

COMPUTATIONAL
METHODS FOR
COMPLEX
LIQUID-FLUID
INTERFACES

PROGRESS IN
COLLOID AND INTERFACE SCIENCE

Series Editors

Reinhardt Miller and Libero Liggieri

Physical-Chemical Mechanics of Disperse Systems and Materials

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Computational Methods for Complex Liquid–Fluid Interfaces

Mohammad Taeibi Rahni, Mohsen Karbaschi, and Reinhard Miller

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Edited by

Mohammad Taeibi Rahni

Mohsen Karbaschi

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Series Foreword

Liquid interfaces are omnipresent in our daily life and represent essential elements in many technologies and real products. Emulsions and foams, for example, consist, to a large extent, of interfaces, and their behavior as material is controlled by the corresponding interfacial properties. Such practical systems are often dealt with under highly dynamic conditions so that, in particular, fluid dynamics comes into play.

To master dynamic technologies, such as high speed coatings, spraying, and emulsification, a detailed knowledge on the specific behavior of interfaces is required. Often, experiments for their quantitative determination are extremely complex and a clear analysis of data gained by various methods appears impossible without the corresponding computational simulations on molecular, mesoscopic, and macroscopic levels. Many experimental methods in surface science have very strong limitations with respect to dynamic conditions, except when adequate computational simulations are available to complement them.

The present book is the fifth volume in the series *Progress in Colloid and Interface Science* published by CRC Press. Its title, *Computational Methods for Complex Liquid–Fluid Interfaces*, indicates that it deals with a very broad spectrum of works at liquid interfaces studied experimentally and described by complementary simulations.

The book is edited by the team of editors from both the Max Planck Institute of Colloids and Interfaces in Potsdam, Germany, and the Sharif University of Technology in Tehran, Iran; The editors, Mohammad Taeibi Rahni, Mohsen Karbaschi, and Reinhard Miller, have been involved in the fields of fluid dynamics simulations and experiments for a very long period of time. In addition, they invited many experts from highly credential institutions from all over the world to write about different aspects of the given topics.

First, introductions to surface science dynamics and various types of simulations are presented, spanning over molecular dynamics to macroscale simulations, based on many different conventional and novel computational techniques. The instructive examples are given to the three different levels of simulations, that is, molecular, mesoscale, and macroscale.

The book is meant for a broad spectrum of readers, starting partly with fundamentals of surface science of interfacial layers and their experimental characterization, passing through more tutorial chapters on various levels of simulations to specific applications, which will be useful to specialists in respective fields.

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The Series Editors

Preface

Many important phenomena in nature, science, and technology contain multiphase flows. Some examples of such flows include emulsification, foaming, coating, spray painting, spray combustion, boiling, coal slurry transport, cavitation, sedimentation, fluidized bed, raining, snowing, and volcanic rock motion. Even though there has been a great deal of research conducted in this important field, the complete dynamics of such flows are not yet fully understood due to their complex inter-phase coupling, whereby different phases strongly affect one another.

Liquid–fluid interfaces are omnipresent in most modern technologies and their quantitative characterization is essential for the optimum use of such technologies. Although an increasing number of specialized related experimental methods exist and many new methods are being developed and improved, the unambiguous data analysis was and still is a bottleneck for further progress in the quantitative understanding of many related phenomena.

In addition, nonequilibrium properties have shown to be very essential in interfacial flows and the interactions between physicochemical properties and hydrodynamics make interfacial dynamics considerably complicated. In particular, processes like emulsification, foaming, or coating require the understanding of highly dynamic properties. Another type of complexity in liquid–fluid interfaces is related to the interactions between the interface and the flow fields of adjacent liquid phases. Thus, any change in the properties of the interface can directly affect the flow fields in both phases. This includes interrelations between the physicochemical properties and hydrodynamics, which usually make interfacial dynamics considerably complicated. Such two-way interactions are of course more complicated in systems containing surface-active molecules, as the mechanisms of transport and adsorption/desorption of surfactant molecules to and from the interface are involved. On the other hand, the quantitative understanding of the mutual dynamical bulk–interface interactions is the main challenge in studying the stability of many systems, such as foams and emulsions. Thus, the properties of the adsorbed layers depend on rather complex mutual bulk–interface interrelations. Especially, the complicated dynamical behaviors existing in both phases (e.g., inside and outside bubbles/drops) have attracted much interest in fundamental and applied research works. This, for example, has led to studying the mechanisms of drop formation and detachment from a capillary tip, which, under certain conditions, are of great interest.

