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# A Two-Fluid Model for Water Transport in a PEM Fuel Cell

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## 1 Introduction and Significance

Proton Exchange Membrane Fuel Cells, PEMFCs, are a promising alternative energy system for a number of applications including automotive and stationary power.

Water management in low temperature PEM Fuel Cells is highly important because of the inherent conflicts between the requirements for efficient low and high power operation. Particularly at low powers, adequate water must be supplied to establish and maintain the membrane humidification for adequate protonic conductivity or resistance losses will decrease the cell efficiency. At high power density operation, more water is produced at the cathode than is necessary for membrane hydration. This excess water must be removed effectively or it will accumulate in the Gas Diffusion Layer (GDL) and block the pathways for reactant transport to the catalysts, introducing mass transport losses and potentially "flooding" the electrode. As power density of the cells is increased to meet the needs of the transportation sector, the challenges arising from water management are expected to become more difficult to overcome simply due to the increased volumetric rate of liquid water generation. Such water management problems are critical for most PEM fuel cell applications. Thus, effectively addressing water management based issues through modeling and experimentation is a key challenge in successful application of PEMFC systems.

Despite the fact that accurate prediction of two-phase transport is critical for optimizing water management in PEMFCs, the understanding of the two-phase transport in fuel cells is still 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 work, but neglects drag between the liquid and the gas phases in the channel. To enable model-based design and optimization of PEM fuel cells, given that proper water management is a key challenge for PEMFC systems, models must address a broad range of conditions including operation with significant liquid water in the channels as droplets or films. This work represents an effort to address the common deficiencies of previous model formulations, introducing a more general multiphase flow model that can serve as the basis for a design tool addressing water management.

## 2 Model Formulation

The model formulation presented is a general form for the Eulerian two-fluid model with extensions to address transport in porous media. After introducing the governing equations, constitutive models for interphase momentum transfer are given and the discretization techniques used within this work are presented.

### Governing Equations

Anderson and Jackson [5] and Ishii [6] derived the multiphase flow equations from first principles by volume averaging the point equations. The key difference between the two is the treatment of fluid-droplet traction term. van Wachem et al. [7] have shown that Anderson and Jackson's formulation [5, 8, 9] is more appropriate for a dispersed phase consisting of solid particles and that Ishii's formulation [9,10] is more appropriate for a dispersed phase consisting of fluid droplets. Since the multiphase flow in fuel cells consists of liquid droplets and films interacting with air, we have chosen Ishii's model for this work, -using averaged continuity and momentum equations in an Eulerian framework.

### Fluid-Solid Momentum Transfer

The drag force exerted on a fluid phase by the solid phase of a porous media is given by a generalized form of Darcy's Law,

### Fluid-Fluid Momentum Transfer

The drag force between two fluids with an interphase transfer coefficient is derived by assuming that one phase is in the form of droplets or bubbles dispersed in the continuous phase.

In this work, we used the Morsi and Alexander model for the drag function [8, 12] which is based calculated using the drag coefficient and the local value of the relative Reynolds number.

### Capillary Pressure in Porous Media

Will be treated as a body force applied to the liquid phase within porous media, and the saturation will therefore correspond to the liquid phase volume fraction [13,14].

Discretization:

The discretization is based on a standard finite-volume method.

### InterPhase Coupling Algorithm.

The drag force for each phase introduces a term depending on the velocity of the other phase into the momentum equations. At higher slip velocities, an implicit treatment of this term is critical for obtaining convergence. The two commonly used approaches are the Partial Elimination Algorithm, PEA, [15] and Simultaneous solution of Non-Linearly Coupled Equations, SINCE, (16). The main advantage of SINCE is the relative ease of extending the algorithm to more than two dynamic phases [17]. However, this comes at a cost of reduced implicitness/convergence. Since fuel cells can be adequately described using two dynamic phases, liquid and gas, the PEA was chosen for this work.

### Continuity Equation

SIMPLE-type methods recast the continuity equation into a pressure-correction equation, the solution of which then provides corrections for velocities and pressures. This work has been adapted to used SIMPLEC [18] algorithm. However, in the two-fluid model, the presence of two phasic continuity equations provides an additional degree of freedom and more complications. Numerical difficulties can arise in the case of large density differences between the fluids, since the continuity equation residuals of the phases would differ by orders of magnitude. The residuals of the denser fluid will then induce false, spurious, corrections in the velocity field for the low-density fluid. To address these issues, the general approach is to form a mixture continuity equation by linearly combining the phasic continuity equations using appropriate weighting factors. In our work, we will investigate using the densities of respective phases as the weighting factors.

**Phase-Fraction Equation**

We followed the approach of composite solution of both phase-fractions mentioned in Vaidya et al. [19]. This approach is based on Carver [20, 21] and derives an equation for the phase fraction by taking the difference of the density-weighted continuity eqations.

**Solution Algorithm**

The most common iterative alogrithm for solving two-phase Momentum and Mass Conservation equations in a segregated finite volume pressure-based framework is the Interphase Slip Algorithm. The algorithm is an extension of Patankar's SIMPLE algorithm [22] and can be summarized as follows:

1. Guess a pressure field P*.
2. Solve the discretized momentum equations for each phase.
3. Solve for the pressure correction equation.
4. Update the pressure and velocity components.
5. Solve the composite equation for phase volume fraction.

