Heat and Mass Transfer

Kuo-Tsung Yu
Xigang Yuan

Introduction to Computational Mass Transfer

With Applications to Chemical Engineering

Second Edition

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Preface

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 became 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.

The research works presented in this book were performed in the State Key Laboratory for Chemical Engineering at Tianjin University under the support of Chinese National Science Foundation (contract number 20136010, 20736005, and 91434204). The help and encouragement from the Chemical Engineering Research Center of Tianjin University is acknowledged.

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

Tianjin, China
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Contents

Chapter 1
Basic Models of Computational Mass Transfer

Abstract The computational mass transfer (CMT) aims to find the concentration profile in a process equipment, which is the most important basis for evaluating the process efficiency, as well as, the effectiveness of an existing mass transfer equipment. This chapter is dedicated to the description of the fundamentals and the recently published models of CMT for obtaining simultaneously the concentration, velocity and temperature distributions. The challenge is the closure of the differential species conservation equation for the mass transfer in turbulent flow. Two models are presented. The first is a two-equation model termed as $\overline{c'^2} - \varepsilon_{c'}$ model, which is based on the Boussinesq postulate by introducing an isotropic turbulent mass transfer diffusivity. The other is the Reynolds mass flux model, in which the variable covariant term in the equation is modeled and computed directly, and so it is anisotropic and rigorous. Both methods are proved to be validated by comparing with experimental data.

Keywords Computational mass transfer (CMT) · Reynolds averaging · Closure of time-averaged mass transfer equation · Two-equation model · Turbulent mass transfer diffusivity · Reynolds mass flux model

Nomenclature

c	Instantaneous mass concentration of species i, kg m^{-3}
	Molar concentration of species i in Sect. 1.4.2, mol s^{-3}
c_t	Total molar concentration of component i per m^3, mol m^{-3}
C	Time average concentration, kg m^{-3}
C^+	Dimensionless concentration
c'	Fluctuating concentration, kg m^{-3}
$\overline{c'^2}$	Variance of fluctuating concentration, kg^2 m^{-6}
D	Molecular diffusivity, m^2 s^{-1}
D_e	Effective mass diffusivity, m^2 s^{-1}
D_t	Isotropic turbulent mass diffusivity, m^2 s^{-1}
$\mathbf{D}_t$	Anisotropic turbulent mass diffusivity, m^2 s^{-1}
g	Gravity acceleration, m s^{-2}
$[I]$	Identity matrix, dimensionless

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Table 1.1 Influence of $\overline{u_i'c'}$ on mass transfer for different processes

Process	S_n	$\left(\frac{\partial \overline{u_i'c'}}{\partial x_i}\right)$	$S_{\text{comb}} = \left(-\frac{\partial \overline{u_i'c'}}{\partial x_i}\right) + S_n$	Process concentration profile and $\overline{u_i'c'}$ profile	Influence on mass transfer
Absorption	+	−	$S_{\text{comb}} > S_n$	Consistent	Favorable
Desorption (regeneration)	−	−	$S_{\text{comb}} < S_n$	Not consistent	Unfavorable
Adsorption	+	+	$S_{\text{comb}} < S_n$	Not consistent	Unfavorable
Desorption (regeneration)	−	+	$S_{\text{comb}} > S_n$	Consistent	Favorable

[a]Absorption process characterized by decreasing concentration profile
Desorption (regeneration) process characterized by increasing concentration profile

J_{w}	Mass flux at wall surface, kg m^{-2} s^{-1}
k	Fluctuating kinetic energy, m^2 s^{-2}
	Mass transfer coefficient, m s^{-1}
$[k]$	Matrix of mass transfer coefficients, m s^{-1}
l	Characteristic length, m
p'	Fluctuating pressure, kg m^{-1} s^{-2}
P	Time average pressure, kg m^{-1} s^{-2}
Pe	Peclet number
r_{c}	Ratio of fluctuating velocity dissipation time and fluctuating concentration dissipation time
S	Source term
Sc	Schmidt number
Sc_{t}	Turbulent Schmidt number
t	Time, s
T'	Fluctuating temperature, K
$\overline{T'^2}$	Variance of fluctuating temperature, K^2
T	Time average temperature, K
u	Instantaneous velocity of species i, m s^{-1}
u'	Fluctuating velocity, m s^{-1}
u_τ	Frictional velocity, m s^{-1}
u^+	Dimensionless velocity, m s^{-1}
U, V, W	Time average velocity in three directions, m s^{-1}
y^+	Dimensionless distance, m
α_{t}	Turbulent thermal diffusivity, m^{-1} s^{-1}
δ	Thickness of fluid film, m
ε	Dissipation rate of turbulent kinetic energy, m^2 s^{-3}
$\varepsilon_{c'}$	Dissipation rate of concentration variance, kg^2 m^{-6} s^{-1}
ε_t	Dissipation rate of temperature variance, K^2 s^{-1}
μ	Viscosity, kg m^{-1} s^{-1}
μ_{t}	Turbulent viscosity, kg m^{-1} s^{-1}