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TWO-PHASE FLOW AND MASS TRANSFER WITHIN THE DIFFUSION LAYER OF A POLYMER ELECTROLYTE MEMBRANE FUEL CELL*

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The membrane of a polymer electrolyte membrane fuel cell must be hydrated with liquid water at all times in order to function effectively. At high current densities, liquid water in the pores of the diffusion layer inhibits oxygen transport to the cathode. The present paper shows the results of an analysis of two-phase flow and mass transfer in the diffusion layer of a fuel cell. A computational fluid dynamics code is adapted to perform calculations assuming Darcy's law applies, with the rate of oxygen diffusion governed by Fick's law. Both relative permeability and capillary pressure are strongly dependent on saturation. A modified version of the interphase slip algorithm is used to perform flow-field calculations. The two phases are each assigned a different pressure. Phase continuity is solved for liquid-phase saturation, from whence capillary pressure, relative permeability, and oxygen exchange coefficients are obtained. Results of numerical calculations are compared to an analytical solution with excellent agreement. Detailed calculations for a typical present-day fuel cells are presented. The results are correlated in terms of gas mass transfer driving force as a function of blowing parameter.

INTRODUCTION

Fuel cells are electrochemical devices that convert chemical energy into electricity and heat. In principle, they are not constrained by the thermodynamic limitations of conventional heat engines, and moreover they can employ hydrogen and hydrogen-rich fuels and thus reduce CO₂ emissions and global dependence on fossil fuels. Although fuel cells have yet to achieve the goals of reliability, efficiency, and cost necessary to compete in the marketplace, they are nonetheless the subject of much active research and development. In order to compete in the future, they must therefore be engineered to a level of performance expectation that exceeds conventional power equipment. Fuel cells are limited by three fundamental factors, namely, charge transfer, ohmic resistance, and mass transfer. The latter predominates at the high current and power densities needed to further achieve market penetration. The polymer electrolyte membrane fuel cell (PEMFC)

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NOMENCLATURE

A	cell area, m^2	Greek Symbols	
b	blowing parameter	α	net drag coefficient
B	driving force	Γ	exchange coefficient, $kg/(m \cdot s)$
g	mass transfer coefficient, $kg/(m^2 \cdot s)$	δ	cell half-width, m
g^*	zero-flux mass transfer coefficient, $kg/(m^2 \cdot s)$	ε	void space, porosity
H	height, m	θ	contact angle, deg
i''	current density, A/m^2	μ	dynamic viscosity, $kg/(m \cdot s)$
J	Leverett function	ν	kinematic viscosity, m^2/s
k	permeability, $/m^2$	ρ	density, kg/m^3
L	length, m	σ	surface tension, N/m
F	Faraday's constant, $96\,485, C/mol$	Subscripts	
M	molecular weight, kg/mol	b	bulk
m	mass fraction	c	capillary
p	pressure, N/m^2	ch	channel
$\dot{S}$	source term, kg/s	dl	diffusion layer
$\dot{S}''$	source term, $kg/(m^2 \cdot s)$	e	electrode (cathode)
s	saturation	eff	effective
Sh	Sherwood number	g	gas
T	temperature, K	H_2	hydrogen
U	superficial velocity, m/s	H_2O	water
u	phase velocity, m/s	l	liquid
x	displacement, m	rel	relative
		O_2	oxygen
		t	transformed substance state
		P	nodal value
		0	ambient, external

is considered to offer potential for mobile applications, and several manufacturers are investing in this technology.

