Modeling of Process Intensification

Edited by
Frerich Johannes Keil

Modeling of Process Intensification

Edited by
Frerich Johannes Keil
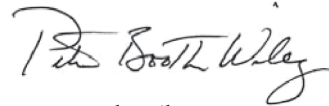
1807–2007 Knowledge for Generations

Each generation has its unique needs and aspirations. When Charles Wiley first opened his small printing shop in lower Manhattan in 1807, it was a generation of boundless potential searching for an identity. And we were there, helping to define a new American literary tradition. Over half a century later, in the midst of the Second Industrial Revolution, it was a generation focused on building the future. Once again, we were there, supplying the critical scientific, technical, and engineering knowledge that helped frame the world. Throughout the 20th Century, and into the new millennium, nations began to reach out beyond their own borders and a new international community was born. Wiley was there, expanding its operations around the world to enable a global exchange of ideas, opinions, and know-how.

For 200 years, Wiley has been an integral part of each generation's journey, enabling the flow of information and understanding necessary to meet their needs and fulfill their aspirations. Today, bold new technologies are changing the way we live and learn. Wiley will be there, providing you the must-have knowledge you need to imagine new worlds, new possibilities, and new opportunities.

Generations come and go, but you can always count on Wiley to provide you the knowledge you need, when and where you need it!

William J. Pesce
President and Chief Executive Officer

Peter Booth Wiley
Chairman of the Board

Modeling of Process Intensification

Edited by
Frerich Johannes Keil

The Editor

Prof. Dr. Dr. h.c. Frerich J. Keil
Hamburg University of Technology
Institute of Chemical Reaction Engineering
Eißendorferstr. 38
21073 Hamburg
Germany

Contents

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

List of Contributors

Eckhard Dinjus
Forschungszentrum Karlsruhe
Institut für Technische Chemie
P.O. Box 36 40
76021 Karlsruhe
Germany

Robert Franke
Degussa AG
Creavis Technologies & Innovation
Project House Process
    Intensification
Rodenbacher Chaussee 4
63457 Hanau
Germany

Parag R. Gogate
Institute of Chemical Technology
Chemical Engineering Department
Matunga, Mumbai-400019
India

Andrzej Gorak
Universität Dortmund
Lehrstuhl für Thermische
    Verfahrenstechnik
FB Chemietechnik
44221 Dortmund
Germany

Steffen Hardt
Leibniz Universität Hannover
Institut für Nano- und
    Mikroprozesstechnik
Callinstr. 36
30167 Hannover
Germany

Dzmitry Hlushkou
Otto von Guericke University
    Magdeburg
Institute of Process Engineering
Chair of Thermal Process
    Engineering
P.O. Box 4120
39106 Magdeburg
Germany

Christian Horst
Infraserv Gendorf
84504 Burgkirchen
Germany

Monika Johannsen
Technische Universität
    Hamburg-Harburg
Institut für Thermische
    Verfahrenstechnik
Eißendorferstraße 38
21073 Hamburg
Germany

Freek Kapteijn
University of Technology
Reactor/Cat. Engineering Group
Julianalaan 136
2628 BL Delft
The Netherlands

Eugeny Y. Kenig
Universität Dortmund
Lehrstuhl für Thermische
  Verfahrenstechnik
FB Chemietechnik
44221 Dortmund
Germany

Frerich J. Keil
Hamburg University of Technology
Institute of Chemical Reaction
  Engineering
Eißendorferstraße 38
21073 Hamburg
Germany

Michiel T. Kreutzer
University of Technology
Reactor/Cat. Engineering Group
Julianalaan 136
2628 BL Delft
Netherlands

Andrea Kruse
Forschungszentrum Karlsruhe
Institut für Technische Chemie
P.O. Box 36 40
76021 Karlsruhe
Germany

Rüdiger Lange
Technische Universität Dresden
Verfahrentechnik / Zi. A208
Münchener Platz 3
01062 Dresden
Germany

