Formulation, Implementation and Validation of a Two-Fluid model in a Fuel Cell CFD Code

Kunal Jain, Vernon Cole, Sanjiv Kumar and N. Vaidya

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 affects 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 and VOF simulation techniques. 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.

Better Decisions, Better Products
Through Simulation & Innovation

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Kunal Jain[a], J. Vernon Cole[b], Sanjiv Kumar[c], Ashok Gidwani[b] and N. Vaidya[a]

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100th AIChE Annual Meeting
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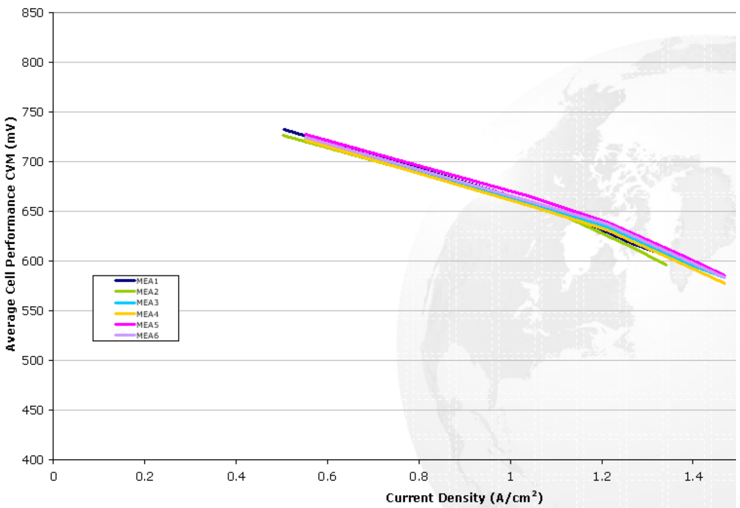
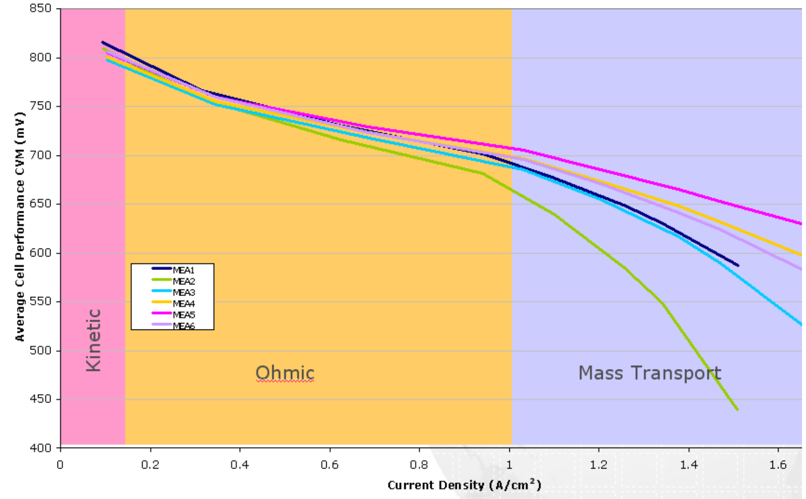
Water Management & Performance

DRY OPERATION



WET OPERATION



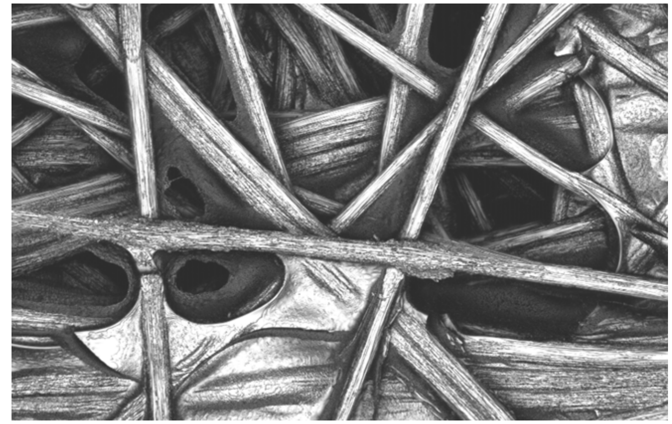
- **Several different MEAs, with different GDL properties and Teflon loadings, perform nearly identically with a given flow field when operated relatively dry, but show markedly different performance above 1 A/cm^2 under relatively wet conditions**
- **Additionally, some flow field designs are better at managing water for a given MEA**

