

Emily M. Ryan

Associate Professor
Department of Mechanical Engineering
Division of Materials Science and Engineering
Boston University

Areas of Specialization:

Meso-scale computational modeling of multiphase reactive systems; multi-scale modeling; validation, verification and uncertainty analysis of complex systems

Education:

Carnegie Mellon University, Pittsburgh, PA, 2005-2009

Ph.D., Mechanical Engineering, December 2009

Dissertation: *A smoothed particle hydrodynamics model of reactive transport in the porous cathode of a solid oxide fuel cell*

M.S., Mechanical Engineering, 2008

Tufts University, Medford, MA, 2000-2004

B.S., Mechanical Engineering, Magna cum Laude

Employment:

- Associate Professor, Department of Mechanical Engineering, Boston University, May 2020 – present
 - Associate Director, Institute for Sustainable Energy, Boston University
 - Founding Faculty Member of Computing and Data Science, Boston University
 - Affiliated Faculty, Materials Science Division, College of Engineering, Boston University
 - Affiliated Faculty, Center for Computational Science, Boston University
 - Affiliated Faculty, Hariri Institute for Computing and Computational Science and Engineering
- Assistant Professor, Department of Mechanical Engineering, Boston University, 2012 –2020
- Computational Scientist, Pacific Northwest National Laboratory, 2010-2011
- Post-Doctoral Research Associate, Pacific Northwest National Laboratory, 2009-2010
- Field Engineer, Select Energy Services, Natick, MA 2004-2005

Awards and Honors:

- Scialog Fellow, Negative Emission Sciences, 2020
- Scialog Fellow, Advanced Energy Storage, 2017-2019
- R&D 100 Award, CCSI Toolset co-developer, 2016
- Hariri Junior Faculty Fellow, 2014
- Kern Faculty Fellow, 2013
- Young Faculty Travel Award, ECS, 2013
- NSF Graduate Research Fellow, 2006-2009

Publications:

Book Chapters

1. E.M. Ryan, M.A. Khaleel, Modeling Solid Oxide Fuel Cells from the Macro-Scale to the Nano-Scale, in: D. Stolten, B. Emonts (Eds.) Fuel Cell Science and Engineering - Materials, Processes and Systems, Wiley, 2012.

Journal Publications

1. A. Cannon, E.M. Ryan (under review). “Heterogeneous Separator Structures in Lithium Batteries and Their Effects on Dendritic Growth”, *ACS Applied Energy Materials*.