Faical Larachi
Laval University
Department of Chemical
  Engineering
Cité Universitaire
Avenue de la Médecine
Pouliot Building
G1K 7P4 Quebec
Canada

Jacob A. Moulijn
University of Technology
Reactor/Cat. Engineering Group
Julianalaan 136
2628 BL Delft
The Netherlands

Andreas Seidel-Morgenstern
Otto von Guericke University
  Magdeburg
Institute of Process Engineering
Chair of Chemical Process
  Engineering
P.O. Box 4120
39106 Magdeburg
Germany

Aniruddha B. Pandit
Chemical Engineering Department
Institute of Chemical Technology
Matunga, Mumbai-400019
India

Ákos Tóta
Otto von Guericke University
  Magdeburg
Institute of Process Engineering
Chair of Thermal Process
  Engineering
P.O. Box 4120
39106 Magdeburg
Germany

Evangelos Tsotsas
Otto von Guericke University
   Magdeburg
Institute of Process Engineering
Chair of Chemical Process
   Engineering
P.O. Box 4120
39106 Magdeburg
Germany

Annelies van Diepen
University of Technology
Reactor/Cat. Engineering Group
Julianalaan 136
2628 BL Delft
The Netherlands

1
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

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), HI-GRAVITEC'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-
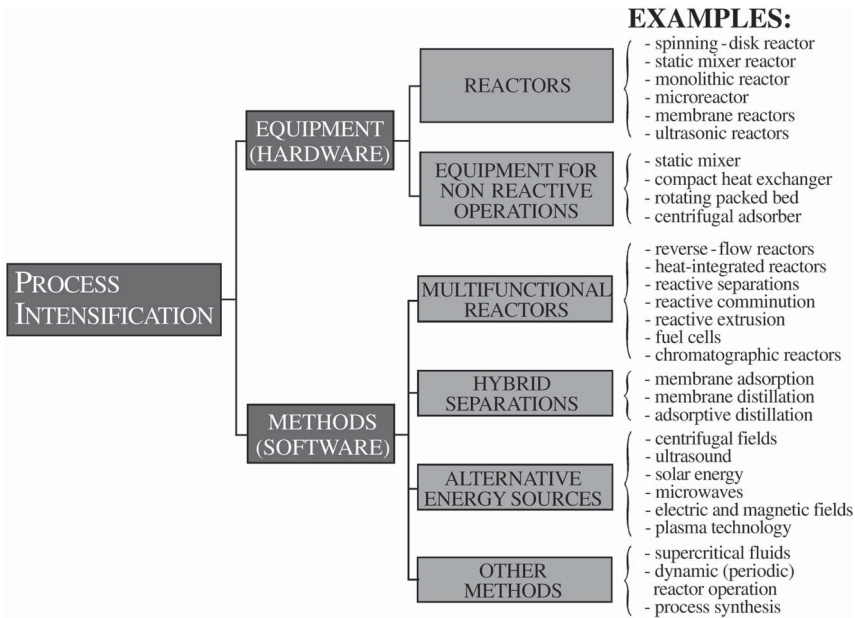
Figure 1.1 Tools of Process Intensification.

proaches. For example, the spinning-disc reactor technology utilizes the effects of high centrifugal force, which is capable of producing highly sheared films on the surface of rotating discs/cones. Convective heat-transfer coefficients as high as $14\,kW\,m^{-2}\,K$ and mass transfer coefficients, K_L values as high as $30 \times 10^{-5}\,m\,s^{-1}$ and K_G values as high as $12 \times 10^{-8}\,m\,s^{-1}$, can be achieved whilst providing micro-mixing and an appropriate fluid dynamic environment for achieving faster reaction kinetics.

A further possibility is offered by external magnetic fields that exert a body force on electrically nonconducting magnetically permeable fluids, and this force can be used to compensate or to amplify the gravitational body force, which can be employed to influence two-phase flow in, for example, trickle-flow reactors.

