THROUGH-THE-ELECTRODE MODEL OF A PROTON EXCHANGE MEMBRANE FUEL CELL

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A one dimensional model for a proton exchange membrane fuel cell was
developed which makes use of independently measured parameters for
predicting single cell performance. Optimization of catalyst layer
formulation and properties are explored. Impact of temperature and cathode
pressure upon system performance is investigated.

INTRODUCTION

Development of a comprehensive mechanistic model is essential for understanding fuel
cell performance and the variables which impact operation. Both through-the-electrode and
down-the channel models have been developed to leverage our experimental effort toward
improving membrane electrode assemblies (MEAs) and defining optimum operating
conditions.

Water management is key to optimal fuel cell operation. High water activity is desired
to obtain maximum ionic conductivity of the membrane and catalyst layers. A significant
improvement in conductivity is apparent when liquid water is in contact with the ionomer.
(1) On the other hand, the presence of liquid water in the backing layer and catalyst layers
will decrease gas phase transport to catalytic sites.

Recent models of proton exchange membrane (PEM) fuel cells include electrode
kinetics, electro-osmotic transport of water and component diffusion through the backing
and cathode catalyst layer. Bernardi et al. developed a comprehensive model from
fundamental transport properties (2). Springer et al. included diffusion limitations which
arise in the backing layer at the cathode (3). Kinetic resistance at the anode was neglected.
Nguyen et al. developed a down-the-channel model to account for mass and heat transfer
between the electrode and gases in the channel (4). A simplified treatment of transport
through the MEA was implemented.

The purpose of the through-the-electrode model is to apply known properties and
relationships to first validate with experimental data and then predict fuel cell behavior.
Key factors include water saturation and transport within backing layers and reaction
kinetics within the cathode catalyst layer. Using this validated model, the impact of cell
temperature and operating pressure will be explored. In addition, use of the model to aid in
design of the catalyst layer is demonstrated.

MODEL DESCRIPTION

A schematic illustration of a PEM fuel cell is shown in Fig. 1. A cation-conducting
polymer membrane is located between two catalyst layers. This structure is in turn placed
next to diffusion backing layers between two flow fields. Hydrogen diffuses through the
backing layer to the anode catalyst layer where
H₂ → 2H⁺ + 2e⁻ \hspace{2cm} [1]

Protons, formed in the reaction, migrate through the cation conducting membrane to the cathode catalyst layer and are consumed by the following reaction

\[
\frac{1}{2} O_2 + 2H^+ + 2e^- \rightarrow H_2O \hspace{2cm} [2]
\]

The difference in electromotive force for electrons produced at the anode and transferred to the cathode converts chemical energy to electrical energy, in a process not limited by the Carnot cycle.

The model attempts to treat the cathode in detail. Kinetics of the oxygen reduction reaction at the cathode is five orders of magnitude slower than hydrogen oxidation in acidic electrolyte. As a result, kinetic resistance at the anode is neglected. Oxygen transport in the cathode requires detailed representation. The presence of liquid water, produced at the cathode, reduces the pore volume available for oxygen diffusion.

Components of the model consist of water transport through the MEA, oxygen diffusion through the cathode backing layer, ionic resistance in the membrane, and transport and kinetics within the cathode catalyst layer. The description of the model is divided into two sections: (a) gas and water transport through the entire MEA structure and (b) cathode catalyst layer kinetics and transport.

**Membrane and Backing Transport**

Diffusive transport through both the anode and cathode backing layers is modeled to obtain the water activity at ionomer interfaces and oxygen concentration at the cathode catalyst layer/backing interface. Within the backing layers, the Stefan-Maxwell equation defines diffusive compositional changes (5)

\[
\frac{dx_i}{dz} = \sum_{j=1}^{s} \frac{1}{CD_q} (x_i N_j - x_j N_i) \hspace{2cm} [3]
\]

where for ideal gases

\[
C = \frac{P'}{RT}
\]

and N_i is the flux of species i in the z direction, D_q^{eff} is the effective binary diffusion coefficient of the pair i-j in the porous medium and C represents the molar gas concentration, P', total pressure, T, absolute temperature, and R, the ideal gas constant.