Optimized water management is a key for performance improvements

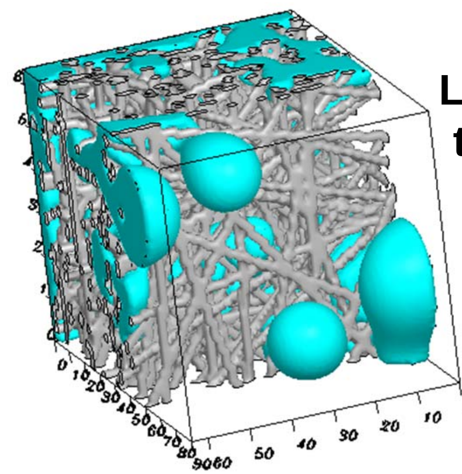
Water Management Issues

- **Conflicting needs:**
  - **Inlet humidification and generation by reaction to adequately wet membrane**
  - **GDL properties must balance need for reactant transport, water removal, and electrical contact**
  - **Removal through small channels – as power density and water generation increases, channel area reduced**

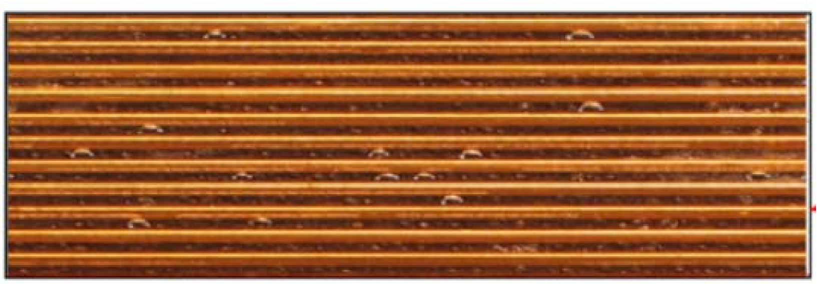
GDL Material



- **Design/Analysis Challenges**
  - **In-situ analysis difficult**
  - **Complex materials, both GDL and catalyst layer**
  - **Channels with large droplets, films, and/or slugs vs. misty flows**



LBM water transport



Visualization of Water in Channels

Model Formulation – Governing Eqns

- **Conservation of Phase k mass**

$$\frac{\partial}{\partial t}(\varepsilon_k \rho_k) + \nabla \cdot \left(\varepsilon_k \rho_k \vec{V}_k\right) = S_k$$

- **Conservation of Phase k momentum**

$$\frac{\partial}{\partial t}\left(\varepsilon_k \rho_k \vec{V}_k\right) + \nabla \cdot \varepsilon_k \left(\rho_k \vec{V}_k \vec{V}_k - \mu_k \nabla \vec{V}_k\right) = \varepsilon_k \left(-\nabla P_k + \rho_k \vec{g}\right) + \vec{I}_k + \vec{B}_k$$

  - **Fluid-fluid drag forces**

$$\vec{I}_{k,m} = -K_{km}\left(\vec{V}_k - \vec{V}_m\right)$$

  - **Porous media drag forces**

$$\vec{I}_{k,s} = -\varepsilon_k^2 \left(\frac{\mu_k}{\kappa_k}\vec{V}_k + \varepsilon_k \frac{C_f \rho_k}{\kappa_k}\left|\vec{V}_k\right|\vec{V}_k\right)$$

  - **Capillary pressure in porous media**

$$P_l - P_g = P_c = \frac{\sigma \cos(\theta_c)}{\sqrt{\kappa / \varepsilon_l}} J(s)$$

Model Formulation – Discretization

- **Discrete Momentum Equation:**

$$\left[a^{u}_{k,p}(1+I)-S^{u}_{k,p}\right]u_{k,p} = \sum\left(a^{u}_{k,nb}u_{k,nb}\right)+B^{u}_{k,p}-K_{p}\left(u_{k,p}-u_{m,p}\right)-\varepsilon_{p}\alpha_{k,p}\nabla P_{p}\cdot\hat{i}$$

  - **Partial Elimination Algorithm: sum momentum equations and solve for phase m velocity in an a cell to eliminate $u_{m,p}$ in u_k equation**

- **Continuity Equation:**
  - **Weighted sum to form pressure correction**

$$\omega_k\left(\frac{\partial}{\partial t}(\varepsilon_k\rho_k)+\nabla\cdot\left(\varepsilon_k\rho_k\vec{V}_k\right)\right)+\omega_m\left(\frac{\partial}{\partial t}(\varepsilon_m\rho_m)+\nabla\cdot\left(\varepsilon_m\rho_m\vec{V}_m\right)\right)=\omega_k S_k+\omega_m S_m$$

