

“In CFD there are no non-solvable problems, there is only the lack of computing time to solve them.”

CFD community

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Introduction

1.1

Heat and Fluid Flows in Materials Science and Engineering

Materials science and engineering is one of the most important and active areas of research in computational heat transfer today. The development of novel materials and innovative processing technologies today is impossible without the assistance of computational *thermo-fluid dynamics* (TFD).¹⁾ For example, fluid flow and heat transfer are extremely important in materials processing techniques such as crystal growing, casting, chemical vapor deposition, spray coating, and welding. For instance, the flows that occur in melts during crystal growing due to temperature and concentration differences can modify the quality of the crystal and, thus, of the semiconductors made from this crystal. The buoyancy-driven flows generated in a melt by casting processes strongly influence micro- and macrosegregation and, ultimately, the microstructure of solidified alloys. As a result, it is important to understand these flows and develop technologies to control such effects. One way to gain such control is through the use of electromagnetic fields [2]. For instance, over the last 30 years electromagnetic fields have become an important part of materials processing technologies [3]. Nowadays the electromagnetic processing of materials (EPM) is one area of engineering where electromagnetic fields are used to process innovative materials such as semiconductors, pure metals, multicomponent alloys, and electrolytes. The background required for this field of engineering is interdisciplinary, basically combining materials science and *magnetohydrodynamics*.²⁾

As a consequence of the importance of fluid flow and heat and mass transfer in materials processing, extensive work has been carried out, presently directed at numerical modeling; see reviews [4, 5]. Following these reviews computer modeling became one of the most crucial elements in the design and optimization of novel technologies in the field of engineering and materials science. However, numerical simulations of flows relevant to materials science and engineering often include complex physical and chemical phenomena. And what is often lacking is a proper

- 1) The field of TFD includes the complete set of governing equations of fluid dynamics coupled with energy and mass conservation equations.
- 2) Magnetofluidynamics, or magnetohydrodynamics (MHD), describes phenomena occurring at the frontier separating fluid mechanics and electromagnetics.

mathematical model capable of adequately describing the physical processes. *But what does it mean to develop a model of any physical process?* As was mentioned at the beginning, practical processes and systems are very often complicated. Thus, to be able to solve a problem, basically we have to simplify some phenomena within this problem through idealizations and approximations. This process of simplifying a given problem is termed *model development*. Once a *mathematical model* is produced, it has to be *implemented* in computer code and then *validated* against experimental data.³⁾ If the model is a good representation of the actual system under consideration, it can be used to study the behavior of the system. This information may be used in the design of new processes or in tuning the performance of existing processes to obtain an optimal design.

One advantage of computer modeling is that the behavior and characteristics of a system may be investigated without actually fabricating a prototype. Thus, the total costs of product development can be reduced. In addition, it should be noted that the simplifications and approximations that lead to a mathematical model also indicate the dominant variables in a problem. This helps in developing efficient physical or experimental models. The best strategy to develop a good working model is to start from a simple model and then to add complexity as the solution proceeds. Then, comparisons with experimental data may provide ways of improvement. By contrast, if one *starts* from a sophisticated model, then not even a converging solution may be obtained. However, even if computational results are obtained (after a long debugging procedure), it would be problematic to identify possible improvements to a such complex model; for example, see [6].

The basic conservation equations describing fluid flow were already available at the end of the eighteenth century. Major contributions were made by Newton, Euler, Lagrange, Navier, and Stokes [7]. However, the numerical methods to solve these equations for engineering applications were developed in the second half of the twentieth century due to the appearance of computers. A historical record of scientists contributing to the development of fluid mechanics can be found in the review written by Durst *et al.* [7]. Since this review, computational fluid dynamics (CFD) has already accumulated the so-called critical mass of computational methods and computational resources such that one can say that *the golden age of fluid mechanics lies ahead of us* [7]. This statement has been demonstrated by the rapid increase of publications devoted to numerical simulations of flow-related problems in all engineering areas from bioengineering to materials science engineering.

