Appendix C: Biographical Information on Subject Matter Experts

Michael Baldea

- Ph.D., Chemical Engineering, University of Minnesota (2006)
- M.Sc., Interface Process Engineering, "Babeş-Bolyai" University, Cluj-Napoca, Romania (2001)
- Diploma, Chemical Engineering, "Babeş-Bolyai" University, Cluj-Napoca, Romania (2000)

Institution

Associate Professor, McKetta Department of Chemical Engineering, University of Texas at Austin

Focus

Modeling, simulation, optimization and control of process and energy systems

Research

Research in our group addresses theoretical challenges and problems of practical importance in the area of process and energy systems engineering. We rely on concepts from multiple fields – nonlinear systems, control, optimization and numerical methods – to develop new theory, algorithms and software tools. Our work follows three major thrusts: integrated decision-making in the chemical and energy supply chains, monitoring and optimizing process performance, and process integration and intensification. Important applications include i) integrating scheduling and control decisions (with a particular focus on chemical plants that interact with the electric grid and can provide ancillary services), ii) quantifying plant-model mismatch for model-based controllers, iii) process data visualization, iv) equation-oriented process simulation and optimization and, v) design and control of intensified processes such as dividing-wall columns and auto thermal reactors. Our research has a strong translational component and we have implemented and validated several of our results on industrial test beds.

Awards

- Outstanding Young Researcher Award, Computing and Systems Technology Division of AIChE (2017)
- NSF CAREER Award (2015-2020)
- Moncrief Grand Challenges Faculty Award, Institute for Computational Engineering and Sciences (2014)

Selected Publications

- C. Tsay, R.C. Pattison, **M. Baldea**, A Dynamic Optimization Approach to Probabilistic Process Design Under Uncertainty, Ind. Eng. Chem. Res., 56, 8606-8621,

2017 http://dx.doi.org/10.1021/acs.iecr.7b00375(invited contribution for the I&EC Research special issue for the 2017 Class of Influential Researchers)

- **M. Baldea**, T.F. Edgar, B. Stanley, A.A. Kiss, Modular Manufacturing: Status, Challenges and Opportunities, AIChE J., 63(10), 4262-4272, 2017 http://dx.doi.org/10.1002/aic.15872(Featured on the journal cover as a Perspective Paper)

- S. Wang, J.M. Simkoff, **M. Baldea**, L.H. Chiang, I. Castillo, R. Bindlish, D.B. Stanley, Autocovariance-based Plant-Model Mismatch Estimation for Linear Model Predictive Control, Syst. Contr. Lett., 104, 5-14, 2017 http://dx.doi.org/10.1016/j.sysconle.2017.03.002

- R.C. Pattison, C. Tsay, **M. Baldea**, Pseudo-Transient Models for Multiscale, Multiresolution Simulation and Optimization of Intensified Reaction/Separation/Recycle Processes, Comput. Chem. Eng., 105(4), 161-172,
2017 http://dx.doi.org/10.1016/j.compchemeng.2016.12.019 (invited paper for *Special Issue on Process Intensification*

- R.C. Pattison, C.R. Touretzky, T. Johansson, **M. Baldea**, I. Harjunkoski, Optimal Process Operations in Fast-Changing Energy Markets: Framework for Scheduling with Low-Order Dynamic Models and an Air Separation Application, Ind. Eng. Chem. Res., 55, 4562-4584, 2016, http://dx.doi.org/10.1021/acs.iecr.5b03499

- Kumar, **M. Baldea**, T.F. Edgar, O.A. Ezekoye, Smart Manufacturing Approach for Efficient Operation of Industrial Steam-Methane Reformers, Ind. Eng. Chem. Res., 54 (16), 4360-4370, 2015 http://dx.doi.org/10.1021/ie504087z (featured as ACS Editors' Choice article on January 12, 2015)

Michael Bradford

- Senior Chemical Engineer, Mid-Atlantic Technology Research and Innovation Center

An innovative and results-oriented senior chemical engineer with subject matter expertise in materials synthesis, materials science, heterogeneous catalysis, solid oxide fuel cells, kinetics, reaction engineering, MEMS packaging, intellectual property, proposal development, stakeholder engagement, and project management. Leverages excellent leadership and communication skills to build and manage cross-functional teams and interface with diverse stakeholders. An entrepreneurial and practical innovator who identifies opportunities and develops intellectual property and solutions to drive organizational success.

