A PARAMETRIC STUDY OF THE PEM FUEL CELL CATHODE

S. Rowshanzamir, M. H. Eikani, M. Khoshnoodi & T. Eshagh Nimvar

Abstract: Most of the overpotential in the solid polymer electrolyte fuel cell is related to the cathode electrode, particularly the cathode catalyst layer. In this research work, a mathematical model for the cathode electrode catalyst layer has been developed. The model is one dimensional, isothermal, pseudo-homogeneous and uses an adjustable parameter. The mathematical model has four nonlinear coupled differential equations that have been solved using MATLAB software. The results obtained by comparing the existing data and model predictions are acceptable. In an optimized fuel cell electrode, it is desirable to achieve higher current densities, lower overpotential and lower catalyst consumption. In this regard, some of design parameters such as overpotential, proton conductivity, catalyst layer porosity and catalyst surface area on the performance of fuel cell have been studied.

Keywords: Solid polymer electrolyte fuel cell, Modeling, Catalyst layer, Gas diffusion electrode

1. Introduction

The proton exchange membrane fuel cell (PEMFC), is one of the most attractive energy conversion devices. It is regarded as a power source for stationary and mobile application. PEM fuel cell is particularly suited to electric vehicle primarily because of its relatively low temperature (70-90°C), efficiency and high power density, quick start-up capability, zero emissions is comparable to existing internal combustion technology. The application of electric vehicle requires a PEMFC offering a high power density and a low catalyst loading to reduce weight, volume and financial costs. Because the thin cathode catalyst layer of PEM fuel cell is the region where the electric power is generated and the largest irreversible losses in cell voltage occur in it, the cell performance depends largely on the optimization of the various processes occurring there[1-3].

Mathematical models are useful for analysis and optimization of the performance of fuel cell and especially for cathode catalyst layer in the case of PEM fuel cell. The mathematical models devoted to the catalyst layer of a fuel cell electrode include the pseudo-homogeneous [4-11], the single pore [12], the thin film [13], and agglomerate models [7, 13]. Among these models the pseudo-homogeneous model, which assumes that the catalyst layer has a uniform thickness and uniform distribution of catalyst particles, ionomer, and gas pores throughout the catalyst layer, is the one most often used, mainly because it’s compares well with experimental results.

The pseudo-homogeneous model has been adopted the following studies in regard to the PEM fuel cell cathode. Bernardi and Verbrugge [4,5] presented a complete model for a gas diffusion cathode bonded to a polymer electrolyte. They incorporated the electro-osmotic and pressure-driven water transport consonant of the PEM fuel cell to investigate the overpotential characteristics, water transport, and catalyst utilization. Springer et al. [6] developed a model considering, in detail, the voltage losses caused by interfacial kinetics at the Pt/ionomer interface, gas transport limitations and proton conduction limitations, in the cathode backing.

Broka and Ekdung [7] studied the discrepancies in polarization curves given by the pseudo-homogeneous model and the agglomerate model under various values of oxygen permeability, conductivities and thickness of the cathode catalyst layer. Srinivason et al. [8] studied the effects of ohmic, diffusion and activation overpotentials on electrode kinetics using both pseudo-homogeneous and agglomerate models. They also compared the kinetics of oxygen reduction reaction on platinum/carbon powders in Nafion film using the
rotating disk electrode and gas diffusion electrode. Marr and Li [9] used a mathematical model to study the performance of the cathode catalyst layer in a PEM fuel cell by including both electrochemical reaction, and mass transport processes. The composition and performance optimization of catalyst platinum has also been investigated. Sui et al. [10] compared both pseudo-homogeneous and agglomerate catalyst models.

Wang et al. considered a spherical flooded-agglomerate model for the cathode catalyst layer of a proton exchange membrane fuel cell, which includes the kinetics of oxygen reduction, at the catalyst/electrolyte interface, proton transport through the polymer electrolyte network, the oxygen diffusion through gas pore, and the dissolved oxygen diffusion through electrolyte [14]. The optimization of distributions of Nafion content and Pt loading in order to get a best performance was presented by Sond et al. [15].

