Edited by K. Sundmacher, A. Kienle,
H. J. Pesch, J. F. Berndt, and G. Huppmann

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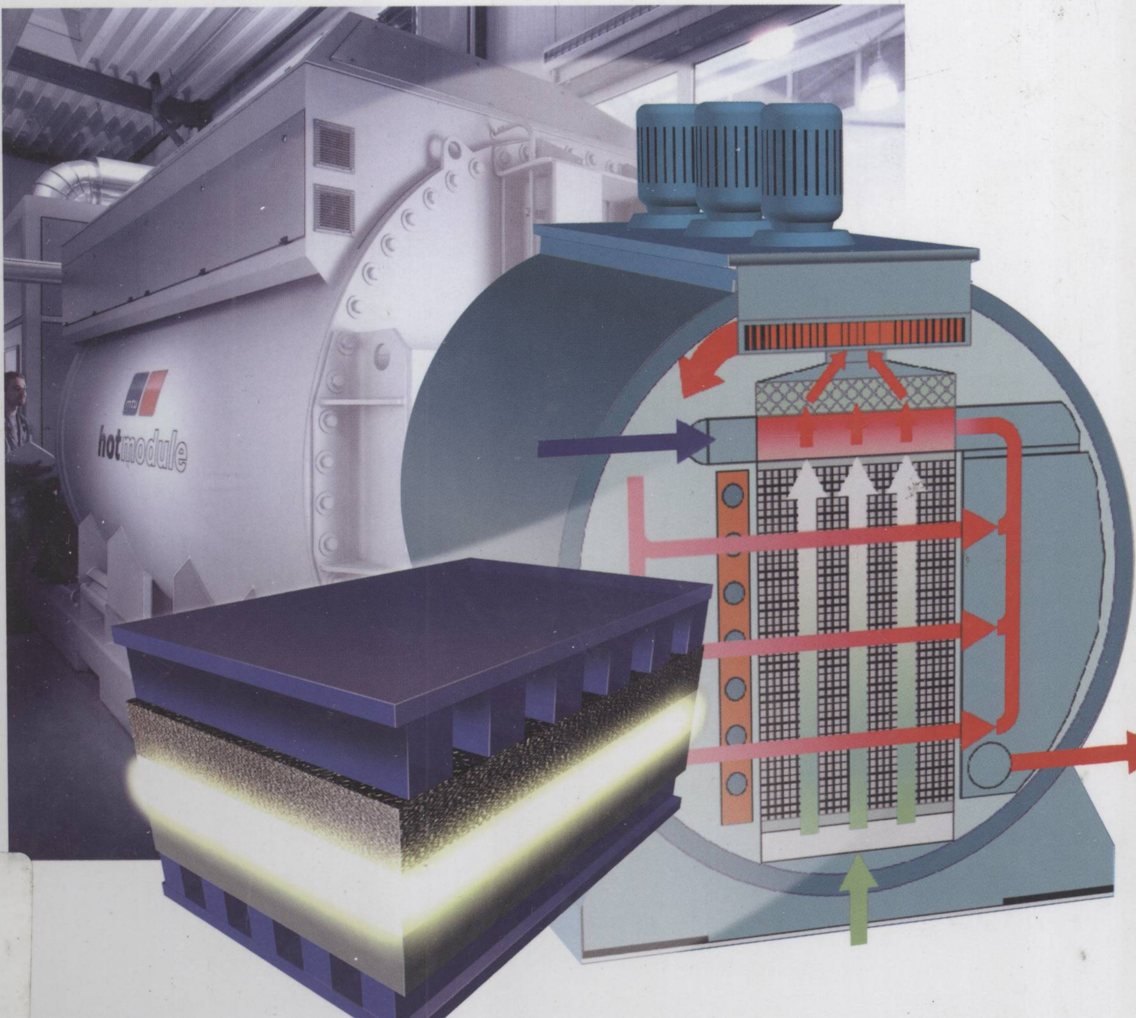
Modeling, Analysis, Simulation, and Control



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Preface

Fuel cells generate electrical energy by electrochemical oxidation of chemical substances such as hydrogen, carbon monoxide, methanol, ethanol, glucose or other hydrocarbons. Due to their functional principle, fuel cells can achieve much higher efficiencies for energy conversion than conventional systems which are based on the Carnot cycle. Because of their high conversion efficiency, fuel cells will play a major role in the future mix of power supply systems.

