Preface

An important problem facing the world today is finding sustainable, cost-effective and ecologically friendly energy sources. In order to meet a growing global energy demand, especially in developing nations, the increased supply of such sources must augment continuing attention to the efficient utilization of energy. Reacting gas-solids flows play an important role in many aspects of efficient fuel production and energy production and energy utilization, *e.g*:

- **Fuel production and processing**: catalytic crackers, H_2 production, S removal, coal gasification, gas clean-up (SOx, NOx, Hg, CO_2), biomass (cellulosic) pyrolysis and gasification, nuclear fuel production
- **Energy production**: fuel cells, coal and biomass combustion, CO_2 separation, nuclear reactors and separation, silicon production and coating for photovoltaic applications, novel combustion technologies like oxy-combustion and chemical looping
- **Energy utilization and efficiency**: polymerization reactors, catalytic reactors, iron and steel making, cement production

These energy sources have to satisfy the current demand but must also meet the projected demand in 2050 (doubled) and at the end of the century (tripled). Considering the inflexibility of the energy markets to even slight fluctuations in demand, this implies an enormous challenge to the scientific community and society in general. This is complicated by the fact that the prevalent technology development process is based on experimentation, using Edisonian approaches which require several iterations to develop the end product. Computational science and engineering, using high performance computers, can accelerate this development process by providing an integration framework which allows scaling between the laboratory experiments and commercial units, facilitates cooperation between various science and engineering disciplines. The topical area of computational gas-solids reacting flows, which is critical to developing new, clean and efficient energy alternatives, is still in its infancy. This book's objective is to bring together the recent advances in all the interdisciplinary fields which impact this area. We believe that this volume provides an intersection of all aspects necessary for understanding computational gas-solids flows and will enable researchers from academia/industry and designers from industry to push the state-of-the-art and find rapid solutions for urgent research and design problems.

The objective of reactor design is to create the right conditions for reactions. The temperature and reactant species distribution, appropriate residence time and removal of products must be considered. Including the effect of a catalyst may be necessary. A comprehensive understanding of all the competing and interacting mechanisms is required to arrive at better designs and improved processes. In particular,

gas-solids reacting flows involve, not only complex interactions of granular materials with gas flow, but also phase-change, heterogeneous and homogeneous reactions, heat and mass transfer. Moreover, the spatial and temporal scales may vary over many orders of magnitude. Thus modeling gas-solids reacting flows requires the integration of the best physics and chemistry models from various science and engineering fields with the most advanced computational algorithms. These algorithms must be scalable to large high-performance computers in order to bear on this important topic. In addition, because of the nascent stage of this field, these theory approaches and numerical techniques are constantly evolving. This book attempts to bring the latest advances into one collection. Specifically, it presents the multiphase continuum formulation for gas-solids flows along with the theory for closure relations for granular stresses, heat and mass transfer correlations, models for chemical reactions, as well as numerical algorithms appropriate for of high-performance computing. The book also illustrates the applications of these computational tools to general gas-solids flows with a focus on energy conversion processes.

This book consists of a comprehensive collection of authoritative works on computational gas-solids flows, encompassing theory, numerical methods and practice. It is distinguished from other books on multiphase flows since it is entirely devoted to all aspects of computational gas-solids flows and also serves as a bridge to the various disciplines critical to further advances of this topic, physics, chemistry, computational science, applied mathematics and various applied engineering fields. A book of this nature is very much needed since computational science is fast becoming the "third pillar" of science and engineering, joining theory and experimentation, due to the rapid advances in both computational hardware and algorithms. It should serve as a commanding reference for researchers in computational gas-solids flows. It is also meant as a text book to train advanced graduate students in the concepts and applications of computational science and engineering that is beginning to transform the study and design of gas-solids reacting systems.

The primary objectives of the authors and editors are to provide:

- A comprehensive book on computational gas-solids reacting flows, which presents the most recent developments in theory and numerical techniques
- Examples of applications where these computational tools have been employed
- A convenient reference book for practicing engineers and researchers in computational gas-solids flows
- A text book for advanced graduate level course in engineering and science

The primary audience of this book is intended to be:

- Advanced graduate students in interdisciplinary science and engineering subject areas or computational science
- Researcher workers and practicing engineers
- Users of multiphase flow software, such as the open-source MFIX or the commercial codes FLUENT®, CFX®, etc.