2. Z. Pollard, A. Roshandelpoor, P. Vakili, E.M. Ryan, J. Goldfarb (submitted Jan 2021). “Tunable, greener polymer foam synthesis in limited data environments”, *Journal of Industrial and Engineering Chemistry*.
3. K. Dong, Y. Xu, J. Tan, M. Osenberg, C. Yang F. Sun, Z. Kochovski, D. T. Pham, S. Mei, A. Hilger, E.M. Ryan, Y. Lu, J. Banhart, I. Manke (submitted Oct 2020). “Unravelling the Mechanism of Lithium Nucleation and Growth and the Interaction with the Solid Electrolyte Interface”, *Nature Communications*.
4. S. Gao, A. Cannon*, F. Sun, Y. Pan, D. Yang, S. Ge, N. Liu, A. P. Sokolov, E. Ryan, H.n Yang, and P. Cao (submitted Jan 2021). “Glass-Fiber Reinforced Polymeric Protective Layers for Stable Li-Metal Electrode: Unraveling the Key Attributes of Artificial Solid-Electrolyte Interface (SEI)”, *Advanced Functional Materials*
5. D. Gopalakrishnan, S. Alkatie, A. Cannon*, N. Bhagirath, **E.M. Ryan**, L.M. Reddy Arava (submitted Sept 2020). “Ionic Liquid Crystalline Electrolyte to suppress dendrite growth in Li metal batteries: An effect of anisotropic mass transport”. *Sustainable Energy and Fuels*.
6. J. Tan, A. Cannon*, E.M. Ryan (2020). “Dendrite growth in Lithium Batteries under Cycling Conditions”, *Journal of Power Sources*, 463: 228187.
7. E. Arai*, A. Tartakovsky, R.G. Holt, S. Grace, E.M. Ryan (2020). “Comparison of Surface Tension Generation Methods in Smoothed Particle Hydrodynamics for Dynamic Systems”, *Computer and Fluids*, 203, 5.
8. E. Arai*, D. Villafranco, S. Grace, E.M. Ryan (2020). “Simulating Bubble Dynamics in a Buoyant System”, *International Journal for Numerical Methods in Fluids*, 93, 3, 169-188.
9. D. Villafranco, A. Gupta, E.M. Ryan, R.G. Holt, S. Grace (2020) “An Assessment of Homogeneous Mixture Method Cavitation Models in Predicting Cavitation in Nozzle Flow”, *Journal of Fluids Engineering*, 143, 1.
10. E.M. Ryan, J. Goldfarb (2019). “Manipulating Dendritic Growth: An Undergraduate Laboratory Experience in the Interplay between Mass Transport, Supersaturated Solutions, and Dendrite Structure”. *Journal of Chemical Education*. <https://doi.org/10.1021/acs.jchemed.8b00962>
11. E.M. Ryan, Z. Pollard, A. Roshandelpoor, Q. Ha*, P. Vakili, J. Goldfarb (2019). “Designing Heterogeneous Hierarchical Material Systems: A Holistic Approach to Structural and Materials Design”. *MRS Communications*, 9, 2, 628-636.
12. K.R. Dupre*, A. Vyas, J.L. Goldfarb, E.M. Ryan (2019). “Investigation of Computational Upscaling of Adsorption of SO₂ and CO₂ in Fixed Bed Columns”, *Adsorption*, 25, 4: 773-782. <https://doi.org/10.1007/s10450-019-00050-4>.
13. E.M. Ryan and P. Mukherjee (2019). “Mesoscale Modeling in Electrochemical Devices – A Critical Perspective”, *Progress in Energy and Combustion Science*, 71, 118-142.
14. K. Dupre*, E.M. Ryan, A. Suleimenov, J. Goldfarb (2018). “Experimental and Computational Demonstration of a Low-Temperature Waste to By-Product Conversion of U.S. Oil Shale Semi-Coke to a Flue Gas Sorbent”, *Energies*, 11, 3195.
15. N. Li, W. Wei, K. Xie, J. Tan*, L. Zhang, X. Luo, K. Yuan, Q. Song, H. Li, C. Shen, E. M. Ryan, L. Liu and B. Wei (2018). “Suppressing Dendritic Lithium Formation Using Porous Media in Lithium Metal Based Batteries”, *Nano Letters*, 18, 3: 2067-2073.
16. W. A. Lane*, E.M. Ryan (2018). “Verification, validation, and uncertainty quantification of a sub-grid model for heat transfer in gas-particle flows with immersed horizontal cylinders”, *Chemical Engineering Science*, 176:409-420.
17. J. Tan*, E.M. Ryan (2016). “Structured Electrolytes to Suppress Dendrite Growth in High Energy Density Batteries”, *International Journal of Energy Research*, 40, 13: 1800-1810.
18. J Tan*, E.M. Ryan (2016). “Computational study of electro-convection effects on dendrite growth in batteries”, *Journal of Power Sources*, 323: 67-77.
19. W. A. Lane*, S. Sundaresan, E.M. Ryan (2016). “Sub-grid models for heat transfer in gas-solid flows with immersed cylinders”, *Chemical Engineering Science*, 151: 7-15.

