

Expert Discussion Panel

Panel Topic: Computational Tools for Polymer Electrolyte Fuel Cell Analysis and Design

- Panel Time and date: 11:00 am - 12:30 pm on August 20, 2021 (EDT)

Panel Session Description:

Polymer electrolyte fuel cell modeling is a multi-disciplinary problem involving physico-chemical phenomena at multiple spatial and temporal scales. The aim of this panel is to highlight recent advancement in computational modeling of polymer electrolyte fuel cells at stack, cell, pore, molecular and atomistic level, and to discuss the advancements necessary to bridge the gap between scales. Topics of discussion will include how to embed advanced membrane electrode assembly (MEA) models into stack models, how new insights from molecular dynamics (MD) and density functional theory (DFT) can improve current MEA membrane and catalyst degradation models, and how can MEA models harness the computational speed of pore-networks to provide better water management predictions in a reasonable time. Finally, the role of open-source software development, standardization, and its role on improving interaction between scales will be addressed.

Panel Moderator: M. Secanell, University of Alberta, Canada

Expert Panelists:

- S. Beale, Forschungszentrum Jülich, Germany
- M. Eikerling, RWTH Aachen University and Forschungszentrum Jülich (IEK-13), Germany
- Weber, Lawrence Berkeley National Laboratory, USA
- J. Gostick, University of Waterloo, Canada
- M. Secanell, University of Alberta, Canada (moderator)

Biography of Panelists:



Steven B. Beale is a scientist and group leader at Forschungszentrum Jülich. His expertise includes fluid flow, heat/mass transfer, and electrochemistry in fuel cells and electrolyzers, physicochemical hydrodynamics in microstructures and porous media, multi-phase flow, and high-performance computing. Dr. Beale was formerly a principal research officer at the National Research Council of Canada. He has 36 years experience in computational fluid dynamics, and 21 years in fuel cells. He is currently operating agent for the IEA Advanced Fuel Cells, Modelling Annex. He holds engineering degrees from McGill, University of California at Berkeley, and a PhD

with Prof. D.B. Spalding FRS, from Imperial College London. An active adjunct Professor at Queen's University since 2003, he is Fellow IMechE (UK) and ASME (USA), from whom he received the dedicated service award. He is currently an editor for J. Electrochemical Energy

Conversion and Storage, Thermopedia, and Computational Thermal Sciences. A former chair ASME Process Industry Division, and former member ASME James Potter thermodynamics medal awards committee, he was also executive director of the CFD society of Canada. Dr. Beale has approx. 150 book chapters, journal articles, peer reviewed conferences proceedings, and technical reports. He has given numerous keynote and invited lectures at LANL, NASA, Imperial College, EU-JSC, ASME, and elsewhere.



Michael Eikerling received his Ph.D. in Physics from Technische Universität München in 1999. From 2003 to 2019, he was Professor of theoretical chemical physics and electrochemical materials science at Simon Fraser University in Burnaby, British Columbia, Canada. Between 2003 and 2013, he held a cross-appointment to the fuel cell institute of Canada's National Research Council in Vancouver, BC, where he shaped a program in physical modeling of fuel cells. As of May 2019, he was appointed as Professor at RWTH Aachen University and Director at the new sub-institute for Theory and Computation of Energy Materials (IEK-13) in Forschungszentrum Jülich, Germany. His research employs a comprehensive spectrum of methods in physical theory and

computation. He has made high impact contributions to: transport phenomena at interfaces and in nanopores, theory and computation of electrocatalytic phenomena, self-organization in electrochemical materials, statistical physics of heterogeneous media, porous electrode theory, and modeling and diagnostics of electrochemical devices. Prof. Eikerling has supervised > 60 highly qualified personnel, including 22 PhD students and 25 postdoctoral fellows. He has published over 150 journal articles (h-index 40), 8 book chapters and 1 textbook. He has delivered 160 invited presentations (including 33 keynote and 8 plenary talks, and 65 seminars). In 2017, he was awarded the Alexander Kuznetsov Prize for Theoretical Electrochemistry of the International Society of Electrochemistry, in recognition of his groundbreaking work on modeling polymer electrolyte fuel cells, with an emphasis on water management, transport and electrocatalysis.