Two classes of water activity profiles can arise and are illustrated in Fig. 1. In Case 1, high relative humidity in the cathode flow channel leads to saturation of gas in the backing layer at the dashed line (a). Water is transported in the liquid phase on the left side of this line through the backing and catalyst layer. The presence of liquid water in the catalytic
layer and high water activity in the membrane tends to increase ionic conductivity. On the 
other hand, the presence of liquid water in the backing layer can reduce the available 
 oxygen partial pressure in the catalyst. These two factors lead to a conflicting impact upon 
fuel cell performance. In Case 2, low relative humidity in the cathode channel yields 
 improved gas phase transport in the cathode backing but lowers ionic conductivity of the 
ionomer phase.

Depending upon whether liquid water is present, water transport in the cathode 
backing occurs by different mechanisms. Eq. [3] describes the mole fraction water when 
water is transported in the gaseous phase. If liquid water partially floods the porous 
structure, the mole fraction of water in the gas phase is constant and is determined by its 
vapor pressure. No water is then transported in the vapor phase. Liquid water saturation 
variations interact with capillary pressure to move liquid water through the backing. In 
addition, the presence of liquid water lowers the gas phase porosity to reduce the effective 
oxgen diffusivity.

Water transport in the membrane results from the sum of electro-osmotic transport and 
diffusion. (7) While electro-osmotic drag is always from the anode to the cathode, 
diffusion follows the concentration gradient and may occur in either direction as illustrated 
in Fig. 1. The applicable equation for net water transport is

\[ N_{H_2O}^{net} = N_{H_2O}^{diff} + \frac{I_n n_d}{F} \]  

where \( I_n \) is the total current density through the cell and \( n_d \) represents the electro-osmotic 
drag coefficient. For the 1-D case, the diffusion equation may be written as

\[ N_{H_2O}^{diff} = -D_{H_2O}^{m} \frac{dC_{H_2O}^{m, w}}{dz_{m, w}} \]  

where subscript or superscript \( m \) designates membrane, \( d \) indicates dry and \( w \) shows a wet 
basis. The derivative in Eq. [5] may be expressed in terms of membrane water content, \( \lambda \), 
which is defined as moles of \( H_2O \) per equivalent of \( SO_3 \)

\[ \frac{dC_{H_2O}^{m, w}}{dz_{m, w}} = \left( \frac{dC_{H_2O}^{m, w}}{d\lambda} \right) \left( \frac{d\lambda}{dz_{m, w}} \right) \]  

Use of \( \lambda \) instead of concentration simplifies integration. Rearrangement of Eq. [6] and 
substitution of Eqs. [4] and [5] yields

\[ d\lambda \]  

\[ dz_{m, w} \] - \[ \frac{N_{H_2O}^{net} - \frac{I_n n_d}{F}}{D_{H_2O}^{m} \frac{dC_{H_2O}^{m, w}}{d\lambda}} \]  

which describes the gradient of water content in the membrane with position.
Use of the diffusion equation is complicated by changes in membrane dimensions with water activity. Assuming that there is no excess volume of mixing between the ionomer and water, a relationship may be derived which describes the change in dimensions with water content. Molar concentration of water on a wet volume basis can be expressed as

\[ C_{H_2O}^{m,w} = \frac{a \lambda}{(c\lambda + 1)} \]  

where

\[ a = \frac{\rho_{m,d}}{E_m} \quad c = \frac{\rho_{m,d} M_w}{\rho_w E_m} \]  

and \( \rho_{m,d} \) represents the density of the dry membrane, \( E_m \), the equivalent weight of the ionomer, \( \rho_w \) and \( M_w \), the density and molecular weight of water, respectively. Assuming that the membrane expands equally in all directions, we can also derive the following relationship between wet and dry membrane thickness

\[ z_{wet} = (c\lambda + 1)^{1/3} z_{dry} \]  