On the other hand, real-world numerical simulations have often been computationally too intensive to predict many flows with large interfaces. However, they have provided necessary insight needed for modeling actual flow problems. In about the past three decades, several numerical works have been performed in which computational fluid dynamics (CFD) has been used. The enormous progress made by various types of such simulations (in molecular, mesoscopic, and macroscopic levels) has provided opportunities for a much better foundation of particularly highly dynamic experimental methods. However, most of these works have not included much details on interfacial thermodynamics, especially variations of molecular properties along the interface, wherein the use of integrated effects can lead to nonphysical solutions.

Of course, if we are dealing with interfacial flows, our mathematical modeling is quite different from multiphase flows in which small interfaces are present, for example, spray flow problems. In interfacial flows, the main concern is to model the transport of liquid–fluid interfaces, which in general are moving and deforming at the same time. One main difference in the mathematical modeling of such flows is having (1) one-fluid (one-field) or (2) two-fluid (two-field) models. In the first type of model, one set of governing equations are used for both phases, while in the latter different sets of equations are used for different phases. Note, the first model type is more common, while in the second one the interface represents a complex boundary condition for both sets of equations used. In conventional CFD techniques of handling large interfaces, the most popular approaches are front tracking, VOF (volume of fluid), and level set methods.

Fortunately, over about the past one and a half decades new CFD ideas, namely, *meshless* methods, such as, smoothed particle hydrodynamics (SPH) method and lattice Boltzmann method (LBM), have been developed and widely used to study interfacial flows. In such methods, the fluid itself is discretized (instead of the media containing it). Then, the mathematical modeling is somehow similar to the one used in molecular dynamics (MD), wherein particle collisions are also taken into account. Due to its numerous advantages, it seems that LBM has been found to be more useful and thus has become more popular in simulations of many interfacial flows. Even though it is not yet fully developed and has some drawbacks for certain flow physics, it seems at the present time that for the simulation of complex liquid–fluid interfaces, it is a rather accurate and relatively simple tool.

The main objective of this book is to highlight the most important computational challenges involved in the two-way coupling of complex liquid–fluid interfaces. In other words, the book is dedicated to present the state of the art of computational methodologies and numerous simulation techniques for the quantification of many interfacial quantities.

The subjects covered in the book are divided into three main aspects of investigations at liquid–fluid interfaces. Section I of the book (Chapters 1 through 5) is dedicated to the fundamentals of liquid–fluid interfaces, that is, the definition of the most important quantities and their experimental investigations. Besides the description of the state of the art of various characterization methods, the theoretical background is described and solutions are presented and discussed.

Section II presents the most important numerical techniques used in interfacial flow problems. It starts with microscale techniques for quantum chemical calculations, treating small systems of molecules by MD computational approaches (Chapter 6). Then, Chapters 7 and 8 cover more modern meshless numerical techniques, that is, SPH and LB methods, which are categorized as state-of-the-art mesoscale CFD techniques. From a macroscale point of view, however, Chapter 9 deals with the most important conventional CFD techniques, which have mostly been used over about the last three decades. These techniques have been tremendously useful in understanding many aspects of interfacial flows.

On the other hand, Sections III and IV deal with different applications of the techniques described in Section II. However, in Section III (Chapters 10 through 18) emphasis is on the technicalities of correctly using the computational techniques developed for interfacial flows, while Section IV (Chapters 19 through 24) emphasizes on the simulation of certain interesting interfacial flow physics, for example, acoustic cavitation-bubble dynamics.

Many people have helped us tremendously during the preparation of this manuscript and of course without their support this work would not have been finalized on time. First, we thank our coauthors, who accepted to work with us and prepared and sent their manuscripts on time. Second, the continuous support of our group members at MPI in Potsdam was a great help in the preparation of the manuscript.

Mohammad Taeibi Rahni

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Reinhard Miller studied mathematics at the University of Rostock, Rostock, Germany, and did his PhD and habilitation at the Berlin Academy of Sciences, Berlin, Germany. He works at the Max Planck Institute of Colloids and Interfaces in Potsdam, Germany. His scientific interests are experimental investigations of adsorption layers at liquid interfaces under dynamic conditions, interfacial rheology, stability of foams, and emulsions.

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