Mass transfer is an interdisciplinary activity, and different approaches abound. In mechanical engineering, the concept of a mass transfer coefficient (Spalding, 1960) is often employed. Conventional fuel cells, such as PEMFCs and solid oxide fuel cells (SOFCs) generally employ gaseous mixtures as reactants and products. Previous work (Beale, 2004) was concerned with single-phase mass transfer and the development of a single-phase SOFC stack model (Beale and Zhubrin, 2005) based on the distributed resistance analogy of Patankar and Spalding (1974). The PEMFC, however, relies on

the membrane being hydrated in order to function effectively, and hence the problem is two-phase—with both liquid and gas present. Lin and Beale (2005) considered transport and electrochemical phenomena in a single commercial PEMFC unit; however, progress in the development of a PEMFC stack model requires extensions of the approach to SOFCs. An important step in the SOFC stack model was the replacement of fine-scale diffusion terms by simple lumped-parameter mass transfer analysis theory. The purpose of the present work, therefore, is to advance previously developed single-phase mass transfer theory so that it can be applied to a two-phase PEMFC. Attention is confined to the cathode-side porous diffusion layer, where liquid water is present. (NB: The term “diffusion layer” enjoys widespread use in the fuel cell literature. However it is something of a misnomer, and is sometimes referred to simply as a “porous transport layer.” We retain the conventional name here while recognizing the shortcomings.)

Figure 1 illustrates the problem schematically: hydrogen molecules are oxidized to form protons at the anode and pass through the hydrated membrane to combine with oxygen and form water at the cathode. These are transported via a channel (the main flow is perpendicular to the cross section shown in Fig. 1). The solid bipolar plate houses the channel and serves as an electric current collector for the fuel cell. The porous diffusion layer allows oxygen to pass from the channel to the cathode, and water to move in the opposite direction. The ratio of the channel width to the diffusion layer width is often chosen as 1:2 with the channel and bipolar plate being of equal width. The protons also drag water molecules across the membrane; thus, water is produced at the cathode by two mechanisms: (i) as a product of the electrochemical reaction and (ii) due to electro-osmotic drag. In this study, it is presumed that the gas in the channel is already saturated with water vapor and that all water produced is in the liquid form.

Figure 1. Schematic of PEMFC assembly.

Previous Work

The difficulties associated with conducting physical experiments on PEMFCs have led many researchers to develop mathematical models. Studies have been based on noncoupled two-phase flow, simplified two-fluid Darcy's law models, and the so-called "mixture" model. However, few correlations exist for two-phase transport properties such as relative permeability and capillary pressure relevant to PEMFC diffusion layers, which restricts the representative accuracy of the models—a notable exception being the work of Gostick et al. (2006).

Bernardi and Verbrugge (1992) give a 1D model in which transport through the cathode diffusion layer is governed by Darcy's law, and liquid and gas flows are assumed to occur in separate pore spaces, i.e., decoupled. Berning et al. (2002) consider a 3D extension of this model. Janssen (2001) presents a model that describes 1D water transport normal to the catalyst layer interface coupled to a 1D along-the-channel mass balance. The model describes two-phase water transport in the diffusion layers using irreversible thermodynamics, and takes into account local equilibrium between the liquid and vapor phases of water at the catalyst layer interfaces.

Nam and Kaviani (2003) present a 1D two-fluid Darcy's law model for hydrophobic diffusion layers based on water vapor condensation dynamics and capillary motion of the condensate. Pasaogullari and Wang (2004) investigate two-phase transport in both hydrophobic and hydrophilic diffusion layers. Simplified definitions of two-phase Darcy's law transport are presented assuming that capillary action is the dominant water transport process. The model is further simplified by assuming that there is no liquid water present in the channels and that the gas phase is fully saturated with water vapor. Natarajan and Nguyen (2001) develop a pseudo-3D, simplified two-fluid Darcy's law model for the cathode with the discretization of the channel into a series of control volumes that are treated as well mixed. In the diffusion layer, Darcy's law for liquid water transport is expressed in terms of capillary pressure using Richard's equation. The vapor and liquid continuity equations are coupled through an interfacial mass transfer rate. The model does not account for momentum effects in the channel.