Dr. Bradford worked for over nine years at Lilliputian Systems, Inc. (no longer in existence), mostly as Director of Chemical Engineering and Director of MEMS SOFC Packaging, focusing largely on reformer and combustion catalyst development, anode development, hermetic seal development, component interdependencies, and SOFC system assembly and testing. Although most work was privately funded and not published, two patents are available in the areas of sealing glass development (US 9,415,569) and system design and operation (US 9,147,899).

Elizabeth J. Podlaha-Murphy

- Ph.D., Colombia University, 1992
- MS, University of Connecticut, 1989
- BS, University of Connecticut, 1986

Elizabeth J. Podlaha-Murphy joined the Clarkson University Department of Chemical and Biomolecular Engineering as Department Chair and Professor in August, 2017. She has held positions as Professor of Chemical Engineering at Northeastern University, and Associate/Assistant Professor at Louisiana State University in the Department of Chemical Engineering. She has served on numerous department and university committees, and was the past Chair of the Electrode position Division of The Electrochemical Society and member of the Board of Directors of The Electrochemical Society. Podlaha-Murphy has made research contributions in the area of electrode position and electrochemistry, forwarding research on the understanding of kinetic-transport phenomena inherent to plating, creating more environmentally friendly electrode position processes, and in generating novel nanoscale structures of alloys and metal matrix composites for components in micro- and nano-size devices. She has been funded by a prestigious NSF CAREER award, and both single and multi-investigator NSF, NIH, DARPA, DOE and industrial grants. Outcomes of this research have been presented in over 90 peer-reviewed journals and proceeding papers including *Nano Letters*, *Journal of The Electrochemical Society* and *Electrochimica Acta*, as well as 130 scientific conference presentations, and 3 patents.

She is a member of The Electrochemical Society (ECS), American Institute of Chemical Engineers (AIChE), Materials Research Society (MRS), American Chemical Society (ACS), American Society for Engineering Education (ASEE), and the American Association for the Advancement of Science (AAAS).

Eric Stuve

- B.S., University of Wisconsin, 1978.
- M.S., Stanford University, 1979.
- Ph.D., Stanford University, 1984.

Research Interests

- Electrocatalysis for Fuel Cells
- Electrochemical Surface Science
- Fuel Cell Engineering

Electrochemical Surface Science

Improving the nation's economic competitiveness and environmental management requires advances in portable power handling, in terms of both energy storage and conversion. This translates to a need for more efficient energy conversion in the form of electrochemical fuel cells. Our research focuses on fundamental issues of fuel cells, specifically on issues of electrocatalysis and water transport in fuel cells.

Direct Hydrocarbon Oxidation in Solid Oxide Fuel Cells

Solid oxide fuel cells (SOFC) provide an opportunity for fuel-flexible fuel cells that operate at higher efficiencies than other types of fuel cells. These advantages arise from the high temperature of SOFC operation, 800–1000 °C, which facilitates direct oxidation and reforming of hydrocarbon fuels and a source of high quality waste heat. Some of the issues faced in direct hydrocarbon oxidation are: (1) avoiding carbon formation on the anode and (2) understanding the role of oxide ions in the reaction mechanism. To address these issues we have developed a SOFC mounted in a vacuum system with facilities for accurate control of fuel and oxygen partial pressures and measurement of reaction products by a calibrated mass spectrometer. The measurements highlight the interplay of fuel oxidation kinetics, carbon deposition on the anode, and transport of oxide ions through the electrolyte. We have examined a wide range of fuels; H_2, CH_4, C_2H_4, CH_3OH, C_2H_5OH, and C_7H_8; reacting at gadolinium-doped ceria (GDC), Pt/GDC, and CoO_3/Pt/GDC anodes at temperatures of 800–1000 K and pressures of 5–50 Torr. The combined mass spectrometry and current measurements show some fascinating behaviors, including induction periods for electrocatalytic oxidation, spontaneous and forced oscillations, and coupled reforming with direct surface reaction. These effects indicate carbon formation on the anode and changes in oxidation state and conductivity in the near surface layers of the electrolyte. The overall implication is that catalyst activity is a strong function of electrolyte structure, ionic flux, and adsorption kinetics of the fuel. This work is funded by the Office of Naval Research.

