NUMERICAL MODELLING OF PEM FUEL CELLS
UNDER PARTIALLY HYDRATED MEMBRANE
CONDITIONS

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Abstract

In proton-exchange membrane fuel cells it is particularly important to maintain appropriate water content and temperature in the electrolyte membrane. The water balance depends on the coupling between diffusion of water, pressure variation, and the electro-osmotic drag in the membrane. In this paper we apply conservation laws for water and current, in conjunction with an empirical relationship between electro-osmotic drag and water content, to obtain a transport equation for water molar concentration and to derive a new equation for the electric potential that strictly accounts for variable water content and is more accurate than the conventionally used Laplace’s equation.

The model is coupled with a computational fluid dynamics model that includes the porous gas diffusion electrodes and the reactant flow channels. The resulting coupled model accounts for multi-species diffusion (Stefan-Maxwell equation); first-order reaction kinetics (Butler-Volmer equation); proton transport (Nernst-Planck equation); and water transport in the membrane (Schlögl equation). Numerical simulations for a two-dimensional cell are performed over nominal current densities ranging from \(i = 0.4A/cm^2\) to \(i = 1.2A/cm^2\). The relationship between humidification and the membrane potential loss is investigated, and the impact and importance of two-dimensionality, temperature and pressure non-uniformities are analysed and discussed.

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Nomenclature

**English letters**

A  Area \([m^2]\)
c  Molar concentration \([mol \cdot m^{-3}]\)
\(D\)  Diffusion coefficient \([m^2 \cdot s^{-1}]\)
\(D\)  molecular diffusion coefficient \([kg \cdot m^{-1} \cdot s^{-1}]\)
f  Membrane swelling coefficient
\(F\)  Faraday’s constant \([96487 \text{coulombs} \cdot mol^{-1}]\)
h  Specific enthalpy \([J \cdot kg^{-1}]\)
\(\vec{i}\)  Current density \([A \cdot m^{-2}]\)
\(i_0\)  Nominal current density \([A \cdot m^{-2}]\)
\(k_p\)  Hydraulic permeability \([m^2]\)
\(k_h\)  Permeability of the membrane \([m^2]\)
\(k_\phi\)  Electric permeability \([m^2]\)
\(M\)  Molecular weight \([kg \cdot mol^{-1}]\)
\(n_d\)  Electro-osmotic drag coefficient
\(\dot{n}\)  Stoichiometric molar flux \([mol \cdot s^{-1}]\)
\(\dot{\nabla}\)  Molar flux \([mol \cdot m^{-2} \cdot s^{-1}]\)
p  Pressure \([Pa]\)
\(\dot{q}\)  Heat source \([W \cdot m^{-2}]\)
\(R\)  Universal gas constant \([8.3143 J \cdot mol^{-1} \cdot K^{-1}]\)
s  Entropy \([J \cdot mol^{-1} \cdot K^{-1}]\)
T  Temperature \([K]\)
\(\vec{u}\)  True (actual) velocity of a species \([m \cdot s^{-1}]\)
u  Velocity component in the \(x\)-direction \([m \cdot s^{-1}]\)
\(\vec{U}\)  Bulk velocity \([m \cdot s^{-1}]\)
v  Velocity component in the \(y\)-direction \([m \cdot s^{-1}]\)
\(V\)  Volumetric flow rate \([m^3 \cdot s^{-1}]\)
\(X\)  Molar fraction of a species in the gas mixture
Z  Charge number

**Greek letters**

\(\alpha\)  Relative humidity
\(\epsilon_m^w\)  Volume fraction of the water in the membrane
\(\eta\)  Overpotential \(V\)
\(\gamma\)  Porosity
\(\Gamma\)  Boundary of computational domain or interface between components
\(\kappa\)  Membrane conductivity \([A \cdot V^{-1} \cdot m^{-1}]\)
\(\lambda\)  Hydration index in the membrane
\(\Lambda\)  Thermal conductivity \([W \cdot m^{-1} \cdot K^{-1}]\)
\(\mu\)  Molecular viscosity \([kg \cdot m^{-1} \cdot s^{-1}]\)
\(\omega\)  Mass fraction of a species in the gas mixture
\(\phi\)  Electric potential \([V]\)
\(\rho\)  Density \([kg \cdot m^{-3}]\)
\(\xi\)  Bulk viscosity \([kg \cdot m^{-1} \cdot s^{-1}]\)
\(\zeta\)  Stoichiometric flow ratio
Sub-scripts for Boundaries or interfaces

\( i_a \) Interface between anode-side channel and anode  
\( i_{an} \) Interface (catalyst layer) between anode and membrane  
\( i_{aw} \) Anode wall boundary  
\( i_c \) Interface between cathode-side channel and cathode  
\( i_{cm} \) Interface (catalyst layer) between cathode and membrane  
\( i_{cw} \) Cathode wall boundary  
\( i_{ina} \) Anode inlet boundary  
\( i_{inach} \) Anode-side channel inlet boundary  
\( i_{inc} \) Cathode inlet boundary  
\( i_{incch} \) Cathode-side channel inlet boundary  
\( i_{inm} \) Membrane inlet boundary  
\( i_{outa} \) Anode outlet boundary  
\( i_{outach} \) Anode-side channel outlet boundary  
\( i_{outc} \) Cathode outlet boundary  
\( i_{outcch} \) Cathode-side channel outlet boundary  
\( i_{outm} \) Membrane outlet boundary

Other super- and sub-scripts

\( i_{ano} \) Anode  
\( i_{cat} \) Cathode  
\( i_{eff} \) Effective quantity  
\( i_{envor} \) Environmental (ambient) condition  
\( i_f \) Fixed charge in the membrane  
\( i_g \) Gas phase  
\( i_l \) Liquid phase  
\( i_m \) Membrane  
\( i_p \) Proton  
\( i_{sat} \) Saturation state  
\( i_w \) Water in the liquid phase

1. Introduction.

Water management of proton exchange membrane fuel cells (PEMFCs) is a critical operation issue. Optimal operation is achieved by carefully balancing the supply and removal of water vapor to ensure that neither flooding of the electrodes nor drying out of the membrane take place. Protonic conductivity is strongly dependent on the membrane water content, and high conductivity required for efficient operation can
only be achieved by maintaining the membrane near full water saturation.