After substitution of the derivative of Eq. [10] into Eq. [7] we obtain

\[ \frac{d\lambda}{dz_{m,d}} = \left( N_{H_2O}^{m} - \frac{I_y}{F} \right) \frac{(c\lambda + 1)^{1/3}}{\varphi_{H_2O} \left( \frac{dC_{H_2O}}{d\lambda} \right)} \]  

where the derivative of Eq. [8] yields

\[ \frac{dC_{H_2O}}{d\lambda} = \frac{a}{(c\lambda + 1)^2} \]  

Through Eq. [11], membrane water content may be calculated.

Effective transport properties for both diffusion and ionic conduction are dependent upon porosity. Formation resistivity, \( R_O \), is related to bulk resistivity, \( R_w \), of the conducting phase by

\[ R_O = F_R R_w \]  

where the formation resistivity factor, \( F_R \), is defined as

\[ F_R = \frac{a}{\phi_m} \]
In this expression, $\phi$ represents porosity, $a$ is a coefficient which varies from 0.6 to 2.0 and $m$ is the cementation factor or tortuosity factor that ranges from 1 to 3 (6). This type of relationship represents ionic conductivity of brine saturated rocks which vary widely in pore characteristics. For sandstone rock, which approximates the types of porosity found in MEA electrodes, the Humble formula sets $m = 2.15$. (6) Thus, effective transport properties may be approximately related to bulk properties by:

$$K_{\text{eff}} = \phi^2 K$$
$$D_{q_{\text{eff}}} = \phi^2 D_{q}$$  \[15\]

Solution for the water distribution through the MEA structure is obtained by integrating from the anode channel to the cathode catalytic layer and from the cathode channel to the cathode catalytic layer. The mole fraction of components is calculated in both the anode and cathode channels. For a given current density, a net flux of water is assumed through the anode backing and membrane. Eq. [3] is used to calculate the gas composition through the anode backing. Binary diffusion coefficients needed in Eq. [3] are calculated from Chapman-Enskog kinetic theory for the gaseous state at low density (5).

At the anode backing / membrane interface, the mole fraction of water is converted to water content in the membrane interface by the following expression (7)

$$\lambda_{(w_c)} = 0.043 + 17.81a - 39.85a^2 + 36.0a^3 \quad 0 < a \leq 1$$  \[16\]

where $a = x_w P' / P_{sat}$. Since this correlation was obtained for membranes treated in boiling water, the relation is assumed to hold to 100°C.

Membrane properties include electro-osmotic drag coefficient, water diffusion coefficient and ionic conductivity. Recent water content and electro-osmotic drag measurements indicate (8)

$$a_w (\text{water vapor}) \leq 1 \quad \lambda \leq 14 \quad n_a = 1.0$$
$$a_w (\text{liquid water}) = 1 \quad \lambda = 22 \text{ to } 25 \quad n_a = 2.5$$

Data for the diffusion coefficient for water in the membrane was obtained from Zawodzinski et. al. (1). The data was correlated in the form given below:

$$D_{H_2O} = C_1 + C_2(1 - \exp(-C_3 \lambda))$$  \[17\]

Water diffusivity is adjusted from 30°C by the following equation:

$$D(\text{at } T_{cell}) = D(30°C) \left[ \frac{E_a}{R} \left( \frac{1}{303} - \frac{1}{273 + T_{cell}} \right) \right]$$  \[18\]
where \( \frac{E_a}{R} = 2416 \) (9). The potential loss in the membrane and catalytic layer is calculated from the ionic conductivity. Conductivity data from Zawodzinski et al. (1) is fitted with the equation

\[
\kappa_i = C_T [C_i^0 + C_i^*(1 - \exp(-C_i^* \lambda))] \tag{19}
\]

where \( C_T \) is the temperature coefficient for temperatures other than 30°C where \( C_T = 1.0 \). While complete curves have not been measured as a function of temperature, membrane conductivity in liquid water is available for NAFION® 117 and DOW ionomers (1). The data is fitted by

\[
C_T = C_i^0 + C_i^* T \tag{20}
\]

Water content is integrated by Eq. [11] through the membrane to the cathode catalytic layer where the water content is assumed to be constant.

