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Publisher's version / Version de l'éditeur:

<https://doi.org/10.1115/1.2039949>

Journal of Fuel Cell Science and Technology, 2, pp. 213-218, 2005

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Numerical Predictions of Transport Phenomena in a Proton Exchange Membrane Fuel Cell

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Transport phenomena play an important role in the performance of the proton exchange membrane fuel cell. Water generated by electrochemical reactions and transported by osmotic drag and back diffusion can cause saturation or flooding, preventing oxygen from reaching catalysis sites. Dehydration may also occur, resulting in poor proton conductivity. Balancing water content within the membrane involves judicious water and heat management strategies. In this paper, detailed mathematical models for the prediction of all significant aspects of physicochemical hydrodynamics for a proton exchange membrane fuel cell are employed. Fully coupled heat and mass transfer and electrochemistry are considered, and the dependence of water transport on these factors is taken into account. Two distinct approaches were considered: a fully three-dimensional approach and a hybrid scheme, whereby the electrochemistry and electric fields are treated as locally one dimensional in the membrane assembly. Comparisons between the two approaches are presented and discussed. The numerical results suggest a dependence of the rate-of-water removal on temperature, current density, and inlet humidification levels, and also that the oxygen concentration in the air channels significantly affects current density distribution. [DOI: 10.1115/1.2039949]

Keywords: Proton Exchange Membrane, Fuel Cell, Computational Fluid Dynamics, Transport Phenomena, Water Transport

1 Introduction

High energy transfer, low pollutant emission, and moderate operating temperature make the proton exchange membrane (PEM) fuel cell an attractive candidate for energy conversion. Potential applications of the PEM fuel cell are in the automotive, residential power supply, and mobile communication sectors, to name but a few. The commercial success of the PEM fuel cell depends on cost reduction, e.g., of catalyst materials, and on increasing the operational efficiency of the device.

A key element of the PEM fuel cell is the membrane, typically Nafion™, with a chemical structure consisting of a fluorocarbon backbone, side chain, and ion cluster composed of sulfuric acid ions. The membrane is a good conductor of H⁺ protons, if and only if it is hydrated, with mobile hydrogen ions in the cluster [1]. Thermal and water management are two critical performance issues for PEM fuel cells [2]. Water generated by the electrochemical reaction, and osmotic drag and back diffusion can cause oversaturation or even flooding on the cathode side, thus preventing oxygen from entering the catalysis sites. On the anode side dehydration may occur, resulting in lower protonic conductivity. Balancing the water content in the membrane involves judicious water and heat management strategies.

The performance of a PEM fuel cell is often characterized in the form of a polarization curve. This is governed by activation, ohmic, and concentration overpotentials. Much attention has been paid in the past to the cathode side of the PEM fuel cell, where the exchange current density is low and the presence of overhydration in the porous cathode and catalyst layers may result in activation and concentration losses.

Mathematical models and numerical analysis of PEM fuel cells play an important role in understanding the physicochemical phenomena and in improving or optimizing PEM fuel cell systems.

Bernardi and Verbrugge [3] proposed a one-dimensional (1D) model for the ion-exchange membrane and gas-diffusion porous electrodes. Springer et al. [1] deployed experimental data for water diffusion coefficient, electro-osmotic drag coefficient, and membrane conductivity (as a function of water content) in a 1D model. These models provided a fundamental framework for the multidimensional models that followed. Fuller and Newman [2] analyzed water and thermal management and fuel utilization in their pseudo two-dimensional (2D) model. Nguyen and White [4] demonstrated the importance of water and thermal management in maintaining high-performance PEM fuel cells, with a pseudo 2D model. Gurau et al. [5] considered transport phenomena in a 2D PEM fuel cell model. Their calculations showed uneven species distributions in the air and/or fuel channels and in the porous diffusion layers. Recent efforts have been toward modeling two-phase flow and transport on the cathode side, with emphasis on PEM fuel cell operation at high current density.

The objectives of this paper are to apply both a detailed three-dimensional (3D) model and a hybrid model to an industrial PEM fuel cell design, in order to predict water transport and distribution within the unit and also the impact of oversaturation and dehydration on either side of the membrane, on the overall performance of the fuel cell. In addition, the two models are compared with a view to using the simpler model to perform performance calculations, in place of the more complex procedure.

