With the rapid development and continuing advances of computer technologies and numerical computation, many new multidisciplinary research areas have emerged, including computational chemistry, computational physics, computational biology, and others. It is recognized that computational methodology has now become one of the three basic methodologies of conducting scientific and engineering research, along with theoretical investigation and experimental studies.

In the 1970s, the cross-disciplinary studies of fluid dynamics and numerical computation had led to the new research area of computational fluid dynamics (CFD). This multidisciplinary development later on extended to heat transfer; and consequently the field of computational heat transfer (CHT) or numerical heat transfer (NHT) was introduced. The establishment of these two new research areas has helped scientists and engineers solve many difficult problems, such as the prediction of flow and heat transfer behaviors in engineering design and applications.

Nevertheless, what chemical engineers deal with includes not only fluid flows and heat transfer but also mass transfer and chemical reactions. The detailed information of mass transfer, especially the concentration distribution, is essential to the design and the assessment of chemical equipment as it serves as the basis in evaluating the process effectiveness or efficiency. The conventional approach to predict the concentration field is by the empirical method which is not only unreliable but also lacking of theoretical foundation. Thus a rigorous method for accurate predictions needs to be investigated.

Mass transfer processes are complicated, usually involving turbulent flow, heat transfer, multiple phases, chemical reactions, unsteady operation, as well as the influences from internal construction of the equipment and many other factors. To study such a complicated system, we propose a novel scientific computing framework in which all the relevant equations on mass transfer, fluid dynamics, heat transfer, chemical reactions, and all other influencing factors are involved and solved numerically. This is the main task and research methodology of computational mass transfer (CMT).
Moreover, all mass transfer processes involve the diffusion through the interface between adjacent phases. Interfacial effects, such as the Marangoni convection and the Rayleigh convection, cannot be ignored. Therefore, the study of interfacial effects is another important aspect of CMT.

In recent years, we explored in this new area on the closure of the differential turbulent mass transfer equation by proposing the two-equation $c^2 - \varepsilon_c$ model and the Reynold’s mass flux (fluctuating mass flux) $u'c$ model. Our approach has been successfully applied to various chemical processes and equipments, including distillation, absorption, adsorption, catalytic reaction, and fluidized chemical processes. The interfacial behaviors of mass transfer were also studied by both simulations and experiments.

This book is chiefly based on our published research work and graduate dissertations in the area of CMT. The purpose of writing this book is first to serve as a textbook for the graduate course titled “Introduction to the Computational Mass Transfer”, offered to the graduate students of Chemical Engineering discipline in Tianjin University; and second as a reference book for those who are interested in this area.

The contents of this book can be divided into two parts. The first part, Process Computation, involves the prediction of concentration, velocity, and temperature distributions in chemical engineering equipment. The second part, Interface Computation, concerns the prediction of interfacial effect on mass transfer behaviors.

Chapter 1 of this book covers the basic equation and models of computational mass transfer. Chapters 2–6 present the application of computational mass transfer to discuss the process computation of various gas–liquid contacting and catalytic reaction as well as fluidized processes and equipment in chemical engineering. Chapters 7 and 8 deal with the multi-component mass transfer and concentration behavior near interface. Chapters 9 and 10 introduce the computation of Marangoni and Rayleigh convections and their influence on mass transfer by using respectively differential equations and the lattice Boltzmann method.

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We warmly welcome any suggestions, discussions, and criticism on this book.

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