Jeff Gostick is an Associate Professor in Chemical Engineering at the University of Waterloo where he runs the Porous Materials Engineering & Analysis Lab. His research is centered around understanding the structure-performance relationship in porous electrodes used in hydrogen fuel cell, redox flow systems, zinc-air cells, Li-ion batteries, and super-capacitors. His group uses a combination of experimental characterization, novel production methods, and advanced custom computational tools. He is the lead developer of the open source pore network modeling project OpenPNM (openpnm.org), as well as PoreSpy, a tool for porous media image analysis (porespy.org). Prof Gostick is a licensed professional engineer, has published over 70 journal articles, and was recently named an Emerging Leader by the Canadian Society for Chemical Engineering.



Adam Z. Weber holds B.S. and M.S. degrees from Tufts University, and a Ph.D. at University of California, Berkeley in chemical engineering under the guidance of John Newman. Dr. Weber is a Senior Scientist and Leader of the Energy-Conversion at Lawrence Berkeley National Laboratory, co-Director of the Million Mile Fuel Cell Truck Consortium and co-Deputy Director of HydroGen consortium. His current research involves understanding and optimizing fuel-cell and electrolyzer performance and lifetime including component and ionomer structure/function studies using advanced modeling and diagnostics, understanding flow batteries for grid-scale

energy storage, and analysis of solar-fuel generators and CO₂ reduction. Dr. Weber has coauthored over 170 peer-reviewed articles and 10 book chapters on fuel cells, flow batteries, and related electrochemical devices, developed many widely used models for fuel cells and their components, and has been invited to present his work at various international and national meetings. He is the recipient of a number of awards including a Fulbright scholarship to Australia, a 2012 Presidential Early Career Award for Scientists and Engineers (PECASE), the 2014 Charles W. Tobias Young Investigator Award of the Electrochemical Society, the 2016 Sir William Grove Award from the International Association for Hydrogen Energy, and a 2020R&D100 award for microelectrode development. He is a Fellow of The Electrochemical Society and the International Association of Advanced Materials.



Marc Secanell is a Professor in the Department of Mechanical Engineering at the University of Alberta, Canada, and the director of the Energy Systems Design Laboratory. He received his Ph.D. and M.Sc. in Mechanical Engineering from the University of Victoria, Canada, in 2008 and 2004, respectively. He holds a B.Eng. degree (2002) from the Universitat Politècnica de Catalunya (BarcelonaTech). In 2008, he was an Assistant Research Officer at the National Research Council of Canada, Institute for Fuel Cell Innovation in Vancouver, Canada and in 2015-16 he was a visiting research scholar in the Energy Conversion Division at the

Lawrence Berkeley National Laboratory, US. His research interests are in the areas of: a) analysis and computational design of polymer electrolyte fuel cells and electrolyzers; b) fabrication and characterization of polymer electrolyte fuel cells and electrolyzers; c) finite element analysis; and, d) multidisciplinary design optimization. His current research projects include the development of the open-source Fuel Cell Simulation Toolbox (OpenFCST - www.openfcst.org), an open-source framework to analyze fuel cells. He has authored over 50 journal articles, 30 conference proceedings and two book chapters receiving over 2,500 citations (h-index: 31 in Google Scholar). He has been an invited speaker at prestigious conferences such as the Electrochemical Society Meeting and the Gordon Research Conference in Fuel Cells. He has received several awards including University of Alberta, Faculty of Engineering Teaching and Research Awards (2020 and 2018) and the Association of Professional Engineers and Geoscientists of Alberta (APEGA) Early Accomplishment Award (2013).