2 Mathematical Model

The traditional planar PEM fuel cell is composed of multilayers of components. A layer of polymer electrolyte membrane is sandwiched by two catalyst layers and two porous gas diffusion electrodes. The membrane is typically made of Nafion™, and the catalyst layer consists of platinum catalyst, ionomer membrane electrolyte, and void space. The membrane-electrode assembly (MEA) is sandwiched between two layers of bipolar plates, containing air and fuel microchannels and possibly water-cooling channels.

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Manuscript received April 8, 2004; final manuscript received March 31, 2005. Review conducted by Nigel M. Sammes.

The physicochemical-hydrodynamic phenomena involved in PEM fuel cells center around four aspects: mass transfer, heat transfer, electric and electrochemical processes. Two models were considered in the present study; (i) a 3D model, as described in [6], using the commercial computational fluid dynamics (CFD) code FLUENT™, and (ii) a hybrid model developed in-house by the present authors and coded as user-defined functions within the same CFD code.

The hybrid model developed here is a combination of a full 3D model for fluid flow, heat and mass transfer, with 1D water and proton transport through the membrane. The way in which the electrochemistry and electric potential fields are treated in the two approaches is different. In the 3D model, two Poisson's equations for the protonic and electronic potentials are solved; in the hybrid model the overpotential is explicitly derived from a Butler-Volmer equation. The models are briefly outlined below.

2.1 Mass Transport. Air and fuel are considered to be multispecies mixtures. Transport of the gas mixtures through the microchannels and porous media is governed by generically similar sets of governing equations. In addition to convection of the fluids, there is diffusion of the gaseous species, which is described by the Stefan-Maxwell equations. Numerical experiments have shown that under many circumstances, a generalized Fick's law approach is an acceptable alternative for engineering applications. The latter was adopted here.

For steady flow, the governing equations for the mixture may be written as follows:

$$\text{div}(\rho \mathbf{u}) = S \quad (1)$$

$$\text{div}(\rho \mathbf{u}; \mathbf{u}) = -\text{grad } p + \text{div}(\mu^{\text{eff}} \text{grad } \mathbf{u}) + \mathbf{S} \quad (2)$$

$$\text{div}(\rho c_p \mathbf{u} T) = \text{div}(k^{\text{eff}} \text{grad } T) + S \quad (3)$$

$$\text{div}(\rho \mathbf{u} y_i) = \text{div}(\Gamma_i \text{grad } y_i) + S \quad (4)$$

where $\mathbf{u}$ is velocity, p is pressure, S is a source term, y_i is mass fraction of species i , μ^{eff} is an effective dynamic viscosity, obtained from the formulation of Wilke [7], $\Gamma_i = \rho D_i^{\text{eff}}$ is an exchange coefficient, D_i^{eff} is an effective diffusion coefficient, and k^{eff} is thermal conductivity.

For fluid flow in porous media (such as electrodes and catalyst layers), the field equations may be multiplied by the porosity ε . Under these circumstances, the effective diffusion coefficient is frequently defined in terms of a tortuosity (and porosity) for the medium. It is assumed that the pore size is much larger than the molecular mean-free path, so that Knudsen diffusion is negligible. The effective diffusion coefficient is obtained using the so-called Bruggmann correction [8],

$$D_i^{\text{eff}} = \varepsilon^{3/2} D_i \quad (5)$$

where D_i is the diffusion coefficient of species i , which is obtained from the Chapman-Enskog equation [9].

Fluid flow in porous media may be written in terms of Darcy's law,

$$\mathbf{U} = \varepsilon \mathbf{u} = -\frac{k_p}{\mu} \text{grad } p \quad (6)$$

where k_p is the absolute permeability. This is achieved by the introduction of a linearized source term, $S = -\mu \mathbf{U} / k_p$ into the momentum equation, (2). Equation (6) may also be applied to multiphase liquid and gas flows by the introduction of the concept of relative permeability [10], to be considered a function of volume fraction.