It is true that the invention of the computer made it possible to obtain particular solutions for typical flows in different engineering applications including phase-change phenomena. Today, a wide range of commercial software is available on the market allowing engineers to predict and optimize heat and fluid flow in various industrial applications. However, there are still many uncertainties in predicting multiphase and phase-change flow problems, for example, gas–liquid or solid–liquid–gas system behavior. At the same time, the use of so-called direct numerical

3) A mathematical model is one that represents the performance and behavior of a given system in terms of mathematical equations.

simulations is limited by the lack of computing power to perform direct numerical simulations of natural multiscale processes including turbulent flow problems for high Re numbers or even the solidification of alloys. Thus, the development of novel mathematical models covering the multiscale and multiphysical nature of many fluid-flow-related problems remains a current task for engineers engaged in CFD. As a result, in spite of the “golden age of fluid mechanics,” much remains to be done for the next generation of CFD scientists.

The main goal of the present work is to sketch out the role of fluid mechanics in phase-change phenomena by way of a combined theory of numerics and solidification including some illustrative examples. Finally, it should be noted that no attempt has been made in this monograph to explore all aspects of solidification and computational TFD. In particular, numerous books dealing with CFD have already been published. Some of the best, by subject matter, are cited below:

- Mathematical fluid mechanics [8],
- Physics of fluid mechanics [9],
- Numerical approaches to heat and fluid flow for beginners [10],
- Computational methods for fluid dynamics (incompressible flows) [11, 12],
- Computational methods for fluid dynamics (compressible flows) [13, 14],
- Fluid flows in magnetohydrodynamics [15, 16].

The same is true of books related to descriptions of solidification. Currently, several books have been published that are devoted to different aspects of solidification modeling including:

- Phenomenological description of solidification processes [17],
- Fundamentals of solidification with numerous examples [18, 19],
- Solidification theory for engineers [20],
- Numerical modeling in material science and engineering including fracture mechanics [21],
- Modeling of moving boundaries with reference to solidification [24–26].

However, none of these books fully discusses the computational schemes and algorithms for the solution of the governing conservation equations for fluid flow and heat and mass transfer coupled with electrodynamic equations. As a result, the theoretical part of this work presents only those aspects of numerical algorithms that are primarily related to fluid flow magnetohydrodynamics and phase-change problems with reference to materials science and engineering applications.

1.2

Overview of the Present Work

This work is about modeling and simulations of different physical processes related to materials science and engineering. In particular, the goal of writing this

monograph is to present recent developments in the modeling of heat- and mass-transfer applications related to phase-change phenomena under the influence of electromagnetic fields. In order to supply the information required for the reader to gain a basic understanding of the methods used in this work for solving fluid-flow-related problems, a summary of the numerical schemes and pressure-based algorithms for the solution of Navier–Stokes equations is provided. In parallel, to illustrate the computational and theoretical issues involved, examples arising from materials processing and fluid-flow-control applications are chosen to give a detailed description of the author’s findings. In the context of each physical phenomenon discussed in this work, the entire scope of the computational setup (including problem and model formulation, code and model validation, scaling, and physical interpretation) is described systematically.

The monograph aims to accomplish the following objectives:

- Present basic conservation equations and boundary conditions used in flow-related problems in materials science and engineering.
- Show basic discretization schemes and algorithms for the numerical solution of convection- and diffusion-related problems including some methods for the solution of a linear equation system.
- Present recent developments in CFD for the treatment of complex geometry problems using fixed Cartesian grids.
- Present the basic aspects of macro- and microscale modeling of pure and binary metal alloy solidification including the control of phase-change phenomena by application of electromagnetic fields.
- Show comparisons between present simulations and experimental data published in the literature.
- Illustrate an interpretation of simulation results devoted to the control of fluids and heat and mass transfer using different combinations of electromagnetic fields related to materials science applications.

In what follows, an overview of the chapters and their content is given.

Chapter 2 briefly reviews basic conservation equations such as the conservation of mass, of momentum, of energy, and of solute. In addition, the standard boundary and initial conditions required for the solution of conservation equations are given and their physical meaning is discussed. Additionally, the equations of electromagnetism are covered in this chapter as clearly as possible. Finally, there is an illustrative example of the calculation of the Lorentz force induced by a rotating magnetic field applied to nonhomogeneous electroconducting media.

Chapter 3 explains the basic discretization approaches and numerical methods used in TFD. Particular attention is paid to finite volume methods as the most popular in the computational heat- and mass-transfer community. After each section illustrative examples are given to demonstrate the advantages and disadvantages of different numerical schemes such as the central difference scheme (CDS), the upwind first-order scheme (UDS), the linear upwind difference scheme (LUDS), the upstream weighted differencing scheme (UWDS), the total variation diminishing

differencing scheme (TVD), the power-law scheme (PDS), and the upwind third-order scheme (QUICK). Finally, an example is introduced to illustrate different iterative methods for the solution of the heat-transfer equation.

