Guest Editorial

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Guest Editorial

Special Issue on Modeling and Experimental Validation of Fuel Cells, Batteries, and Electrolysers

In the 1980s and 1990s, progress in fuel cell and battery research evolved mainly around materials development, empirical approaches, and efforts focusing mostly separately on either the microscale (electrodes and electrolytes) or the macroscale (systems, thermodynamics, and balance-of-plant). Since the 2000s, with the advent of more powerful computing and modeling resources, and the general progress in the field, it has seen a shift to the merging of scales, the possibility of 3D probing and quantification with fuel cell stacks and battery packs becoming the focal point. In parallel, disciplines have merged, too: a holistic and a detailed understanding in the range of underlying phenomena of chemistry, physics, materials science, and mechanical engineering has been combined with the addition of the influence of an electrical field or current. This union is essential to achieve the progress needed for the commercial breakthrough expected from the technologies. It became established that both experimental and modeling aspects deserve simultaneous and an equally weighted consideration, and it is recognized that the correspondences between models and experiments deliver among the most valuable advances to the field, due to the level of confidence and insight they provide.

It was in this spirit that the Symposium on Modeling and Experimental Validation of Fuel Cells (MODVAL) was created in 2004 by Swiss and German fuel cell scientists, supported since its creation by the Swiss Federal Energy Office, to bring together modelers from essentially the polymer electrolyte and solid oxide fuel cell worlds, at first mostly from Switzerland and Germany. The MODVAL Symposium became established as an annual two-day event taking place in March, usually alternating between a German and Swiss academic institution to host it, and it explicitly emphasizes the validation component for submitted contributions, i.e., each paper should appeal or "talk" to modelers and experimentalists and ideally deal with both modeling and experimental aspects in its contribution. Several years ago, the strongly growing battery topic was rather naturally added to the fuel cell topic and, further on, electrolysis. The number of participants has grown over the years, too, to equilibrate itself at around 120–130 people, still dominated by Swiss and German participation, but increasingly Pan-European and international. Covered topics are:

- Modeling on all the scales, 0D to 3D and nano to macro: kinetics, electrode and transport processes, microstructures, cells, repeating units, stacks, and systems; steady state and dynamic; and design, degradation, and performance. Contributions highlight the result or application or the simulation approach and methodology.
- *Validation experiments*: for model parameter determination, in situ/ex situ/post-test characterization techniques; 3D-microstructure quantification and transport phenomena; data interpretation (e.g., impedance spectroscopy); and advanced measurements (electrode segmentation and local diagnostics).
- *Application areas*: flow and thermal management, water management, degradation, reliability, control, stress, fuel processing, etc.

Of the submitted contributions, roughly 2/3rd are presented orally, in parallel sessions, and the remaining 1/3rd in a poster session. In March 2016, the Swiss Federal Institute of Technology in Lausanne (EPFL), through its specialized research Group of Energy Materials (GEM) active in fuel cells, organized the 13th annual MODVAL event, in the SwissTech Convention Center on EPF-Lausanne campus, receiving 60 oral contributions and 35 posters, of which roughly 1/3rd on batteries, 1/3rd on polymer electrolyte fuel cells, and 1/3rd on remaining topics (solid oxide fuel cells, electrolysis, etc.). Five invited talks were included from distinguished international speakers. After the symposium, a series of papers were submitted for the intention of a special issue, of which the present volume is the first one.

In a study on reduced-order models for Li-ion batteries, Gopalakrishnan et al. drastically reduced computation time and memory usage (factor 100) by their new approach of the discrete-time realization algorithm. The improved method helps paving the way toward real-time battery management, implementing a physics-based battery model. Along similar lines, in his paper Shah used dimensionality reduction to develop a surrogate model approach for field variables in fuel cells, based on Gaussian process modeling and principal component analysis to overcome computational issues. In their paper concerned with methanol crossover in direct methanol fuel cells, Bayat and coworkers used a 3D finite element model considering single phases, gas at the cathode (air) and liquid at the anode (methanol). Their model only slightly overpredicts experimental i-V results, remaining useful to predict the fuel cell performance under the influence of temperature, anode-side layers' porosity, and methanol concentration. Yokokawa et al. addressed the persistent and inherent issue of electrolyte conductivity degradation (yttria–zirconia) in high-temperature solid oxide fuel cells, using Raman data for the slow cubic-to-tetragonal transformation, related to NiO dissolution, thermally activated Y-diffusion, and an oxygen potential profile shift within the electrolyte, all affecting the oxygen ion conductivity decay. They highlight the importance of this degradation effect in interpreting ohmic losses in real stacks versus test pellets. Moving on toward the design of SOFC systems, Wagner and Schiffmann in their innovative development design computed and demonstrated what it takes to couple a high-speed miniature fan with an SOFC stack on the 10 kWe scale to recirculate a large part of the anode exhaust to the reformer inlet, reducing the system complexity (no water source needed) without penalizing net electrical system efficiency. Finally, Majerus et al. made the case for the use of SOFCs with biogas as resource, typically of small power scale and totally underused and therefore of immense potential in combination. They compute under which precise circumstances SOFCs become economically

viable to valorize this underestimated resource. These articles comprise the first part of this special issue. Additional articles that comprise the second part of this special issue will be published in a future issue.

We would like to very sincerely thank Professor Dr. W. K. S. Chiu for the kind suggestion to propose the ASME *Journal of Electrochemical Energy Conversion and Storage* to be the platform for this Special Issue of the MODVAL-13 Symposium and his relentless efforts and support in its concrete realization. The reviewers also deserve a special and warm thanks for their essential and demanding work in our epoch where the available time for this task is under ever higher pressure. On the local organizational side, our most sincere gratitude is extended to Mr. Nicolas Borboën, IT-specialist in the EPFL Faculty of Engineering Sciences, and Mrs. Valérie Jacot-Descombes, of the Event Managing Team at EPFL, for their tremendous help and investment in all the organizational matters, announcements, website, invites, circulars, finances, Book of Abstracts, scheduling, catering, accommodation, reception, and back-office, in order to make MODVAL-13 to another successful symposium in the series.

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