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Edited by

Mohammad Taeibi Rahni
Mohsen Karbaschi
Reinhard Miller

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Series Foreword

Liquid interfaces are omnipresent in our daily life and represent essential elements in many technologies and final 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.

Reinhard Miller
Potsdam, Germany

Libero Liggieri
Genoa, Italy
The Series Editors

Preface

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

Liquid– uid 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 ows and the interactions between physicochemical properties and hydrodynamics make interfacial dynamics considerably complicated. In particular, processes like emulsi cation, foaming, or coating require the understanding of highly dynamic properties. Another type of complexity in liquid– uid interfaces is related to the interactions between the interface and the ow elds of adjacent liquid phases. Thus, any change in the properties of the interface can directly affect the ow elds 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 ows with large interfaces. However, they have provided necessary insight needed for modeling actual ow problems. In about the past three decades, several numerical works have been performed in which computational uid 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 ows, our mathematical modeling is quite different from multiphase ows in which small interfaces are present, for example, spray ow problems. In interfacial ows, the main concern is to model the transport of liquid– uid interfaces, which in general are moving and deforming at the same time. One main difference in the mathematical modeling of such ows is having (1) one- uid (one- eld) or (2) two- uid (two- eld) models. In the rst 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 rst 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 uid), 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 ows. In such methods, the uid 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 ows. Even though it is not yet fully developed and has some drawbacks for certain ow physics, it seems at the present time that for the simulation of complex liquid– uid 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– uid interfaces. In other words, the book is dedicated to present the state of the art of computational methodologies and numerous simulation techniques for the quanti cation of many interfacial quantities.

The subjects covered in the book are divided into three main aspects of investigations at liquid– uid interfaces. Section I of the book (Chapters 1 through 5) is dedicated to the fundamentals of liquid– uid interfaces, that is, the de nition 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 ow 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 ows.

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 ows, while Section IV (Chapters 19 through 24) emphasizes on the simulation of certain interesting interfacial ow 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 nalized 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

Mohsen Karbaschi

Reinhard Miller

Editors

Editors

Mohammad Taeibi Rahni received both his BSc and MSc from the University of Texas at Austin and his PhD from the University of Illinois, Urbana-Champaign. He is a guest researcher at the Max Planck Institute of Colloids and Interfaces in Potsdam, Germany, and has a full time faculty member position at Sharif University of Technology, Tehran, Iran. His main area of interest is computational fluid dynamics (CFD), with particular emphasis on the application of various computational techniques to interfacial phenomena.

Mohsen Karbaschi earned his PhD in chemical engineering from Sharif University of Technology, Tehran, Iran, linked to the Max Planck Institute of Colloids and Interfaces in Potsdam, Germany. He has worked as a researcher at the Max Planck Institute since 2011. His primary research interests lie in the area of surface science and multiphase flows, particularly with respect to different applications of computational fluid dynamics simulations and experimental analysis.

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.

Contributors

Eugene V. Aksenenko
Institute of Colloid Chemistry and Chemistry of Water
Ukrainian National Academy of Sciences
Kyiv (Kiev), Ukraine

Alidad Amirfazli
Department of Mechanical Engineering
York University
Toronto, Ontario, Canada

Shelley L. Anna
Departments of Chemical Engineering and Mechanical Engineering
Center for Complex Fluids Engineering
Carnegie Mellon University
Pittsburgh, Pennsylvania

Masoumeh Azadegan
Electrical Engineering Group
School of Engineering
Tarbiat Modarres University
Tehran, Iran

Dariush Bastani
Chemical and Petroleum Engineering Department
Sharif University of Technology
Tehran, Iran

Elena A. Belyaeva
Sechenov Institute of Evolutionary Physiology and Biochemistry
Donetsk National Technical University
Donetsk, Ukraine

Thomas Boeck
Institute of Thermodynamics and Fluid Mechanics
Technical University of Ilmenau
Ilmenau, Germany

Michael R. Booty
Department of Mathematical Sciences
and
Center for Applied Mathematics and Statistics
New Jersey Institute of Technology
Newark, New Jersey

Dieter Bothe
Center of Smart Interfaces, Mathematical Modeling and Analysis
Technical University of Darmstadt
Darmstadt, Germany

Richard A. Campbell
Laue-Langevin Institute
Grenoble, France

Huanchen Chen
Department of Mechanical Engineering
University of Alberta
Edmonton, Alberta, Canada

Mehdi Daemi
Aerospace Engineering Department
Sharif University of Technology
Tehran, Iran

Joël De Coninck
Department of Physics
University of Mons
Mons, Belgium

Kathrin Dieter-Kissling
Center of Smart Interfaces, Mathematical Modeling and Analysis
Technical University of Darmstadt
Darmstadt, Germany

Trang Nhu Do
Department of Chemistry
and
Waterloo Institute for Nanotechnology
University of Waterloo
Waterloo, Ontario, Canada

Kerstin Eckert
Institute of Fluid Mechanics
Technical University of Dresden
Dresden, Germany

Valentin B. Fainerman
Medical Physiochemical Center
Donetsk Medical University
Donetsk, Ukraine

Zhi-Gang Feng
Department of Mechanical Engineering
University of Texas at San Antonio
San Antonio, Texas

Sashikumaar Ganesan
Supercomputer Education and Research Centre
Indian Institute of Science
Bangalore, India

Majid Haghshenas
Mechanical Engineering Department
University of Central Florida
Orlando, Florida

Andreas Hahn
Institute for Analysis and Computational Mathematics
Otto von Guericke University Magdeburg
Magdeburg, Germany