You and Liu (2002) develop a 2D model for the cathode. When the partial pressure of water vapor exceeds the saturated vapor pressure, liquid water is formed, and the resulting flow is modeled using a mixture model. Meng and Wang (2005) present a 3D model including two-phase transport in the diffusion layers, namely, a liquid coverage model at the channel/diffusion layer interfaces, and a two-phase flow model in the channels. A mixture model is employed to describe gas and liquid water transport in the diffusion layers. In the channels, mist flow is presumed. Mazumder and Cole (2003) develop a comprehensive 3D model to treat the formation and transport of liquid water using a mixture model. Slip between the gas and liquid phases is accounted for by the relative mobility of the two phases, and phase change is modeled. Senn and Poulikakos (2005) consider multicomponent two-phase transport in the diffusion layer, while Innoue et al.

(2006) model mass transfer in the diffusion layer ignoring liquid water transport. Sinha and Wang (2007) study liquid water flooding by means of a pore network model.

Experimental data are few, although Yang et al. (2004) examined two-phase flow in a transparent fuel cell and recorded microscopic optical images of the liquid water. Time-series images show liquid water drops emerging from the diffusion layer and migrating along the walls in an annular fashion. For industrial fuel cells made of graphite plates, the behavior is more likely drop or slug flow, the former growing on and detaching from the diffusion layer. None of the models above devised for diffusion layers can readily describe these channel flow regimes. Conversely, established Eulerian-Eulerian techniques (Spalding, 1980), which are appropriate for describing annular-, drop-, or slug-type flows, need to be modified to consider the two-phase Darcy's law flow within the porous diffusion layer.

Present Contribution

The primary goal of the present work is to extend previous results for single-phase mass transfer analysis to consider two-phase mass transfer on the air side of a PEMFC. The purpose here is not to develop detailed models specific to any given design, but rather to reduce the two-phase mass transfer problem to a standard form so that fine-scale diffusion terms may be replaced by simple rate equations. This will enable the future construction of spreadsheet calculation procedures for single PEMFCs as well as CFD-based models for large stacks of cells, where prohibitively expensive fine-grid calculations may be replaced by rate terms (Beale and Zhubrin, 2005). At present, PEMFC stack design is seriously restricted by the inability of the CFD engineer to construct fine meshes within memory limitations and run times typical of present-day computers. A secondary goal of this work is to adapt existing Eulerian-Eulerian methodology to the PEMFC problem so that the deficiencies of the "simplified" models above may be abandoned in favor of more rigorous closure assumptions for future PEMFC models, including channels, diffusion layers, and so forth.

Theoretical Formulation

For fluid flow within the diffusion layer, the incompressible multiphase form of Darcy's law is presumed to apply as follows:

$$U_i = s_i u_i = -\frac{k}{\mu_i} k_{\text{rel},i} \text{grad } p_i \quad (1)$$

where $i = l$ (liquid) or g (gas) as appropriate. In Eq. (1), s_i is the effective (excluding connate fluid) phase saturation with $s_g = 1 - s_l$, U_i is the filter or superficial velocity, u_i is the phase velocity, k is the absolute permeability, and k_{rel} is the relative permeability. (NB: u_i is a superficial velocity, not an interstitial or pore velocity.) This formulation

thus accounts for the volume fractions of gas and liquid, but ignores the solid material entirely. The relative permeability of liquid and gas phases are presumed to be

$$k_{\text{rel,g}} = s_g^3 \quad (2)$$

$$k_{\text{rel,l}} = s_l^3 \quad (3)$$

The difference between the gas and liquid pressures is the capillary pressure. This is computed using a J function (Leverett, 1941) as follows:

$$p_c = p_g - p_l = \frac{\sigma \cos \theta}{\sqrt{k/\varepsilon}} J(s_l) \quad (4)$$

Udell (1983) and Pasaogullari and Wang (2004) suggest

$$J = 1.417(1 - s_l) - 2.120(1 - s_l)^2 + 1.263(1 - s_l)^3 \quad (5)$$

$$J = 1.417s_l - 2.120s_l^2 + 1.263s_l^3 \quad (6)$$

for hydrophilic and hydrophobic media, respectively. Phase continuity, in the absence of phase changes, requires that

$$\text{div}(\rho_i s_i u_i) = 0 \quad (7)$$

Since gradients of liquid pressure are much larger than those of gas pressure and are equal in magnitude to those in the capillary pressure, Eq. (7) may be conveniently rewritten as a diffusion equation for liquid,

$$\text{div} \Gamma_l \text{grad } s_l = 0 \quad (8)$$

where

$$\Gamma_l = \sqrt{k\varepsilon} \frac{k_{\text{rel,l}}}{\nu_l} \sigma \cos \theta \frac{dJ}{ds_l} \quad (9)$$