20. J.Tan*, K. Ferris, A.M. Tartakovsky, E.M. Ryan (2016). “Investigating the effects of anisotropic mixing on dendrite growth in high energy density lithium batteries”, *The Journal of the Electrochemical Society*, 163, 2: A318-A327.
21. C. Storlie, W.A. Lane*, E.M. Ryan, J.R. Gattiker, D.M. Higdon. (2015) “Calibration of Computational Models with Categorical Parameters and Correlated Outputs via Bayesian Smoothing Spline ANOVA”. *Journal of the American Statistical Society*, 110: 68-82.
22. D.C. Miller, M. Syamlal, D. Mebane, C. Storlie, D. Bhattacharyya, N. V. Sahinidis, D. Agarwal, C. Tong, S. E. Zitney, A. Sarkar, X. Sun, S. Sundaresan, E.M. Ryan, D. Engel, C. Dale. (2014). “Carbon Capture Simulation Initiative: A Case Study in Multi-Scale Modeling and New Challenges”. *Annual Review of Chemical and Biomolecular Engineering* 5.
23. W.A. Lane*, C. Storlie, C. Montgomery, E.M. Ryan. (2014). “Numerical modeling and Bayesian calibration of a bubbling fluidized bed with immersed horizontal tubes”. *Powder Technology*, 253: 733-743.
24. J. Tan*, E. M. Ryan (2013). “Dendrite Growth in a Lithium Air Battery System”. *The Electrochemical Society Transactions* 53, 20: 35-43.
25. E.M. Ryan, K.F. Ferris, A.M. Tartakovsky, M.A. Khaleel. (2013). “Computational Modeling of Transport Limitations in Li-air Batteries”. *The Electrochemical Society Transactions* 45, 29: 123-136.
26. E.M. Ryan, D. DeCroix, R. Breault, W. Xu, E.D. Huckaby, K. Saha, X. Sun, S. Sundaresan, S. Darteville. (2013). “Multi-phase CFD modeling of solid sorbent carbon capture system”, *Powder Technology*, 242: 117-134.
27. E.M. Ryan, W. Xu, X. Sun, and M.A. Khaleel (2012) “A damage model for degradation in the electrodes of solid oxide fuel cells: Modeling the effects of sulfur and antimony in the anode”. *Journal of Power Sources*, 210: 233-242.
28. E.M. Ryan, K.P. Recknagle, W. Liu, M.A. Khaleel. (2012). “The Need for Nano-scale Modeling and Experimentation in Solid Oxide Fuel Cells”, *Journal of Nanoscience and Nanotechnology*, 12: 6758-6768.
29. E.M. Ryan, T. Sanquist. (2012). “Validation of Building Energy Modeling Tools Under Idealized and Realistic Conditions”, *Energy and Buildings*, 47: 375-382.
30. E.M. Ryan, A.M. Tartakovsky. (2011). “A Hybrid Micro-Scale Model for Transport in Connected Macro-Pores in Porous Media”, *Journal of Contaminant Hydrology*, 126: 61-71.
31. E.M. Ryan, A.M. Tartakovsky, C. Amon. (2011).” Pore-Scale Modeling of Competitive Adsorption of a Plume in a Porous Medium”, *Journal of Contaminant Hydrology*, 120-121: 56-78.
32. E.M. Ryan, A.M. Tartakovsky, M.A. Khaleel, C. Amon. (2011). “Pore-Scale Modeling of the Reactive Transport of Chromium in the Cathode of a Solid Oxide Fuel Cell”, *Journal of Power Sources*, 196: 287-300.
33. K.P. Recknagle, E.M. Ryan, B.J. Koeppel, M.A. Khaleel. (2010). “Modeling of Electrochemistry and Steam-Methane Reforming Performance for Simulating Pressurized Solid Oxide Fuel Cell Stacks”, *Journal of Power Sources*, 195:6637-6644.
34. E.M. Ryan, A.M. Tartakovsky, C. Amon. (2010).” A Novel Method for Modeling Neumann and Robin Boundary Conditions in Smoothed Particle Hydrodynamics”, *Computer Physics Communications*, 181: 2008-2023.

* Denotes graduate student supported by Prof. Ryan

Peer-Reviewed Conference Publications

1. D. Villafranco, H.K. Do, S. Grace, E.M. Ryan, R. Holt, “Assessment of Cavitation Models in the Prediction of Cavitation in Nozzle Flow”, ASME Proceeding: 53rd Forum on Cavitation and Phase Change, FEDSM2018-83223, V002T16A003, 2018.
2. W.A. Lane*, E.M. Ryan, A. Sarkar, S. Sundaresan. “Sub-Grid Filtering Model for Multiphase