In the hybrid model, the catalyst layers are treated as plane surfaces. Mass source terms for each species are given by

$$S_{\text{H}_2} = -\frac{M_{\text{H}_2}}{2F} i_a \quad (7)$$

$$S_{\text{O}_2} = -\frac{M_{\text{O}_2}}{4F} i_c \quad (8)$$

$$S_{\text{H}_2\text{O}} = \frac{M_{\text{H}_2\text{O}}}{2F} i_c \quad (9)$$

where F is Faraday's constant (96,487 C/mol), i_a is the proton generation rate on the anode side, i_c the cathodic consumption rate (both positive by convention), and M is molecular weight. For the 3D model the catalyst layers are considered to be of finite thickness, thus the source term S and current density i are "per unit volume," with units kg/m³s and A/m³, respectively. In the hybrid model these are "per unit area" (i.e., S is in kg/m²s and i A/m²).

A unique feature of the Nafion membrane is that proton conductivity, electro-osmotic drag, and diffusion coefficients are strong functions of water content [1]. This is attributed to the chemical structure of the material, which consists of fluorocarbon backbone, side chain, and SO₃H⁺ ion cluster. Protons become mobile only when the membrane is hydrated, and they bind to water molecules, and hop from SO₃⁻ site-to-site within the membrane.

If the pressure difference across the membrane is small, then the two major mechanisms involved in water transport through the membrane are electro-osmotic drag and back diffusion. The flow rate through the membrane can then be written as follows [1,4]:

$$N_{\text{H}_2\text{O}} = n_d \frac{i}{F} - D_w \frac{dC_{\text{H}_2\text{O}}}{dz} \quad (10)$$

where $N_{\text{H}_2\text{O}}$ is the molar flow rate of water through the membrane, n_d is the osmotic drag coefficient, D_w is the water diffusion coefficient in the membrane, z is the direction perpendicular to the membrane-electrode interface, and $C_{\text{H}_2\text{O}}$ is water concentration.

Both n_d and D_w can be written as functions of water activity a and temperature T as follows [1,4]:

$$n_d = 0.0049 + 2.024a - 4.53a^2 + 4.09a^3 \quad a < 1 \quad (11)$$

$$n_d = 1.59 + 0.159(a - 1) \quad a \geq 1 \quad (12)$$

$$D_w = (0.0049 + 2.024a - 4.53a^2 + 4.09a^3) D^0 \times \exp \left[2416 \left(\frac{1}{303} - \frac{1}{273 + T} \right) \right] \quad a < 1 \quad (13)$$

$$D_w = [1.59 + 0.159(a - 1)] D^0 \exp \left[2416 \left(\frac{1}{303} - \frac{1}{273 + T} \right) \right] \quad a \geq 1 \quad (14)$$

2.2 Heat Transfer. Heat transfer in the microchannels and porous electrodes is governed by Eq. (3) (assuming pressure work, and viscous dissipation to be negligible). In solid regions, convection is absent, and Eq. (3) reduces to a simple Poisson equation. Latent heat is released by condensation of water vapor into the liquid phase. Heat sources result from the electrochemical reactions on both sides of the membrane, and also from activation, Joule, and contact resistance.

Although heat is generated as a result of a variety of mechanisms, the origin of all heat sources and/or sinks of heat comes from the change in chemical potential of the reactants and/or products. The change in enthalpy of formation ΔH is equal to the sum of heat and electrical energy (assuming mechanical work to be negligible). Thus, the total amount of heat generated could be written as

$$S = i \left(\frac{-\Delta H}{nF} - V \right) \quad (15)$$

The reader will note the value of ΔH is dependent on the fraction of water in the liquid or vapor form. Equation (11) cannot be used to enumerate the various sources of thermal dissipation for the fuel cell; for these, specific closure equations are required.

2.3 Electric and Electrochemical Processes. For the 3D model, the electrochemical reactions at the membrane-electrode interfaces may be written implicitly in terms of local current density in the form of a Butler-Volmer-type equation [11,12] as follows:

$$i_k = i_{0,k}^{\text{ref}} \left(\frac{C_k}{C_k^{\text{ref}}} \right)^{\gamma_k} \left[\exp \left(\frac{\alpha_a F}{RT} \eta \right) - \exp \left(- \frac{\alpha_c F}{RT} \eta \right) \right] \quad (16)$$

where i_k is the volumetric current density in the catalyst layer, and $i_{0,k}^{\text{ref}}$ is a volumetric reference exchange current density, which depends on such parameters as the electrochemical reactions:

as well as temperature and catalyst loading, C_k^{ref} is the reference concentration of hydrogen on the anode side and oxygen on the cathode side, γ_k is a stoichiometric coefficient for species k in the cathodic and anodic reactions, α_a and α_c are transfer coefficients, η is the activation overpotential (which is positive on the anode side but negative on the cathode side). The numerical value of the exchange current is based on the experimental results of Parthasarathy et al. [13]. The anode overpotential may be expressed as follows,

$$\eta_a = (\Phi_e - \Phi_m)_a - E_a \quad (17)$$

A similar expression may be written for the cathode overpotential. Here Φ_e and Φ_m are the local electronic and protonic potentials. The Nernst potential E is just the sum of two half-potentials $E = E_a + E_c$. The half values are not unique; the sum, however, may readily be written as

$$E = \frac{-\Delta G}{2F} + \frac{RT}{2F} \ln \left(\frac{x_{\text{H}_2}^{1/2}}{x_{\text{H}_2\text{O}}} \right) + \frac{RT}{4F} \ln(p_a) \quad (18)$$

where x is mole fraction, ΔG is the change in Gibb's free energy for the reaction, under reference conditions, and p_a is air pressure.

The potential distributions of both Φ_e and Φ_m satisfy Laplace's equation, since there can be no net accumulation of electrical charge within the domain

$$\nabla \cdot (\mathbf{i}_m + \mathbf{i}_e) = 0 \quad (19)$$

and $\mathbf{i}_m$ and $\mathbf{i}_e$ are the proton and electron current density vectors, respectively.

In the hybrid model, a somewhat different approach is taken than that given above: The cathode overpotential changes very little over the catalyst layer in a direction perpendicular to the membrane interface, though the oxygen concentration changes significantly over the thickness of the catalyst layer. Thus, by integration of Eq. (16) across the catalyst layer, one obtains essentially the same equation, other than that $i_{0,k}^{\text{ref}}$ now represents the reference surface current density, C_k is the concentration of the reactant k at the membrane interface, and i_k is the surface current density value.

The absolute value of the overpotential on the cathode side is much larger than that on the anode side, and the overpotential on the anode side is usually neglected. If $|\alpha_c F \eta_c| \gg RT$, Eq. (16) can be rewritten as

$$|\eta_c| = \frac{RT}{\alpha_c F} \ln \left[\frac{i}{i_{0,k}^{\text{ref}}} \left(\frac{C_{\text{O}_2}}{C_{\text{O}_2}^{\text{ref}}} \right) \right] \quad (20)$$

In the hybrid model, Φ_e and Φ_m are not solved for as state variables. The potential losses in the membrane, diffusion layers,

Table 1 Parameters for base case

Membrane thickness	2.3×10^{-4} m
Gas-diffusion layer thickness	2.6×10^{-4} m
Catalyst layer thickness	0.1×10^{-4} m
Channel height	7.62×10^{-4} m
Channel width	1.0×10^{-3} m
Channel rib width	5.0×10^{-4} m

and bipolar plates are computed from ohmic resistance terms. Relatively constant potential distributions were observed on both sides of the membrane interfaces.

3 Results and Discussion

The PEM fuel cell prototype given in Ticianelli et al. [14] was used as the base case for a comparison of the detailed numerical simulation and the hybrid model. Physical parameters and properties are given in Tables 1 and 2, respectively.

3.1 Comparison of 3D and Hybrid Models. The same geometry was used to compare the 3D and hybrid methodologies. The hybrid approach requires that the flux lines of current be primarily oriented in a vertical direction. It is valid when the electronic conductivity of the electrodes is constant, the effective diffusion coefficients of the gas diffusion layers are relatively large, and the reaction rates are slow. Effective diffusion coefficients within the central layers are relatively high, so that the current is evenly distributed throughout the membrane interfaces. Figure 1 shows path lines of current within the fuel cell in a cross-sectional view. It can be seen that the path lines are reasonably evenly distributed, and hence, the hybrid approach would be appropriate in this case.

The hybrid and 3D methodologies were compared under the same average current density and temperature conditions. For mass transfer calculations, precisely the same source and/or sink terms of reactants/products are prescribed, based on Eqs. (7)–(9). The electro-osmotic drag coefficient and diffusion coefficient are indirectly related to the water vapor mole fraction distribution at the interface between the electrodes and the membrane. As the local membrane current density distribution is presumed constant for the hybrid model, a higher water vapor mole fraction is predicted for this model at the anode interface.