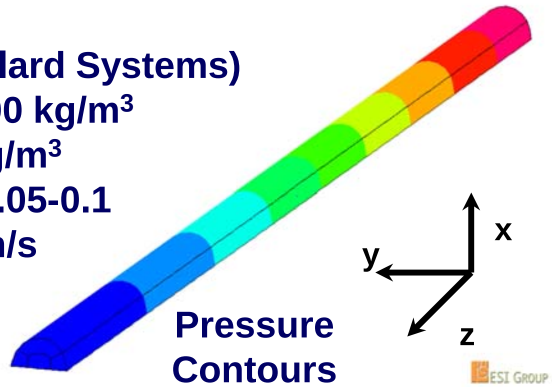
- **Phase Fraction Equation:**
  - **Approaches evaluated include secondary phase only, weighted difference**

$$\omega_k\left(\frac{\partial}{\partial t}(\varepsilon_k\rho_k)+\nabla\cdot\left(\varepsilon_k\rho_k\vec{V}_k\right)\right)-\omega_m\left(\frac{\partial}{\partial t}(\varepsilon_m\rho_m)+\nabla\cdot\left(\varepsilon_m\rho_m\vec{V}_m\right)\right)=\omega_k S_k-\omega_m S_m$$

Model Evaluation: Convergence

Continuity and Phase Fraction Weighting

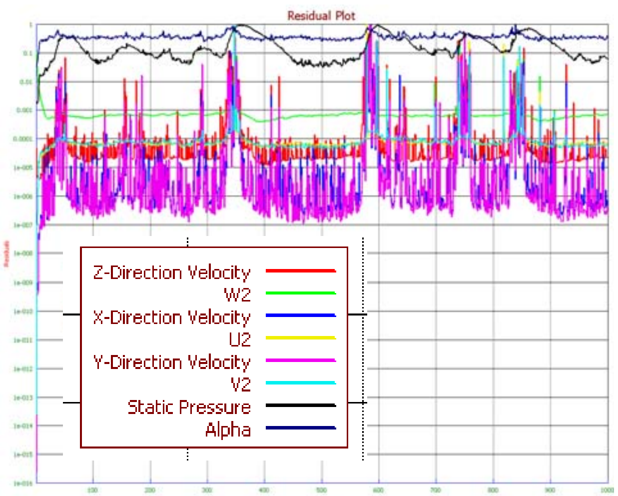
Cathode Channel (Ballard Systems)
- Liquid Density = 1000 kg/m^3
- Gas Density = 3.3 kg/m^3
- Volume-Fraction = 0.05-0.1
- Inlet Velocity = 6.5 m/s



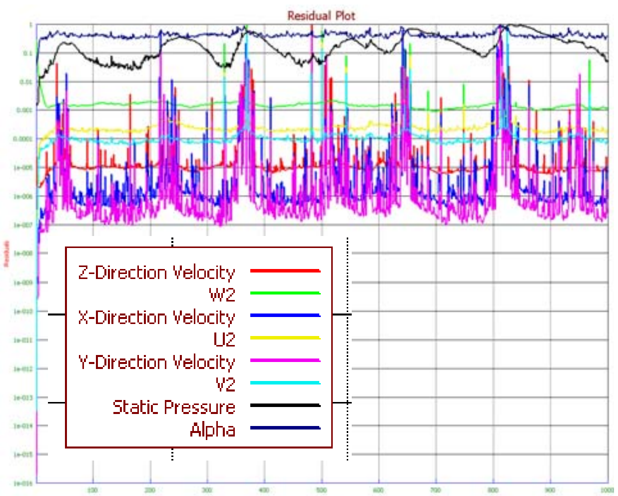
Pressure Contours

	$\omega_{k,p}$	$\omega_{m,p}$	$\omega_{k,\alpha}$	$\omega_{m,\alpha}$
A	$\rho_{m,ref}/\rho_{k,ref}$	1	0	1
B	$1/\rho_{k,ref}$	$1/\rho_{m,ref}$	0	1
C	$1/\rho_{k,ref}$	$1/\rho_{m,ref}$	$1/\rho_{k,ref}$	$1/\rho_{m,ref}$