ORGANIZATION

This book has thirteen chapters in total, divided into three sections: Theory, Numerical Methods, and Practice. Section one, Theory, has five chapters. The first chapter discusses the development of the continuum theories and an overview of the various closures needed to solve gas-solids reacting flows. The second and third chapters provide kinetic theory based closures for granular stresses for mono-disperse and poly-disperse systems. The fourth chapter covers wide-ranging issues related to interfacial drag closures and finally the fifth chapter discusses closures for heat and mass transfer. Section two consists of four chapters and they cover various methods to solve the theoretical descriptions provided in the first section. The first chapter in this section introduces fully coupled implicit solvers for gas-solids flows and how these methods contrast with segregated solvers on staggered grids. The second chapter deals with the use of DQMOM (direct quadrature method of moments) for polydisperse gas-solids flows. The third chapter covers the topic of direct numerical simulations for gas-solids flows where the particle collisions and flow over the particles are resolved. The fourth chapter in this section delves into the mixed Eulerian-Lagrangian hybrid methods based on MP-PIC (Multiphase particle-in-cell). The third section comprises of four chapters that give four illustrative examples of the application of computational gas-solids flows. The first chapter in this section deals with circulating fluidized beds and the recent success of MP-PIC methods in simulating large-scale risers. The second chapter details the simulation of bubbling fluidized beds for group A particles. The third chapter is on the polymerization reactors and illustrates the effectiveness of population balance methods to model particle-size changes. The final chapter details the application of the methods discussed in this book for large-scale simulations of volcanic flows with particular emphasis on verification and validation. Below we provide an overview of these thirteen chapters in this book:

Theory

Multiphase Continuum Formulation for Gas-Solids Reacting Flows

Madhava Syamlal and Sreekanth Pannala

This introductory chapter lays out the formulation of multiphase continuum models for gas-solids flows, including heat and mass transfer with chemical reactions. It presents the basis for the different continuum formulations for mass, momentum, granular energy, thermal energy, and species balance equations for interpenetrating gas and (multiple) solids phases along with the constitutive relationships needed to close the coupled system of equations. This chapter is primarily derived from the authors' extensive involvement in developing an open-source computational platform for gas-solids flows, MFIX (http://mfix.netl.doe.gov). A detailed history of the development of this field over the last 2-3 decades is presented along with extensive references for the interested reader to explore the literature in greater depth. Finally provides an illustrative example explores the effects of exercising the different model and simulation options. The chapter not only serves as a good guide for a widely accepted simulation software but one could also obtain the software along with the example problem to get a "hands-on" experience and, possibly, to contribute to this growing field. The chapter also provides a common context for later chapters.

Hydrodynamic Equations from Kinetic Theory: Fundamental Considerations

James Dufty and Aparna Baskaran

This chapter provides a theoretical description for the dynamics of the granular phase only, with emphasis on the derivation of the macroscopic hydrodynamic fields for the granular phase (species densities, flow velocity, and the granular temperature) for a prescribed microscopic interaction among the grains. This is achieved by introducing the general notion of a kinetic equation to obtain macroscopic balance equations for the fields. The constitutive equations for the fluxes appearing in these balance equations are obtained through specialized solutions to the kinetic equation, resulting in a closed set of hydrodynamic equations. This is demonstrated using the Boltzmann-Enskog kinetic equation for a system of smooth, inelastic hard spheres that leads to granular Navier-Stokes hydrodynamic equations for weakly inhomogeneous fluid states. For gas-solids flows, the role of interstitial gas is important. This effect can be included, along with other body forces, as source terms in the kinetic equations. This chapter also includes a brief discussion about hydrodynamics beyond the Navier- Stokes limit.

