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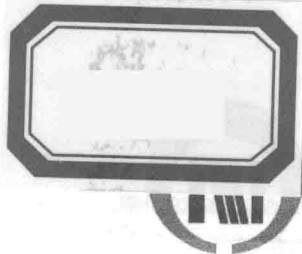
NUMERICAL SIMULATION OF MULTIPHASE REACTORS WITH CONTINUOUS LIQUID PHASE

液相连续多相反应器的数值模拟



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ELSEVIER

本书系统介绍了液相反应器和反应结晶器内多相混合、流动、传质和反应过程的数学模型、数值方法及实验技术等基础研究和工程应用的内容,涵盖了反应器和颗粒尺度(固体颗粒、气泡和液滴)上的气-液、液-固、液-液、气-液-固、液-液-固和气-液-液等多相特性。本书除了介绍作者及合作者在这些领域的研究新成果外,也广泛搜集国内外的前沿研究成果,向读者做全景式的介绍。

本书将为多相流反应器和结晶器(例如搅拌槽、环流反应器和微反应器)的设计、优化和放大提供基础理论和数值方法,作为在化学反应工程、传质与传热、流体力学、结晶学等领域内的科学家和工程师的一本参考书,特别适合于需要掌握先进的计算流体力学和计算反应工程学工具、用数学模型和数值模拟方法来研究搅拌槽、环流反应器和微反应器的读者,也可供广大化工和冶金工程师以及高等学校相关专业师生参考。

图书在版编目(CIP)数据

液相连续多相反应器的数值模拟=Numerical simulation of multiphase reactors with continuous liquid phase: 英文 / 杨超, 毛在砂著.

— 北京: 化学工业出版社, 2014.5

ISBN 978-7-122-19852-5

I. ①液… II. ①杨… ②毛… III. ①液相-多相流
动-反应器-数值模拟 IV. ①TQ052.5

中国版本图书馆CIP数据核字(2014)第 033176 号

本书由化学工业出版社与德国爱思唯尔(Elsevier)出版公司合作出版。版权由化学工业出版社所有。本版本仅限在中华人民共和国境内(不包括中国台湾地区和香港、澳门特别行政区)销售。

责任编辑: 杜进祥 吴 刚 徐雅妮 责任校对: 马燕珠 装帧设计: 韩 飞

出版发行: 化学工业出版社(北京市东城区青年湖南街13号 邮政编码100011)

印 装: 北京京华虎彩印刷有限公司

710mm×1000mm 1/16 印张 20 字数 628 千字 2015年3月北京第1版第1次印刷

购书咨询: 010-64518888(传真: 010-64519686) 售后服务: 010-64518899

网 址: <http://www.cip.com.cn>

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定 价: 280.00 元

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Preface

Multiphase reactors with continuous liquid phase such as stirred tanks and loop reactors are popularly used equipment for multiphase chemical reactions, crystallization and mixing in chemical and petrochemical, hydrometallurgical and pharmaceutical industries, etc. Much effort has been devoted to numerically resolving the hydrodynamics and transport in multiphase reactors with liquid phases and satisfactory progress has been achieved, especially with respect to single-phase liquid systems. The flow and transport in reactors operating in multiphase systems demand more intensive attention, both numerical and experimental. The computational fluid dynamics and computational transport principles have been developed into reliable and efficient tools to study and optimize the macroscopic performance of unit operations in process equipment. Along with the rapid development of physical and chemical technologies, numerical simulation of multiphase flow and mass transfer in multiphase reactors with continuous liquid phase is now faster than ever before. It is now appropriate to present the state-of-the-art knowledge and research in this very active field. We hope this book is able to provide useful knowledge for our colleagues and to facilitate research and development in the field of multiphase reaction engineering.