Mohammad Taghi Hamidi Beheshti
Electrical Engineering Group
School of Engineering
Tarbiat Modarres University
Tehran, Iran

Jari Jalkanen
Forschungszentrum Jülich GmbH
Institute for Advanced Simulation
Jülich Supercomputing Centre
Jülich, Germany

Aliyar Javadi
Max-Planck-Institute for Colloids and Interfacial Research
Potsdam, Germany
and
Chemical Engineering Department
University of Tehran
Tehran, Iran

Mohsen Karbaschi
Max-Planck-Institute for Colloids and Interfacial Research
Potsdam, Germany

Elena S. Kartashynska
Physical and Organical Chemistry Department
Donetsk National Technical University
Donetsk, Ukraine

Mikko Karttunen
Department of Chemistry
and
Waterloo Institute for Nanotechnology
University of Waterloo
Waterloo, Ontario, Canada
and
Department of Mathematics and Computer Science
Institute for Complex Molecular Systems
MetaForum, Eindhoven, the Netherlands

Mehran Kiani
Aerospace Engineering Department
Sharif University of Technology
Tehran, Iran

Thomas Köllner
Institute of Thermodynamics and Fluid Mechanics
Technical University of Ilmenau
Ilmenau, Germany

Nina M. Kovalchuk
Department of Chemical Engineering
University of Loughborough
Loughborough, United Kingdom
and
Department of Micro Kinetics of Native Disperse Systems
Institute of Biocolloidal Chemistry
National Academy of Sciences of Ukraine
Kyiv (Kiev), Ukraine

Volodja I. Kovalchuk
Department of Micro Kinetics of Native Disperse Systems
Institute of Biocolloidal Chemistry
National Academy of Sciences of Ukraine
Kyiv (Kiev), Ukraine

Jürgen Krägel
Max-Planck-Institute for Colloids and Interfacial Research
Potsdam, Germany

Christoph Lehrenfeld
Institute for Geometry and Practical Mathematics
RWTH Aachen University
Aachen, Germany

Libero Liggieri
CNR—Institute for Energetics and Interphases
Genoa, Italy

Bin Liu
Department of Chemistry
and
Waterloo Institute for Nanotechnology
University of Waterloo
Waterloo, Ontario, Canada

Giuseppe Loglio
Department of Organic Chemistry
University of Florance
Florence, Italy

Marzieh Lotfi
Max-Planck-Institute for Colloids and Interfacial Research
Potsdam, Germany
and
Chemical and Petroleum Engineering Department
Sharif University of Technology
Tehran, Iran

Holger Marschall
Center of Smart Interfaces, Mathematical Modeling and Analysis
Technical University of Darmstadt
Darmstadt, Germany

Hamid Reza Massah
Acoustical Engineering Society
Tehran, Iran

Iman Mazaheri
Mechanical and Aerospace Engineering Department
Azad University
Tehran, Iran

Marcel B.J. Meinders
Wageningen University and Research Centre
Top Institute of Food and Nutrition
Wageningen, the Netherlands

Efstathios E. Michaelides
Department of Engineering
Texas Christian University
Fort Worth, Texas

Reinhard Miller
Max-Planck-Institute for Colloids and Interfacial Research
Potsdam, Germany

Zahra Mokhtari-Wernosfaderani
Acoustical Engineering Society
Tehran, Iran

Mahmoud Najafi
Mathematics Department
Kent State University
Kent, Ohio

Stefan Odenbach
Institute of Fluid Mechanics
Technical University of Dresden
Dresden, Germany

Chiara Pesci
Center of Smart Interfaces, Mathematical Modeling and Analysis
Technical University of Darmstadt
Darmstadt, Germany

Mohammad Taeibi Rahni
Aerospace Engineering Department
Sharif University of Technology
Tehran, Iran
and
Max-Planck-Institut für Kolloid- und Grenz ächenforschung
Potsdam, Germany

Arnold Reusken
Institute for Geometry and Practical Mathematics
RWTH Aachen University
Aachen, Germany

Massoud Rezavand
Mechanical and Aerospace Engineering Department
Azad University
Tehran, Iran

Leonard M.C. Sagis
Laboratory of Physics and Physical Chemistry of Food
Department AFSG
Wageningen University
Wageningen, the Netherlands
and
Department of Materials, Polymer Physics
ETH Zurich
Zurich, Switzerland

Karin Schwarzenberger
Institute of Fluid Mechanics
Technical University of Dresden
Dresden, Germany

Michael Siegel
Department of Mathematical Sciences
and
Center for Applied Mathematics and Statistics
New Jersey Institute of Technology
Newark, New Jersey

Kristin Simon
Institute for Analysis and Computational Mathematics
Otto von Guericke University Magdeburg
Magdeburg, Germany

Tian Tang
Department of Mechanical Engineering
University of Alberta
Edmonton, Alberta, Canada

Lutz Tobiska
Institute for Analysis and Computational Mathematics
Otto von Guericke University Magdeburg
Magdeburg, Germany

Ruud G.M. Van der Sman
Wageningen University and Research Centre
Top Institute Food and Nutrition
Wageningen, the Netherlands

Dieter Vollhardt
Max-Planck-Institute for Colloids and Interfacial Research
Potsdam, Germany

Yuri B. Vysotsky
Physical and Organical Chemistry Department
Donetsk National Technical University
Donetsk, Ukraine

Jirasak Wong-ekkabut
Faculty of Science
Department of Physics
Kasetsart University
Bangkok, Thailand