Water content is again estimated for the cathode catalyst layer, but starting at the cathode flow channel. As shown in Fig. 1, gas composition through the cathode backing is integrated with Eq. [3] to the catalyst layer. In this case, however, water condensation can occur at some plane in the backing. From this point toward the catalyst layer, a constant water mole fraction is defined with a lower gas saturation to account for the presence of liquid water.

At the cathode layer / catalyst layer interface, Eq. [16] is again applied to obtain the water content of the ionomer. If the water content after integrating in both directions agrees, convergence is obtained. If they differ, a new net water flux is assumed and the calculation is repeated until convergence is obtained.

The procedure is complicated by non-ideal behavior at the gas - ionomer interface. NAFION® in contact with water vapor at unit activity yields \( \lambda = 14 \). Liquid water with the same activity produces \( \lambda = 22 \). Contact angle measurements show that membrane surface wettability is different for the two cases (10). Small-angle neutron scattering techniques indicate the presence of high kinetic resistance to water transport at the interface for water vapor (11). Thus, it is assumed that a step change occurs at the interface. Concentration gradients within the membrane are unaffected.

**Cathode Catalyst Layer**

A conceptual representation of the catalytic layer is given in Fig. 2. The catalyst layer is represented as a uniform structure with catalyzed carbon black particles covered with a continuous ionomer film. Oxygen reaches the catalyst by diffusion through void volume within the structure. Assumptions for the model include a uniform water content of the catalyst layer, a uniform distribution of components within the layer, and low electronic resistance compared to ionic resistance.

Derivation of the equations describing the current distribution, potential distribution, oxygen flux and oxygen concentration are similar to those by Springer et. al. (12). Four governing equations are as follows:
\[
\frac{dI_z}{dz} = Ai_z^* \left\{ \exp \left( \frac{\alpha_n F \eta}{RT} \right) - \exp \left( -\frac{\alpha_n F \eta}{RT} \right) \right\} \tag{21}
\]

\[
\frac{d\eta}{dz} = \frac{I_z}{\kappa_{ef}^*} \tag{22}
\]

\[
\frac{d(N_{O_2})}{dz} = -\frac{1}{4F} \frac{dI_z}{dz} \tag{23}
\]

\[
\frac{d(C_{O_2})_s}{dz} = \frac{N_{O_2}}{D_{O_2}^0} \tag{24}
\]

where

\[
i_z^* = i_{0,ef}^* \left( \frac{C_{O_2}^f}{C_{O_2}^0,ef} \right) \tag{25}
\]

and \( A_i \) is the catalyst surface area per unit volume of catalyst layer. Since the catalyst layer is assumed to be grain supported, expansion of ionomer with hydration is neglected. Equation [25] assumes that the proton concentration is constant at the catalyst interface. While oxygen diffusion in the “z” direction occurs in both the gas phase and ionomer, fluxes are greater in the gas phase. Thus, diffusion in the ionomer is neglected.

The catalyst is assumed to be covered with an ionomer film to facilitate proton transfer. Calculations indicated that if this film was uniformly distributed over the carbon support, the mass transfer limiting current for oxygen diffusion through the film would be greater than 10 amp/cm² of geometric area. Thus, oxygen diffusion through ionomer is neglected.

Concentration of oxygen in the ionomer as a function of temperature was obtained from the work of Sakai et al. (13). The molar concentration of oxygen in ionomer, \( C_{O_2}^f \), was defined as being proportional to the molar concentration of oxygen in the gas phase, \( C_{O_2}^g \). The proportionality constant was in turn made a function of temperature.