To facilitate the exchange of original research results and reviews on the design, scale-up, and optimization of multiphase reactors, we have written this book entitled *Numerical Simulation of Multiphase Reactors with Continuous Liquid Phase* to address many important aspects of multiphase flow and transport fields. This book aims to embrace important interdisciplinary topics in fundamental and applied research of mathematical models, numerical methods, and experimental techniques for multiphase flow and mass transfer in reactors and crystallizers, operating in gas–liquid, liquid–solid, liquid–liquid, gas–liquid–solid, liquid–liquid–solid, and gas–liquid–liquid systems on the macro-scale and meso-scale (namely the scale of particles including solid particles, bubbles, and drops). Thus, important and interesting topics of research frontiers for a wide range of engineering and scientific areas are presented. We believe that this is a good reference book for readers interested in the design and scale-up of multiphase reactors and crystallizers, in particular stirred tanks, loop reactors, and microreactors, using mathematical modeling and numerical simulation as tools.

We express our sincere appreciation to Jie Chen, Yang Wang, Ping Fan, and Zhihui Wang, who contributed to Chapter 2; Xiangyang Li, Xin Feng, Jingcai Cheng, and Guangji Zhang, who contributed to Chapter 3; Qingshan Huang, Weipeng Zhang, and Guangji Zhang, who contributed to Chapter 4; Yumei Yong, Xi Wang, and Yuanyuan Li, who contributed to Chapter 5; and Jingcai Cheng, Xin Feng, and Yuejia Jiang, who contributed to Chapter 6.

We are very grateful to our many students who have contributed to the book. We wish to thank Prof. Jiayong Chen at our institute, for valuable advice and continuous encouragement. We would like to express our gratitude to our families for their

great support of our work. This work is partly supported by China Sci-Tech projects including 973 Program (2010CB630904, 2012CB224806), National Science Fund for Distinguished Young Scholars (21025627), National Natural Science Foundation of China (20990224, 21106154, 21306197), and 863 Project (2012AA03A606, 2011AA060704). We also look forward to receiving any comments, criticisms, and suggestions from the readership, which would be of benefit to the book and the authors.

Chao Yang and Zai-Sha Mao

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Chao Yang is a professor at the Institute of Process Engineering (IPE), Chinese Academy of Sciences (CAS). He was born in 1971 and received his Ph.D. and B.Sc. degrees in chemical engineering in 1998 and 1993 respectively, both from Nanjing University of Technology, China. He was a postdoctoral fellow at the Institute of Chemical Metallurgy, CAS from 1998 to 2000, and a visiting scientist at Cornell University from 2005 to 2006. He has published about 130 papers in peer-reviewed journals, and holds 28 patents and five computer software copyrights. He won the Asia Research Award from the Society of Chemical Engineers, Japan, and the Hou Debang Chemical Science and Technology Award in 2012, the National Award for Youth in Science and Technology and the Young Scientist Award of the Chinese Academy of Sciences in 2011, the Mao Yi-Sheng Science and Technology Award in 2010, second prize in the China State Natural Science Award and first prize in the Technological Invention Award from the China Petroleum and Chemical Industry Association in 2009. He was granted the National Science Fund for Distinguished Young Scholars in 2010. His research interests include numerical simulation and experimental diagnosis of multiphase flow and transport phenomena in various multiphase reactors such as stirred tanks, loop reactors, microreactors, and membrane reactors.

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As a principal investigator in chemical engineering fundamentals, his main research interests are multiphase flow in chemical reactors, mathematical modeling of multiphase reactors, and numerical simulation of the behavior of drops, bubbles and solid particles. He has written over 170 peer-reviewed technical papers and 20 patent applications on multiphase flow and chemical reactors.

He was awarded the 1991 Award for the Best Fundamental Paper by the South Texas Section of AIChE, first prize from the Science and Technology Progress of China Petroleum & Chemical Industry Federation in 2006, and second prize in the State Natural Science Award in 2009. He is the associate editor-in-chief of the *Chinese Journal of Chemical Engineering* and *Chinese Journal of Process Engineering*. He was an adjunct professor at the Graduate School of Chinese Academy of Sciences, giving graduate courses on Chemical Reaction Engineering and Mathematical Modeling in Chemical Engineering.

