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Three-Dimensional Modeling and Experimental Study of a High Temperature PBI-Based PEM Fuel Cell

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This paper investigates the performance of a high temperature proton exchange membrane (PEM) fuel cell. Both experimental work and numerical simulation are conducted. The high temperature proton exchange membrane is based on polybenzimidazole (PBI) doped with phosphoric acid. A single cell with triple serpentine flow channels was operated at steady state at various levels of temperature, pressure, and air stoichiometry. A three-dimensional model was used to simulate the cell performance, and polarization curves were used to validate the experimental values. The theoretical model accurately predicts the experimental results. A sound knowledge of the impact of various variables at various levels of the cell operation is necessary for unraveling the parametric influence and can prove extremely useful for optimizing the cell operation. © 2009 The Electrochemical Society. [DOI: 10.1149/1.3203309] All rights reserved.

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High temperature proton exchange membrane fuel cells (HT-PEMFCs) with polybenzimidazole (PBI)-based membrane are considered the next generation of power generating devices due to their superior performance compared with the low temperature perflourosulphonated-based membranes. They operate at higher temperatures from 120 to 180°C and exhibit stable voltage output at steady state conditions. The HT-PEMFC is credited with faster electrochemical kinetics, improved water management, and carbon monoxide tolerance.<sup>1-3</sup> As a result of the low electro-osmotic drag and the good proton conductivity of the PBI membrane, the fuel cell design and the routine maintenance could also be significantly simplified.<sup>4</sup>

Both numerical simulation and experimental work on HT-PEMFC were done by various researchers. Savadogo' conducted an extensive study of alternative proton conducting membranes that operate at high temperatures and compared them to the low temperature perfluorinated membranes. The high temperature membranes are credited with high temperature range, tolerance of higher anode poisoning by CO, improved chemical kinetics, and enhancement of the fuel cell efficiency. The ease of using high temperature fuel cells operating above 140°C currently receives wide attention because light hydrocarbon fuels (alcohol, natural gas, and propane) are viewed as future candidates for a PEMFC application. Cheng et al.<sup>6</sup> investigated the high temperature proton exchange membrane using a steady-state electrochemical method at various temperatures (80-120°C); the back-pressure was set to 1-3 atm and relative humidity (RH) of 25-100% at a steady hydrogen crossover. The effect of temperature was larger than that of pressure and RH. Lobato et al.' investigated the influence of various parameters that affect the polycondensation synthesis of PBI and concluded that membranes with high Mw PBIs displayed enhanced mechanical and chemical stability and high thermal stability.

Ma et al.<sup>8</sup> studied the conductivities of PBI membranes for the HT-PEMFC under controlled temperature and RH. Liu et al.<sup>9</sup> conducted studies on performance degradation of the HT-PEMFC based on  $H_3PO_4$ -doped PBI and found physical degradation. Arsenio and Gomez-Romero<sup>10</sup> reported on developments on proton conducting poly(2,5-benzimidazole) (ABPBI) membranes for the HT-PEMFCs and concluded that ABPBI can be very easily sulphonated by sulfuric acid doping and heat-treatment, which increase acid uptake and, consequently, increase conductivity. Cheddie and Munroe<sup>11,12</sup> developed the one- and three-dimensional (3D) numerical models of the high temperature PBI membrane fuel cell to predict the polarization

performance and temperature difference within the PBI membrane fuel cell. The results indicate the temperature difference could be 20 K at a power density of 1000 W/m<sup>2</sup>.

Overall, a few studies have been dedicated to both experimental and theoretical modeling. The absence of experimental data creates a lacuna between idealistic and realistic conclusions, hence the essence of this study. The objective of this paper is to study both numerically and experimentally the HT-PEMFC with a PBI membrane. An experimental approach is adopted here to establish the impact of various parameters on the performance of an HT-PEMFC based on phosphoric acid. A 3D model is developed and validated by comparing the polarization curves of the model with the experimental data. The model agrees with the experimental data throughout the whole operational region. The distribution of reactants in both gas diffusion layer and flow channel is also calculated for the cell at various operating conditions.