Four unknowns, namely \( I_z \), \( \eta \), \( N_{O_2} \), and \( C_{O_2} \), are described by equations [21] to [24]. Boundary conditions are based upon known values of variables. Before integration is begun, the current density, \( I_g \), for the electrode is assumed. Since the water saturation through the MEA has been obtained, ionic conductivity can be calculated. Boundary conditions thus become:

\[
z = 0 \quad I_z = 0 \tag{26}
\]

\[
z = \delta_c \quad \frac{d\eta}{dz} = \frac{I_s}{\kappa_{ef}^*} \tag{27}
\]

\[
z = 0 \quad N_{O_2} = \frac{I_s}{nF} \tag{28}
\]
Solution of Eqs. [21] to [24] involves the use of a Runge-Kutta integration routine with adaptive stepsize control (14). A "shooting" method is implemented where an overpotential is assumed at z = 0 and integration is performed to z = \delta_c. The "shooting" procedure is repeated until the condition specified by Eq. [27] is met.

Cell voltage is then calculated as \( V = V_{\infty} - I \cdot AR_m - \eta_c(z = \delta_c) \). \( V_{\infty} \) is calculated from the free energy of reaction at temperature and pressure. (Cell voltages are generally calculated at currents greater than 0.01 amp/cm² so corrections for electrode corrosion currents, organic impurity oxidation, and hydrogen diffusion and reaction at the cathode may be neglected.) The membrane resistance \( AR_m \) is calculated by integrating over the membrane thickness by the following equation:

\[
AR_m = \delta \int_0^\delta \frac{dz_m}{\kappa(\lambda)} = \int_0^\delta \frac{(c\lambda + l)^{1/3}}{\kappa(\lambda)} \, dz_d
\]

where \( c \) is defined in Eq. [9].

Two Tafel slopes have been measured for oxygen reduction on platinum. Parthasarathy et al (15) found that at potentials greater than 0.75 to 0.8 volts vs the dynamic hydrogen reference electrode, oxygen reduction occurs on a Pt-oxide covered surface. Below this potential, an oxide-free surface is proposed.

Early simulations with data from Parthasarathy et al. (15) yielded high kinetic resistance at low current densities. A subsequent paper by Parthasarathy et al. (16), which explored the effect of pressure upon kinetics, yielded exchange current densities that were ten times larger than in the former paper. Parthasarathy et al. attributed related phenomena to organic contamination (17). Thus, exchange current densities from the later paper were used along with the temperature dependence from the first paper.

Electrode parameters derived from the indicated references are given in Table I. The transfer coefficients were calculated from the mean value of Tafel slopes measured from 30 to 80°C. The catalyst surface area \( A_v \) was calculated from the measured catalyst layer thickness and a platinum surface area on carbon of 100 m²/gm Pt. Reference values were calculated at 80°C. Volume fractions of void and ionomer were obtained from the measured catalyst layer thickness and the ink formulation.

**EXPERIMENTAL**

A single cell and reference test stand were designed and constructed to provide tight control on operating parameters. Key components included mass flow control of gas streams, humidification with HPLC pumps and vaporizers and balances to weigh recovered anode and cathode water. Cell temperature was controlled by water circulation through heat exchangers within the single cell. A data acquisition and control system allowed unattended operation with programmed gas stoichiometries and humidification (18,19). High frequency resistance of the MEA was measured at 1 kHz by a 4 probe method.
Membrane electrode assemblies (MEAs) were assembled by a procedure similar to that described by Wilson et. al. (20). Two decals were coated with a carefully controlled thickness of catalyzed ink in the TBA form and dried in an oven. One decal was placed on each side of the membrane, generally NAFION 112, and pressed under carefully controlled conditions. The catalyzed membrane was then sandwiched between two pieces of Teflonated graphite paper and placed in the test cell. Active area was 46.5 cm².