For steady-state mass transfer in the gas phase,

$$\text{div}(\rho_g s_g u_g m) = \text{div } s_g \Gamma_{\text{eff}} \text{grad } m \quad (10)$$

where m is the mass fraction of any given species. The effective exchange coefficient, Γ_{eff} , is estimated using effective medium theory (Nam and Kaviani, 2003),

$$\Gamma_{\text{eff}} = \Gamma \varepsilon^{3/2} s_g^{1/2} \quad (11)$$

Solution of the system of Eqs. (7)–(10) is obtained in terms of overall continuity (gas pressure correction), phase continuity (saturation), momentum, and scalar transport equations using the interphase slip algorithm (IPSA) (Spalding, 1980) as implemented in the

computer code PHOENICS (Spalding, 2006). This approach differs from previous fuel cell codes in that the two-phase Eulerian-Eulerian system of equations is solved for gas and liquid saturations. It differs from previous IPSA calculations in that the diffusion form of the phase continuity equation, Eq. (8), rather than the convective form, Eq. (7), is solved for the phase saturations. The adopted approach is quite general and may be readily employed in a number of other applications of multiphase flow in porous media. In the PHOENICS code, the phase volume fractions are thus identified as the effective saturations, and the use of “porosities” is thus avoided, although there would be no problem employing these if necessary.

Mass Transfer

Let it be proposed that the diffusive flux in Eq. (10) be replaced by a linear rate term,

$$s_g \Gamma_{\text{eff}} \text{grad } m = s_g g_{\text{dl}} (m_e - m_b) \quad (12)$$

where g_{dl} is a diffusion layer mass transfer coefficient, m_e is the mass fraction of oxygen at the cathodic electrode, and m_b is the bulk mass fraction of oxygen at the channel/diffusion layer interface. The “Ohm’s law” for mass transfer (Spalding, 1960, 1963) may be written as

$$\rho_g U_g = s_g g_{\text{dl}} B = s_g g_{\text{dl}}^* b \quad (13)$$

where $g^* = g$, $\lim \rho U \rightarrow 0$.

$$B = \frac{m_b - m_e}{m_e - m_t} \quad (14)$$

$$b = \frac{\rho_g U_g}{s_g g_{\text{dl}}^*} \quad (15)$$

The cathode and bulk species mass fractions and phase saturation are not constant and must be obtained by integration over the appropriate surface. Many mass transfer problems involving chemical reactions require that g is obtained as a function of either the driving force, B , or the blowing parameter, b . Electrochemical devices are rather unique in that the reaction rate, i.e., the mass flux $\rho_g U_g$, and hence the blowing parameter b , are prescribed (galvanostatic boundary condition). The fuel cell mass transfer problem is thus characterized by knowledge of the driving force B as a function of the blowing parameter b . This allows losses due to charge and mass transfer (so-called activation and concentration overpotentials) to be estimated.

Boundary Conditions

The cathode boundary conditions in the transport equations are for fixed flux (Neumann condition) whereas external values are prescribed at the channel boundary as fixed val-

ues or linearized conditions. At the cathode, a constant mass flux corresponding to the current density of i'' is presumed. The mass sources of oxygen and water are prescribed according to Faraday's law as