Ultrasound can either be used for enhancing mass transfer or reaction engineering [28]. Cavitation generates conditions of locally very high temperatures (>6000 °C) and pressure (>10 000 bars) along with the release of active radicals, which results in intensification of many of the physical and chemical transformations. Sonochemistry opened new possibilities for chemical synthesis. Sonoreactors can be thought of as high-energy microreactors. A compilation of chemistry and extreme and nonclassical conditions was edited by van Eldik and Hubbard [29].

The present book reviews recent developments in modeling of process intensification. It is divided into eleven chapters. After an introduction and overview, Robert Franke from Degussa AG describes in Chapter 2 the efforts on PI from an industrial point of view in their "project house". A special feature is the use

of molecular simulations on various levels, like quantum chemistry, and classical molecular dynamics or Monte Carlo simulations. For liquid/liquid equilibria COSMO/RS is in use. Cash-flow analysis and project valuation under risk are investigated by Monte Carlo approaches.

Chapter 3 has been written by Steffen Hardt from Darmstadt University of Technology on modeling and simulation of microreactors. Flow distributions and heat transfer in various microchannels are described. Fast mass transfer and mixing are key aspects of microreactors. Modeling of micromixers is discussed in detail. The chapter is completed by a review of reacting flows in microchannels. The discussion of modeling and simulation techniques for microreactors shows that the toolbox available at present is quite diverse and goes well beyond the standard capabilities of CFD methods available in commercial solvers. Most of the effects are described by the standard continuum equations, but there are a number of problems that are extremely difficult, and require very fine computational grids. Among these problems is the numerical study of mixing in liquids that often severely suffers from discretization artefacts.

Chapter 4 by Rüdiger Lange from the University of Technology Dresden is on modeling and simulation of unsteady-state operated trickle-flow reactors. The behavior of these three-phase reactors is rather complex due to cocurrent flow of gas and liquid downward through a catalyst packing. Periodic change of reactant-feed concentration and/or volumetric flow rate are suitable for a considerable improvement of reaction conversion. A review of unsteady-state operated trickle-flow reactors is presented and a dynamic reactor model developed by Lange's group, based on an extended axial dispersion model, is described in detail.

Andreas Seidel-Morgenstern's group from the Max-Planck-Institute in Magdeburg presents in Chapter 5 an extensive review of packed-bed membrane reactors (PBMR), and analysis of the properties of this type of reactors by means of models developed in their group. In contrast to conventional tubular fixed-bed reactors, where all reactants together are fed into the reactor inlet, packed-bed membrane reactors allow one or several reactants to be dosed via membranes over the reactor wall along the axial reactor coordinate. Computational results, based on realistic data originating from the important class of partial oxidation reactions, are presented. The oxidative dehydrogenation of ethane to ethylene using a vanadium oxide catalyst was considered. Different membrane permeabilities were studied in the range of currently available porous materials. Investigations by a two-dimensional reactor model revealed that flow maldistribution, caused by increased bed porosity close to the membrane wall, leads to local temperature profiles that result in performance predictions different from an integral reactor. Results of a three-dimensional model using the lattice Boltzmann method are also presented.

In Chapter 6 Jacob Moulijn's group from the Delft University of Technology discusses the advantages and disadvantages of using segmented flow in microchannels to intensify catalytic processes. Once bubbles are formed in microchannels, they can no longer coalesce, and hence no energy is required to break up larger bubbles. As a result, the same gas–liquid mass-transfer behavior can be

obtained at an order of magnitude lower power input. This flow pattern can be used for biochemical conversions using cell cultures, provided the channels are not too small, and the operating conditions are such that biofilm formation is suppressed. If the segmented flow pattern is used for a reaction catalyzed at the walls of the capillary channels, then the mass transfer is actually improved by reducing the amount of energy that is dissipated in the system. This allows the simultaneous achievements of two goals of process intensification: reduction of energy requirement and reduction of equipment size.

