

# Multiphysics, Multiphase and Multiscale Modeling of Polymer Electrolyte Fuel Cells: With a Focus on the Gas Diffusion Layer

Pablo A. García-Salaberri\*, Jeff T. Gostick<sup>†</sup>, Gisuk Hwang<sup>‡</sup>, Marcos Vera\*,  
Iryna Zenyuk<sup>•</sup> and Adam Z. Weber<sup>◦</sup>

\* Dpto. de Ingeniería Térmica y de Fluidos, Universidad Carlos III de Madrid, Leganés, Spain  
e-mail: pagsalab@ing.uc3m.es, mvcoello@ing.uc3m.es - web page: <http://fluidosuc3m.es/>

<sup>†</sup> Department of Chemical Engineering, McGill University, Montreal, Quebec, Canada  
e-mail: jeff.gostick@mcgill.ca - web page: <http://pmeal.com/>

<sup>‡</sup> Department of Mechanical Engineering, Wichita State University, Wichita, Kansas, USA  
e-mail: Gisuk.Hwang@wichita.edu - web page: <http://webs.wichita.edu/?u=gshwang>

<sup>•</sup> Department of Mechanical Engineering, Tufts University, Medford, Massachusetts, USA  
e-mail: iryna.zenyuk@tufts.edu - web page: <http://engineering.tufts.edu/me/people/Zenyuk/>

<sup>◦</sup> Energy Conversion Group, Lawrence Berkeley National Laboratory, Berkeley, California, USA  
e-mail: azweber@lbl.gov - web page: <https://eetd.lbl.gov/people/adam-weber>

## ABSTRACT

Numerical modeling plays a crucial role for the analysis of the complex multiphysics, multiphase and multiscale transport phenomena that take place in the membrane electrode assembly of Polymer Electrolyte Fuel Cells (PEFCs). In particular, thorough understanding of the coupled mass, charge and heat transport processes that occur in thin, heterogeneous, anisotropic, mix-wettability Gas Diffusion Layers (GDLs) is essential to develop novel fuel-cell designs with improved performance and extended durability. In this work, various techniques, such as continuum, lattice Boltzmann and pore network methods, are combined with X-ray tomographic reconstructions of dry and partially-saturated GDLs to perform numerical simulations on the material microstructure [1, 2]. The effects of GDL pore-scale architectures on cell performance and effective transport properties (diffusivity, permeability, and electrical and thermal conductivity) are examined. In addition, the limitations introduced by the widely used volume-averaged approach when modeling finite-size GDL materials are discussed. For this purpose, the predictions of a 3D PEFC model using a fully volume-averaged description are compared with those accounting for the real GDL microstructure. The insight gained from this work-in-progress will be leveraged to develop advanced PEFC models in order to assist the construction of next-generation GDLs, as well as to improve our understanding of PEFC technology.

## REFERENCES

- [1] P. A. García-Salaberri, G. Hwang, M. Vera, A. Z. Weber, J. T. Gostick, “Effective diffusivity in partially-saturated carbon-fiber gas diffusion layers: Effect of through-plane saturation distribution”, *Int. J. Heat Mass Tran.*, Vol. **86**, pp. 319–333, (2015).
- [2] P. A. García-Salaberri, J. T. Gostick, G. Hwang, A. Z. Weber, M. Vera, “Effect of local saturation and application to macroscopic continuum models”, *J. Power Sources*, Vol. **296**, pp. 440–453, (2015).