$$\dot{S}_g'' = \rho_g U_g = -\frac{M_{O_2} i''}{4F} \quad (16)$$

$$\dot{S}_l'' = \rho_l U_l = (1 + 2\alpha) \frac{M_{H_2O} i''}{2F} \quad (17)$$

The gas phase mass flux is negative (suction) and the liquid flux is positive (injection). In Eq. (17), the net drag coefficient, α , is the number of water molecules transported from anode to cathode per proton. It includes both the effects of electro-osmotic drag from the anode to the cathode and back diffusion from the cathode to the anode. Thus, the net drag coefficient is much smaller than that due to electro-osmotic drag alone. According to the experimental results of Janssen and Overvelde (2001), α does not depend significantly on the current density at fixed stoichiometry and varies in the range -0.09 to 0.21 for saturated gases for Nafion 105 and 112 membranes. At the channel/diffusion layer interface, the external pressure is fixed to a constant value, $p_{0,i}$ with $\dot{S}_i'' = k k_{rel,i} (p_{0,i} - p_{p,i}) / \nu_i \delta$, where $p_{p,i}$ is the in-cell pressure. For the gas, it is assumed that $p_{0,g} = 0$; for the liquid, an interfacial saturation $s_{0,l}$ is presumed and used to compute the reference value $p_{0,l}$ by means of Eqs. (4) and (6).

At the cathode, chemical species are presumed to emanate from a reservoir at constant transferred substance state (Spalding, 1960). Since for the gas phase only oxygen is transferred, $m_t = 1$. The liquid is a pure substance, and no phase change is assumed to occur, i.e., the gas is fully saturated. The mass transfer of oxygen at the cathode is $\dot{S}_{O_2}'' = \rho_g U_g (m_t - m_p)$, computed as a fixed source or flux. Mass transfer of oxygen between the bulk fluid in the channel and the diffusion layer is presumed to be governed by a linear rate equation, $\dot{S}_{O_2}'' = s_g g_{ch} (m_b - m_p)$, where m_b is the bulk mass fraction of oxygen in the channel. The value of the channel mass transfer coefficient, g_{ch} , is obtained from a Sherwood number correlation, with $Sh_{ch} = 5.385$ for 1D convection diffusion (planar channel) and $Sh_{ch} = 2.712$ for a square channel with mass transfer at one boundary only (Shah and London, 1978)

RESULTS

One-Dimensional Two-Phase Mass Transfer

The 1D solution corresponds to the case where the channel and diffusion layer are both planar. An analytical solution is possible for the liquid in the 1D case assuming $U_g = 0$ and $\alpha = 0$ (Pasaogullari and Wang, 2004),

$$0.35425 (s_1^4 - s_{0,1}^4) - 0.8480 (s_1^5 - s_{0,1}^5) + 0.6315 (s_1^6 - s_{0,1}^6) - \frac{AM_{H_2O} i''}{2F} \left(\frac{v_l}{\sigma \cos \theta \sqrt{k\varepsilon}} \right) x = 0 \quad (18)$$

where $s_{0,1}$ is the liquid saturation at $x = 0$. Figure 2 is a comparison of the results of calculations performed using the IPSA formulation compared to $s_1(x)$ obtained from Eq. (18) for $s_{0,1} = 0$. Also shown is the absolute value of the capillary pressure $|p_c|$. In both cases agreement is near exact, thus validating the IPSA-based methodology for this class of problem. The saturation gradient drives the liquid flow, which is essentially independent of the gas flow. It can be seen that s_1 and p_c are strongly nonlinear near the origin, where the relative permeability is very small.

Figure 3 shows the results of the mass transfer analysis for the 1D problem in terms of driving force versus blowing parameter. These are both very small for the fuel cell under consideration, and as is readily apparent from Fig. 3, the graph is linear, with

$$B = b \quad (19)$$

This substantially simplifies the PEMFC mass transfer problem. Note however that knowledge of the saturation at the cathode is required in order to compute b in Eq. (15).

Figure 2. Saturation and capillary pressure curves compared to 1D solution.

Figure 3. Mass transfer driving force versus blowing parameter in 1D.