Chapter 4 describes basic algorithms used when simulating incompressible fluid flows coupled with heat and mass transfer. There is a demonstration of the accuracy of different discretization schemes (UDS, LUDS, QUICK, PDS, CDS-DC) modeling convective terms in solving steady incompressible flow and heat transfer in a two-dimensional lid-driven cavity. Recent novelties in the field of fixed Cartesian grid methods, including immersed boundary methods, are discussed. Some of them are illustrated by benchmark tests.

Chapter 5 introduces existing models for the simulation of phase-change phenomena on the macro- and microscales applied to pure materials and binary metal alloys. The so-called *single-domain mixture* model for the macroscale prediction of solidification and the *modified cellular automaton* model for microscale modeling are favored in this work. The modeling of turbulent solidification is reviewed and described. Following the chapter a short benchmark example is given to demonstrate the accuracy of the fixed grid technique, where the solid–liquid interface is treated implicitly with the two-phase region modeled as a porous medium.

Chapter 6 illustrates the performance of the numerical schemes given in previous chapters on the basis of a numerical study of the spin-up of liquid metal driven by a rotating magnetic field. In particular, the transient axisymmetric swirling flow in a closed cylindrical cavity, driven by a rotating magnetic field (RMF), has been studied by means of numerical simulations. Based on the time histories of the volume-averaged azimuthal and meridional velocities, it has been shown that RMF-driven spin-up can be divided into two phases. The spin-up starts with an initial adjustment (i.a.) phase in which a secondary meridional flow in the form of two toroidal vortices is established. The i.a. phase is generally completed on achieving the first local maximum in the volume-averaged kinetic energy of the secondary flow. The second phase has been referred to as inertial, where the establishment of Bödewadt layers at the horizontal walls plays a major role. Additionally, the influence of stable thermal stratification on the spin-up dynamics is studied numerically. It is found that a stable thermal stratification damps the inertial waves and significantly reduces the magnitude of the meridional flow velocities. However, an RMF-driven flow under the action of a stable thermal stratification became unstable earlier in comparison to the isothermal flows. An increase in the Grashof number leads to the occurrence of axisymmetric instability along the side wall in the form of Taylor–Görtler vortices.

Chapter 7 explores the different flow regimes of laminar and weak turbulent rotating fluid flows driven by a rotating magnetic field. Both two-dimensional direct numerical simulations and RANS-based simulations are performed to answer the following questions. How can we define a transition between a viscous Stokes flow and an inertial regime? How relevant is the aspect ratio for the secondary flow intensity? What is the influence of magnetic forcing and the aspect ratio of the cavity on the side wall, and on the top and bottom torques? What is the influence

of Taylor–Görtler vortices induced by the rotation of a melt on a time-averaged flow structure?

Chapter 8 addresses the numerical modeling of transient mass and momentum transport until the homogenization of two miscible fluids is achieved under the action of externally imposed rotating and traveling magnetic fields. The main aim of the study is to investigate the physical mechanisms responsible for enhancing a mixing process using alternating magnetic fields and to explore the role of buoyancy in rotary mixing. Finally, different combinations of a TMF and an RMF are considered in terms of the effectiveness of the mixing. It is shown that the time of the initial adjustment phase is the key parameter for enhancing the mixing processes by the periodic superposition of different electromagnetic fields.

Chapter 9 presents different ways to control binary metal alloy solidification using combinations of electromagnetic fields. In particular, in this chapter two types of electromagnetic stirring (EMS) are considered: contactless EMS and contact EMS. Contactless EMS is demonstrated through the application of rotating and traveling magnetic fields by the unidirectional solidification of an Al-Si alloy and the side-cooled solidification of an Al-Cu alloy. Contact EMS is illustrated by considering the unidirectional solidification of a Pb-Sn alloy under the influence of superimposed steady external magnetic fields and steady electrical currents applied directly to a melt by means of electrodes that have direct contact with the melt. The main purpose of this chapter is to demonstrate the influence of the so-called Lorentz force induced by electromagnetic fields on phase-change phenomena on a micro- and macroscale.

Almost all chapters include examples. They are intended to illustrate the properties of numerical schemes or to explore the role of fluid flows in heat and mass transfer coupled by means of fluid flow. The methods of analysis of the numerical results presented in this monograph can be used for a wide variety of fluid-flow problems encountered in materials science and engineering.