The importance of fuel cells is also reflected by an exponential increase of journal papers and book contributions being published during the last two decades (see Fig. 1). Among the published papers and books, most are focused on polymer electrolyte fuel cells (PEMFC), direct methanol fuel cells (DMFC) and solid oxide fuel cells (SOFC). In comparison to these types of cells, the molten carbonate fuel cell (MCFC) so far has attracted relatively little attention. But this is in total contrast to the current status of system development. While large-scale applications of PEMFC, DMFC and SOFC-systems up to now are still quite rare, more than 20 demonstration plants of the MCFC HotModule type (power range: 250–300 kW) were already installed successfully for various applications by the company CFC Solutions Ltd./Ottobrunn in Germany.

As another trend, the literature analysis clearly reveals that the proportion of publications dealing with the model-based analysis and control of fuel cells is steadily increasing. But this research field is still young and therefore it comprises only about one tenth of the overall number of articles and books in this whole area (see Fig. 1). Designing efficient fuel cell stacks not only requires suitable electrode and membrane materials, but also powerful engineering methodologies and tools. Due to the complex nonlinear behaviour of fuel cells, their design and operation cannot be based on pure intuition. This is why advanced model-based methods for the analysis, control and operation have to be further developed in the next few years.

A comprehensive volume covering all aspects of model-based analysis, control and operation of fuel cell systems is still missing. To fill this gap, the present book was prepared with special focus on the MCFC as an example of high technical relevance. The presented concepts and methods are also transferable to other fuel cell types such as the PEMFC.

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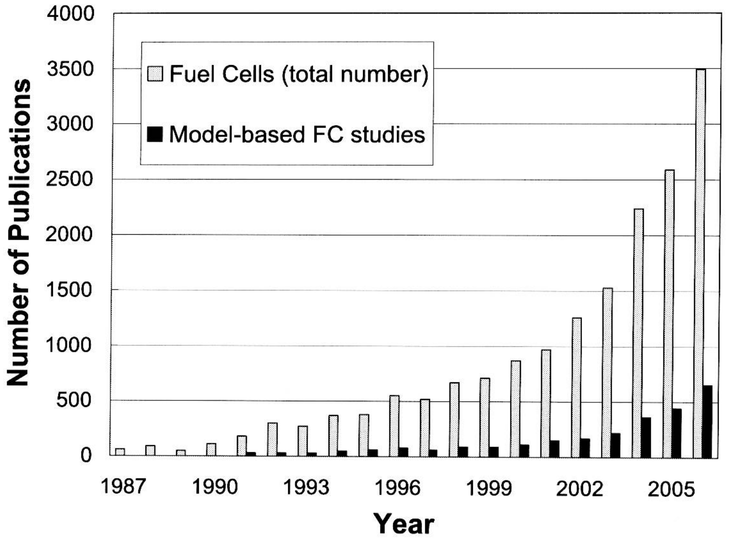

Fig. 1 Journal publications on fuel cells from 1987 to 2006 according to the Science Citation Index.

The book is divided into three parts: Part A surveys the design and operation of MCFC fuel cells with special focus on the HotModule type, which integrates the generation of hydrogen by methane steam reforming and the electrochemical oxidation of hydrogen in one single unit. Part B is dedicated to process analysis by means of mathematical models describing the complex interactions of mass, energy and charge transport phenomena within the fuel cell stack. Part C focuses on how process models can be used for state estimation, for advanced control strategies and for solving steady-state as well as dynamic optimization tasks.

Part A: Design and Operation

Chapter 1 being written by Gerhard Huppmann, who is one of the inventors of *MTU's Carbonate Fuel Cell HotModule*, is concerned with the basic concepts and the key features of the cell design, presents possible applications using natural gas and other fuels, and discusses important economical aspects. Focus in Chapter 2 is on *Operational Experiences* which are reported by Koch et al. The authors collected a series of experimental data at different load scenarios at a 250 kW_{el} MCFC HotModule stack which is installed as part of IPF's power plant at the University hospital in Magdeburg. The data form the basis for the identification of realistic model parameter values being a major prerequisite for reliable fuel cell simulations which are reported in the subsequent chapters.