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Introduction

1

To meet the growing need for bulk chemicals in the national economy and in human life, chemical engineers have been trying to develop the best methodology for scaling up all types of reactors for diversified products. Historically, a larger scale reactor was tentatively designed after a series of cold model experiments and hot model tests. Even though these tests were done carefully and the design was backed up with a wealth of valuable intellectual experience, such a scale-up remains quite risky, because a new or large-sized reactor is the result of *extrapolation* based on tests in limited scopes of reactor configuration and experimental conditions. Better extrapolation would result from a basis of scientific laws that have been proved universally true in many industrial tests in addition to numerous natural phenomena. Mathematical models of chemical reactors are believed to be a sound scientific basis for such extrapolations. A practical model of a reactor is very complicated: phenomenologically involved with multiphase flow, macro- and micromixing, heat and mass transfer, and complex chemical reactions; mathematically with algebraic, ordinary and partial differential equations with strong nonlinearity and mutual coupling. Fortunately, we can utilize numerical simulation to solve such models, and tentatively guide the scale-up of chemical reactors to successful commercial operation. This explains why we are advocating the approach of mathematical modeling and numerical simulation so ardently, both in chemical engineering fundamental research and in industrial innovation.

Many interesting methods may be complemented with mathematical modeling and numerical simulation – for example, optimized operation for higher productivity or better product quality, upgrading the performance of reactors already on the process line, etc. There is one further comment here on scaling-up a reactor. Strictly speaking, we are not sure if the present reactor type and configuration are suitable for a larger scale reactor, as judged by our previous experience on extrapolation. A chemist can conduct a reaction successfully in a lab beaker (a small stirred tank), but this does not mean all commercial reactors for the same reaction should be conducted in large beakers. Using the approach of mathematical modeling and numerical simulation, we can conduct many virtual (numerical) tests of several reactor types and configurations on different scales, with the confidence that the capability of such a first-principles-based approach can achieve an optimized extrapolation of reactors. This approach may ultimately resolve the methodology of reactor renovation and

innovation. The approach relies heavily on an in-depth quantitative understanding of the mechanisms occurring in chemical reactors for building the mathematical models and the various numerical techniques for solving the established models, as itemized and exemplified in this book.

This book is primarily focused on chemical engineering sciences and technologies, and aims to be a reference book for scientists and engineers in the fields of chemical reaction engineering, mass/heat transfer, hydrodynamics, crystallization, etc. The book will provide design, optimization, and scale-up concepts and numerical methods for multiphase reactors and crystallizers such as stirred tanks, loop reactors and microreactors for different application purposes. There are five subsequent chapters on various topics relevant to multiphase reactors with liquid phases.

Chapter 2 deals with the multiphase flow and interphase mass transfer on a particle scale. The mechanism of multiphase flow and mass transfer on the mesoscale is vital to the design and scale-up of reactors and crystallizers. The orthogonal boundary-fitted coordinate system-based simulation and level set method are improved to compute the motion and mass transfer of bubbles and drops, and also the mirror fluid method for motion of solid particles is developed. Thereafter, the modified cell model is proposed to examine the flow and transport behavior of particle swarms. The study on the motion and mass transfer of a solute to/from a single drop with a surfactant adsorbed on the interface and the Marangoni effect is expounded to better understand the liquid extraction and reaction processes. Also, the principal research results for the transport process of a spherical particle in pure extensional and simple shear flows are introduced in this chapter.

Chapter 3 deals with the numerical simulation of multiphase stirred tanks, which are the most used reactors or crystallizers in continuous, batch, or fed-batch modes. Good mixing in stirred tanks is important for minimizing investment and operating costs, providing high yields when mass/heat transfer is limiting, and thus enhancing profitability. Multiphase flow and transport in stirred tanks demand more intensive attention with combined numerical and experimental approaches. In this chapter, we present extensive experimental and numerical simulation results of recent developments for stirred tanks. Multiphase flows (including two- and three-phase flows) are discussed in detail based on numerical methods using the Eulerian multifluid approach and RANS (Reynolds average Navier–Stokes)-based turbulence models (e.g., k - ϵ model). Novel surface aeration configurations are introduced for better gas dispersion and high pumping capacity, and the hydrodynamic characteristics of multi-impellers and numerical simulation of gas hold-up in surface-aerated stirred tanks are also addressed. Some new advances in numerical simulation are also presented. The algebraic stress model (ASM) and large eddy simulation (LES) are recommended for future research on multiphase flows in stirred reactors.