RESULTS AND DISCUSSION

Single cell performance was measured as a function of temperature, pressure, anode and cathode humidification levels. A comparison between the measured performance and modeling results is given in Fig. 3. Cathode stoichiometry is represented by calculating an mean effective oxygen concentration. The only parameters adjusted to obtain this match are the gas saturation in the catalyst layer and cathode backing. These variables induce a slight downturn at high current density. The measured high frequency resistance was consistently higher than the calculated value. The calculated value only included resistance from the membrane. The difference may be attributed to interfacial resistance and a portion of the ionic resistance of the catalyst layer.

A model with independently defined parameters can aid in studies on the effect of MEA structure upon performance. Two key parameters in MEA optimization include carbon black packing density and NAFION® to carbon ratio within the catalyst layer. Carbon packing density is determined from micrographs of MEA cross sections after testing is complete. A series of simulations were run to explore the relationship between cell voltage and cathode catalyst loading. Cases included three thicknesses of catalyst layer at 5 different carbon packing densities.

In Fig. 4, cell voltage at 1 amp/cm² increases at carbon packing density increases from 0.5 g/cm². After reaching a maximum, a decrease is performance is predicted. At higher packing densities, $A_v$ increases to improve kinetics. A decrease in void fraction increases the ionomer volume fraction which in turn improves ionic conductivity through Eq. [15]. As packing density continues to increase, a point is reached where the void fraction reduction begins to impact oxygen diffusion through the catalyst layer. A downturn in performance is then predicted.

Good performance is predicted even at low catalyst loading. For instance, for a 5 μM layer, 0.59 volts is predicted at 1 amp /cm². This value may be compared to the experimental results by Ferreira et al. who found that at a Pt loading of 0.05 mg/cm², 0.56 volts was obtained at 1 amp/cm² with 1 atm air (21). Thus, reasonable agreement is obtained, particularly when the differences in air pressure and unknowns in Ferreira's MEA structure, are considered.

Inferences may also be made concerning the relative performance of supported platinum catalysts and platinum black at low catalyst loadings. Platinum surface area of a 20% Pt /C catalyst is approximately 100 m²/gm Pt compared to around 30 m²/gm for platinum black (22). Higher performance might be expected for the supported catalyst at the same loading. This indeed appears to be true at catalyst loadings below 0.2 mg/cm². Other factors tend to predominate at higher catalyst loadings. Carbon occupies space which may be better utilized by ionomer to increase ionic conductivity or void volume to improve oxygen access. The advantage that platinum black holds above 0.5 mg/cm² may be
partially lost through the use of carbon with higher platinum loadings. Lower Pt surface area, however, reduces potential gains.

The ionomer to carbon ratio was explored as another laboratory adjustable variable. The weight of carbon was used in the ratio since it correlates with pore volume available for ionomer addition in a grain supported structure. Fig. 5 illustrates that at low current densities, the benefits of ionomer addition reach an asymptote. A mass transfer limit is not reached. At high ionomer loadings, mass transfer limitations are reached at higher current densities. It should be noted that ionomer addition may also impact wettability characteristics of the structure. While carbon surfaces, formed at elevated temperature, tend to be hydrophobic, ionomer in contact with liquid water is hydrophilic. Additional ionomer may be expected to increase liquid water saturation. Compared to model predictions, a mass transfer limit is anticipated at lower ionomer loadings.

Operating temperature and pressure affect system performance. As shown in Fig. 6, a slight improvement in cell voltage is predicted at elevated temperature. Higher reference exchange current densities, ionic conductance, and gas diffusivity tend to increase performance. Above 100°C, a reduction in performance is generally observed at lower pressure (23). As the boiling point of water at pressure is approached, the oxygen mole fraction is reduced significantly by dilution with water vapor. Similar behavior is predicted at low and high current densities.

Cell voltage is dependent on cathode pressure. A series of simulations was performed to explore the effect of cell pressure and air stoichiometry upon performance. Stoichiometry is represented by lowering the average oxygen concentration in the cathode channel. This approach was found to be approximately correct (3). While higher total cathode pressure is expected to improve oxygen transport and kinetics, other factors reduce its effectiveness. First, the diffusivity of oxygen is inversely proportional to pressure. In addition, water condensation, that reduces oxygen transport, is facilitated by higher pressure.