## Experimental

*Experimental setup.*— The experimental setup consisted of a Schatz Energy Research Center multitest bench with four test stations on a single bench with a central control of the individual test stations. The data acquisition system is National-Instrument-based. The membrane electrode assembly used was phosphoric acid PBI membrane from BASF Co., USA. The catalytic loading was different on each side of the membrane. The single cell had an active area of 45 cm<sup>2</sup> with a triple serpentine flow channel on Poco-graphite plates. The cell was assembled in-house and was compressed to maintain an adequate contact pressure between the cell components.

The hydrogen supply was of 99.997% purity from a dedicated in-house electrolyzer, while compressed air was supplied from a compressor. The hydrogen flowmeter was rated from 0 to 2 slpm, while the air flowmeter was rated from 0 to 10 slpm. The backpressure was set at two pressure levels, atmospheric and 25 psig. The air stoichiometry was set at three levels: 200, 250, and 300%. The hydrogen stoichiometry was kept constant at 120% throughout the entire testing procedure. All tests were conducted at steady-state conditions at four temperature settings of 120, 140, 160, and 180°C.

Before the start of the experiment, the cell was run for 100 h at 160°C at a load of 9 A to break in the membrane. Three replicates of each data point were collected within an interval of 3–4 min waiting time. The variability of the three replicates was observed to be around 1 mV, as the output of high temperature membrane was very stable and repeatable. The average values of the voltages and current densities were used for the plots of polarization curves. At the end of the experiment, the cell was purged with nitrogen gas on both hydrogen and air sides before shutdown. This was done to prevent leaching of the acid into the cell, thereby degrading the performance of the membrane.

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**Figure 1.** (Color online) Polarization and power density curves at P = 25 psig; air stoichiometry = 200% and H<sub>2</sub> stoichiometry = 120%.

*Experimental test results.*— Figures 1 and 2 present the plots of polarization and power density curves for two different pressure levels: (*i*) At P = 25 psig (172.4 kPa) and (*ii*) at atmospheric pressure. Both tests were set at variable temperatures of 120, 140, 160, and 180°C, air stoichiometry of 200%, and hydrogen stoichiometry of 120%. The cell voltage increased with temperature and pressure. At atmospheric pressure, the cell could only be tested up to 35 A as against 45 A for the 25 psig pressure setting.

At a current density of  $300 \text{ mA/cm}^2$  and above, the voltage increase was more pronounced and uniform than at lower current density and a very predictable trend was observed from the data collected. Figure 3 describes the effects of air stoichiometry on the cell performance at two operational temperatures. Different from low temperature fuel cell, there is no transport loss at high current density. Therefore, the air stoichiometry seems to play an invisible role in the cell performance for a high temperature fuel cell as long as an adequate amount of air is supplied for the chemical reaction.

In summary, the cell voltage was more sensitive to temperature and pressure increase than with stoichiometry in all three levels of stoichiometry tested. In conclusion, the above test proved that the HT-PEMFCs operate more efficiently at higher temperature around 180°C than at lower or medium temperatures.

#### Modeling

A 3D single-phase isothermal model is developed here to predict the performance of the HT-PEMFC with a PBI membrane.

*Model assumptions.*—Because the HT-PEMFC is operating above  $100^{\circ}$ C at around 2 atm pressure, the water exists in vapor form only.<sup>13</sup> Because of the property of the PBI membranes, the



Figure 2. (Color online) Polarization and power density curves at P = Patmos; air stoichiometry = 200% and H<sub>2</sub> stoichiometry = 120%.



Figure 3. (Color online) Polarization curves at P = Patmos and  $H_2$  stoichiometry = 120%.

water drag coefficient from anode to cathode is assumed to be zero, which is different from the typical low temperature PEMFC with a Nafion membrane.<sup>14-16</sup> Also, as the membrane is doped with phosphoric acid, the mechanism of proton transfer is through the acid in the membrane.<sup>17</sup> The gas mixture is treated as an ideal gas. The flow is laminar due to the low Reynolds number. The gas diffusion layer (GDL) is made of isotropic and homogeneous porous materials.