Kinetic Theory for Granular Materials: Polydispersity

Christine M. Hrenya

In this chapter, existing kinetic theory based models for granular flows are critically evaluated in the context of polydisperse granular flows. The species segregation predicted by these kinetic theory models is reviewed and rigorous extensions of these models for polydisperse gas-solids flows are discussed. There has been significant recent progress in advancing the state-of-the-art for polydisperse, kinetic-theory models for granular flows and many of the simplifications associated with earlier models (*e.g.*, equipartition of energy) are now treated in a more rigorous fashion. However, for gas-solids flows, the incorporation of gas effects into polydisperse models is just beginning and further work is needed to improve their predictive capabilities.

Interfacial Interactions: Drag

Wei Ge, Ning Yang, Wei Wang and Jinghai Li

The drag interaction between gas and solids not only acts as a driving force for solids in gas-solids flows but also plays as a major role in the dissipation of the energy due to drag losses. This leads to enormous complexities as these drag terms are highly non-linear and multiscale in nature because of the variations in solids spatio-temporal distribution. This chapter provides an overview of this important aspect of the hydrodynamic interactions between the gas and solids and the role of spatio-temporal heterogeneities on the quantification of this drag force. In particular, a model is presented which introduces a mesoscale description into two-fluid models for gas-solids flows. This description is formulated in terms of the stability of gas-solids suspension. The stability condition is, in turn, posed as a minimization problem where the competing factors are the energy consumption required to suspend and transport the solids and their gravitational potential energy. However, the lack of scale-separation leads to many uncertainties in quantifying mesoscale structures. The authors have incorporated this model into computational fluid dynamics (CFD) simulations which have shown improvements over traditional drag models. Fully resolved simulations, such as those mentioned in this chapter and the subject of a later chapter on Immersed Boundary Methods, can be used to obtain additional information about these mesoscale structures. This can be used to formulate better constitutive equations for continuum models.

Mass and Heat Transfer Modeling

Ronald W. Breault

This chapter focuses on the important topic of mass and heat transfer models and closures for continuum gas-solids reacting flows. The previous three chapters have primarily focused on the hydrodynamics of gas-solids flows, However, in addition, accurate models for heat and mass transfer must be constructed to allow predictive simulations of reacting gas-solids flows. As mentioned before, the goal of an ideal reactor is to establish the best temperature, reactant species distribution and residence time conditions for reactions. This, obviously, requires an accurate understanding the heat and mass transfer within the gas and also across the gas-solids interface. This chapter provides an overview of this topic for dilute and dense gas-solids systems. Specifically, it covers diffusional mass transfer, turbulent dispersion, and convective heat transfer between the different phases and, also, at the boundaries. Again in this case, there is a lack of scale-separation. Thus, there are large uncertainties in the models available in the literature. Fully resolved simulations can lead to a reduction of this uncertainty.

Numerical Methods

Coupled Solvers for Gas-Solids Flows

Berend van Wachem

Segregated solvers commonly used in most gas-solids flow software converge one variable at a time and ensure overall convergence through non-linear iterations through the variables. On the contrary, the main advantage of collocated, non-Cartesian, coupled solvers, the approach discussed in this chapter, is an increased robustness due to the implicit treatment of the pressure-velocity coupling or in general all the variables. Although the equations describing multiphase flows appear similar to those of single-phase flows, their solution is usually much more difficult since the coupling between equations is often more important than the coupling between terms in each equation, which is the default case for single-phase flow. This is due to the presence of volume fractions which are constrained to sum to unity, and large source terms, as well as their gradients. This makes the availability of a robust solution method extremely desirable. A number of approaches for a fully coupled solution approach are discussed in this chapter and application of coupled solvers for gas-solids flows is still in its initial phase.

Quadrature-Based Moment Methods for Polydisperse Gas-Solids Flows

Alberto Passalacqua, Prakash Vedula, and Rodney Fox

Common Eulerian-Eulerian two-fluid models assume that the particle phase to be dominated by collisions and employ kinetic theory even when the particle volume fraction is low. Since collisions do not dominate in the extremely dilute regime, this assumption leads to erroneous predictions of the particle phase flow patterns and the models cannot capture phenomena like particle trajectory crossing for finite Stokes numbers. In this chapter, an Eulerian quadrature-based moment method (QMOM) for the direct solution of the Boltzmann kinetic equation for the particle phase coupled with Eulerian fluid solver is described. This is a more fundamental approach to treat non-zero Knudsen-number and finite Stokes-number conditions for dilute gas-particle flows. The chapter details the derivation of QMOM method for moment transport equations and the coupling procedure with the fluid solver. The predictions of the method are shown for a lid-driven cavity flow with particles, at finite Stokes and Knudsen numbers, and compared with both Eulerian-Eulerian two-fluid model predictions and with Eulerian-Lagrangian simulations.