- Heat Transfer With Immersed Tubes”, ASME 2014 International Mechanical Engineering Congress and Exposition, 8A, V08AT10A060, 2014.
3. W.A. Lane*, C. Storlie, C. Montgomery, E.M. Ryan. “Modeling and Validation of a Large Scale, Multiphase Carbon Capture System”, ASME Fluids Engineering Division Summer Meeting, 2, V002T06A006, 2013.
 4. W.A. Lane*, E.M. Ryan, C. Montgomery, C. Storlie, J. Wendelberger. “Numerical modeling and Bayesian calibration of a bubbling fluidized bed with immersed horizontal tubes”, ASME Fluids Engineering Division Summer Meeting, 2013.
 5. J. Tan*, E. M. Ryan. “Dendrite Growth in a Lithium Air Battery System”. The Electrochemical Society Transactions 53, 20: 35-43, 2013.
 6. E.M. Ryan, K.F. Ferris, A.M. Tartakovsky, M.A. Khaleel. “Computational Modeling of Transport Limitations in Li-air Batteries”. The Electrochemical Society Transactions 45, 29: 123-136, 2013.
 7. E.M. Ryan, X. Sun, W. Xu, D. DeCroix, E.D. Huckaby, S. Darteville, S. Sundaresan, K. Saha. “Multi-Phase CFD Modeling of A Solid Sorbent Carbon Capture System”, ASME Fluids Engineering Summer Meeting. 2012.
 8. E.M. Ryan, X. Sun, D.S. DeCroix, E. Huckaby, S. Darteville, C.J. Montgomery, W. Xu, K. Saha, A. Sarkar, W. Pan, S. Sundaresan. “Multi-Phase CFD Modeling of a Solid Sorbent Carbon Capture System”, ASME Fluids Engineering Summer Meeting, 2012.
 9. K.P. Recknagle, E.M. Ryan, M.A. Khaleel. “Numerical Modeling of the Distributed Electrochemistry and Performance of Solid Oxide Fuel Cells”, ASME 2011 International Mechanical Engineering Congress & Exposition. 2011.
 10. E.M. Ryan, K.P. Recknagle, M.A. Khaleel. ”Modeling the Electrochemistry of an SOFC through the Electrodes and Electrolyte”, The Electrochemical Society Transactions. 2011.
 11. S. Adami, X. Hu, N. Adams, E.M. Ryan, A.M. Tartakovsky, A Fully Coupled 3D Transport Model in SPH for Multi-Species Reaction-Diffusion Systems, in: 6th International SPHERIC Workshop, Hamburg 2011.
 12. E.M. Ryan, C. Amon. “Modeling the Species Transport and Reactions in an SOFC Cathode using Smoothed Particle Hydrodynamics”, Proceedings of the 6th Annual ASME International Fuel Cell Science, Engineering, and Technology Conference. 2008.
 13. M. Pickering, B. Gravel, M. Portsmore, E.M. Ryan. “The Benefit of Outreach to Engineering Students”, Proceedings of the American Society of Engineering Education Annual Conference and Exposition. 2004.
 14. K. Clark, E.M. Ryan. “The Undergraduate Experience in Engineering Educational Outreach”, Proceedings of the American Society of Engineering Education Annual Conference and Exposition. 2003.
 15. E. Milto, E.M. Ryan. “Gender Differences in Approaching Design Problems at LEGO Camp”, Hawaii International Conference on Education. 2004.

* Denotes graduate students supervised by Dr. Ryan

Presentations:

Invited

1. *Mesoscale Separator Design to Mitigate Dendrite formation in lithium batteries*, TMS, San Diego, CA, February 26, 2020.
2. *Computational Modeling and Upscaling for Post Combustion Carbon Capture*, CleanTech Club, Boston University, Boston, MA, December 9, 2019.
3. *Understanding Interfacial Stability in High Energy Density Batteries*, Research on Tap, Boston University, Boston, MA, December 4, 2019.
4. *Computational Modeling and Upscaling for Post Combustion Carbon Capture*, Cornell University, Ithaca, NY, October 28, 2019.

