Journal of Fuel Cell Science and Technology

Guest Editorial

Modeling and Simulation of PEM Fuel Cells

The operation of fuel cells with polymer electrolyte membranes (PEMs) is based on complex interactions of physical, chemical, and electrochemical processes on multiple scales. Understanding these basic processes and their interactions is a key issue for the improvement of cell performance and for the identification of critical issues to be addressed by research for new materials and construction principles. A qualitative and quantitative understanding of this complex matter is possible only on the base of mathematical models.

In this issue, we focus on the processes on the scale of a single cell. The spatial distribution of the species is modeled by systems of partial differential equations describing coupled transport and reactions. The so created models are rather complex, and do not admit readily available analytical solutions. A mathematical analysis of these models is possible only after strong simplifications, while putting the focus on a small set of basic features, or using approaches such as boundary layer theory classically known to electrochemists.

An alternative is to use numerical simulations as a tool to approximate the solutions of the partial differential equation. Current numerical models are able to handle rather complex interactions, and therefore are an indispensable tool already for the qualitative understanding. Their predictive capabilities strongly depend on the availability of parameters and on the proper link between the different scales. Here, the situation is not really satisfactory, calling for mathematically sound upscaling approaches and for the mathematical support of the measurement process itself.

At the workshop "Modeling and Simulation of PEM Fuel Cells," these topics were addressed and discussed by an international group of scientists. The workshop took place in Berlin, Germany on Sept. 18–20, 2006 at the Weierstrass Institute for Applied Analysis and Stochastics (WIAS) in Berlin. It was organized jointly by Fuhrmann and Holzbecher (WIAS) as well as by Haasdonk, and M. Ohlberger (Institute for Applied Mathematics of Freiburg University).

It was an event of the interdisciplinary network "H2 and Direct Methanol PEM Fuel Cells" supported by the German Federal Ministry of Education and Research within its funding program "Networks in Basic Research for Renewable Energy and Efficient Energy Usage," and as such received financial support from the Ministry.

The meeting had 50 international participants, among them several company representatives, and 5 invited speakers. The entire program of the workshop is available in the internet (http://www.mathematik.uni-freiburg.de/IAM/News/workshops/PEMSIM2006/). Special topics of the workshops were the modeling and simulation of H_2 and methanol fuel cells and stacks, with special emphasis on bubble transport, the mathematical description of porous transport layers and the three phase boundary, molecular dynamic simulations of new types of polymer membranes, and the analysis, control, and reduction of complex nonlinear systems.

This special issue collects a selection of original contributions to the workshop with respect to different fields, which roughly can be grouped into three categories.

The first group of papers deals with the development and application of mathematical approaches to the handling of complex nonlinear systems in the context of fuel cells. This includes sensitivity analysis (Sternberg) and bifurcation analysis (Groetsch).

A second group of papers is devoted to transport models. These concern two phase material parameters (Becker), two phase transport in cathodes (Gurau), and membrane modeling (Steinkamp). All three papers have in common the modeling of transport in multiple phases.

Finally, a third group handles coupling between transport and reactions: catalytic reaction kinetics measured in flow cells (Fuhrmann) and upscaling at the triple phase boundary between catalyst, membrane, and pore space in the porous catalyst layer (Berg).

These topics show prominently the width of the field of PEM fuel cell modeling. In this complex situation, a common point of the papers is that they emphasize the strength of the mathematical modeling approach. They go beyond "simple forward calculations." Advanced topics of the mathematical modeling approach such as upscaling, inverse estimates, bifurcation analysis, sensitivity analysis, or model reduction are discussed in this special issue.

We hope that the publication of these papers in the *Journal of Fuel Cell Science and Technology* will stimulate further research and discussion of mathematical modeling and simulation for fuel cells. This research can only be performed jointly by mathematicians, natural scientists, and engineers.

J. Fuhrmann
Weierstrass Institute for Applied Analysis and Stochastics,
Berlin, Germany

B. Haasdonk
Albert-Ludwigs-Universität Freiburg,
Freiburg im Breisgau, Germany

E. Holzbecher
Weierstrass Institute for Applied Analysis and Stochastics,
Berlin, Germany

M. Ohlberger
Universität Münster,
Münster, Germany

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