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Modeling Gas Diffusion Layers in Polymer Electrolyte Fuel Cells Using a Continuum-based Pore-network Formulation

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#### **Abstract**

A pore-network formulation is presented to model gas diffusion layers (GDLs) in polymer electrolyte fuel cells (PEFCs) using a continuum-based approach. The formulation can easily be integrated into macroscopic models in CFD codes, thus improving the modeling predictions while keeping a moderate computational cost.

The continuum-based pore-network formulation is based on a cubic lattice [1], which is divided into control volumes (cubes) of prescribed size. Pores and throats are placed inside the control volumes, and "connectors" of negligible volume interconnect the control volumes. The "connectors" are used to regulate the invasion-percolation pattern according to the size of the throat that links the pores within neighboring control volumes. Hence, the formulation can account for both invasion-percolation between pores as well as evaporation/condensation in the pore volume inside each control volume. This is a major advantage compared to traditional pore-network models based on a fully discrete formulation where phase-change phenomena are difficult to implement. Local anisotropic effective transport properties (permeability and diffusivity) are determined using a 1D resistor network analogy inside each control volume according to the size of the pore and throats in it.

The model is validated against capillary pressure curves and effective transport properties (effective diffusivity and permeability) measured ex situ. In addition, water saturation profiles are compared with distributions obtained using X-ray computed tomography [2].

- [1] Jeff T. Gostick, Marios A. Ioannidis, Michael W. Fowler, Mark D. Pritzker, Pore network modeling of fibrous gas diffusion layers for polymer electrolyte membrane fuel cells, J. Power Sources 173 (2007) 277-290.
- [2] 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 throughplane saturation distribution, International Journal of Heat and Mass Transfer 86 (2015) 319–333