Chapter 7 focuses on chemical-reaction modeling in supercritical fluids, in particular in supercritical water. This contribution is from Eckhard Dinjus' group at the Research Center Karlsruhe. The contribution gives detailed presentations of modeling of systems by elementary reactions and their reaction engineering.

Chapter 8 consists of two parts. The first contribution by Christian Horst explains some fundamentals of cavitation and its modeling applied to a so-called "High Energy Density Crevice Reactor". The Grignard reaction of chlorobutane isomers was used as an example. The sound field inside sonochemical reactors can be modeled by treating the liquid bubble mixture as a pseudofluid. The Kirkwood–Bethe–Gilmore equations were used to calculate the bubble motions of bubbles with different sizes. Knowing the bubble-size distribution at a given sound pressure by calculating cavitation thresholds and using this information in an equation for the local total bubble number, the calculation of the complex bulk modulus of the bubbly mixture is possible. The resulting sound velocities and the damping coefficients can be used for calculating the sound field by finite-element codes. The simulation results have been employed to optimize reactor geometries and to interpret some surprising effects. Sonochemical effects for Grignard reactions were also modeled.

The second contribution, written by Pareg Gogate and Anniruddha Pandit from the Institute of Chemical Technology in Mumbai, stresses important factors for efficient scaleup of cavitational reactors and subsequent industrial applications based on the theoretical and experimental analysis of the net cavitational effects. Guidelines for selection of an optimum set of operating parameters have been presented and hydrodynamic cavitation has also been discussed.

Chapter 9 on simulated moving-bed chromatography has been written by Monika Johannsen at Hamburg University of Technology. Simulated moving-bed (SMB) chromatography is a powerful purification process allowing the continuous separation of a feed mixture into two product streams. Most of these separations are performed using liquid chromatography. The complexity of preparative chromatography results in highly complex models for the quantitative description compared to analytical chromatography. The models are based on the adsorption theory and the theory of nonlinear chromatography. Various simulation tools for the SMB technique have been developed, which can be used for optimization of the column length, column configuration, flow rates, feed concentration, and switch times. Applications of SMB chromatography and modeling of this process are reviewed.

Chapter 10 reviews modeling of reactive distillation. This contribution is written by Kenig and Gorak at the University of Dortmund (Germany). In reactive distillation, reaction and distillation take place within the same zone of a distillation column. Reactants are converted to products with simultaneous separation of the products and recycle of unused reactants. The process basics and peculiarities are discussed in detail. Up-to-date applications, reactive distillation modeling and design issues are presented. The theoretical description is illustrated by several case studies and supported by the results of laboratory-, pilot- and industrial-scale experimental investigations. Both, steady-state and dynamic issues are treated, and the design of column internals is addressed. An outlook on future research requirements is given.

Faïçal Larachi from the Laval University in Quebec (Canada) presents in Chapter 11 experimental and theoretical investigations on artificial gravity (micro- or macrogravity) generated by strong gradient magnetic fields that could potentially open up attractive applications, especially in multiphase catalytic systems where a number of factors can be optimized in an original manner for improving process efficiency. For example, inhomogeneous and strong fields applied to trickle-bed reactors are capable of affecting their hydrodynamics. Liquid holdup can be improved that results in better contacting between a liquid and a catalyst surface. Additionally, a theoretical framework is developed based on the application of the volume-averaging theorems in multiphase porous media to analyze the flow of ferrofluids in a special class of porous media presenting pronounced effects of wall-bypass flows. Limitations of the present models are discussed.

To sum up, process intensification is a rapidly developing field that has already inspired many ideas in modeling and design of new equipment and operating modes, and whose potential is by far not fully tapped.

