and fast melting phase-change RB system  $(2.1 \times 10^5 \le \text{Ra} \le 2.1 \times 10^7)$ , and stability maps are constructed to mark the onset event. It is found that unlike the classical RB system in the phase-change RB system, the onset of buoyancy-driven driven convection depends on the Stefan number, Ste (defined as the ratio between the sensible heat to the latent heat) and Fourier number  $\tau$  in addition to the Rayleigh number *Ra*.

Problem (b) deals with the comparative study of the phase-change (RB) convection system and the classical RB convection system. Here, the role of Ste  $(1.1 \times 10^{-2} \le \text{Ste} \le 1.1 \times 10^{2})$  and the Rayleigh number based on the averaged fluid layer height  $\text{R}a_f$  (3.96 × 10<sup>4</sup>  $\le$   $\text{R}a_f \le 9.26 \times 10^{7})$  is systematically explored. There are two distinct RB flow configura-

tions at low  $Ra_f$  independent of Ste. The ratio of the Nusselt number for phase-change RB convection to the Nusselt number for classical RB convection  $\overline{Nu_h}/\overline{Nu_h^{RB}}$  is always greater than one except for Ste>1 in turbulent regime. The results may turn out to be of immense consequence for understanding and altering the transport characteristics in the phase-change RB convection systems.

The problem (c) deals with the comparison of the heat transfer and thermodynamic performance of natural convection driven melting process inside the square-shaped thermal energy storage system with three different heating configurations: isothermal heating from left side-wall or bottom-wall or top-wall and with three adiabatic walls at low Pr (~ 0.02), low Stefan number, Ste = 0.014 and moderate Rayleigh number ( $Ra \approx 10^5$ ).

**Keywords**: Melting and solidification, multi-scale solidification, grainstructure modelling, phase-change Rayleigh-Bénard convection, onset of convection, thermal energy storage systems.