ABSTRACT

Melting and solidification of pure metals and alloys are important research areas due to its practical applications, where the study of dynamic evolution of the interface offers a challenging task to the researchers. For the last two decades, lattice Boltzmann method (LBM) has been extensively used to model transport phenomena for melting and solidification problems involving complex boundary at the phase interface because of high computational efficiency and cost effectiveness of LBM.

In the present work double distribution function (DDF) with single relaxation time based lattice Boltzmann method (LBM) is used to perform the solid-liquid phase change simulation. D2Q9 lattice stencil is used for the prediction of flow and thermal field. However, in order to overcome numerical instabilities for simulation of low *Pr* fluids, modification of lattice Boltzmann Bhatnagar-Gross-Krook (LBGK) models for incompressible Navier-Stokes equation and the energy equation are proposed in this study. The present work reports development of a lattice Boltzmann model to overcome the numerical instability associated in handling convection in low *Pr* fluids. This modification has been employed to analyze very low *Pr* liquid metals $Pr \in [0.001, 0.1]$. In a systematic analysis, the thermo-fluidic behavior of liquid metals in the melt zone is examined in a square cavity at a wide range of Rayleigh number $Ra \in [10^4, 10^6]$. Transport phenomena in a side heated cavity undergoing melting has been reported where wall and interface heat flux, melting rate and length of interface was studied up to a Rayleigh number of 10^6.

In next part of the work, the melting dynamics has been studied for investigating the flow instability in the melt zone. The parameters are taken as Prandtl number in the range of 0.005-0.05 and Rayleigh number between 10^5-10^6. The presence of different flow circulation in the melt zone is investigated as the flow transition is observed from steady to transition regime. The time series plots of velocity components in the entire melt zone are investigated and peak frequency mapping is performed using Fast Fourier Transform (FFT) analysis to characterize the non-linear flow dynamics in an evolving melt one.

In corner melting/solidification, heating or cooling is performed on two adjacent sides of the cavity. Studies on corner melting for bottom side heated and top side heated melting were undertaken where the related physics was explored and improved melting phenomena was noted. The improved melting performance was explored for corner melting and at the same time the complex physics of natural convection under corner melting could be unveiled. The natural convection effect in corner melting problem is investigated based on enthalpy

based lattice Boltzmann model (ELBM). The investigation is performed for two distinct cases. In the first one the left wall and the bottom wall form the corner (case 1). The counterpart is where the right wall and the top wall form the corner (case 2). The main focus of the work includes capturing the effect of natural convection in melt zone and predicts the evolution of the melt zone dynamics. The effect of Rayleigh number in the range of $Ra=10^2$ - 10^7 on the convective flow field is evaluated for a typical parametric values of Stefan number of 0.01 and Prandtl number of 0.025. Results show distinct convection rolls which also include Rayleigh-Benard cells at the melt zone for the cases under investigations. Evolution of flow fields in the melt zone has been described by presenting sets of isotherms and streamlines. The modified lattice Boltzmann model to simulate melting in low *Pr* materials was also applied in the case of corner melting problems for very low *Pr* number liquid metals $Pr \in [0.001, 0.01]$. The main focus of the work includes the tracing of transient interface movement, calculation of average heat flux at the interface; determine the effect of natural convection in melt zone, distribution of isotherms in the cavity and variation of average melt fraction with time.

As solidification process has numerous applications in metallurgy, geology and other disciplines where environment may not be always predictable and the boundary conditions may vary with time and space, investigation of mushy region dynamics and segregation within an alloy is of special interest where the progress of LBM is still very limited. A hybrid LBM is developed to study the solidification phenomena of *Ni-Cu* alloy in which the flow field is simulated using LBM combined with finite different method (FDM) to solve for thermal and species continuity equation. In the present work, 2-D simulation of *Ni-Cu* (50-50%) alloy has been taken up to understand the effect of boundary conditions on the morphology of mushy region dynamics. Capability of the code is demonstrated to a limited extent due to huge demand on computation time.

To summarize, the thesis demonstrated the capability of LBM for solution of solid to liquid phase change problems. A modified LB model is developed to handle low Pr materials. Studies were performed for melting in side heated cavities as well as for corner melting. Corner solidification and segregation of binary alloy are the other highlights of the work.