5. *Modeling Multiphase, Multi-physics Phenomena in Energy Systems*, Mechanical Engineering, Boston University, Boston, MA, April 12, 2019.
6. *Modeling Multiphase, Multi-physics Phenomena in Energy Systems*, Schlumberger-Doll, Cambridge, MA, March 14, 2019.
7. *Mesososcopic Phenomena in Electrochemical Systems*, Greater Boston Area Statistical Mechanics Society, Brandies University, October 27, 2018.
8. *Interfacial Mesoscopic Phenomena in Electrochemical Systems*, BU Materials Day, Boston University, October 26, 2018.
9. *Materials Science is All Around Us*, AMS Materials Science Day, Boston University, May 21, 2018.
10. *Modeling Multiphase, Multi-physics Phenomena in Energy Systems*, Northeastern University, Department of Mechanical and Industrial Engineering Seminar Series, December 8, 2017.
11. *Modeling Multiphase, Multi-physics Phenomena in Energy Systems*, University of Massachusetts Amherst Department of Mechanical Engineering Seminar Series, October 27, 2017.
12. *Materials Science is All Around Us*, AMS Materials Science Day, Boston University, May 22, 2017.
13. *Modeling Multiphase, Multi-physics Phenomena in Energy Systems*, Tufts University Department of Mechanical Engineering Seminar Series, Medford, MA, March 31, 2017
14. *Suppressing Dendrite Growth in high energy density batteries through anisotropic transport*, TMS, San Diego, CA, March 2, 2017
15. *Modeling and Experimental Studies of Cavitation in Fuel Injectors*, DOE Advanced Engine Combustion Meeting, Livermore, CA, February 2017
16. *Advancing High Energy Density Batteries through Controlled Mass Transport*, BU Research on Tap Materials Science and Engineering: The Science of Stuff, February 2017
17. *Modeling the Physics and Performance Issues in Advanced Battery Technologies*, Hariri Institute for Computing and Computational Science and Engineering, Boston, MA, December 2015
18. *Developing Energy Technologies for the Future: Micron to Device Scale*, Center for Computational Sciences, Boston, MA, May 2015
19. *Filtered Model Development for Solid Sorbent Systems*, Carbon Capture Simulation Initiative Industry Advisory Board Meeting, Reston, VA, September 2015.
20. *Sub-Grid Heat Transfer Models for Gas-Solid Flows*, Carbon Capture Simulation Initiative Industry Advisory Board Meeting, Webinar, July 2015.
21. *Coarse Graining methods for multiphase fluidized beds*, Carbon Capture Simulation Initiative Industry Advisory Board Meeting, Reston, VA, September 2014.
22. *Modeling and Calibration of a bubbling fluidized bed*, Carbon Capture Simulation Initiative Industry Advisory Board Meeting, Reston, VA, September 2013.
23. *High-Fidelity Models of Solid Sorbent Carbon Capture Equipment*, 11th Annual Conference on carbon Capture and Sequestration, Pittsburgh, PA, May 1, 2012.
24. *Using Numerical Methods to Engineer the Next Generation of Energy Systems*, Center for Computational Sciences, Boston University, MA, May 2015.
25. *Detailed Secondary Reaction Modeling of SOFC electrodes*, SECA-NETL Program Review, Morgantown, WV, April 2010.
26. *Electrode Level Modeling of Secondary Reaction in a Solid Oxide Fuel Cell*, Fuel Cell Workshop, PNNL, Richland, WA, October, 2009.
27. *Smoothed Particle Hydrodynamics Modeling of Reactive Transport in a Solid Oxide Fuel Cell Cathode and Porous Media*, Mechanical Engineering Department, University of Toronto, Toronto, CA, May 2009.
28. *Chromium Poisoning in the Cathode of a Solid Oxide Fuel Cell*, PNNL, Richland, WA, January, 2007.

Professional Memberships:

- American Society of Mechanical Engineers
- Sigma Xi
- The Electrochemical Society

- TMS

Professional Service:

- Associate Editor, ASME Journal of Fluid Engineering (2020-present)
- Executive Committee Member at Large, High Temperature Materials Division, Electrochemical Society (2013-present)
 - Attend executive committee meetings, engage in and vote on division decisions
- Conference Session Organization
 - Organizer, Re-envisioning Chemistry's Role in Environmental Sustainability: Perspectives on Progress & Future Directions, ACS, Spring 2020.
 - Chair, Advanced Materials for Energy and the Environment: Design, Fabrication and Application Symposium, ACS, Fall 2018.
 - Vice Chair, International Union of Pure and Applied Physics Conference on Computational Physics, Fluid Dynamics, Turbulence, Nano-fluidics, Magnetohydrodynamics Session, August 2014.
 - Co-Organizer, The Electrochemical Society, Computational Studies on Battery and Fuel Cell Materials, May 2014
 - Co-Chair, Fuel Cell Session, ASME IMECE, 2012
- Tufts University, Department of Mechanical Engineering, Alumni Advisory Board, Member (2015-present)
 - Attend meetings to discuss curriculum, direction, ABET, etc.
- Proposal Reviewer
 - NSF Proposal Panelist, 2012, 2015, 2016, 2017
 - U.S. Department of Energy, Nuclear Energy University Programs, 2013, 2014, 2015, 2016, 2017, 2018
 - U.S. Department of Energy, Office of Advanced Scientific Computing Research, 2014.
 - Canada Foundation for Innovation, 2012
 - U.S. Department of Energy SBIR Phase I Grants, 2011
- Reviewer for Scientific Journals:
 - Computer Physics Communications
 - Nature Communications
 - Journal of The Electrochemical Society
 - Journal of Power Sources
 - Powder Technology
 - Journal of Contaminant Hydrology
 - Applied Energy
 - Elsevier
 - International Journal of Sustainable Energy
 - Energy and Fuel
 - Fuel Cells
 - Biomass and Bioenergy
- Conference Proceedings Reviewer
 - ASME 2012 Fluids Engineering Summer Meeting
 - ASME 2011 Fuel Cell Science, Engineering and Technology Conference