Berg et al., developed a macroscopic model for a non-isothermal cathode catalyst layer (CL) in a proton exchange membrane (PEM) fuel cell is presented, in which liquid water in the CL pores is neglected. The model couples three phases: an electrically conductive carbon/platinum phase, gas pores, and a proton-conducting Nafion phase [16]. A steady-state mathematical model for the ordered cathode of proton exchange membrane fuel cells is developed to investigate the dependence of the cathode performance on the structural parameters of the catalyst layer by Du et al. [17].

Wang et al. presented a pore-scale model for oxygen, water vapor and proton transport through a three-dimensional, random catalyst layer microstructure [18]. A model-based control structure is proposed that comprises a multivariable control of the cathode pressure and the excess ratio of oxygen using the mass flow controller and the outlet throttle as actuators by Danzer et al. [19]. A three-dimensional, steady-state, multi-agglomerate model of cathode catalyst layer in polymer electrolyte membrane (PEM) fuel cells has been developed to assess the activation polarization and the current densities in the cathode catalyst layer by Das et al. [20].

Liu and Eikerling accounted for the full coupling of random porous morphology, transport properties, and electrochemical conversion in cathode catalyst layers. It relates spatial distributions of water, oxygen, electrostatic potential, and reaction rates to the effectiveness of catalyst utilization, water handling capabilities, and voltage efficiency [21]. In this paper, a pseudo-homogeneous model similar to You et al. [11] is used to study the cathode catalyst layer. The model is derived from a basic mass current balance by the control volume approach. The two-point problem is solved using shooting method with Matlab software (version. 6.5) and the model results are compared with open literature data [11].

2. Model Description

Fig. 1 presented a schematic of the cathode bonded to a proton exchange membrane in a PEM fuel cell. The system can be divided into three regions: a membrane region of hydrated solid polymer electrolyte, an active catalyst layer that provides catalytic site for reduction of hydrated solid polymer electrolyte, and a gas diffusion region (gas diffusion layer) composed of highly porous and conductive materials.

The gas diffusion layer is located adjacent to the gas chamber (air/ pure oxygen) and the current collector. Its open pores and electronically conductive materials transport O\textsubscript{2} and electrons to the catalytic layer, respectively.

Membrane is an electronic insulator, but an excellent conductor of protons. The protons produced at the anode go through membrane to the catalyst layer of the cathode, where they react with electrons and O\textsubscript{2} to form H\textsubscript{2}O.

$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$$ (1)

The catalyst layer is formed as a thin layer of proton conductive ionomer (e.g. Nafion), a carbon supported catalyst (e.g. Pt/C), and a void space.

The ionomer portion of the catalyst layer forms the transport avenue for protons, the matrix portion consisting of carbon and catalyst plays the role of electronic conductor and the void space portion transport O\textsubscript{2} to active site [6, 7].

In the present study we focus on the catalyst layer of the cathode, which is in the region of $0 \leq z \leq \delta$ and describe a macro-pseudo-homogeneous model with the following assumptions:

1. The fuel cell is operating under a steady state.
2. The distribution of oxygen concentration, current density, oxygen transport flux, and the overpotential in the catalyst layer is considered to be one dimensional.
3. The catalyst layer is isothermal.
4. The ionomer is considered as being completely saturated of water.
5. The oxygen permeation through the PEM is negligible.
6. The diffusion coefficient is constant.
7. The electron conductivity of carbon matrix is substantially greater than the proton conductivity of ionomer, and the potential drop among solid matrix carbon is negligible compared to the potential drop in the electrolyte phase [4,6,9].
8. The anodic overpotential is disregarded with respect to the cathode ones [4,5]. Consequently, the voltage across the anode is considered to be negligible.
We consider the catalyst layer in Fig. 1 as a homogeneous medium. Consider a small control volume as shown in Fig. 2.

