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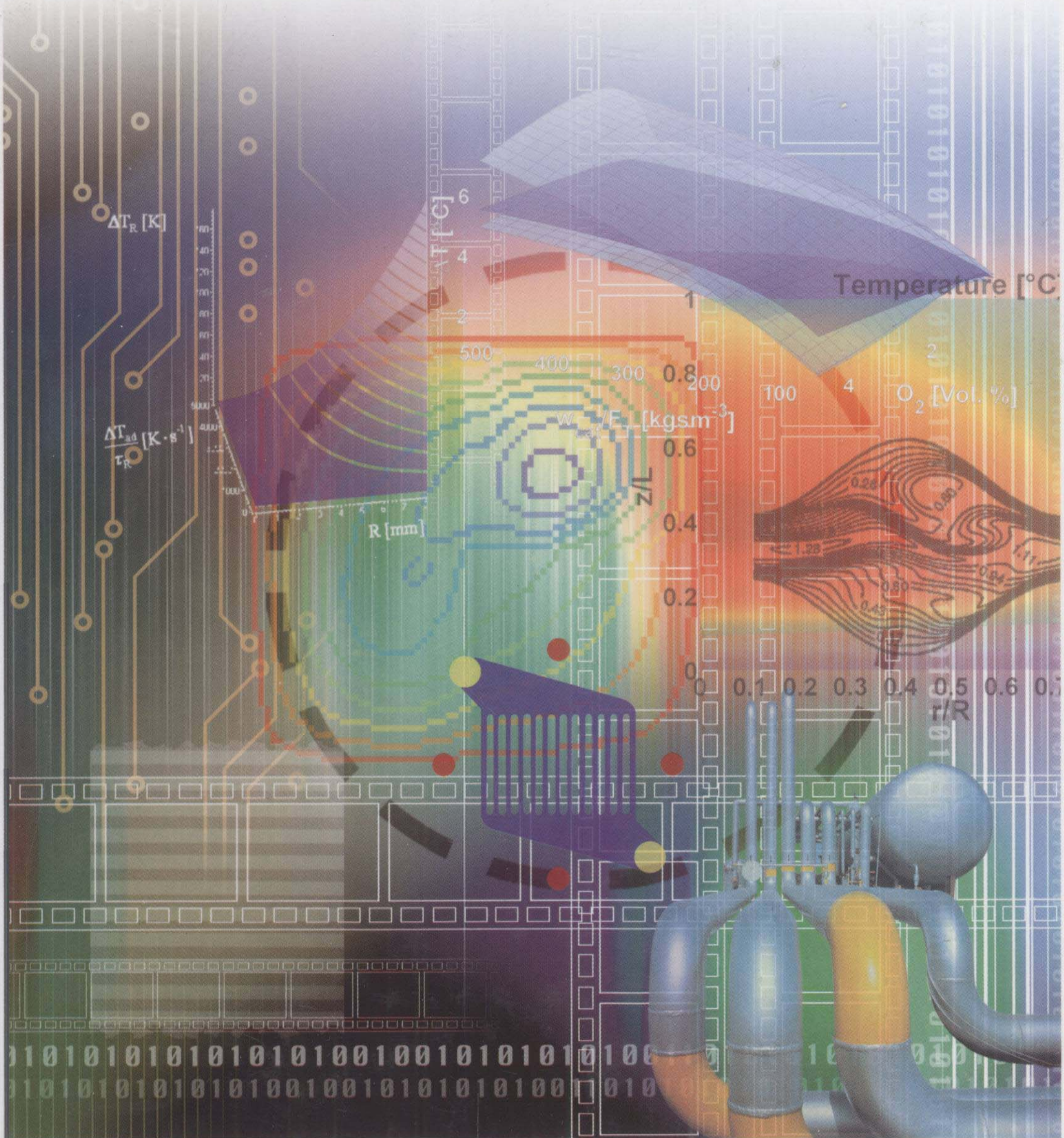
Modeling of Process Intensification



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Preface

Process intensification has been on the upswing since a review written by A. Stankiewicz and J. Moulijn was issued in 2000. Meanwhile, companies and academia are addressing problems in process intensification, organizing workshops and even establishing departments on this subject. Process intensification is a very broad discipline and includes expertise in many diverse fields. It is applied to the development of novel apparatuses and techniques that either dramatically improve chemical or biological processes with respect to reduced equipment size, increased energy efficiency, less waste production, improved inherent safety, or even break new ground in process engineering by introducing newly developed equipment and production procedures. The present book focuses on modeling in process intensification. Experts in various areas of process intensification, from both industry and academia, have contributed to this book, which does not cover all the developments in this field; rather it demonstrates the activities in modeling for some representative problems. New equipment like microreactors, membrane reactors, ultrasound reactors, and those in simulated moving-bed chromatography, magnetic fields in multiphase processes or reactive distillation, requires new modeling approaches. The same applies to nonstationary process operation or the use of supercritical media. Process intensification is an emerging discipline that will result in many surprising developments in the future.