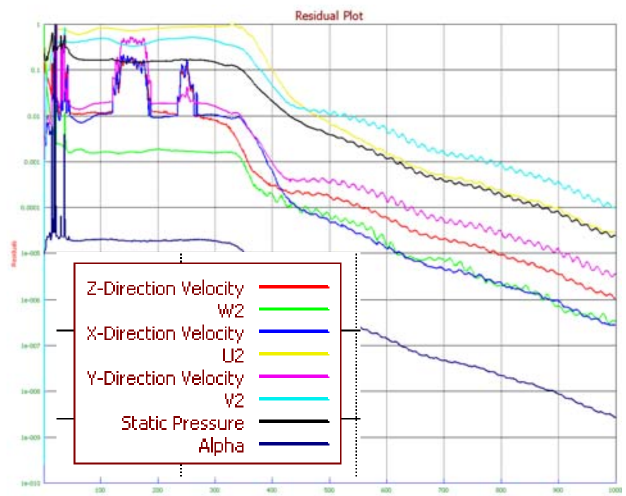
Convergence (Residuals) Plots



Formulation (A)

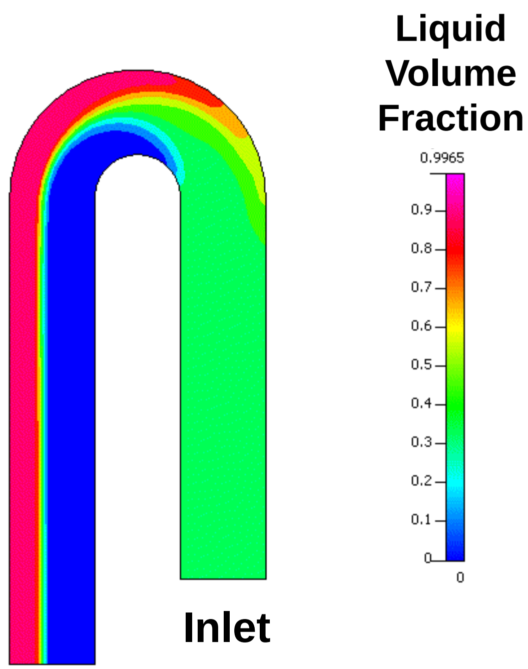


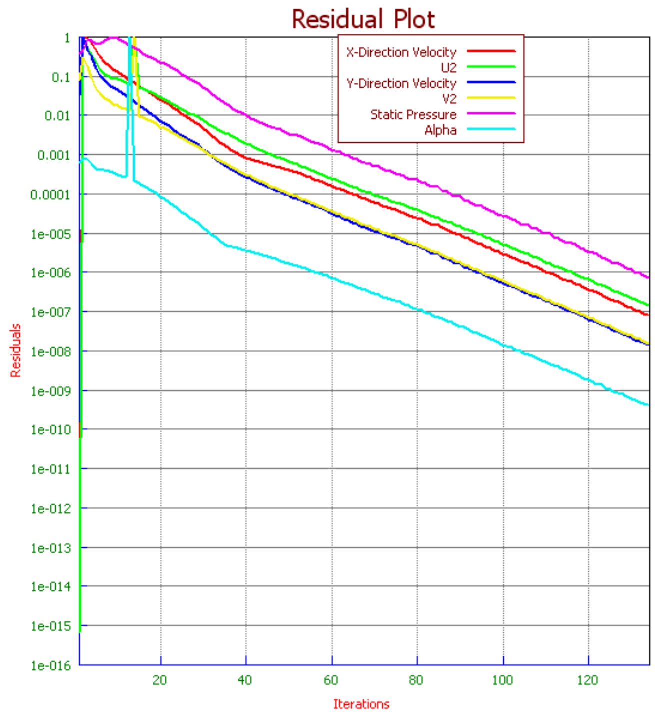
Formulation (B)



Formulation (C)