\[ \text{The decrease of oxygen molar flux should be balanced by the increase of proton current density. From Fig. 2, the oxygen consumption rate in the control volume is:} \]

\[ m_z = N_z - N_{z+dz} = -\frac{dN}{dz} \quad (2) \]

The balance of current density is:

\[ I_{z+dz} = I_z + m_z 4F = I_z - 4F \frac{dN}{dz} \quad (3) \]

or

\[ \frac{dI_z}{dz} = -4F \frac{dN}{dz} \quad (4) \]

When the electrochemical reaction (1) take place at cathode, the electrode potential deviates from equilibrium potential, and it is defined as:

\[ \eta = E - E_{eq} = \phi_{\text{solid}} - \phi \quad (5) \]

The electrochemical reaction rate (oxygen reduction per unit volume) in the catalyst layer can be described using the Butler-Volmer rate expression with the assumption that reduction current is positive [4].

\[ i = -i_0^c \left[ \exp\left(\frac{-\alpha_c F \eta}{RT}\right) - \exp\left(\frac{\alpha_a F \eta}{RT}\right) \right] \quad (6) \]

Where, \( i_0^c \) is the exchange current density at the equilibrium potential. Since, the catalyst layer is assumed to be grain supported, expansion of ionomer with hydration is neglected and assumes that the proton concentration is constant at the catalyst layer. Therefore, the exchange current density is function of dissolved oxygen concentration:

\[ i_0^c = i_0^{c_e} \left( \frac{C_{O_2}}{C_{O_2}^{e}} \right)^{\gamma} \quad (7) \]

The change in current is proportional to reaction current density and catalyst surface area per unit volume, \( a_t \).

\[ \frac{dI_z}{dz} = i \alpha \quad (8) \]

or

\[ \frac{dI_z}{dz} = -a_i^c \left[ \frac{C_{O_2}^{e}}{C_{O_2}^{e}} \right] \exp\left(\frac{-\alpha_c F \eta}{RT}\right) \exp\left(\frac{\alpha_a F \eta}{RT}\right) \quad (9) \]

When water velocity is neglected, the equation of Ohm’s law for ionomer phase expressed as:

\[ \frac{d\phi}{dz} = -\frac{I_z}{k_{eff}} \quad (10) \]

Where, the proton current is related to the ionomer phase potential difference. From Eqs. (5), (10) and assuming the matrix of solid phase to be equipotential (as assumption 7), changes in overpotential can be expressed as:

\[ \frac{d(-\eta)}{dz} = \frac{I_z}{k_{eff}} \quad (11) \]

The oxygen diffusion in the “z” direction occurs in both the gas phase and ionomer, fluxes in the gas phase are greater than ionomer phase. Thus, diffusion in the ionomer is a controller parameter, because the oxygen reduction reaction takes places in the ionomer. Finally, according to Fick’s law, the oxygen flux in the ionomer is related to dissolve oxygen concentration in the ionomer by:

\[ N_{O_2} = -D_{O_2}^{eff} \frac{d(C_{O_2})}{dz} \quad (12) \]

Where \( D_{O_2}^{eff} \) is the effective oxygen diffusion coefficient, and can be determined from:

\[ D_{O_2}^{eff} = D_{O_2} \varepsilon_m^{1.5} \quad (13) \]

There are four dependent variables, \( I_z, \eta, N_{O_2}, C_{O_2} \) involved in four first-order differential equations, Eqs. (4), (9), (11) and (12). The appropriate boundary conditions are listed below. At interface between the cathode gas diffuser and catalyst layer (z = 0):

\[ I_z = 0 \quad (14) \]

\[ N_{O_2} = \frac{I_z}{4F} \quad (15) \]

\[ C_{O_2} = C_{O_2}^{eq} \quad (16) \]
At interface between the membrane and catalyst layer \((z = \delta)\):
\[
I_{\delta-1} = I_\delta
\]  
(17)