*Modeling domain.*— The 3D computational domain includes a section of the PBI membrane and both cathode and anode gas flow channels, GDLs, and catalyst layers. Figure 4 shows the computational domain of this model.

Governing equations.— Conservation of mass and momentum.— With the preceding assumptions, the HT-PEMFC operation is governed by the following conservation equations

conservation of mass 
$$\nabla \cdot u = \frac{Q}{\rho}$$
 [1]

conservation of momentum

$$\rho u \cdot \nabla u = \nabla \left\{ -pI + \mu [\nabla u + (\nabla u)^T] \right\}$$
[2]

where *u* is the gas mixture velocity vector (m/s),  $\rho$  is the gas mixture density (kg/m<sup>3</sup>), *Q* is the source term [kg/(m<sup>3</sup> s)], *p* is the pressure (N/m<sup>2</sup>), and  $\mu$  is the dynamic viscosity of the mixture [kg/(m s)] and is calculated as



Figure 4. A 3D HT-PEMFC model computational domain.

#### Table I. Properties in kinetic parameters in Butler-Volmer equation.

Parameter description	
Exchange current density $\times$ ratio of reaction surface to catalyst layer volume in anode side, $ai_{0,a}^{\text{ref}}$	
Exchange current density $\times$ ratio of reaction surface to catalyst layer volume in cathode side, $ai_{0,c}^{\text{ref}}$	

Reference hydrogen molar concentration,  $C_{H_2-ref}$ 

Reference oxygen molar concentration,  $C_{O_2-ref}$ 

Anodic and cathodic transfer coefficient for hydrogen oxidation reaction

Cathodic transfer coefficient for oxygen reduction reaction

$$\mu = \sum_{i} x_{i} \cdot \mu_{i}$$
[3]

In the porous GDL, the pressure drop is proportional to the gas velocity if the flow is laminar, and it is modeled as

$$(\mu/\kappa)u = \nabla \left\{-pI + (1/\varepsilon)\mu[\nabla u + (\nabla u)^T]\right\}$$
[4]

where  $\kappa$  is the permeability of the GDL  $(m^2)$  and  $\epsilon$  is the porosity of the GDL.

*Conservation of species.*— The multispecies mass transports in the whole computational domain (including the gas channels and GDL) are described by the Maxwell–Stefan equation. It solves for the fluxes of each species in terms of mass fraction. The general form of the Maxwell–Stefan equation is shown below

$$\nabla \left\{ -\rho w_{i} \sum_{j=1}^{N} D_{ij} \left[ \frac{M}{M_{j}} \left( \nabla w_{j} + w_{j} \frac{\nabla M}{M} \right) + (x_{j} - w_{j}) \frac{\nabla P}{P} \right] + w_{i} \rho \vec{u} \right\}$$
  
=  $R_{i}$  [5]

where  $D_{ij}$  is the binary diffusion coefficient, *x* is the molar fraction, *w* is the mass fraction, *M* is the molecular mass, *R* is the universal gas constant [8.314 J/(mol K)], and *T* is the cell operating temperature (K).  $\rho$  is the gas mixture density described by

$$\rho = \left(\sum_{i} x_{i} \cdot M_{i}\right) P/(R \cdot T)$$
[6]

The subscripts i and j represent different species.  $R_i$  is the reaction rate, which accounts for the consumption of reactants and the production of products during electrochemical reactions in the catalyst layer, and  $R_i$  was calculated as

$$R_{\rm H_{2}} = -\frac{j_{\rm a}}{2F}M_{\rm H_{2}}$$

$$R_{\rm O_{2}} = -\frac{|j_{\rm c}|}{4F}M_{\rm O_{2}}$$

$$R_{\rm H_{2}O} = \frac{|j_{\rm c}|}{2F}M_{\rm H_{2}O}$$
[7]

On the cathode side, only oxygen and water are solved because the third species can always be obtained from the mass balance equation given as follows

$$w_{\rm N_2} = 1 - w_{\rm O_2} - w_{\rm H_2O}$$
 [8]

On the anode side, hydrogen is solved and the mass fraction of water is

$$w_{\rm H_2O} = 1 - w_{\rm H_2}$$
 [9]