Model Validation: U-Bend Benchmark



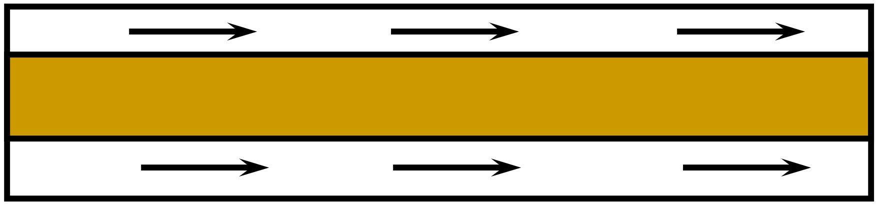


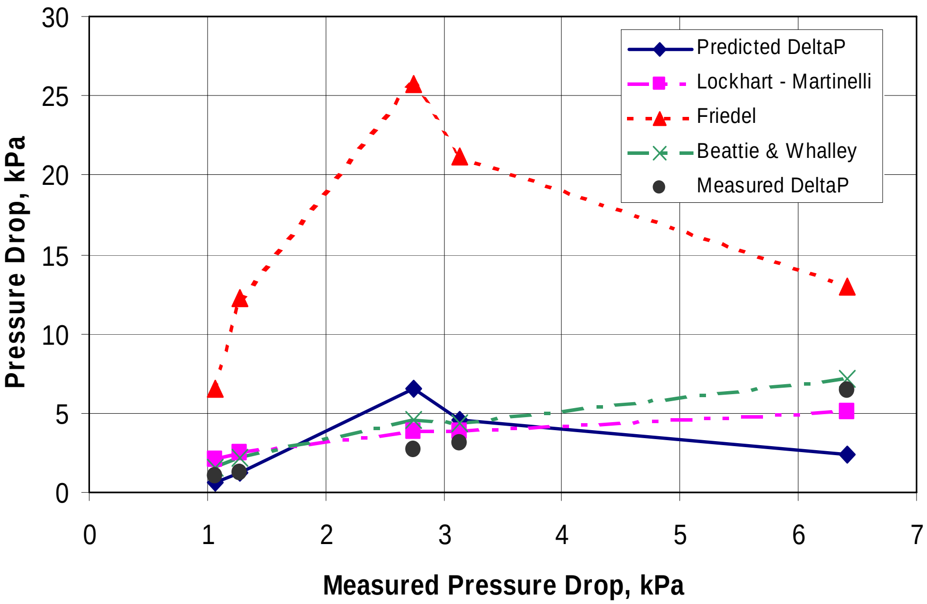
- Benchmark relevant to fuel cells with serpentine channels, expect phase separation due to varying densities and inertia
- Properties are air and water, inlet velocity for both phases 1m/s and the liquid fraction 0.5
- Excellent convergence with Difference of Volume Fractions formulation of phase fraction equation (algorithm C)
- Good agreement with benchmark results of Vaidya et al†

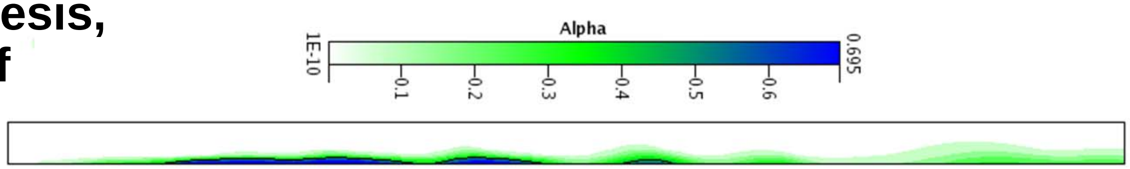
† N. Vaidya, P.J. Dionne, and A.K. Singhal, ASME FED Gas Liquid Flows, 225, 179 (1995)

Model Validation: Annular Flow

- **Predicted and measured pressure drops for two-phase water/air flow in an annulus for liquid volume fractions in the range 10^{-3} to 10^{-1}, mixture Re 100-800**
- **Excellent agreement at lower pressure drops (Re order 100) using Morsi-Alexander Drag model, dp=10μm**
- **Wavy liquid films, likely transient at ΔP=2.74kPa (inlet alpha 4×10^{-3}, Re 112), Re=830 at highest ΔP**
- **Data from C.M. Dillon, Two-Phase Flow within Narrow Annuli, Masters Thesis, Georgia Institute of Technology (2004)**





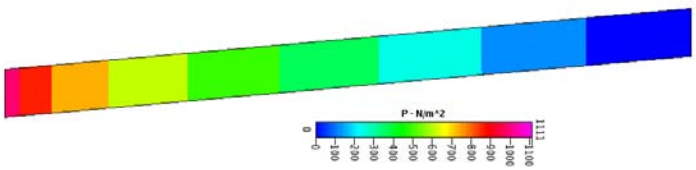


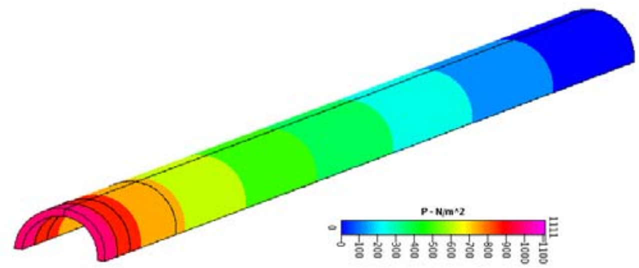
ΔP=2.74kPa, figure scaled 10x in the radial direction