References

1 Hüther, A.; Geißelmann, A.; Hahn, H.: Chem. Ing. Tech., **77** (2005), 1829

2 Kleemann, G.; Hartmann, K.: Wiss. Z. Tech. Hochschule "Carl Schorlemmer", Leuna Merseburg, **20** (1978), 417

3 Ramshaw, C.: Chem. Eng. (London), **389** (1983), 13

4 Cross, W.T.; Ramshaw, C.: Chem. Eng. Res. Des., **64** (1986), 293

5 Stankiewicz, A.I.; Moulijn, J.A.: Chem. Eng. Prog., **96** (2000), 22

6 BHR Group: www.bhrgroup.com/pi/aboutpi.htm

7 see Chapter 2, this book

8 Machhammer, O.: Chem. Ing. Tech., **77** (2005), 1635

9 Stankiewicz, A.I.; Moulijn, J.A. (Eds.): Re-engineering the chemical processing plant: process intensification, Marcel Dekker, New York (2004)

10 Hessel, V.; Hardt, S.; Löwe, H.: Chemical Micro Process Engineering, Wiley-VCH, Weinheim (2004)

11 Marcano, J.G.S.; Tsotsis, T.T.: Catalytic Membranes and Membrane Reactors, Wiley-VCH, Weinheim (2002)

12 Koch, M.V.; VandenBussche, K.M.; Christman, K.M.: Micro Instrumentation in High Throughput Experimentation and Process Intensification, Wiley-VCH, Weinheim (in preparation, January 2007)

13 Wang, Y.; Holladay, J.D. (Eds.): Microreactor Technology and Process Intensification (ACS Symposium Series No. 914), ACS Publ. (2005)

14 Jachuck, R. (Ed.): Process Intensification in the Chemical and Related Industries, Blackwell, Oxford (in preparation)

15 Charpentier, J.-C.: Chem. Eng. Technol., **28** (2005), 255

16 Jachuck, R.: Chem. Eng. Res. Des., **80** (2002), 233

17 Nigam, K.D.P.; Larachi, F.: Chem. Eng. Sci., **60** (2005), 5880

18 Agar, D.: Chem. Eng. Sci., **54** (1999), 1299

19 Burns, J.R.; Jamil, J.N.; Ramshaw, C.: Chem. Eng. Sci., **55** (2000), 2401

20 Kreutzer, M.T.; Kapteijn, F.; Moulijn, J.A.; Heiszwolf, J.: Chem. Eng. Sci., **60** (2005), 5895

21 Liu, T.; Gepert, V.; Veser, G.; Chem. Eng. Res. Des., **83** (2005), 611

22 Gavriilidis, A.; Angeli, P.; Cao, E.; Young, K.K., Wan, Y.S.S.: Eng. Chem. Res. Des., **80** (2002), 3

23 Matlosz, M.: Chem. Ing. Tech., **77** (2005), 1393

24 Kreutzer, M.T.; Kapteijn, F.; Moulijn, J.; Ebrahimi, S.; Kleerebezem, R.: Ind. of Eng. Chem. Res., **44** (2005), 9646

25 Drioli, E.; di Profio, G.; Fontananova, E.: Fluid/Particle Separ. J., **16** (2004), 1

26 Iliuta, J.; Larachi, F.: Can. J. Chem. Eng. **81** (2003), 776

27 Muthukumaram, S.; Kentish, S.E.; Stevens, G.W.; Ashokkumar, M.: Rev. Chem. Eng., **22** (2006), 155

28 Keil, F.J.; Swamy, K.M.: Rev. Chem. Eng., **15** (1999), 85

29 van Eldik, R.; Hubbard, C.D. (Eds.): Chemistry under Extreme and Non-classical Conditions, Wiley & Spektrum Akademischer Verlag, New York, Heidelberg (1997)

2
Process Intensification – An Industrial Point of View

Robert Franke

2.1
Introduction

Process intensification aims at drastic improvements in performance of a process by rethinking the process as a whole. Modeling of process intensification relies partly on well-established engineering software tools that include process simulators and codes on computational fluid dynamics. However, process intensification goes beyond process optimization making the modeling tools – or the modeling Ansätze generally – much more versatile. This chapter will begin with a brief discussion of process intensification from the conceptual and management points of view. In the second section we will report on process-intensification strategies for gas-phase processes based entirely on relatively simple model calculations. Finally we will discuss molecular and financial simulation approaches that are important in the practical work on process-intensification projects.