### 3. Solution Technique

The governing equations and the corresponding boundary conditions together pose a boundary-value problem. This boundary-value problem can be reduced using the following relations:

\[
\xi = \frac{z}{\delta}
\]

(18)

\[
x = \frac{C_{O_2}'}{C_{O_2,\text{gas}}}
\]

(19)

Because of the resistance of porous electrode, the oxygen transport flux across the catalyst layer is limited. The maximum oxygen flux can be defined as:

\[
N_{\text{max}} = D_{O_2,\text{gas}}^{\text{eff}} \frac{C_{O_2,\text{gas}}^{\text{c}}}{\delta}
\]

(20)

\[
N^* = \frac{N_{\text{max}}}{N_{\text{max}}}
\]

(21)

The corresponding current density is defined as the limiting current density

\[
I_{\text{lim}} = 4FN_{\text{max}} = \frac{4FD_{O_2,\text{gas}}^{\text{eff}} C_{O_2,\text{gas}}^{\text{c}}}{\delta}
\]

(22)

\[
I^* = \frac{I}{I_{\text{lim}}}
\]

(23)

By using the dimensionless variables, \(I^*, N^*, x, \eta\), the governing equations take the following form

\[
dN^* = \frac{dI^*}{d\xi}
\]

(24)

\[
dI^* = -\frac{\alpha I^*}{I_{\text{lim}}} \delta \left( \frac{C_{O_2,\text{gas}}^{\text{c}}}{C_{C_2,\text{gas}}} \right) \left( \frac{\exp(-\alpha F \eta RT)}{\exp(-\alpha F \eta RT)} \right)
\]

(25)

\[
d(-\eta) = \frac{I_{\text{lim}}}{k_{\text{eff}}} \delta I^*
\]

(26)

\[
dx = -\frac{D_{O_2,\text{gas}}^{\text{eff}}}{S D_{O_2,\text{eff}}} N^*
\]

(27)

The corresponding dimensionless boundary conditions become:

At \(\xi = 0\)

\[I^* = 0\]

(28)

\[N^* = I^*\]

(29)

\[x = 1\]

(30)

At \(\xi = 1\)

\[
I^* \bigg|_{\xi=1} = I^*_\delta
\]

(31)

The governing equations, 24-27 represent the four dependent variables: \(I^*, N^*, x\), and \(\eta\). Once their values at \(\xi = 0\) are designated, the nonlinear first-order initial-value problem can be solved to yield \(I^*, N^*, x\), and \(\eta\) profiles using numerical methods (e.g. the Runge-Kutta method at Matlab). Before integration is begun, the current density, \(I^*_\delta\) for the electrode is assumed. We have the initial values of \(I^*, N^*, x\) from Eqs. (28), (29) and (30). However, the value of overpotential of the cathode gas diffuser layer /active catalyst layer interface must be chosen to ensure that the solution profiles satisfy Eqs. (31).

### 4. Results and Discussions

After the solution of equations 24-27 and with neglecting the overpotential loss in the anode side, the cell output voltage, is calculated as:

\[
U = U_{\text{w}} - IAR_a - \eta_{\text{loss}}\bigg|_{\xi=0}
\]

(32)

Fig. 3 compares the calculated fuel cell potential as a function of current density with open literature data for the base-case conditions (Tab.1). The model parameter was adjusted to yield model results that suitably mimic the open literature data. With this one adjustable parameter, the agreement between model and open literature data[11] is quite good.