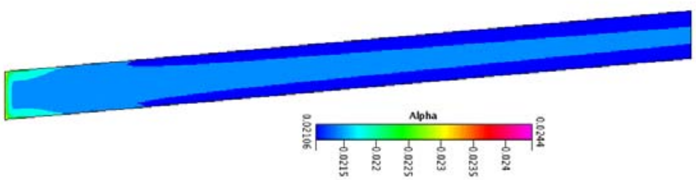
Model Validation: Annular Flow

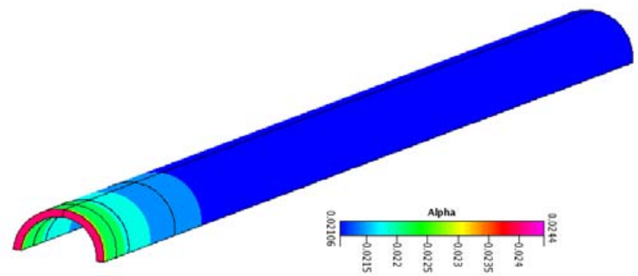
2D-AxiSymmetric

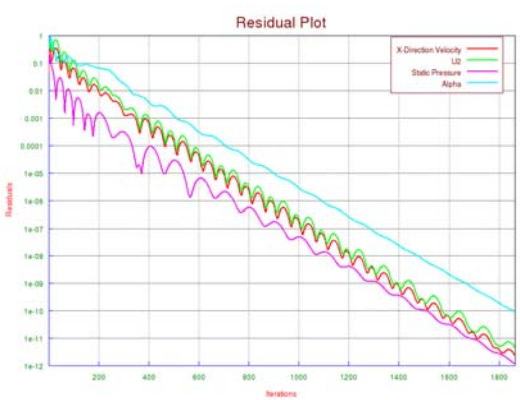
3D



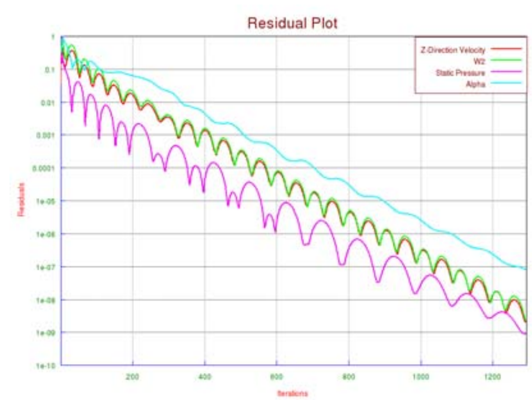








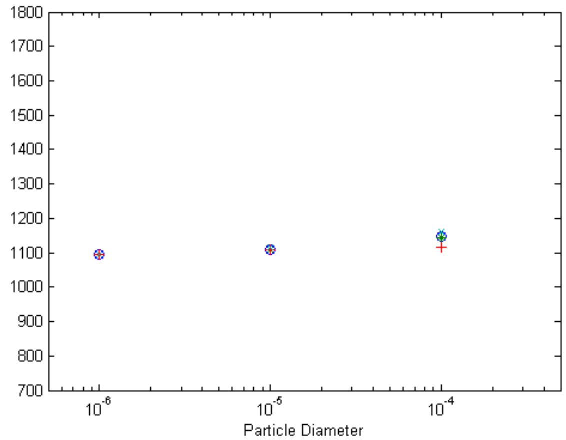
Model	P-Drop
HEM	13.2
BW	2.2
LM	2.11
Exp	1.27
ACE	1.11



