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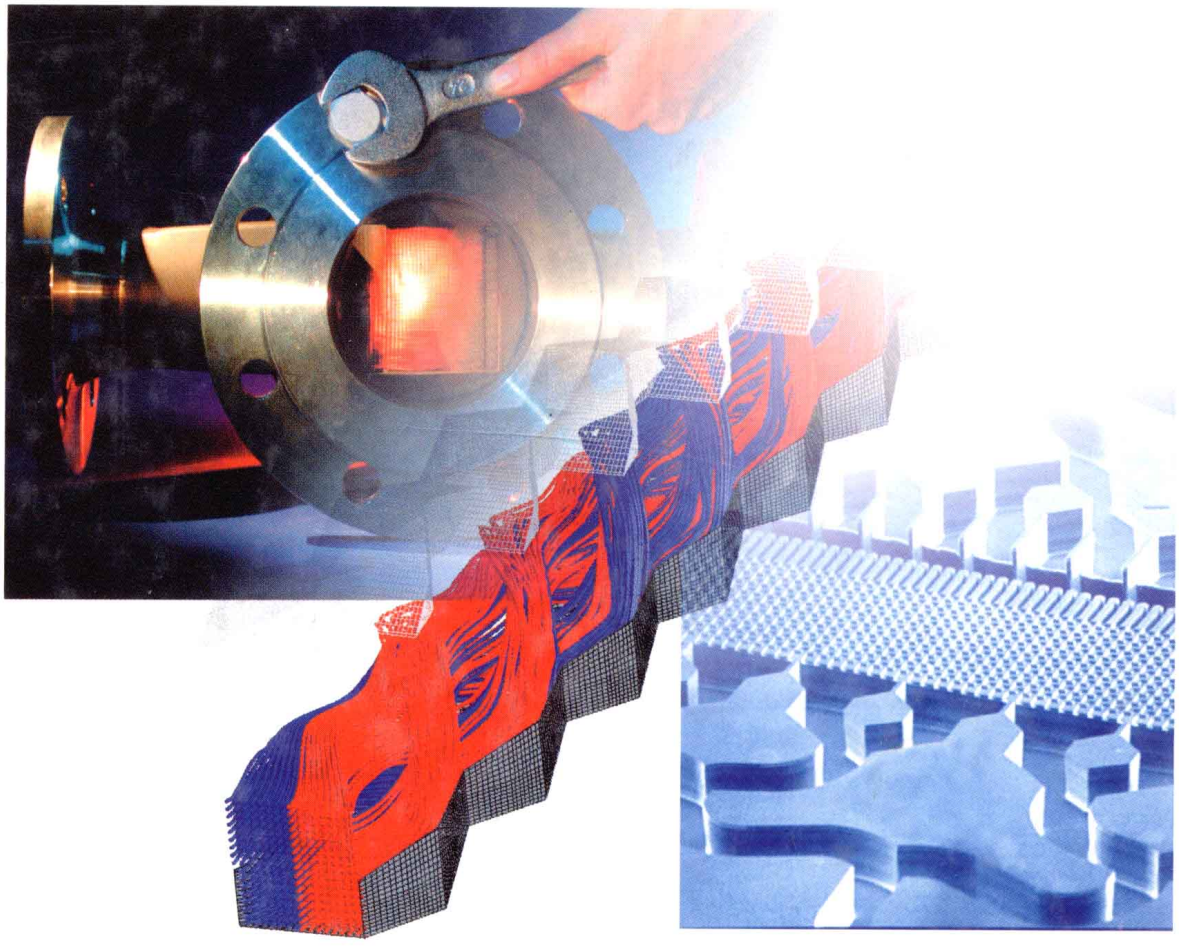
Chemical Micro Process Engineering

Fundamentals, Modelling and Reactions



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Cover Illustration

Upper left: Production- and pilot-scale gas/gas counter-flow heat exchanger comprising microstructured channel arrays. The device (including flanges about 36 kg heavy and 54 cm long), made of stainless steel, is designed for gas throughput in the range of m^3/min at 100 mbar pressure drop for a power of about 10 kW. The internals consist of a stack of microstructured plates having multi-channel arrays of a channel width of 2 mm, depth of 250 μm, and length of 240 mm. Totaling, 6685 micro channels are operated in parallel in this device. The flange-type connection allows installation in large-scale industrial plants (IMM Mainz-Hechtsheim, Germany).

Center: CFD simulation of streamlines of a liquid flow in a caterpillar micro mixer. This device utilizes the split-recombine principle leading to distributive mixing. It is seen that by multiple repetition of this principle the entanglement of the streams increases (IMM Mainz-Hechtsheim, Germany).

