Environmental Engineering and Management Journal *July/August 2007, Vol.6, No.4, 331-333*
http://omicron.ch.tuiasi.ro/EEMJ/

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Book review

MODELING OF PROCESS INTENSIFICATION

Frerich J. Keil (Ed.)

WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany
ISBN: 978-3-527-31143-9, 2007, XV+405 pags.

The book ***Modeling of Process Intensification*** combines the knowledge involved in process engineering and process modelling, in order to ensure a significant reduction of investment and operational costs, through the integration of several unit operations into one single unit of major importance.

Process intensification gains more and more in importance and interest in many fields, leading to the development of novel apparatuses, equipment and techniques which improve the chemical and biological processes with respect to decreased costs with reduced equipment size, increased energy efficiency, less waste and pollution, improved safety.

The book editor, Prof.Dr.Dr.h.c. Frerich J. Keil from the Institute of Chemical Reaction Engineering of the Hamburg University of Technology begins the book with Chapter 1 – *Modeling of Process Intensification – An Introduction and Overview,* offering a presentation of the book. First, he explains the concept of "process intensification", which is "used to describe the strategy of reducing the size of chemical plant needed to achieve a given production objective", but some other definitions of this concept are given. The author also briefly describes the strategies employed by several companies to achieve the goals of process intensification.

The chapter continues with short descriptions of the other chapters of the book.

Chapter 2 – *Process Intensification – An Industrial Point of View*, by author Robert Franke – describes the process intensification concept and actions from an industrial point of view, considering microreaction technology, which is based on chemical microprocessing, characterized by a continuous flow of matter through well-defined structures of specific dimensions. Also, catalytic wall reactors are taken into consideration, offering a short overview of research and process development in several directions, such as partial oxidation. The simulation is analyzed through process intensification, a special feature being the use of molecular simulations on various levels, such as quantum chemistry and classical molecular dynamics or Monte-Carlo simulations.

Chapter 3 – *Modeling and Simulations of Microreactors*, author Steffen Hardt – contains a discussion on modeling and simulation techniques for microreactors and shows that the currently available toolbox is quite diverse and goes well beyond the standard capabilities of computational fluid dynamics (CFG) methods available in commercial solvers.

In microreactors, most of the effects are described by the standard continuum equations, while the special methods needed for the modeling of noncontinuum physics play only a minor role. It is recognized that even in the laminar flow there are a number of problems which are extremely difficult and require very fine computational grids. As further development of modeling and simulation techniques for microreactors, the author recommends the elaboration of system-level models which allow a coupling to CFD simulations, so that the commercial application of microreactors could also gain additional drive.

Chapter 4 – *Modeling and Simulation of Unsteady-State-Operated Trickle-Flow Reactors*, author Rüdiger Lange – describes the behavior of these three-phase reactors, which is rather complex due to cocurrent flow of gas and liquid downward through a catalyst packing. A review of unsteady-state-operated trickle-flow reactors and a dynamic reactor model is presented. The author considers that the modeling of the periodic process management is based mainly on the extension of steady-state models for trickle bed reactors. Their applications for non-steady-state systems have several drawbacks, summarized by the author in the following points.

Chapter 5 – *Packet-Bed Membrane Reactors,* authors Ákos Tóta, Dzmitry Hlushkou, Evangelos Tsosas and Andreas Seidel-Morgenstern – is an

extensive review of this type of reactor (PBMR) and analyzes their properties by means of original models. A specific type of membrane reactor, the so-called "distributor" was analyzed theoretically. In contrast to conventional tubular fixed-bed reactors (FBR), where all reactants are introduced together at the reactor inlet (cofeed mode), PBMRs allow dosing of one or several reactants via membranes over the reactor wall, along the axial coordinate. The concept can be considered an interesting option in the current attempts to improve and intensify reaction processes. This can be a way to improve the performance of complex chemical reactions together with the theoretical framework that allows rapid first estimations in early development stages as well as for more detailed studies required for process design and operation.

Chapter 6 – *The Focused Action of Surface Tension versus Brute Force of Turbulence - Scaleble Microchannel-based Process Intensification using Monoliths,* authors Michiel T. Kreutzer, Annelies van Diepen, Freek Kaptejin, Jacob A. Moulijn – is a contribution concerned with gas-liquid and gas-solid reactors, considering that processes that need such a reactor should be designed in such a way that drastically higher rates based on reactor volume can be achieved while maintaining or improving the selectivity towards the desired product. The discussion is extended on the advantages and disadvantages of using segmented flow in micro-channels in order to intensify catalytic processes. The catalyst quality is not considered and the focus is on the hydrodynamics and the transport phenomena. Using a simple scaling analysis, which takes into account the viscous pressure drop, hydrostatic pressure drop, interfacial pressure drop and penetration theory for mass transfer, it has been demonstrates that two-phase laminar bubble-train flow in small channels can exhibit better mass transfer for a given power input than turbulent contactors. This flow pattern is recommended for biochemical conversions using cell cultures as well, provided that channels are not too small and the operating conditions are such that biofilm formation is suppressed.