The binary diffusivities  $D_{ij}$  used in the Maxwell–Stefan equations were calculated from the empirical correlation<sup>18</sup>

$$D_{ij} = D_{ij_0} \left(\frac{T}{T_0}\right)^{1.5}$$
[10]

where  $T_0$  is the reference temperature and  $D_{ij_0}$  is the reference binary diffusivity as listed in Table I. In the porous media, the ef-

fective binary diffusivity is modified to account for the effect of the porosity of the porous  $\text{GDL}^{19}$ 

$$D_{\rm ii\ eff} = D_{\rm ii}(\varepsilon)^{1.5}$$
[11]

Value  $1.0 \times 109 \text{ A/m}^3$  $3.0 \times 103 \text{ A/m}^3$ 

40.88 mol/m3

40.88 mol/m<sup>3</sup>

 $\alpha_a = \alpha_c = 1$ 

 $\alpha_c = 1$ 

*Conservation of electric charge.*— In a PEMFC, the current can be split into two parts: ionic current and electronic current. Protons travel through the ionic conductor (membrane) to form an ionic current, while electrons transfer only through the solid matrix of electrodes, which results in an electronic current. The current continuity equations are obtained by using Ohm's law

$$\nabla \cdot (-\sigma_{\rm s} \nabla \cdot \phi_{\rm s}) = S_{\rm s}$$
$$\nabla \cdot (-\sigma_{\rm m} \nabla \cdot \phi_{\rm m}) = S_{\rm m}$$
[12]

where  $\varphi$  is the phase potential,  $\sigma$  is the effective electric conductivity (S $m^{-1}$ ), S is the current source term (A $m^{-3}$ ), and the subscript s denotes the property of the solid phase while m denotes that of the membrane. The source terms in the electron and proton transport equations result from the electrochemical reaction, which occurs only in the catalyst layers of anode and cathode sides, and are given as

anode catalyst layer: 
$$S_m = j_a$$
  $S_s = -j_a$   
cathode catalyst layer:  $S_m = j_c$   $S_s = -j_c$  [13]

where  $j_a$  and  $j_c$  are the transfer current density corresponding to the electrochemical reaction at the anode and cathode catalyst layers, respectively.

*Constitutive relations.*— The source terms in both species and charge equations are related to the transfer current density  $j_a$  and  $j_c$ , which was calculated by using a simplified Butler–Volmer equation given as

$$j_{a} = a t_{0,a}^{\text{ref}} \left( \frac{C_{\text{H}_{2}}}{C_{\text{H}_{2},\text{ref}}} \right)^{0.5} \left( \frac{\alpha_{a} + \alpha_{c}}{RT} F \eta_{a} \right)$$
[14]

$$i_{\rm c} = a i_{\rm 0,c}^{\rm ref} \left( \frac{C_{\rm O_2}}{C_{\rm O_2,ref}} \right) \exp \left( -\frac{\alpha_{\rm c}}{RT} F \eta_{\rm c} \right)$$
[15]

where  $\eta$  represents the potential difference between solid matrix and electrolyte and is defined as

anode side: 
$$\eta_a = \varphi_s - \varphi_e$$

athode side: 
$$\eta_c = \phi_s - \phi_e - U_{oc}$$
 [16]

The other coefficients in the Butler–Volmer equation (Eq. 13 and 14) are described in Table I.

*Boundary conditions.*— The inlet gas velocity is calculated based on the stoichiometric ratio, fuel cell active area, and the flow channel dimensions, and is given as

$$U_{\text{in\_cathode}} = \lambda_{\text{c}} \frac{1}{4F} x_{\text{O}_2} RT / (P \cdot A_{\text{channel}} \cdot n_{\text{channel}})$$
[17]