Water transport in the membrane is driven by diffusion, pressure gradient, and electro-osmotic drag. Water is produced at the membrane-cathode catalyst interface. The dragging of water molecules from anode to cathode by migrating proton is counteracted by back diffusion of water from cathode to anode. In particular, at high current densities electro-osmotic drag is dominant leading to potential dehydration on the anode side of the membrane. The overall mechanism is further complicated by the globally exothermic electrochemical reaction [10]. The heat generated increases water evaporation rates at the cathode and, in situations where the membrane is allowed to dehydrate, can combine with ohmic heating in the membrane leading to a deterioration of the membrane-electrode bond.

To avoid membrane dehydration, water management schemes that rely on the humidification of the hydrogen and air streams are usually employed. Such schemes require careful implementation in order to avoid excessive water condensation in the gas diffusion electrodes (flooding) that would plug the pores and prevent reactants from diffusing towards the reaction site, thereby starving the cell.

Since *in-situ* measurements are often difficult, a number of modeling studies have been conducted to better understand how the water and heat management is affected by the physical processes and mechanisms of PEMFCs. Bernardi and Verbrugge (cf. [2, 3, 4]) developed a comprehensive model that couples appropriate thermodynamic conservation laws with a set of four basic phenomenological equations: the Stefan-Maxwell equation for the description of multi-species diffusion, the Butler-Volmer equation for the description of first-order reaction kinetics, the Nernst-Planck equation for the calculation of proton flux through membrane, and the Schlögl equation for the calculation of water velocity in membrane. The model proposed by Springer *et al.* (cf. [15, 14]) to account for a partially hydrated membrane is more empirical in nature. In this model, the Stefan-Maxwell equations along with a correction that accounts for porosity are employed in the diffusion layer; the pressure-diffusivity products for
the Stefan-Maxwell relations are calculated with an empirical formula; the net flux of water across the membrane is calculated using the electro-osmotic drag and diffusion coefficients of water, both of which are functions of the membrane water content. Springer et al. use their model to calculate the water flux across the membrane first and then deduce the membrane resistance and the potential drop across it. Their results show that the water content drops from anode to cathode, and decreases significantly with increasing current. Sena et al. (cf. [12]) considered low operating temperature conditions with dry hydrogen and developed a one-dimensional model to account for water content variation in the membrane. Their model accounts for diffusion and drag of water, and provides satisfactory agreement with experiments for Nafion membranes.

Most existing models are one-dimensional and assume the system is under isothermal and isobaric conditions. Furthermore, they are restricted to the Membrane-Electrode Assembly (MEA) and do not consider convective mass and heat transport in the gas flow channels, but rather prescribe approximate boundary conditions (prescribed concentration) at the flow channel-porous electrode interfaces.

One-dimensional isothermal models, though useful for fundamental understanding, remain applicable only to small single cells with relatively simple geometries and flow channel configurations. Gurau et al. [8] and Singh et al. [13] have clearly shown in their two-dimensional models the importance of transport along the direction of the reactant flow as well as across the MEA. Variation in temperature and pressure is also an important issue: heat transfer and pressure variation can strongly affect water transport and phase change in the porous gas diffusion electrodes. In stack modeling, multi-dimensional convective and diffusive heat and mass transfer has to eventually be taken into account if realistic simulation and design tools are to be obtained over a range of operating conditions and scales.

Recently, [9, 17, 11, 16] presented their two- and three-dimensional PEMFC modeling work, some of which also accounted for the role of water content in determining
the membrane performance. Building upon earlier modeling studies, in this paper we present a two-dimensional, non-isothermal, and non-isobaric model for a complete fuel cell, in which convective transport in the flow channels and water content variation in the membrane are taken into account. Section 2 describes relevant mass and heat transfer processes in PEMFCs. Modelling assumptions are discussed next and the detailed transport models are presented in Section 3, using established conservation laws for mass, momentum, and energy in conjunction with the phenomenological equations developed in Bernardi and Verbrugge’s work [2, 3, 4] which are extended here to two-dimensions and for non-isothermal conditions. The focus of the paper is placed on the study of partial hydration in the membrane. For this purpose, we develop our membrane model partly based on empirical relationships proposed by Springer et al. [15, 14] to explicitly account for water diffusion, pressure distribution, and electro-osmotic drag; thermal effects are introduced implicitly via the variation of membrane transport parameters as functions of temperature. The model is solved numerically using a finite volume method, and a series of numerical experiments are presented and analyzed in Section 4 along with discussion focusing on the effect of two-dimensionality, pressure-gradient, and relative-humidity on PEMFC operation. Finally, some concluding remarks on this study are made in Section 5.

2. Transport processes in fuel cell.

A two-dimensional schematic of a PEMFC is shown in Fig. 1. The Membrane-Electrode Assembly (MEA) is mounted between the anode-side and cathode-side gas distribution channels. The MEA, which is the core of a PEMFC, consists of a polymer electrolyte membrane sandwiched between two catalyzed porous electrodes. The operation of a PEMFC involves the following transport processes:

- A humidified hydrogen fuel mixture \((H_2, CO_2, H_2O(g))\) flows into the

  anode channel.
• Hydrogen diffuses through the porous gas-diffusion anode;
• An electrochemical reaction takes place at the anode-side catalyst:

\[
H_2 \rightarrow 2H^+ + 2e^-
\]

• Electrons flow through the external circuit, providing useful electrical power; meanwhile, protons migrate through the membrane towards the cathode side;
• Humidified air \((O_2, N_2, H_2O_{(g)})\) enters the cathode channel;
• Oxygen diffuses through the porous gas-diffusion cathode;
• A reduction reaction takes place at the cathode-side catalyst producing water and heat:

\[
\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O (+\text{Heat})
\]

In our model, all the above heat and mass transport processes are represented, including the depletion of oxygen and hydrogen at the catalyst layers, the generation
of heat, and the additional water generated as a result of the reduction reaction occurring at the cathode-side catalyst layer.


In order to make the model tractable, we invoke the following assumptions:

1. the transport processes are steady-state and two-dimensional;

2. on the cathode side, the gaseous mixture consists of $O_2$, $N_2$, and $H_2O_{(g)}$ only, while on the anode side, the gaseous mixture consists of $H_2$, $CO_2$ (due to incomplete purification of the hydrogen product), and $H_2O_{(g)}$ only;

3. all gases obey the ideal gas law;

4. the flow in the gas-distribution channels is laminar;

5. the water in the pores of the gas diffusion electrodes is considered separate from the gases, i.e., the gas and liquid water are at different pressures [19];

6. the catalyst layers are sufficiently thin to be considered as interfaces contributing only source/sink terms to the mass and heat transfer processes;

7. no phase change is taken into account for water transport within each component of the PEMFC;

8. water in the membrane is in the liquid phase only, and the water pressure varies linearly in the membrane.