The overpotential at the interface between the cathode and the membrane determines the reaction rate of the PEM fuel cell. The reader will note that the physical meaning of the exchange current densities in the two models are different in as much as the values are either per unit volume or per unit surface area. These are a function of catalyst loading.

The relationship between overpotential and local current density can be seen from Fig. 2. A lower local current density for the hybrid model results in a lower overpotential value. The difference between the two approaches is less than 10%. Figure 2 also shows the variation in ohmic loss as a function of average current density. It can be seen that the hybrid method underpredicts the voltage loss by around 10% when compared to the 3D model.

Table 2 Physical properties at 80 °C

Membrane permeability	1.58×10^{-18} m ²
Porous electrode permeability	3.03×10^{-16} m ²
Saturated water vapor pressure	0.467×10^5 Pa
Electrode volume fraction	0.5
Cathodic transfer coefficient	2
Anodic transfer coefficient	2
Proton reference concentration	1.2×10^3 mol/m ³
Oxygen reference concentration	4.6 mol/m ³
Cathode exchange current density	4×10^6 A/m ³

Fig. 1 Cross-sectional view of the path lines of electric current in a PEM fuel cell

This is because current is more evenly distributed across the membrane for the 1D model; while the actual situation is such that the current density varies locally from the regions located near the air channel to those adjacent to the ribs, depending on the rate of diffusion of oxygen (i.e., concentration), which affects the gradient of the local potential field. For the case considered here, the local variations of current density are relatively small and good agreement between the two methods is seen in Fig. 2. Local current density variations depend not only on the mass-transfer conductivities (exchange coefficients), but also on geometric factors, such as the thickness of the layers and the ratio of channel width to that of the ribs.

Figure 3 shows polarization curves obtained with both hybrid and 3D methods. Agreement between the two models is quite reasonable, with the hybrid method overpredicting cell voltage by a maximum of around 5%. This is because of the flatter current

Fig. 2 Cathodic overpotential and ohmic voltage loss predicted by different approaches

Fig. 3 Polarization curve predictions

density distribution obtained with the hybrid method.

Heat generated within the fuel cell comes from a variety of sources: energy associated with the thermodynamics of the electrochemical reaction, heat of activation, Joule heating, and heat due to contact resistance. If both V and i are close for the two models, a similar net heat source term will arise.

3.2 Water Transport in an Industrial PEM Fuel Cell. Numerical simulations of water transport through the membrane were conducted for a commercial PEM fuel cell prototype. Geometric details of the flow channel configuration are, by necessity, of a proprietary nature. Physical properties of the solid and fluid layers are given in Table 2. The thickness of the various layers together with the widths of the channels and ribs are given in Table 3.

Both 3D and hybrid models were used to predict the performance of a single PEM fuel cell. Comparisons were made at constant temperature, in the absence of species source terms. Under the above conditions, the cathodic overpotential and ohmic voltage loss were compared so that the hybrid model could be used to perform further numerical calculations.

Water transport was examined by taking into consideration the temperature variation in the PEM fuel cell, together with the electro-osmotic drag, and the back diffusion of liquid water through the membrane. A fixed temperature is presumed at both the top and bottom walls.

A typical membrane temperature distribution is shown in Fig. 4. The highest temperatures are located near the air exit zone. Because constant temperature values are prescribed at both the top and bottom walls and the bipolar plates are high conductors of heat, the temperature distribution within the PEM fuel cell varies little over the membrane. Air flows from the bottom-left to the top-right corner, whereas fuel flows from the top-left to the bottom-right corner. Since both gases are heated higher temperature values at the exits are to be anticipated.

Figure 5 shows the membrane current density distribution at the membrane interface. The highest current density is found to occur

Table 3 Physical parameters

Membrane thickness	1.0×10^{-4} m
Gas-diffusion layer thickness	2.0×10^{-4} m
Catalyst layer thickness	0.1×10^{-4} m
Channel height	1.0×10^{-3} m
Channel width	1.5×10^{-3} m
Channel rib width	1.0×10^{-3} m

Fig. 4 Temperature (°C) distribution in the membrane

at the air-fuel inlet region. The reactant concentrations and, hence, the Nernst potential, are both a maximum at the inlet region. The lowest current density is located near the air-fuel exit regions. The current density distribution is related to both the cathodic overpotential and the membrane conductivity, as shown in Figs. 6 and 7. It can be seen that the water-vapor mass fraction reaches a minimum near the exit region, thus resulting in lower protonic conductivity and, hence, a decrease in local current density. The lower overpotential in the exit region is related to the low current density and higher oxygen concentration at the membrane interface resulting from diffusion occurring here.