Chapter 4 deals with the hydrodynamics and transport in loop reactors. Airlift internal loop reactors are commonly used in petrochemical, hydrometallurgical, energy, environmental, and bio-engineering processes due to their excellent advantages of simple structure, high gas–liquid mass and heat transfer rates, good solid suspension, homogeneous shear distribution, and good mixing. Although great achievements have been made on loop reactors, the design and scale-up of these reactors

still remain difficult due to the nature of complex multiphase flow. In this chapter, investigations of the flow and mixing characteristics by experiments and computational fluid dynamics simulations are presented on airlift reactors with very high and low height-to-diameter ratios. Also, as an intrinsic element of the new technology of coal liquefaction in China, an internal airlift loop reactor pilot test is introduced on the feasibility of replacing the bubble column reactor on the industrial process line of direct coal liquefaction.

Chapter 5 deals with the preliminary investigation of numerical methods and experiments for flow and mixing in two-phase microreactors. The miniaturization of chemical engineering devices has recently brought significant changes, and the progress in microreactors opens doors to more efficient, economic, and safer process intensification. The selectivity of fast chemical reactions depends on the quality of macro- and micromixing. In this chapter, the flow, pressure drop, mass transfer, and mixing of two-phase flow in microchannels with different wetting properties are investigated for different flow patterns. Immiscible two-phase flows, thermal transfer, and mass diffusion in microchannels are numerically studied by a lattice Boltzmann method based on field mediators.

Chapter 6 deals with the mathematical models and numerical simulation of solid-liquid crystallizers. Crystallizers are widely used to produce fine and bulk chemicals. Most of the theoretical and experimental studies are aimed at understanding important mechanisms in the crystallization process in order to stabilize process control, and ultimately to obtain products with desired crystal size distribution (CSD), morphology, and mean size. In this chapter, numerical simulations towards predicting the full CSD directly in a more practical crystallization reactor are presented in a Eulerian framework, and nucleation, growth, and aggregation are considered. The effects of aggregation, feeding concentration, agitation speed, mean residence time, and the CSDs of different locations are studied numerically. Reaction crystallizations are mixing-sensitive multiphase processes, so macro- and micromixing in crystallizers and some other multiphase reactors are also presented.

Fluid flow and mass transfer on particle scale

2

2.1 INTRODUCTION

Fluid flow of and mass transfer from/to drops, bubbles, and solid particles are often observed in nature and various areas of engineering. Chemical and metallurgical engineers rely on bubbles and drops for unit operations such as distillation, absorption, flotation and spray drying, while solid particles are used as catalysts or chemical reactants. In these processes, there is relative motion between bubbles, drops or particles on one hand, and a surrounding fluid on the other. In many cases, transfer of mass and/or heat is also of importance. Owing to rapid progress of computer techniques and numerical methods in fluid mechanics and transport phenomena, the application of numerical simulation has recently become increasingly popular in understanding multiphase flow and transport on a particle (a generic term including drops and bubbles) scale.