Fig. 2 shows a schematic of the entire computational domain along with associated boundaries and interfaces. Next, the mathematical formulation for the transport processes in a PEMFC will be described on a component-by-component basis.
3.1. In channels.

In the gas flow channels, the first four assumptions are used. The fluid flow behavior is represented by the steady-state Navier-Stokes equations:

\[ \nabla \cdot (\rho_g \vec{U}_g) = 0 \]  
\[ -\left( \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} \right) + \rho_g (\vec{U}_g \cdot \nabla) u_g - \frac{\partial p_g}{\partial x} = 0 \]  
\[ -\left( \frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} \right) + \rho_g (\vec{U}_g \cdot \nabla) v_g - \frac{\partial p_g}{\partial y} = 0 \]  
\[ -\nabla \cdot (\Lambda_g \nabla T_g) + \nabla \cdot (\rho_g \vec{U}_g H) = 0 \]

In the above four equations, (1) is the mass conservation equation, in which \( \rho_g \) and \( \vec{U}_g = (u_g, v_g)^T \) are the density and velocity of the gaseous mixture, respectively. (2) and (3) are the momentum conservation equations for the \( x \)-direction and \( y \)-direction, respectively.
In these two equations, \( p_g \) is the pressure of the fluid, \( \sigma_{xx} \), \( \sigma_{yy} \), and \( \sigma_{xy} \) are stresses expressed as:

\[
\sigma_{xx} = 2\mu \frac{\partial u_g}{\partial x} + (\xi - \frac{2}{3}\mu) \left( \frac{\partial u_g}{\partial x} + \frac{\partial v_g}{\partial y} \right) 
\]

\[
\sigma_{yy} = 2\mu \frac{\partial v_g}{\partial y} + (\xi - \frac{2}{3}\mu) \left( \frac{\partial u_g}{\partial x} + \frac{\partial v_g}{\partial y} \right) 
\]

\[
\sigma_{xy} = \sigma_{yx} = \mu \left( \frac{\partial u_g}{\partial x} + \frac{\partial v_g}{\partial y} \right) 
\]

with \( \mu \), molecular viscosity, and \( \xi \), bulk viscosity. (4) is the energy conservation equation, in which \( H \) is the total enthalpy, given in terms of the static (thermodynamic) enthalpy \( h \) by:

\[
H = h + \frac{1}{2} |\vec{U}_g|^2 
\]

and \( \Lambda_g \) is the thermal conductivity. We remark that the subscript \( g \) here represents “gas”.

The five equations (1) - (4) and (8) involve seven unknowns: \( \rho_g, u_g, v_g, p_g, T_g, H, \) and \( h \). Note that these physical variables are used to describe the behavior of bulk flow, that is, they represent the behavior of the gaseous mixture instead of that for a certain individual species in the mixture.

The system is closed with the addition of two thermodynamic relations. One is the constitutive equation, relating static enthalpy to temperature and pressure:

\[
h = h(T_g, p_g) 
\]

Since here the fluid is assumed to obey the ideal gas model, \( h \) is a function of temperature only, that is:

\[
\Delta h = C_p \Delta T_g 
\]

if \( C_p \) is approximately viewed as constant.

The other auxiliary equation is the state equation, relating density to temperature and pressure. That is, for each ideal gas \( i \) contained in the gaseous mixture, which
represents one of the three species $O_2$, $N_2$, and $H_2O_{(g)}$ in the cathode-side channel, or one of $H_2$, $CO_2$, and $H_2O_{(g)}$ in the anode-side channel, it obeys:

$$\rho_i = \frac{p_g M_i}{RT_g}$$  \hspace{1cm} (11)

where $M_i$ is the molecular weight of $i$, and $R$ is the universal gas constant (8.3143 J mol$^{-1}$ K$^{-1}$). The relationship between the average density $\rho_g$ and the density of components in the mixture, $\rho_i$, is:

$$\frac{1}{\rho_g} = \sum_{i=1}^{3} \frac{\omega_i}{\rho_i}$$  \hspace{1cm} (12)

In (12), $\omega_i$ is the mass fraction of the species $i$ in the mixture. Each species obeys the following generic advective-diffusive mass transfer equation:

$$- \vec{\nabla} \cdot (D_g \vec{\nabla} \omega_g) + \vec{\nabla} \cdot (\vec{U}_g \rho_g \omega_g) = 0$$  \hspace{1cm} (13)

where, $D_g$, is the molecular diffusion coefficient. In a binary mixture of two species ($A$ and $B$), $D_{gA} = D_{gB} = \rho D_{AB}$, with $D_{AB}$, binary diffusivity of $A$ in $B$. However, our case is a ternary mixture on both cathode and anode sides. We may choose to approximately view the three species as existing in three pairs - $O_2$ and $N_2$, $N_2$ and $H_2O_{(g)}$, $H_2O_{(g)}$ and $O_2$ in the cathode-side channel, and this treatment can similarly apply to the anode-side channel. Thus, each 2-species pair can be considered as a binary mixture so that we can treat our ternary mixture by simply using binary-mixture-related approaches.

The model equations represent a mathematically well-posed system that can be solved to obtain the quantities of interest: $\vec{U}_g$, $\rho_g$, $p_g$, $T$, and $\omega_g$. Note again that here $\vec{U}_g$ is the bulk velocity rather than the diffusion velocity of each species, $\vec{U}_i$, defined as:

$$\vec{U}_i = \vec{u}_i - \vec{U}_g$$  \hspace{1cm} (14)

with $\vec{u}_i$, the true (actual) velocity of the species $i$. To investigate in details the diffusion of each species of the ternary mixture, we need to solve the Stefan-Maxwell
equations (cf. [5]):

\[ \vec{\nabla} X_{g_i} = - \sum_{j=1(j\neq i)}^{3} \frac{X_{g_i} X_{g_j}}{D_{ij}^{eff}} (\vec{U}_i - \vec{U}_j) \]  

