

Water management is one of the main challenges in PEM Fuel Cells. While water is essential for membrane electrical conductivity, excess liquid water leads to flooding of catalyst layers. Despite the fact that accurate prediction of two-phase transport is key for optimal water management, understanding of the two-phase transport in fuel cells is relatively poor. Wang et. al. [1], [2] have studied the two-phase transport in the channel and diffusion layer separately using a multiphase mixture model. The model fails to accurately predict saturation values for high humidity inlet streams. Nguyen et. al. [3] developed a two-dimensional, two-phase, isothermal, isobaric, steady state model of the catalyst and gas diffusion layers. The model neglects any liquid in the channel. Djilali et. al. [4] developed a three-dimensional two-phase multicomponent model. The model is an improvement over previous models, but neglects drag between the liquid and the gas phases in the channel.

In this work, we present a comprehensive two-fluid model relevant to fuel cells. Models for two-phase transport through Channel, Gas Diffusion Layer (GDL) and Channel-GDL interface, are discussed. In the channel, the gas and liquid pressures are assumed to be same. The surface tension effects in the channel are incorporated using the continuum surface force (CSF) model. The force at the surface is expressed as a volumetric body force and added as a source to the momentum equation. In the GDL, the gas and liquid are assumed to be at different pressures. The difference in the pressures (capillary pressure) is calculated using an empirical correlations. At the Channel-GDL interface, the wall adhesion effects need to be taken into account.

SIMPLE-type methods recast the continuity equation into a pressure-correction equation, the solution of which then provides corrections for velocities and pressures. However, in the two-fluid model, the presence of two phasic continuity equations gives more freedom and more complications. A general approach would be to form a mixture continuity equation by linearly combining the phasic continuity equations using appropriate weighting factors. Analogous to mixture equation for pressure correction, a difference equation is used for the volume/phase fraction by taking the difference between the phasic continuity equations. The relative advantages of the above mentioned algorithmic variants for computing pressure correction and volume fractions are discussed and quantitatively assessed.

Preliminary model validation is done for each component of the fuel cell. The two-phase transport in the channel is validated using empirical correlations. Transport in the GDL is validated against results obtained from LBM/VOF simulation techniques [5-8]. The Channel-GDL interface transport will be validated against experiment and empirical correlation of droplet detachment at the interface.

References

- [1] Y. Wang S. Basu and C.Y. Wang, Modeling two-phase flow in PEM fuel cell channels, *J. Power Sources*, 179:603-617, 2008.
- [2] P. K. Sinha and C. Y. Wang, Liquid water transport in a mixed-wet gas diffusion layer of a polymer electrolyte fuel cell, *Chem. Eng. Sci.*, 63:1081-1091, 2008.
- [3] Guangyu Lin and Trung Van Nguyen, A two-dimensional two-phase model of a PEM fuel cell, *J. Electrochem. Soc.*, 153(2):A372-A382, 2006.
- [4] T. Berning and N. Djilali. A 3d, multiphase, multicomponent model of the cathode and anode of a PEM fuel cell, *J. Electrochem. Soc.*, 150(12):A1589-A1598, 2003.
- [5] S. Mukherjee, J.V. Cole, K. Jain, and A. Gidwani, Lattice-Boltzmann Simulations of Multiphase Flows in Gas-Diffusion-Layer (GDL) of a PEM Fuel Cell. 2008 AIChE Annual Meeting, Philadelphia, PA, Nov. 16-21 (2008).
- [6] S. Mukherjee, J.V. Cole, K. Jain, and A. Gidwani, Lattice-Boltzmann Simulations of Multiphase Flows in PEM Fuel Cell GDLs and Micro-channels, 214th Meeting of Electrochemical Society, Honolulu, HI, Oct. 12-17 (2008).
- [7] S. Mukherjee and J. Abraham, Investigations of Drop Impact on Dry Walls with a Lattice-Boltzmann Model, *Journal of Colloid and Interface Science*, 312:341-354 (2007).
- [8] S. Mukherjee and J. Abraham, Liquid Crown behavior in Drop Impact on Wet Walls, *Physics of Fluids*, 19:052103 (2007).