In this chapter, this topic is discussed in detail in the following six sections. Firstly, the theoretical basis and numerical methods frequently adopted are summarized in Sections 2.2 and 2.3 respectively. We choose to focus mostly on three methods: simulation on orthogonal boundary-fitted coordinates, an improved level set method, and a mirror fluid method. This choice reflects our own background, as well as the fact that these methods are deemed successful and reliable for computing the motion and mass transfer of fluid particles (bubbles and drops) or solid particles. The validity of these methods is demonstrated and compared with the reported experimental data in Section 2.4. Also, considering the trace quantities of surfactants unavoidable in most industrial systems, study of the motion and mass transfer of a solute to/from a single drop with a surfactant adsorbed on the interface is carried out to better understand the liquid extraction processes and for the scientific design of relevant equipment. The Marangoni effect, one of the most sophisticated interphase transport phenomena, interests researchers due to its influence on transport rates and it has been mathematically formulated and numerically simulated to shed light on these mechanisms. Recent studies relating to the Marangoni effect are presented in Section 2.5. In Section 2.6, numerical simulation methods on particle swarms are discussed briefly and modified cell models are introduced to examine the flow and transport behaviors of particle swarms. Section 2.7 incorporates related progress on particle motion controlled by fluid shear or extension.

2.2 THEORETICAL BASIS

The mathematical formulation of two-phase particle flow may be exemplified using two-fluid systems in which a liquid drop or a gas bubble moves in another continuous liquid as it follows in this section. The fundamental physical laws governing the motion of and mass transfer from/to a single particle immersed in another fluid are Newton's second law, the principle of mass conservation, and Fick's diffusion law. So the flow field and solute transport in both fluid phases must be formulated using the first principles of fluid mechanics and transport phenomena. When a solid particle is involved, the flow in the solid domain is usually not necessary and the particle is tracked mechanically as a rigid body. In this context, two-phase flow with a solid particle is a simplified case of general two-phase systems.

2.2.1 Fluid mechanics

The motion of a small particle (drop, bubble or solid particle) of around 1 mm size under gravity through an immiscible continuous fluid phase can be resolved using the following assumptions: (1) the fluid is viscous and incompressible; (2) the physical properties of the fluid and the particle are constant; (3) the two-phase flow is axisymmetric or two-dimensional; (4) the flow is laminar at low Reynolds numbers.

The flow in each fluid phase is governed by the continuity and Navier–Stokes equations:

$$\nabla \cdot \mathbf{u} = 0 \quad (2.1)$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \rho \mathbf{g} + \nabla \cdot \boldsymbol{\tau} + \mathbf{S} \quad (2.2)$$

where $\boldsymbol{\tau}$ is the stress tensor defined as

$$\boldsymbol{\tau} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \quad (2.3)$$

and the source term \mathbf{S} is formulated differently in different cases.

Boundary conditions for the governing equations are essential when an interface exists between the two phases. For a bubble or a drop, the normal velocity in each phase is equal at the interface. If the gas in a bubble is taken as inviscid, the bubble surface is mobile and not subject to any shear force. However, if the gas is taken as a viscous fluid, both the velocity vector and shear stress should be continuous across the interface. For a solid particle, both the normal and tangential velocity components of the continuous phase must be zero at the particle surface; that is, the solid surface should satisfy the “no-slip” condition.

For the case with constant physical properties of both fluid phases, including that on the interface, the solution for mass transfer will be decoupled from the problem of fluid flow. Thus, the information of the flow field, required for solution of convective diffusion problems, whether for steady or unsteady mass transfer, can be provided directly from numerical simulation of steady-state fluid flow only once.

2.2.2 Mass transfer

In general, the transient mass transfer to/from a drop (or a bubble) is governed by the convective diffusion equation in vector form:

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = D \nabla^2 c \quad (2.4)$$

in each phase subject to two interfacial conditions:

$$D_1 \frac{\partial c_1}{\partial n_1} = D_2 \frac{\partial c_2}{\partial n_2} \quad (\text{flux continuity at the interface}) \quad (2.5)$$

$$c_2 = mc_1 \quad (\text{interfacial dissolution equilibrium}) \quad (2.6)$$

In the above equations, subscript 1 indicates the continuous phase and 2 the dispersed phase. The solution of Eq. (2.5) is reliant on the resolved fluid flow both in the dispersed and the continuous phases, as addressed by Li and Mao (2001). In accordance with Fick's first law, for steady external mass transfer the local diffusive flux across the interface is calculated by

$$N_{\text{loc}} = -D_2 \frac{\partial c_2}{\partial n_2} = k_{\text{loc}} (\bar{c}_2 - mc_1^\infty) \quad (2.7)$$

where the remote boundary concentration c_1^∞ and the only available measurement of the bubble/drop concentration \bar{c}_2 (averaged over the whole drop, taking a drop as an example) are used to define the driving force and the mass transfer coefficient. The latter may be expressed in terms of dimensional concentration gradient as

$$k_{\text{loc}} = -\frac{D_2}{(\bar{c}_2 - mc_1^\infty)} \frac{\partial c_2}{\partial n_2} \quad (2.8)$$