Lower right: Cross-flow catalyst screening device with multiple short mini-fixed beds. The fixed-bed catalyst section is fed by bifurcation-channel flow architectures that serve for flow equipartition. This device is a typical example for the class of smart chip reactors, widely employed for analytical-chemistry, kinetic studies and process/catalyst screening purposes on a lab-scale level, and is fabricated using MEMS technology based on silicon micromachining (Courtesy K. S. Jensen, MIT Cambridge, USA).

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Preface

Carrying out chemical reactions in volumes as small as possible is *a priori* not a completely new idea. In the beginnings of chemical experimentation, dating back to the age of alchemy, chemical substances like sulphuric acid or ammonia were much more valuable than gold, and very small reaction vessels were used to economize on the precious materials. When analytical chemistry was established as a second, independent discipline, the desire to make do with ever less material was very strong in order to avoid consuming large portions of the product for analysis. Establishing increasingly sensitive analytical techniques has therefore been one of the most significant driving forces in analytics research.

The beginning of the industrial age saw a substantial increase in demand for basic materials and chemicals, and the chemical industry was established to satisfy these demands for high production volumes. The tall and impressive silhouettes of modern chemical plants dominate industrial estates, visible from afar as symbols for the vast capabilities and capacities of today's chemical industry. Without this industry and its equipment of enormous proportions, our economic wealth would be quite inconceivable.

Bearing all this in mind, what is the purpose of Chemical Micro Process Technology?

Conventionally, the development of chemical manufacturing processes takes place subsequently *via* a sequence of different intermediate stages. Approaching the final process design, the reaction volume is successively increased from laboratory scale to reaction vessel dimensions suitable for production outputs of several kilotons *per annum*. This procedure, known as "scale-up", is expensive and time-consuming. During the scale-up, new and previously unencountered problems often crop up and have to be solved. It may even occur that the complete development process has to be re-initiated in order to cirumvent severe obstacles. Furthermore, the developed industrial process is laid out for a specific, predefined throughput, a fact which constrains the later flexibility of production significantly.

The solution of these problems is based on a simple idea: the developed laboratory-scale process is used for manufacturing of a chemical product by parallelization of many small units. Although promising great advantages over scale-up, this procedure, denoted "numbering-up", is not trivial by far. It cannot be carried out in a simple way due to the tremendous technological effort necessary: a chemical plant with hundreds or even thousands of small-scaled vessels, stirrers, heaters, pumps,

etc. would be impractical. A new way of engineering and new technologies had to be developed to combine the advantages of lab-scale processing with the necessities associated with production-scale throughput. First steps into this direction have been taken, and despite some remaining throughput restrictions, first successes have become visible. Also, economical and ecological reasons create increasing demand for further steps in process intensification and sustainable development.

The present book is devoted to both the experimentally tested micro reactors and micro reaction systems described in current scientific literature as well as the corresponding processes. It will become apparent that many micro reactors at first sight "simply" consist of a multitude of parallel channels. However, a closer look reveals that the details of fluid dynamics or heat and mass transfer often determine their performance. For this reason, besides the description of the equipment and processes referred to above, this book contains a separate chapter on modeling and simulation of transport phenomena in micro reactors.

Using specific examples of gas-phase, gas/liquid and liquid-phase reactions, the advantages of microstructured reactors are highlighted in comparison to conventional equipment. At the same time, known problems are pointed out and some processes are listed for which micro reactors so far failed to show superior performance. Furthermore, the book is conceived as a compendium. Processes, microstructured reactors and chemical reactions are described in an integrated manner, providing in each case the relevant original citations. Equipped with the data given in this book, readers will be able to identify the most suitable reactor to successfully perform a given chemical reaction on the micro scale.

By now, Chemical Micro Process Technology has been established as an independent discipline, bringing forth over 1500 publications in the last few years, and an end is not foreseeable. The surge of scientific cognitions encouraged the authors to write this book, which should provide a deeper insight into this new and fascinating subject.

We are very grateful to those who helped this project become reality. In particular, we would like to mention K. Bouras, T. Hang, C. Mohrmann, and L. Widarto, who prepared electronic versions of many of the figures appearing in this book. We also wish to thank C. Mohrmann and L. Widarto for handling the copyright transfer formalities and T. Hang for taking pictures of some of IMM's micro devices. A special thanks goes to B. Knabe and R. Schenk for helping us with literature retrieval. Last but not least, we are indebted to K. S. Drese and F. Schönfeld for the thorough checking of parts of our manuscript.

Mainz, November 2003 *The authors*

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