The dissolved oxygen concentration is calculated by equations:

\[
x_{\text{sat}}^w = \frac{P_{\text{sat}}^w}{P^c}
\]

(33)

\[
K_{O_2,2} = K_{O_2,2} \exp \left[ -\frac{G}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right) \right]
\]

(34)

The constant Henry in Nafion at 50 °C is 0.265 atm.cm\(^3\)/mol [22].

\[
C_{O_2}^{\text{sat}} = (1 - x_{\text{sat}}^w) \frac{P^c}{K_{O_2,2}^2} \text{ or },
\]

(35)

\[
C_{O_2}^f = \frac{P_{\text{gas}}^{O_2}}{K_{O_2,2}^2}
\]

(36)

The effective oxygen diffusion coefficients in gas phase, effective proton conductivity, and open circuit potential are calculated by:

\[
D_{O_2,\text{gas}}^{\text{eff}} = D_{O_2} \varepsilon^{1.5}
\]

(37)

\[
k_{\text{eff}} = \varepsilon_m k
\]

(38)

\[
U_{\text{w}} = 1.23 - 0.9 \times 10^{-3} (T-298) + 2.4 \frac{RT}{4F} \log(P_{H_2}^2 P_{O_2})
\]

(39)
4.1. The Effects of Overpotential

Fig. 4 show the effects of overpotential (at catalyst layer/membrane interface) on the proton current, oxygen concentration and overpotential distribution across the catalyst layer, respectively. Other parameters are given in Table 1. The electrochemical reaction rate depends on the local oxygen concentration and overpotential. Across the catalyst layer, from the gas diffuser/catalyst layer interface ($\xi=0$) to the catalyst layer/membrane interface ($\xi=1$), the dimensionless current density increase; dimensionless oxygen concentration decrease, and the absolute overpotential increases due to ohmic losses across the catalyst layer. When overpotential at catalyst layer/membrane interface is small, ($|\eta|<0.1$), the oxygen reduction rate is very low, little oxygen is consumed, and the oxygen concentration remains almost unchanged. Thus, only a small current density can be produced (across the catalyst layer, the dimensionless current density increase). Since the gradient of overpotential is inversely proportional to the current density when proton conductivity is assumed as constant, the potential loss in the electrolyte is small, and the overpotential across the width catalyst layer remains almost unchanged.


<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catalyst layer porosity, $\epsilon$</td>
<td>0.25 [-]</td>
</tr>
<tr>
<td>Catalyst layer thickness, $\delta_c$</td>
<td>0.00129 cm</td>
</tr>
<tr>
<td>Reference kinetic parameter/ Oxygen reference concentration, $ai_{0,\text{ref}}/C_i^{1/2}$</td>
<td>5.0174×10² A/mol</td>
</tr>
<tr>
<td>Cathodic transfer coefficient, $\alpha_c$</td>
<td>0.52 [-]</td>
</tr>
<tr>
<td>Anodic transfer coefficient, $\alpha_a$</td>
<td>0.54 [-]</td>
</tr>
<tr>
<td>Oxygen diffusion coefficient in plain medium, $D_o^2$</td>
<td>0.0056 cm²/s</td>
</tr>
<tr>
<td>proton conductivity, $\kappa$</td>
<td>0.05 1/Ω cm</td>
</tr>
<tr>
<td>$O_2$ concentration parameter for $i_0, \gamma$</td>
<td>1 [-]</td>
</tr>
<tr>
<td>Cell temperature, $T$</td>
<td>330 K</td>
</tr>
<tr>
<td>$O_2$ Henry’s constant, $K_{O2}$</td>
<td>3.078×10¹ atm-cm/mol</td>
</tr>
<tr>
<td>Air-side pressure, $P$</td>
<td>3 bar</td>
</tr>
<tr>
<td>Fuel-side pressure, $P$</td>
<td>1 bar</td>
</tr>
<tr>
<td>Relative humidity of inlet air and fuel</td>
<td>100% [-]</td>
</tr>
<tr>
<td>Inlet fuel and air temperature, $T_o$</td>
<td>333 k</td>
</tr>
<tr>
<td>Thermodynamic open-circuit potential, $U$</td>
<td>1.174 V</td>
</tr>
<tr>
<td>Volume fraction membrane in active layer, $\epsilon_m$</td>
<td>0.78 mol/cm³</td>
</tr>
<tr>
<td>Ratio of oxygen concentration in ionomer to gas phase, $C_{O2}/C_{G2}$</td>
<td>0.96 mol/cm³</td>
</tr>
<tr>
<td>Activation energy, $G$</td>
<td>5.21 kJ/mol</td>
</tr>
<tr>
<td>Overpotential at catalyst/membrane interface</td>
<td>0.3 V</td>
</tr>
</tbody>
</table>