Here, \( D_{ij}^{eff} \) is the binary effective diffusivity for each 2-species pair, \( X_{g_i} \) is the molar fraction of the \( i \)-species in the gas mixture, which can be readily calculated from \( \omega_{g_i} \) as follows:

\[ X_{g_i} = \frac{\omega_{g_i}}{\sum_{j=1}^{3} \omega_{g_j} M_j} \]  

which can also be inverted:

\[ \omega_{g_i} = \frac{X_{g_i} M_i}{\sum_{j=1}^{3} X_{g_j} M_j} \]  

In practice, we replace the distribution of \( X_{H_2O(g)} \) by employing the saturation assumption:

\[ X_{H_2O(g)} = 0 \]  

here, the saturation pressure, \( p_g^{sat} \), can be expressed using the following empirical formula (cf. [15]):

\[ p_g^{sat} = 10 \left(-2.1794+0.02953(T-273) - 9.1837 \times 10^{-5}(T-273)^2 + 1.4454 \times 10^{-7}(T-273)^3\right) \]  

and \( \alpha \) is relative humidity, which is 1 if the gaseous mixture is fully humidified. After replacing \( X_{H_2O(g)} \), \( \omega_{H_2O(g)} \) is also to be accordingly updated by using (17) for \( H_2O(g) \), which replaces the solution resulting from (13).

On the two channels (see Fig. 2), boundary conditions are prescribed as follows. Along \( \Gamma_{aw} \) and \( \Gamma_{cw} \), the ambient temperature, \( T_{envir} \), and no-slip velocity condition are prescribed. At the two inlets \( \Gamma_{inach} \) and \( \Gamma_{incch} \), the horizontal inflow velocity, \( u \), the ambient temperature, \( T_{envir} \), and the mass fractions \( \omega_{O_2}, \omega_{H_2}, \) and \( \omega_{H_2O(g)} \) should be also specified. Based on the mechanism of cell reactions that requires \( \frac{1}{2} \) mole of \( H_2 \) and \( \frac{1}{4} \) mole of \( O_2 \) to produce one electron with the charge of one Coulomb, we have the following relationships between the stoichiometric mole fluxes and the value of the desired current density, \( i_0 \), which is also called the nominal current density:

\[ \dot{n}_{H_2,\text{required}} = \frac{1}{2} \frac{i_0 A_{MEA}}{F} \]
\[ \dot{n}_{O_2,\text{required}} = \frac{1}{4} \frac{i_0 A_{MEA}}{F} \]

with \( A_{MEA} \), active section area of the membrane electrode assembly (MEA), and \( F \), Faraday constant \( (96487 \text{coulomb/mol}) \). The volume is related to the molar flux by the ideal gas law in its differential form:

\[ p \dot{V} = \dot{n}RT_{\text{envir}} \]

in which \( p \) and \( \dot{V} \) are the pressure and volumetric flow rate corresponding to the gas component, respectively, and \( R \) is the gas universal constant \( (8.3143 \text{J/mol·K}) \). Rearranging equations (20) and (21) with (22) leads to the volume flow ratios of the inlet streams at the cathode and the anode as follows:

\[ \dot{V}_{\text{cat}} = \zeta_{\text{cat}} \frac{1}{4} \frac{i_0 A_{MEA} R T_{\text{envir}}}{X_{O_2}^{\text{in}}} p_{\text{cat}}^{\text{g}} \]

at \( \Gamma_{\text{inach}} \), and

\[ \dot{V}_{\text{ano}} = \zeta_{\text{ano}} \frac{1}{2} \frac{i_0 A_{MEA} R T_{\text{envir}}}{X_{H_2}^{\text{in}}} p_{\text{ano}}^{\text{g}} \]

at \( \Gamma_{\text{inach}} \), with \( \zeta \) denoting the stoichiometric flow ratio. The volume flow in (23) and (24) divided by the section area of the inlet yields the horizontal inflow velocity, \( u \), at \( \Gamma_{\text{inach}} \) and \( \Gamma_{\text{inach}} \). Finally, at the two outlets \( \Gamma_{\text{outach}} \) and \( \Gamma_{\text{outcch}} \), we need to set two different pressure values, \( p_{\text{ano}}^{\text{g}} \) and \( p_{\text{cat}}^{\text{g}} \), which have appeared in (24) and (23), respectively, representing a pressure drop over the MEA. \( \Gamma_a \) or \( \Gamma_c \) are interfaces between channels and electrodes. As described later in Section 3.2 for the electrodes, all the modeling equations presented here will be slightly modified to account for porosity, therefore, we do not specify any particular boundary conditions at \( \Gamma_a \) or \( \Gamma_c \), assuming continuity for the velocity and the pressure of the gas phase at these two interfaces.

### 3.2. In electrodes.
The equations described in Section 3.1 are applicable to the transport phenomena in electrodes with the introduction of the porosity $\gamma$ of the material. Consequently, the continuity equation becomes:

\begin{equation}
\nabla \cdot (\rho g \gamma \vec{U}_g) = 0
\end{equation}

and the momentum equation is reduced to the Darcy’s law:

\begin{equation}
\gamma \vec{U}_g = \frac{k_{g,p} \nabla p_g}{\mu_g}
\end{equation}

where $k_{g,p}$ is the gas-phase hydraulic permeability. Boundary conditions are not required at the interfaces between electrode and channel since electrodes are here considered as extension of the computational domain from channels.

Since Assumption 5 states that the liquid water pores are considered decoupled from the gas pores, the liquid water satisfies the following incompressibility condition:

\begin{equation}
\nabla \cdot (\gamma \vec{U}_l) = 0
\end{equation}

and the Darcy’s law is used for liquid water as well:

\begin{equation}
\gamma \vec{U}_l = \frac{k_{l,p} \nabla p_l}{\mu_l}
\end{equation}

here $k_{l,p}$ is the liquid-phase hydraulic permeability. Note that here the subscript $l$ represents “liquid”.

Again, accounting for the porous nature of the electrodes, the energy equation reads:

\begin{equation}
-\nabla \cdot (\Lambda_g \gamma \nabla T_g) + \nabla \cdot (\rho g \gamma \vec{U}_g H) = 0
\end{equation}

while the generic advective-diffusive mass transfer equation is written as:

\begin{equation}
-\nabla \cdot (D_{g,i} \gamma \nabla \omega_{g,i}) + \nabla \cdot (\vec{U}_g \rho g \gamma \omega_{g,i}) = 0
\end{equation}

We note that, given $\gamma = 1$, equations (29) and (30) are identical to equations (4) and (13) in Section 3.1.
For equations (27) - (30), generally we only need to keep the pressure drop, which is from \( p_{\text{cat}}^g \) at \( \Gamma_c \) to \( p_{\text{ano}}^g \) at \( \Gamma_a \) (see Fig. 2), and set \( T_{\text{envir}} \) for both \( \Gamma_a \) and \( \Gamma_c \); also, we impose homogeneous condition for the mass fractions \( \omega_{O_2}, \omega_{H_2}, \) and \( \omega_{H_2O(g)} \) at these two borders.