CFD Results

The results for the case corresponding to the data of Table 1 are shown in Figs. 4–10. These results were obtained with a mesh of 40×80 computational cells. Figures 4 and 5 show the gas and liquid phase pressures, respectively. The negative relative pressure is indicative of vacuum conditions (with respect to the channel) inside the diffusion layer. It can be seen that the gas pressure field is harmonic (Laplacian) in nature and that the gas and liquid pressure gradients are in opposite directions, since liquid is being injected whereas gas is being removed at the cathode, i.e., the two fluids are in counterflow. Figures 6 and 7 are corresponding pictures of the gas and liquid phase velocities, where the nature of the counterflow for the two phases is readily apparent. Figure 8 shows level lines of the liquid phase saturation, while Fig. 9 illustrates values of the oxygen mass fraction.

The mass transfer driving force B is shown as a function of the blowing parameter b in Fig. 10. It can be seen that, as was observed in Fig. 3, the driving force versus blowing parameter characteristic is linear. In this case, the saturation used to compute the blowing parameter, Eq. (15), is just the arithmetic mean of the gas saturation s_g at the channel.

DISCUSSION

Flow Field Results

Inspection of the results of Figs. 4–7 show that for the gas, there is suction into the diffusion layer due to the consumption of gaseous oxygen at the cathode. The gas flow vectors are normal to isobars of p_g , which decrease from the channel to the cathode. The

Table 1. Physical details for the particular problem considered

Quantity	Value	Quantity	Value
H_{dl} , mm	0.19	α	0.1
L_{dl} , mm	2	ρ_g , kg/m ³	4.803
H_{ch} , mm	1	μ_g , kg/(m s)	2.048×10^{-5}
p , atm	5	ν_g , m ² /s	4.264×10^{-6}
T , °C	80	Γ , kg/(m s)	6.096×10^{-6}
ρ_{H_2O} , kg/m ³	0.290	ρ_l , kg/m ³	971.97
ρ_{O_2} , kg/m ³	1.051	μ_l , kg/(m s)	3.5445×10^{-4}
ρ_{N_2} , kg/m ³	3.462	ν_l , m ² /s	3.6467×10^{-7}
m_{H_2O}	0.06	θ , deg	120
m_{O_2}	0.22	σ , N/m	0.0644
m_{N_2}	0.72	k , /m ²	1.45×10^{-11}
$s_{0,l}$	0	ε	0.84

Figure 4. Gas vacuum pressure (Pa) relative to channel for $i'' = 5,000$ A/m².

Figure 5. Relative liquid pressure (Pa) for $i'' = 5,000$ A/m².

Figure 6. Gas velocity for $i'' = 5,000$ A/m².

Figure 7. Liquid velocity for $i'' = 5,000 \text{ A/m}^2$.

Figure 8. Gas saturation for $i'' = 5,000 \text{ A/m}^2$.

Figure 9. Oxygen mass fraction for $i'' = 5,000 \text{ A/m}^2$.

Figure 10. Two-dimensional mass transfer driving force versus blowing parameter.

converse is true for vectors of the liquid phase where there is injection at the cathode with p_l decreasing away from the cathode toward the channel. Thus, the two phases are in counterflow, with the magnitude of the gradient in the liquid pressure greater than that of the gas, especially near the channel interface. The liquid velocities are smaller in magnitude than the gas velocities. The water saturation, which is presumed to be very small in the channel, rises substantially within the diffusion layer. The saturation gradient effects a gradient in the capillary pressure, Eqs. (4) and (6), which drives the counterflow of the liquid water in the opposite direction to the gas. Inspection of the liquid saturation, Fig. 8, reveals that the contours are more highly concentrated near the channel boundary, as was shown to be the case in Fig. 2. The boundary value of the liquid saturation s_l is an important parameter. When this is small, i.e., $s_{0,l} \sim 0$, the saturation gradient driving the flow near the channel is correspondingly high. However, if the boundary liquid saturation becomes too large, the saturation and capillary pressure gradients are then too small to permit effective transport through the gas diffusion layer. Thus, if there is sufficient buildup of liquid at the diffusion layer–channel interface, performance will be degraded due to lack of water transport (flooding), i.e., a purely capillary-related effect. This is in addition to any “starvation” effects associated with oxygen being unable to reach the electrolyte due to the presence of liquid water within the pores. Flooding in the channels and/or diffusion layers of PEMFCs is a major concern with negative implications, and it is of much importance that fuel cell scientists develop predictive models to further develop effective and reliable products that do not flood.