The water vapor distribution at the membrane-cathode interface is shown in Fig. 7. For the present case, little oversaturation of water is found; however, it is noted that a higher water vapor mass fraction distribution occurs near the air exit: Water is generated along the air channels. A fraction of this water diffuses back to the anode side; however, it was observed that this mechanism is sub-

Fig. 5 Current density for $\bar{i}=5000 \text{ A/m}^2$

Fig. 6 Cathodic overpotential (V) distribution for $\bar{i}=5000 \text{ A/m}^2$

ordinate to forward transfer of water by electro-osmotic drag over a wide range of observed current densities, which is especially true at large current densities.

Figure 8 shows the water vapor distribution. It can be seen that water is being depleted along the fuel flow path, as the electro-osmotic dominates water transport through the membrane. Protonic conductivity is a function of both water content and temperature. It is critical that there be enough water on the anode side for the proper functioning of the membrane.

4 Conclusions

Hybrid and full 3D models were applied to both a straight-channel and an industrial PEM fuel cell design. Both global and local current density distributions were analyzed. The local cur-

Fig. 7 Water vapor mass fraction distribution at the cathode catalyst interface for $\bar{i}=5000 \text{ A/m}^2$

Fig. 8 Water vapor mass fraction distribution at the anode catalyst interface for $\bar{i}=5000 \text{ A/m}^2$

rent density reaches a maximum under the channels or under the ribs of the bipolar plates. The main factors affecting this are the oxygen diffusion rate and the protonic conductivity of the membrane. Since these local-scale phenomena can affect the overall results, future studies will address this matter.

Good agreement was obtained in terms of cell voltage, overpotential, species mass fraction distributions, and ohmic losses. Full-scale numerical simulations performed with both methods were used to perform calculations for temperature, current, overpotential, and water mass fraction distributions over the whole unit cell. The issue of water transport is important to maintain the proper functioning of the membrane.

Acknowledgments

The authors would like to thank the staff of Palcan Fuel Cells Ltd. for providing us with the geometry of an industrial-scale fuel cell. Financial support of the NRC fuel cell program and the Institute of Chemical Process and Environmental Technology is appreciated.

Nomenclature

- C_k = concentration of species k , mol/m^3
 C_k^{ref} = reference concentration, mol/m^3
 D_i^{eff} = effective diffusion coefficient of species i , m^2/s
 D_w = water diffusion coefficient in the membrane, m^2/s
 E = Nernst potential, V
 F = Faraday's constant, $96,487 \text{ C/mol}$
 ΔG = change in Gibb's free energy of formation, J/mol

- ΔH = change in enthalpy of formation, J/mol
 i = current density, A/m^2 , A/m^3
 i_a = proton generation rate, A/m^2 , A/m^3
 i_c = cathodic consumption rate, A/m^2 , A/m^3
 $\mathbf{i}_m, \mathbf{i}_e$ = proton and electron current density vectors, A/m^2 , A/m^3
 $i_{0,k}^{\text{ref}}$ = volumetric reference exchange current density, A/m^2 , A/m^3
 k^{eff} = effective thermal conductivity, W/m K
 k_p = absolute permeability, m^2
 M = molecular weight, kg/mol
 $N_{\text{H}_2\text{O}}$ = molar flow rate of water through the membrane, $\text{mol/m}^2 \text{ s}$
 n_d = osmotic drag coefficient
 p = pressure, Pa
 p_{O_2} = partial pressure of oxygen, Pa
 $\bar{S}$ = general source terms
 $\mathbf{u}$ = velocity, interstitial velocity, m/s
 $\mathbf{U}$ = superficial velocity, m/s
 y_i = mass fraction of species i
 α_a, α_c = transfer coefficients
 ε = porosity
 Φ_e, Φ_m = local electronic and protonic potentials, V
 Γ_i = exchange coefficient, kg/m s
 γ_k = stoichiometric coefficient for species k
 η = activation overpotential, V
 μ^{eff} = effective dynamic viscosity, kg/m s

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