### 3.3. At catalysts.

Here, we do not explicitly give specific modeling equations due to complexities of physics and chemistry at catalysts. However, as stated in Assumption 6 in the beginning of Section 3, we treat the two catalyst layers located at \( \Gamma_{am} \) and \( \Gamma_{cm} \) (see Fig. 2) as interfaces, along which certain source and/or sink terms have to be added to keep balances for mass and heat.

To account for two-dimensionality in our modeling work, in this section, the current density is vectorized as \( \vec{i} = (i_x, i_y)^t \) (see Fig. 1 for the setting of the coordinate system) though the component of the current density in the \( x \)-direction is practically nil.

On the cathode side, a sink term is used to account for the depletion of oxygen at \( \Gamma_{cm} \):

\[
S_{O_2} = -\frac{\vec{\nabla} \cdot \vec{i}}{4F} M_{O_2} \tag{31}
\]

while on the anode side the depleted hydrogen at \( \Gamma_{am} \) is:

\[
S_{H_2} = -\frac{\vec{\nabla} \cdot \vec{i}}{2F} M_{H_2} \tag{32}
\]

with \( F \), Faraday constant (96487 \( \text{coulomb/mol} \)). Corresponding to the two boundaries \( \Gamma_{cm} \) and \( \Gamma_{am} \), these two sink terms will be added to the right hand side of (30) for the oxygen and hydrogen, respectively.

To determine \( i_y \), variable \( y \)-direction component of the current density, the reaction kinetics is taken to be first-order and thus can be described by the Bulter-
Volmer equation (cf. [1]):

\[ i_y = i_0(e^{-\theta nF\eta/RT} - e^{(1-\theta)nF\eta/RT}) \]

where \( i_0 \) is the nominal current density; \( \theta \) is the exchange coefficient measuring the symmetry of the energy barrier; \( n \) is the number of electrons transferred; \( \eta \) is the overpotential; and \( R \) is universal gas constant (8.3143 \( \text{J mol}^{-1} \text{K}^{-1} \)). Then, for the energy equation (29), the heat generated at \( \Gamma_{cm} \) can be calculated using [10]:

\[ \dot{q}_r = \left[ \frac{T(-\Delta s)}{2F} + \eta \right] i_y \]

where \( \Delta s \) is the entropy change of the reaction.

For the liquid water continuity equation (27), the source terms at \( \Gamma_{cm} \) and \( \Gamma_{am} \) are:

\[ S_{H_2O\text{cathode}} = \nabla \cdot \left( \frac{\vec{i}}{2F} + \vec{N}_{H_2O(g)} \right) \frac{M_{H_2O}}{\rho_{H_2O}} \]

\[ S_{H_2O\text{anode}} = \left( \nabla \cdot \vec{N}_{H_2O(g)} \right) \frac{M_{H_2O}}{\rho_{H_2O}} \]

where \( \vec{N}_{H_2O(g)} \) is the molar flux of water vapor, which is all transformed here into liquid water (refer to Assumption 8 that states water in the membrane is in the liquid phase only); the term \( \frac{\vec{i}}{2F} \) represents the molar flux of the water produced due to electrochemical reaction at the cathode-side catalyst.

### 3.4. In membrane.

An improved model is formulated here to allow quantitative assessment of fuel cell operation with a partially hydrated membrane. Some preliminary results using this newly developed approach have been presented in [6]. In our work, we consider liquid water and protons as the only two mobile species in the membrane. Each of these two species should obey the mass conservation principle. Thus, we have:

\[ \nabla \cdot \vec{N}_{w} = 0 \]
and

\[ \nabla \cdot \vec{N}_p = 0 \]  

where, \( N_w \) and \( N_p \) are the molar flux of water and that of protons, respectively.

### 3.4.1. Water transport.

The molar flux of water is taken to be governed by the balance between diffusion, pressure gradient, and electro-osmotic drag, i.e.:

\[ N_w = -D_w \nabla c_w - c_w \epsilon_w^m \frac{k_h}{\mu_l} \nabla p + \frac{n_d \vec{i}}{F} \]  

where, \( c_w \) is the molar concentration of water, which is the variable of interest; \( D_w \) is the diffusion coefficient; \( \epsilon_w^m \) is the volume fraction of the water in the membrane; \( k_h \) is the permeability of the membrane due to hydraulic quantity; \( \mu_l \) is the viscosity; \( p \) is the pressure; \( n_d \) is the electro-osmotic drag coefficient, which will be further discussed later in this Section; and \( \vec{i} \) is the 2-component current density vector as remarked in Section 3.3. Note that the subscript \( w \) here uniquely represents “water”.

Taking into account current conservation:

\[ \nabla \cdot \vec{i} = 0 \]  

and the assumed linear profile of pressure:

\[ \nabla^2 p_l = 0 \]  

the divergence of \( \vec{N}_w \) in (39) reduces to:

\[ \nabla \cdot \vec{N}_w = -D_w \nabla^2 c_w - c_w \epsilon_w^m \frac{k_h}{\mu_l} (\nabla c_w \cdot \nabla p_l) + \frac{\nabla n_d \cdot \vec{i}}{F} \]  

On account of (37), we get:

\[ -D_w \nabla^2 c_w - c_w \epsilon_w^m \frac{k_h}{\mu_l} (\nabla c_w \cdot \nabla p_l) + \frac{\nabla n_d \cdot \vec{i}}{F} = 0 \]
The determination of the electro-osmotic drag coefficient, \( n_d \), follows the work of Springer et al. [15] who propose a functional relationship between this coefficient and membrane water content for Nafion 117:

\[
n_d = \frac{2.5}{22} \lambda
\]

where \( \lambda \) is the hydration index, which is defined as the number of moles of water per equivalent sulfonic acid group, \( SO_3^- \), in the membrane; the numeric values 2.5 and 22 correspond to the number of water molecules dragged per migrating \( H^+ \) ion and the possible maximum hydration index, respectively. They also present an empirical formula relating \( c_w \) to \( \lambda \) as follows:

\[
c_w = \frac{e \lambda}{f \lambda + 1}
\]

here, \( f \) is an experimentally determined swelling coefficient for the membrane, \( e \) is expressed as:

\[
e = \frac{\rho_{m}^{dry}}{E_m}
\]

with \( \rho_{m}^{dry} \), dry membrane density, and \( E_m \), equivalent membrane weight.