Mass Transfer

The fact that the driving force versus blowing parameter graph is linear for a PEMFC of typical contemporary construction is encouraging, and useful for the future construction of simplified-cell or stack-level models. The linear characteristic is due to the fact that the driving force is very small. Since by definition the blowing parameter is the ratio of convection to diffusion, the linear characteristic is a statement to the effect that diffusion is dominant. A corollary is that the mass transfer coefficient, g , is constant, i.e., $g = g^*$ (for small b). This will allow for a simplified mass transfer methodology to be constructed, including multiphase effects. A methodology for performing electrochemical and mass transfer calculations for single-phase flow using a spreadsheet-type analysis was described in the appendix of the paper by Beale (2007), and will not be repeated here. The extensions to the present situation are natural and obvious, provided the mean saturation at the diffusion layer–channel interface can be estimated. Knowledge of the driving force B allows the mass and mole fractions at the cathode to be calculated from the bulk value in the channel, and enables estimates for activation and concentration polarizations to be obtained. In general, the gas saturation must be less than, but near to, unity since, as has already been discussed, if $s_l \gg 0$, the PEMFC is not going to function properly.

Numerical Accuracy

It was found that better numerical stability was obtained when the diffusive form of the continuity equation, Eq. (8), as opposed to the convective form, Eq. (7), was solved for the liquid. The reasons for this are not entirely clear; however, this approach is consistent with those of previous workers (Nam and Kaviani, 2003; Pasaogullari and Wang, 2004) and has the advantage of being second-order accurate. In the PHOENICS code, a convective and/or a diffusive formulation may be adopted since the steady-state phase continuity equation is presumed to be of the form,

$$\text{div}(\rho s u) = \text{div} \Gamma \text{grad } s \quad (20)$$

NB: The origin of the diffusion term in Eq. (20) is in turbulent multiphase flow where a gradient diffusion assumption, $-\overline{\rho s' u'} = \Gamma \text{grad } s$, is sometimes presumed. Equation (8) was conveniently obtained by setting the convection terms in Eq. (20) to be zero, and prescribing Γ_1 according to Eq. (9).

A number of assumptions have been made in the construction of the simplified PEMFC diffusion layer—in particular that (i) the local current density at the cathode does not vary significantly and (ii) the liquid saturation at the channel wall is known. The former will only be true at low current densities; however, at high current densities there will be substantial variations in $i''(x)$. Future studies are required to parameterize the impact of the current density profile on performance in an appropriate nondimensional manner. For the latter, only a detailed analysis of the interfacial phenomena at the channel surface can quantify this important issue.

CONCLUSIONS

The results of this study suggest that it is possible to extend the IPSA (or multiphase SIMPLE) methodology to the analysis of two-phase Darcian flow in PEMFCs. Counter-flow occurs in the diffusion layer of a PEM fuel cell as the result of the production and consumption of liquid water and oxygen gas at the cathode. The motion of the liquid is driven by the capillary pressure, or saturation gradient, and is essentially independent of the gas flow. It is shown that for the reaction rates typical of PEM fuel cells, the mass transfer driving force is small and is a linear function of the blowing parameter. Thus, a standard mass transfer technique (Spalding, 1963) may readily be applied to this particular two-phase flow problem. This will assist in the future development of large-scale two-phase stack simulations based on a distributed resistance analogy, where the construction of CFD grids and solution times are otherwise prohibitively expensive.

The methodology developed here is quite general and thus shows that conventional CFD codes based on standard finite volume techniques may readily be applied to other general-purpose two-phase porous media flows; numerous examples abound in the nat-

ural environment such as groundwater hydrology, petroleum engineering, food processing, and many other applications. Situations where both multiphase Darcy's law and conventional viscous flows (drop, slug, annular, etc.) are simultaneously present are thus amenable to analysis.

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