The editor is grateful to all the authors who contributed to this volume, and to Dr. Rainer Muenz from Wiley-VCH.

F. J. Keil
Hamburg, January 2007

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Modeling of Process Intensification – An Introduction and Overview

Frerich J. Keil

As noted by Hüther et al. [1], the term "process intensification" (PI) was probably first mentioned in the 1970s by Kleemann et al. [2] and Ramshaw [3]. Ramshaw, among others, pioneered work in the field of process intensification. What does "process intensification" (PI) mean? Over the last two decades, different definitions of this term were published. Cross and Ramshaw defined PI as follows: "Process intensification is a term used to describe the strategy of reducing the size of chemical plant needed to achieve a given production objective" [4]. In a review of PI, Stankiewicz and Moulijn [5] proposed: "Any chemical engineering development that leads to a substantially smaller, cleaner, and more energy-efficient technology is process intensification". The BHR Group describes PI as follows [6]: "Process Intensification is a revolutionary approach to process and plant design, development and implementation. Providing a chemical process with the precise environment it needs to flourish results in better products, and processes which are safer, cleaner, smaller, and cheaper. PI does not just replace old, inefficient plant with new, intensified equipment. It can challenge business models, opening up opportunities for new patentable products and process chemistry and change to just-in-time or distributed manufacture". To bring forward PI, Degussa established a so-called "project house" whose research activities are focused on PI. Degussa expanded the meaning of the concept "process intensification": "Process intensification defines a holistic approach starting with an analysis of economic constraints followed by the selection or development of a production process. Process intensification aims at drastic improvements of performance of a process, by rethinking the process as a whole. In particular it can lead to the manufacture of new products which could not be produced by conventional process technology. The process-intensification process itself is "constantly financially evaluated" [1, 7]. As can be recognized from the above definitions, process intensification is a developing field of research and far away from a mature status. The chemical industry and academia are very interested in PI developments. For example, some German chemical engineering associations (DECHEMA, VDI-GVC) established a subject division on process intensification, which has already more than 180 members. In the opening session of this division

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several sceptical questions arose, like: "Are any new options offered by PI which are not known already from other fields of chemical engineering, e.g. optimization or process integration?" "How large should be the improvement of a process for PI?" "What is the difference between the aims of PI and neighbouring disciplines?" [8]. There is an agreement that PI is an interdisciplinary field of research that needs an integrated approach. In PI, the journey is the reward.

PI has inspired already many new developments of equipment, process-intensifying methods and design approaches. As thermodynamic equilibrium and reaction kinetic properties are fixed values for given mixtures under fixed conditions like temperature, pressure and catalysts, most efforts were directed towards the improvement of transport properties, alternative energy resources, and process fluids. Examples of new equipment are the Sulzer SMR static mixer, which has mixing elements made of heat-transfer tubes, Sulzer's open-crossflow-structure catalysts, so-called Katapaks, monolithic catalyst supports covered with washcoat layers, microreactors, ICI's High Gravity Technology (HIGEE), HIGRAVITEC's rotating packed beds, centrifugal adsorbers made by Bird engineering, BHR's improved mixing equipment and HEX reactors, high-pressure homogenizers for emulsifications, the spinning-disc reactor (SDR) developed by Ramshaw's group at Newcastle University, and the supersonic gas/liquid reactor developed by Praxair Inc. (Danbury). Various ultrasonic transducers and reactors are now commercially available. The efforts in PI have been compiled in several books [9–14]. A general introductory paper was presented by Stankiewicz and Moulijn [5]. Process intensification by miniaturization has been reviewed by Charpentier [15]. Jachuck [16] reviewed PI for responsive processing. Other subjects related to process intensification have also been reviewed, for example, trickle-bed reactors [17], multifunctional reactors [18], rotating packed beds [19], multiphase monolith reactors [20], heat-integrated reactors for high-temperature millisecond contact-time catalysis [21], microengineered reactors [22, 23], monoliths as biocatalytic reactors [24], membrane separations [25], two-phase flow under magnetic-field gradients [26], and applications of ultrasound in membrane separation processes [27].

In Fig. 1.1 an overview of equipment and methods employed in PI is presented. PI leads to a higher process flexibility, improved inherent safety and energy efficiency, distributed manufacturing capability, and ability to use reactants at higher concentrations. These goals are achieved by multifunctional reactors, e.g. reactive distillation or membrane reactors, and miniaturization that can be done by employing microreactors and/or improving heat and mass transfer. Microfluidic systems enable very high heat- and mass-transfer rates so that reactions can be executed under more severe conditions with higher yields than conventional reactors. New reaction pathways, for example, direct fluorination of aromatic compounds, are possible, and scaleup of reactors is easier. This feature may enhance instationary reactor operation, like reverse flow, in industrial applications. These are just a few examples.

Intensification of heat and mass transfer can be achieved by using supersonic flow, strong gravitational magnetic fields, improved mixing, among other ap-