Steps 1-5 are repeated till convergence. The system of equations and the solution algorithm presented in the previous sections were implemented into a commercial CFD code (CFD-ACE+) [11]. The linear equations were solved using either a Conjugate Gradient or an Algebraic Multigrid solver.

## 3 Results and Discussion

The two-fluid model formulation has been implemented and evaluated for simulation of two-phase flows relevant to fuel cell analysis. The benchmark model cases for measuring accuracy and robustness was the predicted phase-fraction profiles obtained by Oliveira et al. [23] for the development of stratification of two fluids with different densities.

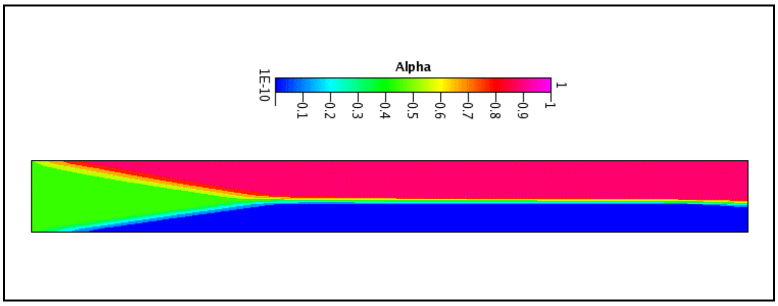


**Figure 1: Alpha contours for stratification for 2d channel case.**

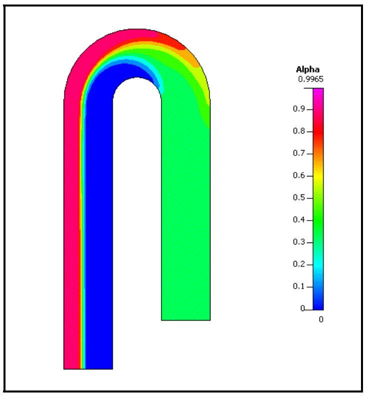

**Figure 2: Liquid fraction, alpha, contours for a U-bend (2d) case.**

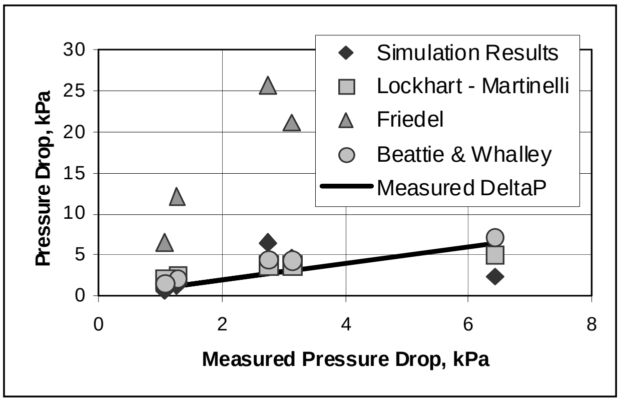


**Figure 3: Comparison of predicted and measured pressure drops for two-phase flow in an annulus, documented by Dillon [24].**

## Two-Phase Transport in Porous Media

The fluid-solid momentum transfer implementation was verified by comparison of predicted pressure drops during one-dimensional, two-phase, flow through porous media with the corresponding analytical solutions, -described in the characterization studies of Nguyen [25].

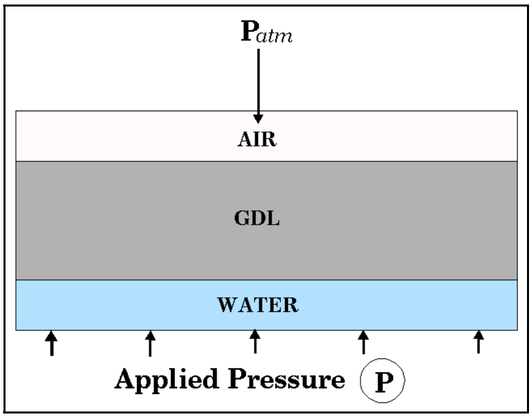


**Figure 4: Schematic of model domain used to assess capillary pressure prediction.**

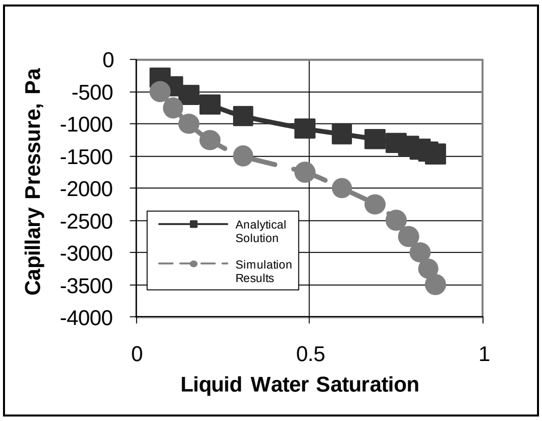


**Figure 5: Comparison of predicted capillary pressure and the analytical value as a function of volume-averaged saturation.**

A saturation gradient is present at the water reservoir – porous media interface, due to the unity liquid phase fraction in the water reservoir. This gradient increased the local value of the capillary pressure at that interface, and caused an over-prediction of the capillary pressure at the volume averaged saturation level. This deficiency of the implementation will be addressed in future work.

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