Formula (45) can be re-written as:

\[
\lambda = \frac{c_w}{e - f c_w}
\]

Thus, for Nafion 117, the electro-osmotic drag coefficient \( n_d \) in (44) can be eventually expressed as:

\[
n_d = \frac{2.5}{22} \frac{c_w}{e - f c_w}
\]

Substituting \( n_d \) in (43) by (48), we get:

\[
-D_w \nabla^2 c_w - c_w \frac{k_l}{\mu_l} (\nabla c_w \cdot \nabla p_l) + \frac{5}{44} \frac{e}{F(e - f c_w)^2} (\nabla c_w \cdot \vec{t}) = 0
\]

Given the solutions of pressure \( p \) and current density \( \vec{i} \), (49) can be viewed as an equation for \( c_w \). For a specific membrane hydration study, we may specify a constant \( c_w \) value along \( \Gamma_{am} \) (see Fig. 2), while prescribing the water content behavior at \( \Gamma_{cm} \).
in such a way that the water balance condition described by (35) and (36) is satisfied on point-by-point basis throughout the length of the membrane.

### 3.4.2. Proton transport.

The flux of protons through the membrane is given by the *Nernst-Planck equation*, indicating that the contributions to the net molar flux of protons come from migration, diffusion, and convection of the dissolved protons (see [3], [13], and [18] for details):

\[
\vec{N}_p = -Z_p \frac{F}{RT} D_p c_p \vec{\nabla} \phi - D_p c_p \vec{\nabla} \phi + c_p \vec{U}_l
\]  

(50)

where, \(Z_p\) is the charge number of ion, \(D_p\) is the diffusion coefficient, \(c_p\) is the molar concentration of protons, \(\phi\) is the electric potential, and \(\vec{U}_l\) is the convective velocity of the liquid water. Note that here the subscript \(p\) uniquely represents “proton”.

The velocity of liquid water in the pores of the membrane can be estimated by the Schlögl equation [13, 18] which states that the convection is driven by the electric potential and the pressure gradient:

\[
\vec{U}_l = \epsilon_m \left( \frac{k_\phi}{\mu_l} Z_f c_f F \vec{\nabla} \phi - \frac{k_p}{\mu_l} \vec{\nabla} p_l \right)
\]  

(51)

where \(k_\phi\) is the electric permeability; \(k_p\) is the hydraulic permeability; \(Z_f\) is the charge number of the fixed charges; and \(c_f\) is the fixed-charge concentration.

The flow of charged species is related to the current density by:

\[
\vec{i} = F \sum Z_i \vec{N}_i = F \vec{N}_p
\]  

(52)

because \(Z_i = 1\) for the only mobile ions which are the hydrogen ions in this scenario.

The membrane conductivity is defined as:

\[
\kappa = \frac{F^2}{RT} \sum Z_i^2 D_i c_i
\]  

(53)
We also have the electroneutrality condition:

$$Z_f c_f + \sum Z_i c_i = 0 \quad (54)$$

Here, we remark that the only mobile ions in the membrane are the hydrogen ions, and for $H^+$ we have

$$Z_p = 1 \quad (55)$$

so (54) can be written as:

$$Z_f c_f = -c_p \quad (56)$$

Hence, equations (50) - (53) are re-written as:

$$\vec{N}_p = -F \frac{RT}{D_p} c_p \vec{\nabla} \phi - D_p \vec{\nabla} c_p + c_p \vec{U}_l \quad (57)$$

$$\vec{U}_l = -\epsilon_m \left( \frac{k_m}{\mu_l} c_p F \vec{\nabla} \phi + \frac{k_p}{\mu_l} \vec{\nabla} p_l \right) \quad (58)$$

$$\vec{N}_p = \frac{i}{F} \quad (59)$$

and

$$\kappa = \frac{F^2}{RT} D_p c_p \quad (60)$$

Re-arrangements through taking the divergence of equation (57) and using equations (58) - (60) along with (38) lead to:

$$-\Delta \phi = -\frac{1}{\kappa} \left( \vec{\nabla} (\ln c_p) \cdot \vec{i} \right) + \frac{RT}{F} \vec{\nabla} \cdot \left( \vec{\nabla} (\ln c_p) \right) \quad (61)$$

The membrane swells due to presence of internal liquid water. Therefore, $c_p$ becomes a function of hydration instead of a constant. Since in the membrane the hydration index, $\lambda$, is defined as the number of moles of water per equivalent sulfonic acid group, $SO_3^-$, for Nafion 117, the proton concentration can be described as:

$$c_p = \frac{c_w}{\lambda} \quad (62)$$

Substituing (45) into (62) results in:

$$c_p = \frac{e}{f \lambda + 1} \quad (63)$$
The comparison between (45) and (62) shows the relationship between these two variables as follows:

\[ c_p = e - f c_w \] (64)

Substituting (64) into (61), we get:

\[ -\Delta \phi = \frac{1}{\kappa} \frac{f}{e - f c_w} (\nabla c_w \cdot \vec{i}) - \frac{RT}{F} \frac{f}{e - f c_w} \Delta c_w - \frac{RT}{F} \left( \frac{f}{e - f c_w} \right)^2 (\nabla c_w \cdot \nabla c_w) \] (65)

Furthermore, we substitute (49) into (65) so that \( \Delta c_w \), i.e., \( \nabla^2 c_w \) can be eliminated. Finally, the electric potential in the membrane, \( \phi \), obeys the following equation:

\[ -\Delta \phi = \frac{f}{e - f c_w} \left( \frac{1}{\kappa} - \frac{5}{44} D_w F^2 \frac{R T e}{(e - f c_w)^2} \right) (\nabla c_w \cdot \vec{i}) \]

\[ + \frac{RT}{F} \frac{f c_w}{e - f c_w} \frac{c_m k_h}{D_w \mu_l} (\nabla c_w \cdot \nabla p_l) \]

\[ - \frac{RT}{F} \left( \frac{f}{e - f c_w} \right)^2 (\nabla c_w \cdot \nabla c_w) \] (66)

Thus, accounting for the variation of the water molar concentration in the membrane yields a more complex equation compared to the commonly employed Laplace's equation, \( -\Delta \phi = 0 \).