2.1.1
Remarks on the Term Process Intensification

The definition of process intensification is still an ongoing process. In 1986 Cross and Ramshaw offered the definition: "Process intensification is a term used to describe the strategy of reducing the size of chemical plant needed to achieve a given production objective" [1]. In 2000 Stankiewicz and Moulijn proposed: "Any chemical engineering development that leads to a substantially smaller, cleaner, and more energy-efficient technology is process intensification" [2]. These definitions restrict process intensification to *engineering* methods and equipment and explicitly exclude the development of a new chemical route or the change in composition of a catalyst (see, e.g., [2]). We are convinced that these narrow definitions are inadequate for the description of process-intensification projects in industry. Following Hüther et al. [3] our working definition is: process intensification defines a *holistic* approach starting with an analysis of economic constraints followed by the selection or development of a production process. As

stated above, process intensification thus 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. In view of this definition, modeling in process intensification also includes the employment of methods such as computer-assisted organic synthesis or financial modeling software suites.

2.1.2
Management Aspects

A central precondition of process intensification is creative thinking. Creativity is an active process by which a genuinely new idea takes form. Creativity needs to be distinguished from innovation. In industry, an innovation is the introduction of new products or application processes or services *to the market*. It characterizes the generation of new ideas in order to produce a new product, process or service. Creativity is required if innovation is to be possible. In industrial R&D creativity is usually a product of prior knowledge and thinking, but truly creative acts in science are mostly unplanned. This does not mean that they happen by chance but that they are quite unpredictable and not guaranteed. Although exceptions may exist, significant inventions are usually the results of many years of constant research in a certain field and the accumulation of vast amounts of data. An enormous number of publications exist that discuss how to create an environment for creativity and innovation (see, e.g., [4] and references therein). Since R&D in industry takes place almost exclusively in teams, team work is the key for running a successful research process. Two types of teams seem to be particularly suitable for creative R&D work: crossfunctional and multidisciplinary teams. Crossfunctional teams consist of members who have different functions and specialisms, for instance in research, marketing, controlling and production. In these teams expertise in developing *and* launching new products or technologies are linked. Multidisciplinary teams are especially suited to developing new technologies by pooling the expertise of, for instance, chemists, physicists and engineers.

The organization of R&D addressed to process intensification can be briefly illustrated by considering Degussa's approach where it is realized in the form of a so-called "project house". Project houses have been developed by Degussa for multiunit research. They are a part of *Creavis Technologies & Innovation*, the Degussa R&D unit that attends to crosscompany and crossportfolio research activities to develop new fields of business and technologies. Project houses are formed for a limited time period of three years with the participation of several Degussa business units and Creavis and are linked into internal and external research networks. They include multidisciplinary project teams whose members are recruited from different business and service units. Since process intensification addresses the drastic improvement of a process using novel technologies by rethinking processes as a whole, knowledge of actually existing and realized

technologies and products must be brought together with special knowledge in novel equipment and process technology. The concept of project houses is ideally tailored to these requirements. Sustainability is guaranteed because at the end of a project house's existence, either the business units market the results generated in the form of new products and processes or (in cases where concepts cannot be developed within the business units) internal start-ups for business development are founded.