CFD Modeling of Bubbling Fluidized Beds of Geldart A Powders

Todd Pugsley, S. Karimipour and Z. Wang

In this chapter, the role of fluidized beds in a range of industrial sectors, from oil refining and coal combustion to pharmaceutical manufacture and ore roasting is described. Even after 80 years of experience using these systems in the industry and extensive experimental research at academic/research institutions, the fundamental understanding of fluidized bed hydrodynamics is still far from complete. This chapter details the role of advanced modeling using CFD as one tool for improving this understanding and focuses on the application of CFD to fluidized beds containing fine Geldart A powders. One of the main features of these beds is the formation of clusters that reduce the drag below that for non-cohesive particles. This chapter discusses the role of mesoscale clustering on the predictions of the macroscale fluidized behavior and emphasizes the fact that approaches to reduce drag such as the one described in this chapter are *ad hoc.* Thus, there is a pressing need for an improved understanding of cluster formation (possibly through methods such as IBM described before) and for robust models describing their effect that can be utilized in coarse grid simulations of industrial scale fluidized beds

Computational Modeling of Gas-Solids Fluidized Bed Polymerization Reactors

Ram G. Rokkam, Rodney Fox and Michael Muhle

This chapter discusses the fluidization process used for production of polyethylene, one of the most widely used thermoplastics. The gas-phase process is based on fluidized-bed reactors (*e.g.*, UNIPOL™ PE PROCESS and Innovene process) for the polymerization units. In this chapter, a detailed CFD model that incorporates the catalyst size distribution along with polymerization kinetics is employed. A quadrature method of moments (QMOM) is employed to predict the final polymer size distribution and temperature. The chapter details the Eulerian-Eulerian model based on the kinetic theory of granular flow that is used to solve the fluidized-bed dynamics and the predictions of particle segregation, slug formation and other non-ideal phenomena.

Validation Approaches to Volcanic Explosive Phenomenology

Sébastien Dartevelle

This chapter deals with natural large scale gas-solids flows unlike the commercial/laboratory devices at smaller scales described before. This chapter describes the fact that volcanic explosive phenomenology is poorly understood in terms of its fundamental physical processes as it is difficult to collect data because of the inherent uncertainties about the location and occurrence of volcanic eruptions and any placement of measurement devices. In addition, the accuracy of any simulation tools is severely constrained because of the limitations on the initial, boundary, and inflow conditions. As such it is important to conduct detailed verification and validation to increase the benefits of simulations. This chapter presents a two step approach for validating volcanology models. The first part involves validation against simple and well-constrained analog (small scale) experiments targeting the key physics controlling volcanic cloud phenomenology. The second "geo-validation" step requires comparing against well characterized (as much as possible) geophysical-geological (large scale) events. The author points out that this last step can only be qualitative as the natural system is not fully characterized. However, it is a necessary step to have reasonable confidence that the models describe large scale volcanic phenomenology and be of use to policy-makers and others to make decisions based on these models.

In conclusion, this book brings together the latest work on theory, numerical techniques and applications for gas-solids reacting flows from the experts in the various interdisciplinary fields. This book is meant for interdisciplinary students and researchers from diverse fields, like physics, chemistry, applied mathematics and various engineering disciplines. It also articulates unresolved issues within these fields which should be addressed in order to advance the entire area of computational science and engineering for gas-solids reacting flows. This would have great relevance to the design of industrial processes, particularly in energy related industries. To our knowledge, this will be the first book on this topic which brings together literature from different fields and, thus, act as a bridge between these fields, serving as a vehicle of knowledge dissemination. This book is also unique in that it comprehensively relates the subject of computational gas-solids flows with modern high-performance computing and the general area of computational science.