Part B: Model-Based Process Analysis

In Chapter 3, Heidebrecht et al. present a rigorous *MCFC reference model* which accounts for the most important physico-chemical phenomena within the cell and also for the special recycle structure of the HotModule process. The model consists of a coupled set of hyperbolic and parabolic partial differential equations along with further ordinary differential and algebraic equations, completed by an integral equation expressing the overall charge conservation condition. The numerical treatment of these model equations, using finite volume discretization methods, results in a set of differential-algebraic equations (DAE) whose *index analysis* is performed by Chudej et al. in Chapter 4.

As outlined by Gundermann et al. in Chapter 5, *parameter identification* at an industrial-scale MCFC stack requires a special stepwise strategy which has to account for measurement errors as well as for possible leakages at the plant. With regard to cell dynamics, the solid heat capacity is the key parameter to be determined. Once realistic fuel cell model parameters have been identified, one can simulate the steady-state behaviour, particularly the current-voltage performance curve. Furthermore, the *process* analysis presented by Heidebrecht et al. in Chapter 6 includes the dynamic cell voltage decline after a load increase which can occur when the fuel cell is moved from a low-current operating point to a higher current load.

In Chapter 7, Krasnyk et al. present theoretical predictions of *hot spot formation and steady-state multiplicities* in high-temperature fuel cells. The discovered phenomena are relevant for the MCFC as well as for the SOFC and arise from the increase of the ion conductivity of electrolytes at increasing operating temperatures.

In the final chapter of part B, Heidebrecht et al. analyse and compare different *conceptual designs and reforming concepts* by means of a simple along-the-channel anode model. From this study it turns out clearly that the highest current yields are attainable by direct internal reforming within the anode channels.

Part C: Optimization and Advanced Control

The efficient operation of industrial scale fuel cell plants such as the MCFC HotModule requires continuous monitoring of key state parameters. In particular, for safe load changes one would like to know the spatially distributed temperature field within the fuel cell stack. But the experimental accessibility of internal temperatures is quite limited. Therefore, as a very promising monitoring alternative, Grötsch et al. in Chapter 9 show how to develop a model-based observer via *model reduction and state estimation* for tracing the dynamic evolution of the MCFC temperature field.

The subject of Chapter 10 which was written by Sternberg et al. are *optimal control strategies* for load changes between two predefined steady-state operating points. The aim of control is to attain the new steady state as fast as possible after load change. This leads to a so-called boundary control problem which can be tackled with the help of the software package NUDOCCCS.

In the final contribution, Heidebrecht et al. show that the *optimization of the reforming catalyst distribution* can lead to significant improvements of the fuel cell efficiency. Since methane steam reforming is an endothermic reaction, it can be used as an internal cooling element for the exothermic electrochemical reactions.

In the appendix, the complete set of equations and related parameters is given for the *MCFC reference model* which is the "mother" of all reduced model variants being used for simulation, analysis, control and optimization as discusses in preceding chapters. This information will serve as a source of information for readers who are interested to get all details in order to start their own comparative studies.

Book History and Acknowledgements

The present book presents the outcome of the joint research project "Optimised control of fuel cell systems using methods of nonlinear dynamics" which was performed from 2002 until the end of 2005 in close collaboration of five German research groups from academia and industry. The project was coordinated and organized by the editors of this book and their colleagues at the Otto-von-Guericke-University Magdeburg, the Max-Planck-Institute for Dynamics of Complex Technical Systems in Magdeburg, the University of Bayreuth, the power plant operating company IPF Heizkraftwerksbetriebsgesellschaft Ltd., and the Molten Carbonate Fuel Cell producing company MTU CFC Solutions Ltd. in Ottobrunn. The financial support of the joint project from the Federal Ministry of Education and Research (BMBF) in Germany is very gratefully acknowledged. Intermediate results were discussed in 2004 on a MCFC workshop with financial support from the German Competence Network Pro3 e.V. which is also gratefully acknowledged.

The editors like to thank particularly their colleagues Peter Heidebrecht, Matthias Gundermann, Michael Mangold, Markus Grötsch, Mihai Krasnyk, Kurt Chudej, Kati Sternberg and Mario Koch for their excellent support during the project work and in preparing the manuscripts being the basis for the present book publication. Last but not least, we are very thankful to Dr. Rainer Münz from Wiley-VCH for his helpful assistance during the production of this book.

March 2007

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Further Reading

Sundmacher, K., Kienle, A., Seidel-Morgenstern, A. (Eds.)

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