With the increase of overpotential, current density increase, more oxygen is consumed, and the corresponding of high current density, the electrolyte phase potential loss across the catalyst layer is high and so absolute overpotential increases across the catalyst layer. While $|\eta|$ is close to 0.35, the current density reaches the “limiting current density”, and oxygen concentration becomes zero at catalyst layer/membrane interface. With further increase of overpotential, the oxygen reduction rate increase, most oxygen is consumed in a thin region of the catalyst layer, the active catalyst layer and because of the oxygen mass-transport limitation; the current density cannot increase.

4.2. The Effect of Proton Conductivity

Fig. 5 show effects of proton conductivity on the proton current, oxygen concentration and overpotential distribution across the catalyst layer, respectively. The comparison is based on the same overpotential at the catalyst layer/membrane interface (total activation and concentration overpotential is 0.3) and in this case the highest possible current is desired to improve fuel cell performance. When proton conductivity at catalyst layer decrease, ohmic resistance increases and the corresponding potential loss in the electrolyte phase from catalyst layer/membrane interface to the catalyst layer/gas diffuser interface increases. At low proton conductivity ($\kappa=0.005 (\Omega cm)^{-1}$), the reaction is proton conduction controlled and oxygen consumption, current generation rate are low in the region $\xi<0.5$, and most of the current generation in a thin region closest the catalyst layer/membrane interface. While when proton conductivity is high, oxygen reduction is diffusion controlled, and most of the reaction occurs in a thin region closest to the catalyst layer/gas diffuser interface. High proton conductivity can be achieved by increasing water content and ionomer fraction in the catalyst layer. While water content is mainly related to operating conditions, ionomer fraction in the catalyst layer is a design parameter. As shown in Fig. 5, when $\kappa=0.5(\Omega cm)^{-1}$, the overall current density approaches the limiting current density at about $\xi=1$, which means an optimum ionomer fraction exists in the catalyst layer, because enough carbon particle, catalyst particle and porosity for oxygen transport should also be provided in the catalyst layer.
and enough polymer electrolyte for proton transport, thus pores in the catalyst layer for oxygen transport is limited. The oxygen transport resistance depends on the effective porosity. As seen in Fig.6, when the effective porosity of the catalyst layer decrease from 0.35 to 0.15, the oxygen transport resistance increase and oxygen is quickly consumed at catalyst layer, limiting current density decrease.

4.3. The Effects of Effective Porosity of the Catalyst Layer

Fig. 6 shows the influences of effective porosity on the performance of the catalyst layer. Oxygen can reach to surface catalyst through the hydrophobic pores of solid matrix. Therefore, the catalyst layer must have enough carbon matrix for good electron conductivity, enough Pt particle surface for electrochemical reaction, enough polymer electrolyte for proton transport, thus pores in the catalyst layer for oxygen transport is limited. The oxygen transport resistance depends on the effective porosity. As seen in Fig.6, when the effective porosity of the catalyst layer decrease from 0.35 to 0.15, the oxygen transport resistance increase and oxygen is quickly consumed at catalyst layer, limiting current density decrease.
4.4. The Effects of the Active Catalyst Surface Area