To approximate the effect of air compression upon overall system performance, cell voltage may be reduced by an amount equivalent to the compression penalty. Fig. 7 illustrates the predicted net cell voltage versus cathode pressure and air stoichiometry. It is apparent that at an air stoichiometry of 3, atmospheric pressure operation would be preferred. At lower stoichiometries, cell voltage is less sensitive to pressure. Below an air pressure of 2 atm, other factors such as humidification requirements and equipment size may become predominant factors. It should be noted, however, that water rejection behavior of an MEA can also affect the optimum pressure.

CONCLUSION

A through-the-electrode model, based upon independently measured or calculated parameters, has expanded our ability to predict the impact of variables upon PEM fuel cell performance. After model validation, it was found that cell performance increases with carbon backing density up to a maximum. As indicated in the literature, moderate performance is predicted at Pt catalyst loadings below 0.1 mg/cm². Finally, platinum black electrodes are predicted to compete effectively with supported catalysts at loadings above 0.2 to 0.5 mg/cm².
Increased operating temperature at two atm pressure is predicted to increase cell performance up to about 100 °C. As the boiling point of water is reached, performance drops because of reduced oxygen mole fraction. Higher air pressure also improves cell performance. Once a voltage penalty is subtracted to account for compression costs, maximum system performance appears to occur between 1 and 2 atm pressure at air stoichiometries less than 3.

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Table 1. Parameters for the Cathode Catalytic Layer

| Parameter                                                                 | Tafel Slope at 80°C | Tafel Slope at 80°C |
|---------------------------------------------------------------------------|---------------------|---------------------|
| Cathodic transfer coefficient for O₂ electrode, α_c                       | 0.86 (15)           | 0.52 (15)           |
| Exchange current density at reference O₂                                  | 4.9E-7 (15,16)      | 1.3E-5 (15,16)      |
| Catalyst surface area per unit volume, cm²/cm³, λ_v                        | 1.40E+5             |                     |
| Anodic transfer coefficient for O₂ electrode, α_a                         | 0.54 (24)           |                     |
| Reference concentration of O₂ in ionomer, mole/cm³, C₀                    | 1.21E-5             |                     |
| Volume fraction ionomer                                                  | 0.17                |                     |
| Volume fraction void                                                     | 0.53                |                     |
| Ratio of Oxygen concentration in ionomer to gas phase, Cₒᵛ / Cₒᵣ          | 0.07 (13)           |                     |

Figure 1. Schematic illustration of a proton exchange membrane fuel cell.
Figure 2. Schematic illustration of the Cathode Catalyst Layer.

Figure 3. Validation of model with experimental results, temperature: 95°C, H₂/air pressure: 1.8 atm, anode RH: 100%, anode stoich: 1.5, cathode RH: 96%, cathode stoich: 3.3, gas saturation - catalyst layer / cathode backing 0.4 / 0.65.
Figure 4. Predicted fuel cell performance for 20% Pt on Vulcan XC-72 and platinum black catalyst, membrane: NAFION® 112, temperature: 95°C, H₂/air pressure: 1.8 atm.

Figure 5. Predicted cell voltage versus ionomer to carbon ratio, 20% Pt /C, membrane: NAFION® 112, carbon packing density: 0.6 gm/cm³, Temp: 95°C, air/H₂ pressure: 1.8 atm, catalyst gas saturation: 0.4, backing gas saturation: 0.6.
Figure 6. Predicted impact of cell operating temperature upon cell voltage, H₂ / air pressure: 1.8 atm, Anode RH: 100%, cathode RH: 96%, catalyst gas saturation: 0.4, backing gas saturation: 0.6.

Figure 7. Predicted impact of operating pressure and cathode stoichiometry upon cell voltage corrected for air compression penalty, 80°C, 70% Adiabatic Compressor Efficiency.