Chapter 7 – *Chemical Reaction Modelling in Supercritical Fluids in Special Consideration of Reactions in Supercritical Water,* authors Andrea Kruse and Eckhard Dinjus get a better understanding of the chemical reactions by means of systems of elementary reaction, widely used in gas-phase kinetics, especially in oxidation reactions, and also explains how they are influenced by the properties of the supercritical fluids. The discussion is focused on chemical reaction modelling in supercritical fluids, in particular in supercritical water. These models could be a helpful tool to project processes in supercritical fluids in industrial applications.

Chapter 8 – *Ultrasound Reactors* – Christian Horst, Parag G. Gogate and Aniruddha B. Pandit is organized in two parts.

The first is written by Christian Horst and deals with some fundamental aspects of cavitation and its modeling. The sound field inside sonochemical reactors recommended to be modeled by treating the liquid bubble mixture as a pseudofluid with mean values. In order to calculate the properties of this mixture it is proposed to evaluate the bubble motion of bubbles with different sized using the Kirkwood-Bethe-Gilmore equation. The resulting speeds of sound and the damping coefficients can be integrated in the equation for the acoustical approximation neglecting convective terms in the mass and momentum balance. The results of the simulation have been employed to optimize reactor geometries and to interpret unexpected effects. Sonochemical effects for Grignard reactions were also modeled.

The second part stresses the importance of some factors which determine an efficient scale up of cavitational reactors and their industrial applications based on the theoretical and experimental analysis of the net cavitational effects. Cavitation generates conditions of high temperature and pressure along with the release of active radicals, which results in intensification of many of the physical and chemical transformations. It is highlighted that the cavitation phenomena can be effectively exploited for a variety of physical/chemical transformations including chemical synthesis, biotechnology, environmental engineering, polymer engineering, and the rate of the transformations are at times, orders of magnitude higher than in the conventional approach and also the energy consumption is relatively lover. Guidelines for the selection of an optimum set of operating parameters have been presented.

Chapter 9 – *Modeling of Simulated Moving-bed Chromatography*, author Monica Johannsen shows that this technique is a powerful purification process allowing the continuous separation of a feed mixture into two product streams. The developed models are based on the adsorption theory and the theory of nonlinear chromatography. For optimization of Simulated Moving-bed (SMB) chromatography the influence of column length, column configuration, flow rates, feed concentration and switching times is studied. For each large-scale application a comparison of discontinuous elution chromatography and continuous SMB process is recommended to be made. Application of SMB chromatography and modelling of this process are reviewed.

Chapter 10 – *Modeling of Reactive Distillation*, authors Eugeny Y. Kenig and Andrzej Górak analyses modeling of reactive distillation. This operation, combining the separation and reaction steps inside the same zone of a single column, is often advantageous compared to traditional sequential unit operation. A detailed discussion of the process basics and peculiarities is given, considering the up-to-date applications and RTD modeling and design issues.

The theoretical illustration uses several case studies and supported by the results of laboratory, pilot and industrial scale experimental investigations. Both steady-state and dynamic issues are treated together with the design of column internals. The modeling of RD processes is demonstrated by the heterogeneous catalyzed syntheses of some compounds using different catalytic internals. These processes are described based on the pseudo homogeneous approach for the reaction kinetics. Both steady-state and dynamic issues are treated and the design of column internals is addressed. An outlook on future research requirement is given.

Chapter 11 – *Experimental and Theoretical Exploration of Weak- and Strong-gradient Magnetic Fields in Chemical Multiphase Processes*, author Faiçal Larachi deals with experimental and theoretical investigations on artificial gravity generated by strong gradient magnetic fields, which could be applied in multiphase catalytic systems wherea number of factors can be optimized for improving process efficiency.

A theoretical framework based on the application of the volume-average theorems in multiphase porous media is developed, to analyze the flow of ferrofluids in a special class of porous media presenting pronounced effects of wall-bypass flows.

Each chapter ends with a rich list of references. Also, the subject index at the end of the book is a very good searching engine.

The book is a very useful tool for experts in various area of process intensification, from both industry and academics.

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