2.2
Microreaction Technology

2.2.1
Principal Features

Microreaction technology is based on chemical microprocessing that is characterized by a continuous flow of matter through well-defined structures with dimensions that characteristically lie in the interval 0.1–1000 µm. When comparing microreaction technology with (conventional) reaction technology the distinguishing phenomena are usually described as "microeffects" or "scaling effects". Important microeffects are the strongly intensified heat and mass transport in directions of the small lateral dimensions of the apparatus due to diffusion and heat conduction. These are no longer negligible in comparison to convection and are responsible for drastically enhanced heat and mass transfer. Both result in specific advantages over conventional process technology. For example, the usage of microreactors prevents the occurrence of hot spots due to the greatly improved heat dissipation. This makes possible higher reactant concentrations, higher catalyst loading or the use of highly active catalysts when dealing with exothermic reactions. For a comprehensive introduction we refer to [5].

Microreaction technology is used in each of the three phases of product or process development. In the development laboratory it is especially useful in providing precisely defined conditions. Another advantage is its usage in high-throughput experiments. In process development the characteristics mentioned above turn microreaction systems into powerful tools even if the process itself is to be realized using conventional technology. Microreaction technology is particularly useful here in searching for optimal process parameters and in providing benchmarks. A drastically accelerated process development is possible if microstructured equipment is used in production. It is not necessary to perform time-consuming studies for the scale up because the production scale can be realized *in principle* by parallelization; i.e. by multiple repetitions of the microstructured *elements* ("numbering up" the elements). To date, such chemical microprocesses have only been built as pilot plants, largely due to the formidable challenges that must be overcome in the development of technical concepts, and that go beyond the requirements for conventional processes.

2.2.2
Catalytic Wall Reactors

This section offers a short overview of research and process development in a field that is the target of one of the key projects in Degussa's project-house process intensification. Most of this survey has been published recently by Hüther et al. [3].

Partial oxidations are one of the most important classes of gas-phase reactions in the chemical industry. Usually these reactions are highly exothermic and solid catalysts are used. Since the product is generated by an only partial oxidation of the reactant, total oxidation has to be avoided as either a side reaction or an elementary step in a series of reactions. The control of residence time and especially reaction temperature are essential for the enhancement of the selectivity of partial oxidations. A brief look at the reaction enthalpies of ethylene oxide, one of the major intermediate products based on ethylene (in 1999 the world capacity was 14.5 million tonnes per year [6]) illustrates the crucial importance of heat control. The reaction enthalpy of the partial oxidation of ethylene to ethylene oxide is –105 kJ/mol, while the total oxidation of ethylene resulting in carbon dioxide and water is more than one order of magnitude larger at –1327 kJ/mol. Consequently this side reaction causes the occurrence of regions of extremely high temperatures (hot spots) with negative impact on the selectivity and the lifetime of catalysts.

In order to enhance space-time yields of catalytic gas-phase reactions, two strategies are in principle possible: the improvement of catalyst activity or the implementation of more intense process conditions. This usually leads to an increase of heat production that can only be partially released, if at all, using conventional reactor technology.

A simple estimation of the temperature profile inside a tube reactor starts from an energy balance for the system [7]. Since we are particularly interested in the performances of a tube reactor and a catalytic wall reactor the following simplifying assumptions are made:

1. A constant heat conduction and viscosity is achieved.
2. Heat conduction in the longitudinal direction is neglected.
3. Friction in the bed of solid catalyst pellets is neglected.
4. It is assumed that the reactor is an ideal tubular flow reactor.
5. The temperature dependence of the reaction is neglected.

The final assumption is a drastic simplification that leads to an *underestimation* of the temperature increase. The temperature T of an arbitrary point in the catalytic bed may be related to the effective thermal conductivity λ, the heat of reaction ΔH_R and the rate of reaction $\tilde{r}$ by the differential equation

$$\lambda \left(\frac{\partial^2 T}{\partial r^2} \right) - \Delta H_R \cdot \tilde{r}(c, T) = 0 \tag{2.1}$$