Consistent with the boundary condition prescription for equation (49), where a constant \( c_w \) value is specified along \( \Gamma_{am} \) (see Fig. 2), a nil electric potential is set at \( \Gamma_{am} \) (see Fig. 2), and at \( \Gamma_{cm} \) we have:

\[ \nabla \phi = -\frac{\vec{i} - F c_f U_l}{\kappa} \] (67)

According to [15], here the conductivity, \( \kappa \), for the Nafion 117 membrane can be expressed as a function of both water content, \( \lambda \), and temperature, \( T \):

\[ \kappa = \left( 0.5139 \frac{c_w}{e - f c_w} - 0.326 \right) \exp \left( 1268 \left( \frac{1}{303} - \frac{1}{T} \right) \right) \] (68)

In our computation, \( \kappa \) in (66) and (67) is updated using (68).

The complete mathematical model was implemented into the CFX-4 commercial CFD package. This CFD code uses finite volume discretization, providing a platform for solving the conservation form of the equations for mass, momentum, energy, and multispecies. Additional phenomenological equations developed in this paper to account for specific fuel cell transport processes were implemented by writing an extensive suite of user subroutines. Customized iterative procedures were also designed to ensure an effective coupling between the electrochemistry and the various transport processes.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>gas channel length (half) (x-direction in Fig. 1)</td>
<td>m</td>
<td>0.025</td>
</tr>
<tr>
<td>gas channel width (z-direction, not shown in Fig. 1)</td>
<td>m</td>
<td>0.001</td>
</tr>
<tr>
<td>$A_{MEA}$: full active MEA area</td>
<td>m²</td>
<td>0.00005</td>
</tr>
<tr>
<td>anode-side channel thickness (y-direction in Fig. 1)</td>
<td>m</td>
<td>0.001</td>
</tr>
<tr>
<td>anode thickness (y-direction in Fig. 1)</td>
<td>m</td>
<td>0.00026</td>
</tr>
<tr>
<td>wet membrane thickness (y-direction in Fig. 1)</td>
<td>m</td>
<td>0.00023</td>
</tr>
<tr>
<td>cathode thickness (y-direction in Fig. 1)</td>
<td>m</td>
<td>0.00026</td>
</tr>
<tr>
<td>cathode-side channel thickness (y-direction in Fig. 1)</td>
<td>m</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Table 1. Dimensions of a PEMFC (refer to Fig. 1).

The PEM fuel cell physical dimensions and key boundary conditions used in this study are listed in Tables 1 and 2, and are based on the design and operating conditions reported by Bernardi and Verbrugge [3]. In practice, the hydrogen fuel injected into the anode-side channel must be humidified to help maintain a satisfactory level of hydration in the membrane portion that is adjacent to the anode; therefore, a higher vapor mass fraction ($\omega_{H_2O(g)} = 0.623$) has to be assigned for the anode-side channel. At the other end, a lower vapor mass fraction ($\omega_{H_2O(g)} = 0.006$) corresponds to the minor component of the vapor in the slightly humidified air that enters the cathode-side channel.
Table 2. Boundary conditions.

The transport properties and physical parameters of the membrane correspond to Nafion 117 and are listed in Table 3.

<table>
<thead>
<tr>
<th>Property/Parameter</th>
<th>Unit</th>
<th>Value/Expression</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_{\text{dry}}$: dry membrane density</td>
<td>kg $m^{-3}$</td>
<td>1980</td>
<td>[7]</td>
</tr>
<tr>
<td>$E_w$: equivalent membrane weight</td>
<td>kg mol$^{-1}$</td>
<td>1.1</td>
<td>[7]</td>
</tr>
<tr>
<td>$e = \frac{E_m}{E_w}$: equation (46)</td>
<td>mol $m^{-3}$</td>
<td>1800</td>
<td>[15]</td>
</tr>
<tr>
<td>$f$: membrane swelling coefficient</td>
<td></td>
<td>0.0126</td>
<td>[15]</td>
</tr>
<tr>
<td>$D_w$: water diffusion coefficient</td>
<td>$m^2 s^{-1}$</td>
<td>$2.5 \times 10^{-7} \left(\frac{e^{\frac{273}{T}} - 1}{e^{\frac{273}{T}} - 1} \right)$</td>
<td>[20]</td>
</tr>
<tr>
<td>$\epsilon_w$: volume fraction of water</td>
<td></td>
<td>$\frac{48(e - f_{\text{w}})}{18(e - f_{\text{w}})}$</td>
<td>[15]</td>
</tr>
<tr>
<td>$k_h$: hydraulic permeability</td>
<td>$m^2$</td>
<td>$1.58 \times 10^{-18}$</td>
<td>[7]</td>
</tr>
<tr>
<td>$k_{\phi}$: electrokinetic permeability</td>
<td>$m^2$</td>
<td>$7.18 \times 10^{-20}$</td>
<td>[4]</td>
</tr>
<tr>
<td>$\mu$: water viscosity</td>
<td>$kg m^{-1} s^{-1}$</td>
<td>$1.788 \times 10^{-5} \left(5.704 - 5.306 \left(\frac{273}{T} - 1\right)^2\right)$</td>
<td>[21]</td>
</tr>
<tr>
<td>$\kappa$: membrane conductivity</td>
<td>$A V^{-1} m^{-1}$</td>
<td>Eqn. (68)</td>
<td>[15]</td>
</tr>
</tbody>
</table>

Table 3. Properties and parameters used in the membrane model.

The results presented in this paper are plotted using the following conventions:

- In Figs. 3 - 5 and 9 - 12, the membrane thickness (0.00023m) and longitudinal dimension (0.025m) are presented in non-dimensional form;
- In Figs. 6 - 8, for both $x$- and $y$-coordinates, the actual dimensions of the cell and components are used (refer to Fig. 1 and Table 1).