Investigation of Water Transport in Proton Exchange Membrane Fuel Cells

One of the most pressing problems in operating proton exchange membrane (PEM) fuel cells is knowledge and control of the flow of water within the fuel cell. To maintain good conductivity, and hence good performance, the PEM electrolyte must be adequately hydrated at all times. Different operating conditions create different modes of water transport, because protons must be hydrated as they move through the electrolyte. At low current densities (e.g., idle conditions), water must be supplied with the anode gas (hydrogen) for adequate hydration. At high current densities, water must be effectively removed at the cathode to prevent flooding. At intermediate current densities, it is sometimes necessary to remove water from both the anode and cathode. We are investigating how water flows in a PEM fuel cell as a function of operating conditions and fuel cell design. These studies focus on spatio-temporal characteristics of water flow. That is, we desire to understand the time dependence of water transport during, for example, a change from high to low current or vice versa, as well as the spatial characteristics, namely, whether water prefers to through some areas of the membrane, but not others. This information will lead to improved electrolytes and fuel cell designs as well as improved control systems for operating fuel cell cells under dynamic conditions. This work is supported by the Seattle Foundation.

Teaching Interests

Eric Stuve's teaching interests include process design and fuel cell engineering. Since 1992, Stuve has supervised undergraduate research projects in fuel cell engineering. This lead to establishment of the Fuel Cell Locomotive interdisciplinary senior design project, which ran from 1996 to 2004. Working with Professors Stu Adler and Dan Schwartz, he developed a curriculum in fuel cell and electrochemical engineering, consisting of both introductory and advanced courses: CHEM E 345, 445, 446, and 461.

Other Information

Eric Stuve has published over 50 technical papers in catalytic and electrochemical surface science. He is a member of the American Institute of Chemical Engineers, the American Chemical Society, the American Society of Engineering Education, the American Vacuum Society, and the Electrochemical Society. He serves on review panels for the National Science Foundation, Environmental Protection Agency, and Department of Energy.

Recent Publications

- Medvedev, V.K., S. B. Adler, Stuve, E.M. Electrocatalysis and Reforming in Oscillatory Reaction of Methane on a Pt-LSC/Ceria Anode for Solid Oxide Fuel Cells. to appear in *Twelfth International Symposium on Solid Oxide Fuel Cells (SOFC-XII)* **2011**, ECS.

- Árnadóttir, L., Stuve, E.M., Jónsson, H. Adsorption of water monomer and clusters on platinum(111) terrace and related steps and kinks I. Configurations, energies, and hydrogen bonding. *Surface Science* **2010**, 604: pp. 1978-1986.

- Manghani, R. Stuve, E.M. Enhanced Field Ionization of Water Adsorbed on a Carbon Monoxide Platinum Field Emitter Tip. *Surface Science* **2009**, 603: pp. 165-172.

- Árnadóttir, L., Jónsson, H., Stuve, E.M. The Effect of Coadsorbed Water on the Stability and Configuration of Formyl (HCO) and Hydroxymethylidyne (COH) Intermediates on Pt(111): A Density Functional Theory Study, in *Proton Exchange Membrane Fuel Cells, Vol. 8*, **2008**, T. Fuller (Ed.), Electrochemical Society Transactions, Pennington, New Jersey.

- Roen, L. M., Stuve, E.M. Design and Characterization of an On-line Electrochemical Mass Spectrometry System for Measurement of Multi-step Reaction Kinetics, to appear in *Proton Exchange Fuel Cells 6*, T. Fuller (Ed.), ECS Transactions, Vol. 3 **2006**.

- Rothfuss, C. J., Medvedev, V.K., Stuve, E.M. The Influence of the Surface Electric Field on Water Ionization: a Two Step Dissociative Ionization and Desorption Mechanism for Water Ion Cluster Emission from a Platinum Field Emitter Tip. *Journal of Electroanalytical Chemistry* **2003**, 554-555: pp. 133-143.

- Madden, T. H., Stuve, E.M. Development of an Electrochemical Flow Cell

- Technique for Studying Methanol Electro-Oxidation at Elevated Temperatures. *Journal of the Electrochemical Society* **2003**, 150: E1-E10.

- Rothfuss, C. J., Medvedev, V.K., Stuve, E.M. Temperature and Field. Dependence of Protonated Water Cluster Emission from Field Adsorbed Water Layers on Platinum. *Surface Science* **2002**, 501: 169-181.

- Scovell, D. L., Pinkerton, T.D., Medvedev, V.K., Stuve, E.M. Phase Transitions in Vapor Deposited Water under the Influence of High Surface Electric Fields. *Surface Science* **2000,** 457: pp. 365-376.

- Jarvi, T. D., Madden, T.H., Stuve, E.M. Vacuum and Electrochemical Behavior of Vapor Deposited Ruthenium on Platinum (111). *Electrochemistry and Solid State Letters* **1999,** 2: pp. 224-227.