### Table II. Base model parameters.

Parameter		Value
Humidified temperature (°C) Fuel cell temperature (°C) Anode inlet gas flow rate Cathode inlet gas flow rate Backpressure (Pa) Mass fraction of H <sub>2</sub> O_cathode Mass fraction of O <sub>2</sub> _ cathode Mass fraction of H <sub>2</sub> _ anode Anode reference voltage (V) Open-circuit voltage (V) Dynamics viscosity_anode at 180°C (Pa s) Dynamics viscosity_cathode at 180°C (Pa s)	Operating conditions	28 180 Stoic = 1.2 Stoic = 2.0 101325 0.023 (calculated) 0.228 (calculated) 0.743 (calculated) 0 0.93 1.19 $\times$ 10 <sup>-5</sup> (calculated) 2.46 $\times$ 10 <sup>-5</sup> (calculated)
Ionic conductivity, $\sigma_m$ (S m <sup>-1</sup> ) PBI membrane thickness ( $\mu$ m)	Membrane properties	9.825 S/m (tuned based on) <sup>21</sup> 100 μm (BASF)
Electrical conductivity, $\sigma_{d}$ (S m <sup>-1</sup> ) Porosity Permeability, $k_{p}$ (m <sup>2</sup> ) Thickness ( $\mu$ m)	GDL properties	222 S/m (E-TEK) <sup>22</sup> 0.4 $1.18 \times 10^{-11}$ m <sup>2</sup> <sup>12</sup> 380 µm (BASF)
Simulated length (cm) Channel cross section (mm <sup>2</sup> ) Width of the shoulder (mm) Channel patterns	Gas channel dimensions	2 0.7874 × 1 mm 0.90932 mm Serpentine
Catalyst layer thickness ( $\mu$ m) Anode exchange current density (A m <sup>-2</sup> ) Cathode exchange current density (A m <sup>-2</sup> )	Catalyst layer information	
$\begin{array}{l} D_{{\rm O}_2\_{\rm N}_2} \mbox{ at } 293.2 \ {\rm K}({\rm m}^2/{\rm s}) \\ D_{{\rm O}_2\_{\rm H}_2{\rm O}} \mbox{ at } 308.1 \ {\rm K}({\rm m}^2/{\rm s}) \\ D_{{\rm H}_2{\rm O}\_{\rm N}_2} \mbox{ at } 307.5 \ {\rm K}({\rm m}^2/{\rm s}) \\ D_{{\rm H}_2{\rm O}\_{\rm N}_2} \mbox{ at } 307.5 \ {\rm K}({\rm m}^2/{\rm s}) \\ D_{{\rm H}_2{\rm H}_2{\rm O}} \mbox{ at } 307.1 \ {\rm K}({\rm m}^2/{\rm s}) \end{array}$	Binary diffusion coefficient <sup>23</sup>	$\begin{array}{c} 2.2 \times 10^{-5} \\ 2.82 \times 10^{-5} \\ 2.56 \times 10^{-5} \\ 2.56 \times 10^{-5} \\ 9.15 \times 10^{-5} \end{array}$

$$U_{\text{in\_anode}} = \lambda_{a} \frac{I}{2F} x_{\text{H}_{2}} RT / (P \cdot A_{\text{channel}} \cdot n_{\text{channel}})$$
[18]

where  $U_{\rm in\_cathode}$  and  $U_{\rm in\_anode}$  are the average inlet velocity on the cathode and anode sides, respectively,  $A_{\text{channel}}$  is the channel crosssectional area, and  $n_{\text{channel}}$  is the channel number, which is 3 for the triple serpentine configuration.

The species fraction at the inlet is calculated based on the humidified air and corresponding temperature. At the outlet of the flow channel, back-pressure is set to the atmospheric pressure. The flow is assumed to be fully developed. The boundary in the middle plane of the land area is set symmetrical, while the no-slip boundary condition is applied to other impermeable walls and surfaces.

The anode current collector is set to 0 V and the cathode current collector is equal to the fuel cell operating voltage. The rest of the boundaries are set to be insulated or symmetrical (Table II).

### Results

The aforementioned fuel cell model is solved using finiteelement-based commercial software COMSOL Multiphysics. A second-order hexahedral element was adopted and a total of 120,513 degrees of freedom was solved using the PARDISO solver.

