

Abstract

Phase change processes encompass a wide range of engineering and scientific disciplines, and occur in many materials processing applications such as casting, welding, surface alloying, glass forming, energy storage in phase change materials and crystal growth; as well as in natural phenomena such as formation of icebergs and evolution of igneous rocks. Computational modeling (or process modeling) of such processes becomes important in assisting product/process design, which often can give insight into certain issues that could be expensive and sometimes impossible to achieve in experiments. Some computationally challenging aspects in numerical simulation of phase change materials processing is considered to be the central theme behind the present work. While some standard mathematical models in this regard have been well established, certain aspects of phase change modeling are yet to be extensively explored in materials processing applications, mainly because of the associated computational complexity. Primary aim of this thesis is to investigate some of these relatively unexplored areas, such as turbulence modeling in materials processing and Lattice Boltzmann simulation of melting/solidification problems.

As a first step, a generalized three dimensional transient turbulence modeling framework is presented, which incorporates morphological and thermodynamic features of solid-liquid phase change. The standard $k-\epsilon$ model is chosen as a basis, to start with, for its inherent simplicity and adaptability to common CFD codes. The set of volume-averaged equivalent single-phase governing equations (mass, momentum, energy, species conservation, turbulent kinetic energy and dissipation rate of turbulent kinetic energy) are numerically solved following a pressure-based Finite Volume Method according to the SIMPLER algorithm. Phase change aspects of the problem are addressed using a modified enthalpy-porosity technique along with an appropriate enthalpy-updating scheme. In order to assess the performance of the formulated turbulence model, the same is subsequently utilized to simulate a generic high power laser surface alloying process, where effects of turbulent transport can actually be realized. Also, the simulation is further extended to assess the influences of various significant processing parameters such as laser power, scanning speed and powder feed rate on pool geometry and dynamics of the molten pool, cooling rates, as well as species concentration distribution inside the substrate. In order to investigate the overall effects of turbulence, the present turbulent model predictions are compared with the corresponding laminar model results, and significant differences in the molten pool morphology as well as parametric results are observed. Further, a fairly good matching is observed between the present turbulence model predictions and the reported benchmark experimental results.

In order to explore further possibilities of more sophisticated turbulence modeling for materials processing applications, a large eddy simulation (LES)

scheme is used for modeling isothermal phase change processes in laser surface melting applications. While satisfactory results are obtained in this respect, and more detailed information are obtained with regard to capturing of larger eddies, it is observed to be computationally too costly to take into account all intrinsic aspects of materials processing applications. In fact, for all practical purposes, these simulation results do not reveal too much of additional information over system length scales, which could otherwise justify the use of such an involved modeling approach, especially in the perspective of heavy computational costs that need to be paid.

For an order-of-magnitude assessment of predictions from the numerical model, a systematic approach is subsequently presented for scaling analysis of three-dimensional transient turbulent momentum, heat and mass transfer pertaining to the case of a typical laser surface alloying process. With suitable choices of non-dimensional parameters, the governing equations, coupled with appropriate boundary conditions, are first scaled, and the relative significance of various terms appearing in them are accordingly analyzed. The analysis is then utilized to predict the orders of magnitude of some important quantities, such as the velocity scale at the top surface, velocity boundary layer thickness, temperature rise in the pool, turbulent kinetic energy and its dissipation rate at the top surface. The scaling predictions are also assessed by comparison with numerical and experimental results, and an excellent agreement is observed in an order-of-magnitude sense.

In order to reduce high computational costs involved with the numerical simulation, a highly efficient parallel algorithm, based on $k-\varepsilon$ model, is utilized to simulate the three dimensional, transient, turbulent transport phenomena in case of a typical laser surface alloying process. The parallelization of the code is done following the pipelining method, which uses temporal parallelism in a distributed computing environment and the code is run on a cluster of workstations (COW) connected with local area networking (LAN). Equal partitioning of the spatial domain into subdomains along the longer geometric dimension is performed to decompose the computational domain. The message passing interface (MPI) utility is used for communications among the subdomains on each processor. To demonstrate the parallel performance, a systematic analysis is carried out with up to 16 nodes and various grid sizes. It is found that the overall parallel performance improves up to a certain number of processors and then degrades with an increase in the processor number. However, it is revealed that irrespective of parallelizing the CFD code, dramatic improvements in computational efficiency may not be achievable in reality.

Concerned with the computational complexities associated with the conventional CFD approach for modeling complicated phase change problems in materials

processing mentioned as above, the second part of this thesis attempts to devise an entirely different elegant computational modeling approach which can lead the research community towards simulation of large scale melting/solidification systems within affordable time frames, which has still remained an unrealistic proposition, even with the advanced computational resources that are available these days. The specific idea here is to develop an alternative Lattice Boltzmann (LB) approach, which potentially retains simplicity, accuracy and parallelizability of the classical LBM and at the same time overcomes most of the practical computational constraints and restrictions imposed by the conventional CFD method.

To start with, a hybrid lattice Boltzmann scheme is presented initially to solve a conduction based phase change problem. The model essentially combines the classical Boltzmann transport equation with the conventional enthalpy formulation of phase change. The pertinent macroscopic variable (temperature) is obtained through solution of a single particle density distribution function. The proposed model is subsequently utilized to simulate formation of an industrial ice block and a good agreement is found with the available results in the literature.

In order to further extend the present modeling philosophy for the case of generalized convection-diffusion phase change situation, a novel lattice Boltzmann scheme is proposed to numerically simulate practical melting-solidification problems, often encountered in materials processing. For the purpose of formulating this novel scheme, an enthalpy based thermal lattice Boltzmann model is proposed which is subsequently coupled with a fixed-grid enthalpy-porosity approach, consistent with the microscopic solvability theory. The macroscopic density and velocity fields are obtained through solution of an evolution equation of a single particle density distribution function in the lattice Boltzmann framework, whereas, the macroscopic temperature field is obtained by solving another evolution equation of a total enthalpy density distribution function. The phase change aspects are numerically handled by an enthalpy-porosity technique, with a modified enthalpy updating closure scheme. The present scheme is observed to be accurate and stable for a wide range of relaxation times. The model is subsequently applied to test cases reported in benchmark studies of solid-liquid phase change modeling, such as problems involving melting of pure gallium in a rectangular cavity, crystal growth during equiaxed solidification of an undercooled melt and Rayleigh-Benard convection in presence of directional solidification of a freezing substance kept in a top-cooled enclosure. A fairly good agreement is found with the numerical and experimental results available in the literature. It is, therefore, expected to evolve as an attractive and efficient proposition for numerical modeling of complicated phase change problems, over the years to come.