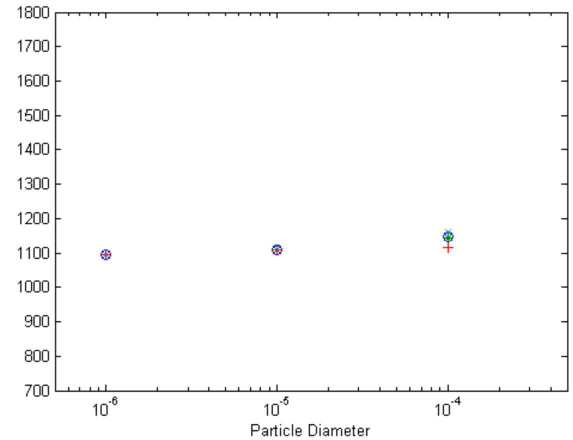
Model Sensitivity: dP & Drag Model

5% quality

2d

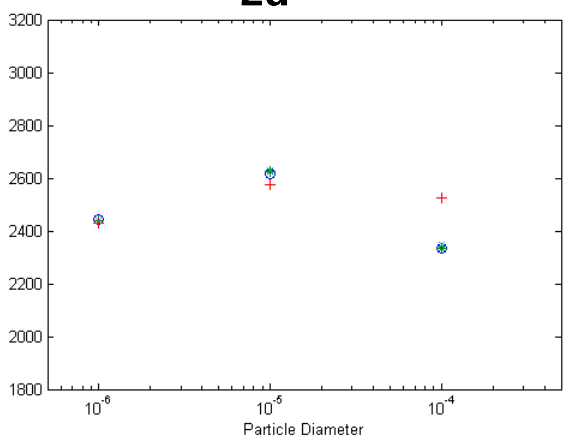


3d

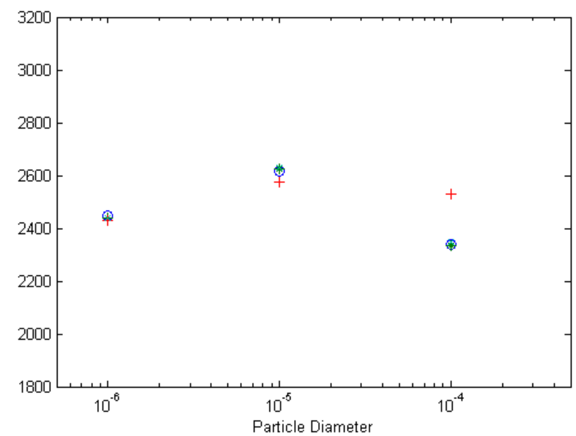


10% quality

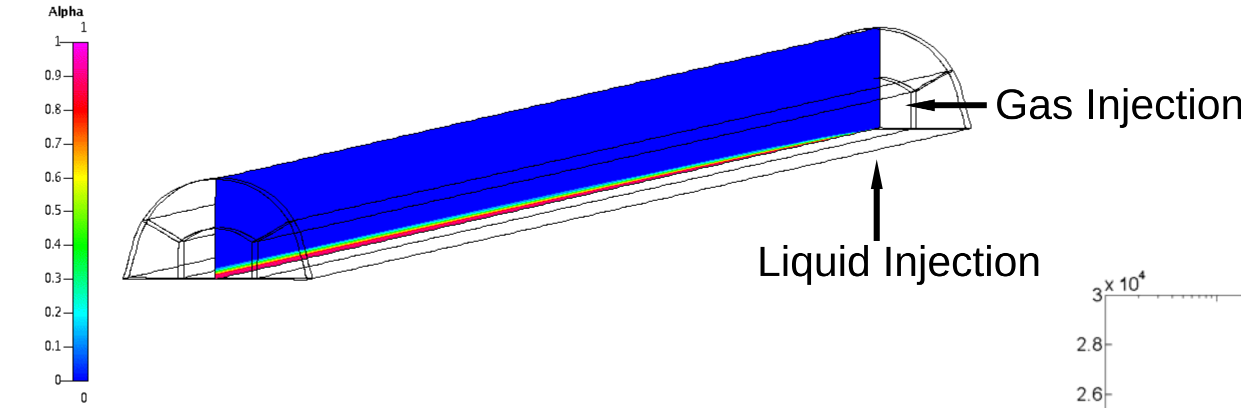
2d

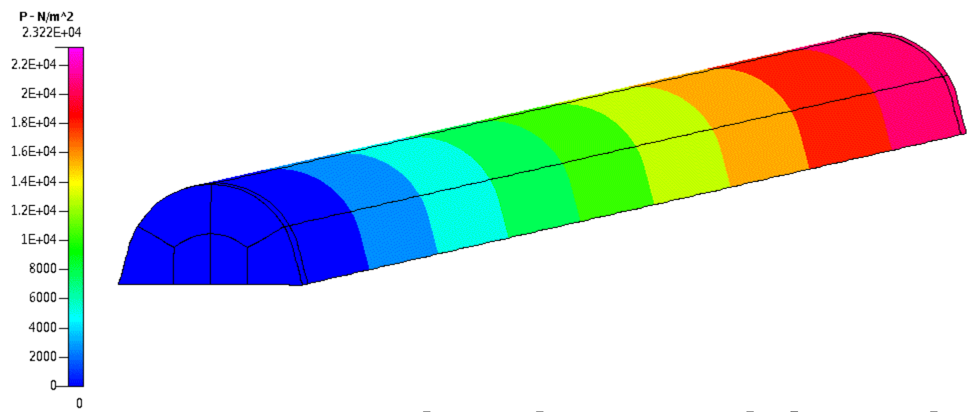


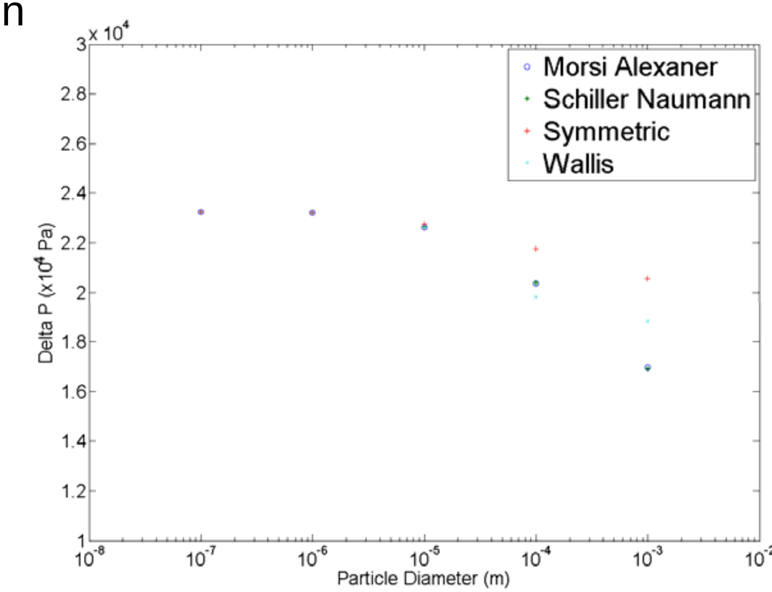
3d



Model Sensitivity: Ballard Channel





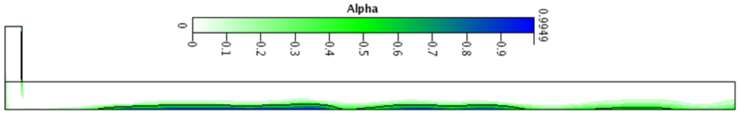


- **Assessing drag models and dispersed (liquid) phase drop size effects for model with liquid injection to mimic cathode channel during operation**

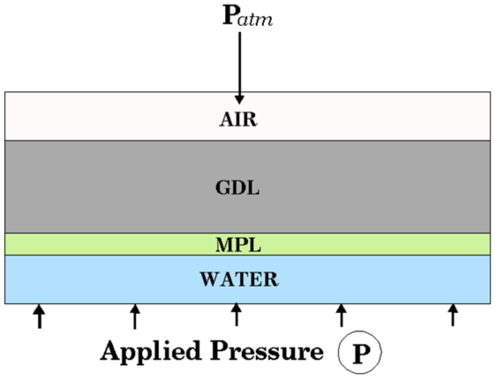
Fuel Cell Model Physics

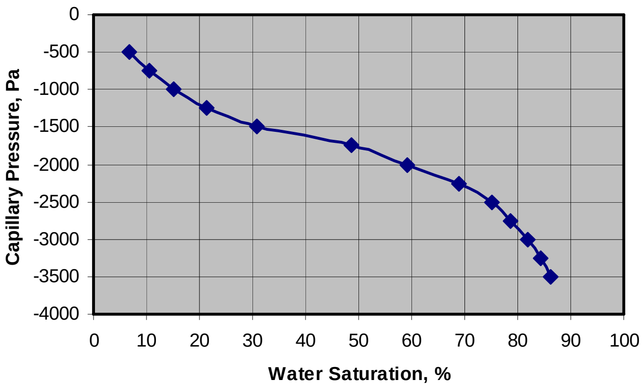
- **Implemented capillary pressure effects in porous media**
  - Leverett function for saturation dependence, extensible to other fitting functions
  - Testing against measured imbibing/drainage and equilibrium saturation dependence, numerical issues at porous – open interfaces
- **Integrated two-phase solution with chemical species transport and reaction**
  - Effective diffusivity in porous media and channels
  - Electrochemical and catalytic reactions in porous media

Annular Flow Pressure Drop



Porous Media Capillary Pressure





Summary and Conclusions

- **Implemented and validated robust two-fluid model formulation for multiphase flows in fuel cell channels**
  - **Demonstrated good agreement against experiment and benchmark simulations**
  - **Evaluated sensitivity to dispersed phase droplet diameter and drag models**
- **Initiated extension to porous media effects (solid drag and capillary pressure), coupling with reacting flow and species conservation**

- **Resulting model is a suitable foundation for addressing water management issues through modeling and simulation**

Acknowledgments

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Outline (Necessary?)

- **Introduction and Significance**
  - **Need for water management**
  - **State-of-the-art?**
- **Model Formulation**
- **Validation Studies**
- **? Fuel Cell application?**
- **Conclusions**