PREFACE

Fuel cells are energy converters able to transform chemically stored energy directly to electrical energy at high thermodynamic efficiencies. From the point of view of chemical engineers, fuel cells are electrochemical membrane reactors featuring a high degree of complexity due to the interaction of multistep electrode reactions with simultaneous (and often multiphase) mass, charge, and energy transport phenomena. In spite of significant progress during the past two decades, further improvements of performance, durability, and controllability are necessary for translating fuel cell technologies into commercial products. For this purpose, a detailed understanding of the steady state and dynamic behavior of fuel cells—on electrode level, the single cell level, and the system level—is of fundamental importance. This can be achieved only by physical–chemical modeling of all relevant processes involved in the operation of fuel cell systems. Thus, the present issue of *Advances in Chemical Engineering* is focused on the model-based analysis, control, and optimization of fuel cells.

Chapter 1 gives an overview on different chemical routes for converting hydrocarbon fuels to hydrogen or hydrogen-rich gas mixtures usable for operating different types of fuel cells. Apart from fuels, fuel processors, and fuel requirements, quantitative modeling and simulation approaches are reported, aiming at the description of the molecular processes during fuel conversion and the prediction of chemical reactions on catalytic surfaces in combination with heat and mass transport phenomena between surfaces and gaseous fluids.

Chapter 2 is focused on polymer electrolyte fuel cells (PEFCs) which receive the most attention for automotive and small stationary applications because of their high electrical efficiency and power density. The governing conservation equations, transport equations, electrochemical reaction kinetics, and thermodynamic relations are examined with regard to performance-related issues. The chapter is written as a guide toward understanding the complex interactions that occur within PEFCs.

While conventional PEFCs are operated with high purity hydrogen gas as anode feed, direct methanol fuel cells (DMFCs) are fed with aqueous methanol solutions. This makes DMFCs attractive for mobile and portable applications. Chapter 3 reports the principles of operation and models which have been developed to create viable DMFCs.

In particular, models which describe the dynamic cell response are reviewed to aid in development of control strategies.

Chapter 4 is focused on PEFC fuel cell system modeling and controller design. The formulation of lumped parameter models, able to capture the essential dynamics of fuel cell stacks and systems, is discussed. The design of controllers for hydrogen purge, heat management, and air supply is described. Conventional PID controllers as well as advanced control methods (Model Predictive Control) are presented. Moreover, selected approaches for fuel cell fault diagnosis are presented.

Chapter 5 briefly summarizes the physical phenomena responsible for the degradation phenomena occurring in various parts of PEFC fuel cells. It is mainly targeted at the experimental techniques and models used by engineers for evaluating aging processes. The operating conditions applied in long-term tests of fuel cell components are presented and a selection of typical aging situations is discussed.

While Chapters 2–5 cover different aspects of low-temperature PEFCs, the following contributions are focused on high-temperature solid oxide fuel cells (SOFCs). Chapter 6 presents a modeling framework for SOFCs, including the transport phenomena and chemical and electrochemistry reactions. Using tubular and planar cells as examples, model problems are solved to illustrate and discuss both steady state and dynamical behaviors. The latter are highly relevant for the interpretation of electrochemical impedance spectra and for the development of control strategies, as well as for coordinating multiple sensors and actuators.

Chapter 7 discusses SOFCs at the system level, that is, the integration of a cell stack with the so-called balance-of-plant components (BoP: reformer, pumps, blowers, heat exchangers, burner, etc.). Understanding and predicting the exchange of matter and energy among the BoP components is essential for system design and control. In addition to system efficiency, one has to perform a careful analysis of the life-cycle costs in order to optimize the overall system performance.

Of course, this collection of chapters does not represent a comprehensive compendium of the whole area of fuel cell engineering. But I hope that this sampling of work will provide graduate students and experienced practitioners with a helpful introduction to the current state of model-based fuel cell analysis, control, and optimization.

Finally, I would like to thank the series editor Prof. Guy Marin and the publisher Elsevier for the invitation to organize this topical issue. And, of course, I am very thankful to the authors of the seven chapters for taking time to contribute to this volume.

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