Then, the local Sherwood number is

$$Sh_{\text{loc}} = \frac{dk_{\text{loc}}}{D_2} = -\frac{d}{(\bar{c}_2 - mc_1^\infty)} \frac{\partial c_2}{\partial n_2} \quad (2.9)$$

and the drop area averaged Sh_{od} is

$$Sh_{\text{od}} = \frac{\oint Sh_{\text{loc}} ds}{\oint ds} \quad (2.10)$$

On the other hand, the overall mass transfer coefficient k_{od} may be evaluated from the overall solute conservation based on the drop as follows:

$$k_{\text{od}} (c_2^* - \bar{c}_2) A = V_d \frac{d\bar{c}_2}{dt} \quad (2.11)$$

where \bar{c}_2 is the average concentration of the drop at any time instant, which is almost the only available measure of solute concentrations of drops in conventional

experiments. If the time interval $t_{\text{out}} - t_{\text{in}}$ is chosen small enough, k_{od} may be evaluated approximately from integration of the above equation as

$$k_{\text{od}} = -\frac{V_d}{A} \frac{1}{t_{\text{out}} - t_{\text{in}}} \ln \left(\frac{c_2^* - \bar{c}_{2,\text{out}}}{c_2^* - \bar{c}_{2,\text{in}}} \right) \quad (2.12)$$

where A and V_d are the volume and the surface area of the drop, and for a spherical drop $V_d/A = d/6$. The corresponding Sherwood number is

$$Sh_{\text{od}} = \frac{d}{D} k_{\text{od}} \quad (2.13)$$

2.2.3 Interfacial force balance

When the drop or bubble shape is to be determined, the force balance over the interface must be satisfied. Moreover, the interface that separates two contacting phases is the common boundary of two phases. The interface status must be compatible with the motion of either phase. Thus, the equations governing the momentum and mass balances are often used as the boundary conditions for the governing equations of motion and transport in each phase.

In general macroscopic hydrodynamic formulations, the interface is taken realistically as a weightless layer of zero thickness. Therefore, all forces exerted over an infinitesimal section of the interface have to be summed to be zero, whether the particle is in steady or accelerating motion. As illustrated in Figure 2.1, the pressure and stress tensor in both fluids and the surface force are involved. The overall force balance is as follows:

$$(-p_1 \mathbf{I} + \boldsymbol{\tau}_1) \cdot \mathbf{n} + \mathbf{f}_s = (-p_2 \mathbf{I} + \boldsymbol{\tau}_2) \cdot \mathbf{n} \quad (2.14)$$

where the surface force \mathbf{f}_s is the sum of normal and tangential force components:

$$\mathbf{f}_s = -\sigma \kappa \mathbf{n} + \nabla_s \sigma \quad (2.15)$$

in which $\kappa = -\nabla \cdot \mathbf{n}$ is the mean curvature of the interface, \mathbf{n} is the outward normal unit vector, and ∇_s is the surface gradient operator. The interfacial tension σ is generally a function of temperature, solute concentration at the surface, surfactant

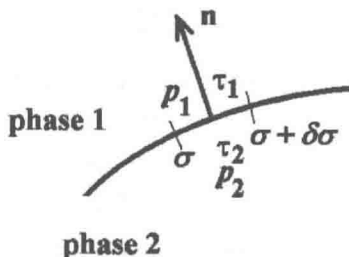


FIGURE 2.1 Interfacial force balance over an interface segment.