Figure 5 presents the polarization curve obtained from both numerical simulation and experimental test. The experimental data

were obtained at 1 atm and 180°C as described earlier. The model is trained by tuning the open-circuit voltage and membrane conductivity. The inlet velocity was calculated based on the channel dimension, stoichiometric ratio, and the current density from the experi-



Figure 5. (Color online) Base case polarization curve comparison.

mental testing. The current density predicted by the numerical model was very close to the experimental current density used to calculate the corresponding input velocity. The maximum difference between the numerical current density and experimental current density is within 0.04  $A/cm^2$  only at the high current density regions.

The mass fraction of the anode reactant  $H_2$  is shown in Fig. 6. The mass fraction of  $H_2$  decreases along the flow direction. In the cross-sectional view, the mass fraction of  $H_2$  is high in the channel and low in the porous GDL, where diffusion dominates the species mass transport in the porous media. The arrow indicates the direction of the diffusion flux.

Figure 7 shows the mass fraction of  $O_2$  on the cathode side. The  $O_2$  mass fraction is high in the channel and low near the reaction site due to the consumption of reaction. No obvious  $O_2$  mass fraction reduction was identified along the flow direction because that cathode is running at a higher stoichiometric ratio and the flow channel is very short.

Figure 8 shows the molar fraction of the water vapor on both anode and cathode sides. Because both fuel and oxidant are humidified at a relatively low temperature  $(28 \,^\circ\text{C})$ , the water vapor enters the fuel cell with a low concentration. As water is produced on the cathode catalyst layer, it has a high molar fraction at the cathode GDL near the catalyst. On the anode side, because there is no osmotic drag effect on the PBI membrane, there is no water transfer from the anode to the cathode as the proton moves that way. As a result, the anode water molar fraction increases slightly due to the consumption of hydrogen. Because hydrogen has relatively small molar mass compared with water, the mass fraction of water in the anode does not change much on the anode GDL.

Figure 9 shows the local current density distribution at both cathode and anode catalyst layers. The high current density region was identified under the gas channel upstream, while the low current density was identified under the bipolar plate shoulder downstream along the channel. Figure 10 shows the polarization curve at different back-pressures. By changing the operating pressure, the validated numerical model fits the experimental data at a back-pressure of 25 psig. In both low and high current density regions, the current numerical model fits the experimental results very well.

### Conclusions

Both experimental testing and numerical simulation were conducted to study an HT-PEMFC with PBI membrane. The HT-PEMFC research was conducted in the temperature range of  $120-180^{\circ}$ C on a single cell with an active area of 45 cm<sup>2</sup> PBI membrane made by BASF Co., USA. The hydrogen stoichiometry was set at 120%, while the air stoichiometry was varied from 200, 250, to 300%, and the pressure was adjusted from atmospheric to 25 psig. A 3D single-phase isothermal model was developed to predict the HT-PEMFC performance.

From this work, the following conclusions can be drawn: There seems to be no drastic drop of cell voltage at high current density. This is presumed to be because the water exits only in the vapor form at high operating temperature. The need to humidify the reactants is not required as proton conductivity in the high temperature membrane depends on impregnation in an acid and conduction of protons through the solid matrix, which eliminates fully hydrating the membrane as is the case with a low temperature Nafion membrane.

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Figure 6. (Color online) Anode  $H_2$  mass fraction distribution at different cross sections along the channel direction [vector: hydrogen diffusive flux, kg/(m<sup>2</sup> s)].

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Figure 7. (Color online) Cathode  $O_2$  mass fraction distribution at different cross sections along the channel direction [vector: oxygen diffusive flux, kg/(m<sup>2</sup> s)].

Figure 8. (Color online) Water vapor molar fraction along the channel direction (z). Top: cathode; bottom: anode.

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Greek



Figure 9. (Color online) Local current density (A/cm<sup>2</sup>) distribution at the cathode catalyst layer.



Figure 10. (Color online) Effect of back-pressure on polarization curve: P = 1 atm and P = 25 psig.