Simulations at $i = 0.8 A/cm^2$ are first examined since this is the highest current density reported in the study of Springer et al. [11]. Fig. 3 shows the distribution...
Fig. 3. Comparison between one-dimensional and two-dimensional water content results corresponding to $|\vec{i}| = 0.8A/cm^2$ with both thermal and pressure-drop effects turned off.

obtained with the present model when constant pressure and temperature ($T = 353K$) conditions are maintained. In order to compare our 2D simulations with the one-dimensional results of Springer et al. (cf. [15]), the distribution corresponding to a section midway between the cell inlet and outlet is presented. The water content drops more steeply near the cathode and less rapidly near the anode for the one-dimensional case, but for both cases the overall trends are similar.

Next, we examine the impact of the non-uniformity of pressure on the two-dimensional predictions. Fig. 4 and Fig. 5 show water content profiles at various
Fig. 4. Water content distribution at constant pressure corresponding to $|\vec{u}| = 0.8\text{A/cm}^2$.

locations from the inlet (dimensionless $x = 0$) to the outlet (dimensionless $x = 1$). Both figures demonstrate that the water content decreases from the inlet to the outlet. This is because the highest oxygen mass fractions occur near the inlet, leading to a more complete reduction reaction that generates more water (see the 2nd chemical reaction equation in Section 2). In Fig. 4, we switch off the pressure-gradient terms in (49), and observe the steep drop in water content from the cathode to the anode. On the other hand, when the pressure-gradient terms in (49) are switched on, radically altered distributions are obtained as shown in Fig. 5. With a pressure drop of 2
Fig. 5. Water content distribution with pressure drop corresponding to $|\vec{i}| = 0.8\text{A/cm}^2$.

*atm* from the cathode to the anode, much higher levels of hydration are maintained through most of the membrane, and virtually uniform water content is maintained over 75% of the membrane thickness.

In Fig. 6, the temperature distribution in the cell is illustrated. The locations of the boundaries are indicated with respect to Fig. 2 and Table 1. The higher temperatures arise close to the inlet at the membrane-cathode interface, where the thickness is $h = 0.00126m$, as the air stream is oxygen rich in that region and the exothermic electrochemical reaction is strongest. The temperature maxima reach 367
Fig. 6. Temperature distribution in the cell (refer to Fig. 2 and Table 1 for locations of interfaces: $\Gamma_c$ at $y = 0.001\, m$; $\Gamma_{cm}$ at $y = 0.00126\, m$; $\Gamma_{am}$ at $y = 0.00149\, m$; $\Gamma_a$ at $y = 0.00175\, m$).

$K$, which is $14\, K$ above the nominal operating temperature of $353\, K$. The variation of temperature is here implicitly taken into account through the coefficients in equations (49) and (66) (see Table 3).

Next, we examine our membrane electric potential predictions. First, we switch off all the source/sink terms in (66), i.e., the potential field is computed using the conventional Laplace’s equation. The resulting electric potential distribution in the membrane is shown in Fig. 7, in which the maximum membrane electric potential loss reaches $0.152\, V$. When water content variation is accounted for by using our new
model, i.e., with the source/sink terms in (66), a potential loss maximum of 0.148 V is predicted and differences of up to 3% are obtained in the distribution as shown in Fig. 8. Though the 2D effects look generally weak in the center and on the anode side of the membrane, the changes in both temperature and potential along the cathode side are appreciable. It should also be noted that the 2D effects are attenuated on the anode side as a constant water concentration is prescribed along the anode side in the simulations presented here.

With all source/sink terms switched on in equation (66), we also apply our model
to a series of tests corresponding to different nominal current density values ranging from $i = 0.4\, A/cm^2$ to $i = 1.2\, A/cm^2$. For $i = 0.4\, A/cm^2$, Fig. 9 and Fig. 10 shows the water flux behavior along the membrane-cathode interface at relative humidities of 60% and 90%. The water flux decreases nonlinearly from the inlet to the outlet, and the trends for both cases look similar. Again, this longitudinal decrease of water flux is related to the local current density which is highest close to the inlet, and hence generates more water there (see the reaction equation shown at the end of Section 2).

When the current density is increased to $i = 0.6\, A/cm^2$, the water flux distri-
Fig. 9. Water flux distribution along membrane length on the cathode side ($i=0.4\ A/cm^2$, at relative humidity of 60%).

Distributions exhibits an approximately linear drop as shown in Fig. 11 and 12, for both relative humidity values (60% and 90%). The drop rate near the inlet is less severe than in the lower current density cases as shown in Figs. 9 and 10.

Fig. 13 shows effects of relative humidity on membrane electric potential loss and, hence, on cell voltage. We still use the case of $i = 0.4\ A/cm^2$ as example. As relative humidity increases, the electric potential loss in the membrane decreases, and this is most evident over the interval of $[0.5, 0.8]$.

Fig. 14 depicts the membrane electric potential loss curves over a current den-
Fig. 10. Water flux distribution along membrane length on the cathode side ($i=0.4$ A/cm$^2$, at relative humidity of 90%).

... interval of [0.4A/cm$^2$, 1.2A/cm$^2$] and at different relative humidities. To a good approximation, the potential increases linearly with the current density; however, the higher the relative humidity of the incoming streams, the smaller the slope of the membrane electric potential loss.

In Fig. 15, we plot polarization curves at different relative humidities ranging from 30% to 100%. For the high/low relative humidity cases, the numerical procedure failed to converge in the extremes of low current densities (activation regime) or high current density (mass transport limited regime). This is not critical as in normal oper-
Fig. 11. Water flux distribution along membrane length on the cathode side (\(i=0.6\ A/cm^2\), at relative humidity of 60%).
shows that the cell can only operate at a very low current density.

5. Concluding remarks.

The membrane model developed in this study provides a physically realistic description of water content variation in the membrane. The predictive abilities of the model are also significantly enhanced by the two-dimensional formulation and by
Fig. 13. Cell voltage and membrane potential loss behaviors at different relative humidities ($i=0.4 \text{ A/cm}^2$).

The results show that significantly improved water content distributions can be maintained in the membrane when the cell is operated with a higher pressure on the cathode side than on the anode side. The simulations using our model also clearly highlight the importance of maintaining higher relative humidities in fuel cell operation.

Although temperature variations were also accounted for in our model, we have not accounted for phase change of water in the electrodes. Evaporation and condensa-
Fig. 14. Membrane potential loss curves corresponding to three different relative humidities.

...tion rates are expected to be strongly affected by temperature and pressure. Further developments that account for phase change would enhance the capabilities of the model.

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Fig. 15. Polarization curves corresponding to different relative humidities.

Berning for their contribution to the computational framework used in this study.

REFERENCES