Fig. 7 shows the influences of the active catalyst surface area per unit volume on the performance of the catalyst layer. The active catalyst surface area increases by using finer catalyst particles (such as Pt) and/or by increasing catalyst loading, which usually comes higher capital. As shown in Fig. 7(a), when active catalyst surface area is increased, the current density increased, though the overall current density is still controlled by the limiting current density. Fig. 7(b) shows the variations of oxygen concentration with surface area. When \( \alpha = \text{base case}/2.5 \), the electrochemical reaction will not be strong enough, and the overall current density will be lower than \( \alpha = \text{base case} \). Thus, there also exists an optimum catalyst surface area. Fig. 7(c) provides the variations of overpotential with catalyst surface areas. There are other parameters that influence the performance of the catalyst layer, the exchange current density, cathodic transfer coefficient and anodic transfer coefficient. Increasing exchange current density and cathodic transfer coefficient can increase the current density when the overpotential is given. These parameters are related to the electrochemical reaction and can be improved by controlling electrochemical reaction conditions, such as temperature, concentration, and favored electrochemical reaction paths.

Fig. 6. The variation of current density, oxygen concentration with porosity across the catalyst layer.

Fig. 7. (a) The variation of current density with catalyst surface area, (b) the variation of oxygen concentration with catalyst surface area, (c) the variation of overpotential with catalyst surface area across the catalyst layer.
5. Conclusions

A pseudo-homogeneous model of proton exchange membrane fuel cell for cathode catalyst layer has been proposed and described in details. This model has been solved by Matlab software. Although the model is relatively straightforward, fuel cell performance predicted by this model compared well with the open literature data [11]. The parametric effects on the performance of the cathode catalyst layer in a proton exchange membrane fuel cell are systematically studied. Based on the modeling results are as:

- Before reaching to limiting current density, increasing the overpotential leads to increasing the current density.
- Increasing of the proton conductivity increases the current density and decreases the variation of overpotential in the catalyst layer and also decreases the catalyst layer effective thickness.
- By decreasing the catalyst layer porosity, the oxygen mass transfer, the limiting current density, the ratio of transfer to consumption of oxygen and the catalyst layer effective thickness are decreased.
- By increasing the catalyst surface area, the current density, the rate of oxygen consumption, the ratio of consumption to transfer of oxygen and the variation of overpotential are increased and the catalyst layer effective thickness is decreased.
- It should be mentioned that in the low limiting current densities (low oxygen transfer), increasing of catalyst surface area has no influence on the fuel cell performance.
- Based on the results, the design parameters for the cathode catalyst layer can be optimized for different working conditions.

6. Nomenclature

- a: surface area per unit volume of catalyst layer, cm$^2$/cm$^3$
- $AR_m$: membrane resistance, Ω cm$^2$
- C: concentration, mol/cm$^3$
- D: diffusion coefficient, m$^2$/s
- E: potential, V
- F: Faraday constant, 96487 C/mol
- G: activation energy, kJ/mol
- $i_0$: catalyst exchange current density, A/cm$^2$
- I: current density, A/cm$^2$
- $m_T$: Oxygen consumption rate, mol/s
- N: molar flux, mol/cm$^2$.s
- R: universal gas constant, 8.314 J/mol.K
- S: ratio of oxygen concentration in ionomer to gas phase, $C_{O_2}/C_{O_2}$
- T: absolute temperature, K
- U: voltage, V
- $z$: dimension through the catalyst layer, cm

Greek symbols

- $\alpha$: Cathodic charge transfer coefficient
- $\chi$: Dimensionless oxygen concentration
- $\xi$: Dimensionless length through catalyst layer
- $\gamma$: $O_2$ concentration parameter for $i_0$
- $\delta$: catalyst layer thickness, cm
- $\phi$: potential, V
- $\varepsilon$: Porosity
- $\kappa$: ionic conductivity, (Ω Cm)$^{-1}$
- $\eta$: overpotential, V

Subscripts and superscripts

- c: cathode catalyst layer
- eff: effective property which accounts for porosity
- eq: equilibrium
- f: ionomer film
- lim: limiting current density
- m: membrane
- $O_2$: oxygen
- oc: open circuit
- Solid: electrode surface
- sat: saturation
- w: water
- z: dimension through catalyst layer

References