## List of Symbols

- concentration, mol m-3 С
- D diffusion coefficient, m2/s
- F Faraday constant, coulomb/mol
- local current density, A/m2
- I identity matrix
- 1 thickness,  $\mu m$
- М molar mass, kg/mol
- Ν mass flux, kg/(m<sup>2</sup> s)
- pressure, Pa Р
- 0 source term in mass conservation equation, kg/(m<sup>3</sup> s)
- R universal gas constant, 8.314 J/(mol K)
- $R_{\rm i}$ reaction rate of specie i, kg/(m<sup>3</sup> s)
- catalyst layer specific area,  $m^2/m^3$
- temperature, K Τ
- velocity vector, m/s и
- $U_{\rm oc}$ open-circuit voltage, V
- mass fraction

- GDL porosity ε
- overpotential, V η
- GDL permeability of electrode, m<sup>2</sup>
- μ dynamic viscosity, Pa s
- density, kg/m3 ρ
- electrical conductivity, S/m σ
- φ electrical potential, V

Subscripts

- а anode
- с cathode
- electrolyte phase e
- species reference condition
- ref solid carbon

Superscripts

- 0 standard/reference condition
- agglomerate property agg eff effective coefficient

# References

- 1. J. Zhang, Y. Tang, C. Song, X. Cheng, J. Zhang, and H. Wang, Electrochim. Acta, 52, 5095 (2007).
- 2. Z. Liu, J. S. Wainright, M. H. Litt, and R. F. Savinell, Electrochim. Acta, 51, 3914 (2006)
- Q. Li, R. He, J. A. Gao, J. O. Jensen, and N. J. Bjerrum, J. Electrochem. Soc., 150, 3. A1599 (2003).
- 4. J. T. Wang, R. F. Savinell, J. Wainright, M. Litt, and H. Yu, Electrochim. Acta, 41, 193 (1996).
- O. Savadogo, J. Power Sources, 127, 135 (2004).
- X. Cheng, J. Zhang, Y. Tang, C. Song, J. Shen, D. Song, and J. Zhang, J. Power 6. Sources, 167, 25 (2007).
- J. Lobato, P. Canizares, M. A. Rodrigo, J. J. Linares, and J. A. Aguilar, J. Membr. Sci., 306, 47 (2007).
- 8. J. L. Ma, J. S. Wainright, M. H. Litt, and R. F. Savinell, J. Electrochem. Soc., 151, A8 (2004).
- 9. G. Liu, H. Zhang, J. Hu, Y. Zhai, D. Xu, and Z. G. Shao, J. Power Sources, 162, 547 (2006).
- 10. J. A. Asensio and P. Gomez-Romero, Fuel Cells, 5, 3 (2005).
- 11. D. F. Cheddie and N. D. H. Munroe, Energy Convers. Manage., 47, 1490 (2006).
- 12. D. F. Cheddie and N. D. H. Munroe, J. Power Sources, 160, 215 (2006).
- 13. T. J. Schmidt and J. Baurmeister, J. Power Sources, 176, 428 (2008).
- 14. J. Zhang, Y. Tang, C. Song, and J. Zhang, J. Power Sources, 172, 163 (2007). 15. D. Weng, J. S. Wainright, U. Landau, and R. F. Savinell, J. Electrochem. Soc., 143,
- 1260 (1996). X. Ren, W. Henderson, and S. Gottesfeld, J. Electrochem. Soc., 144, L267 (1997). 16
- F. P. Incropera and D. P. DeWitt, Fundamentals of Heat and Mass Transfer, John 17. Wiley & Sons, New York (1996).
- R. B. Bird, W. E. Stewart, and E. N. Lightfoot, Transport Phenomena, John Wiley 18. & Sons, New York (1960).
- 19. J. Bear and J. M. Buchlin, Modeling and Applications of Transport Phenomena in Porous Media, Kluwer Academic, Boston (1991).
   K. Broka, Techn. Lic. Thesis, Royal Institute of Technology, Stockholm, (1995).
- 21. H. L. Lin, T. L. Yu, W. K. Chang, C. P. Cheng, C. R. Hu, and G. B. Jung, J. Power Sources, 164, 481 (2007).
- http://www.etekinc.com/standard/index.php, last accessed March 27, 2008. 22.
- 23. E. L. Cussler, Diffusion-Mass Transfer in Fluid Systems, Cambridge University Press, London (1969).



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