Modeling and simulation study on the complex seepage mechanism of porous electrode for a proton exchange membrane fuel cell

Hui He¹, Pengtao Sun² and Yousheng Xu¹,a

¹Department of Physics, Zhejiang Normal University, Jinhua, 321004, China
²Department of Mathematical Sciences, University of Nevada Las Vegas, 4505 Maryland Parkway, Las Vegas, NV 89154, USA

aCorresponding E-mails: ysyou@zjnu.cn

Keywords: Fuel cell, Complicated seepage mechanism, Numerical simulation

Abstract. In this paper, a three-dimensional, complex seepage model of a proton exchange membrane fuel cell (PEMFC) is studied, the corresponding finite element method and numerical simulation are given as well, where species transport, fluid flow, charge transport, heat transfer and electrochemical reaction in the PEMFC are simultaneously addressed. The domain to be studied includes porous gas diffusion layers, catalyst layers, gas channels, bipolar plates, and membrane. The fluid transportation phenomena arising in the whole fuel cell are described by the referred model, different physical parameters and source terms are reflected in different areas. The chemical components, flow characteristics and distributions of temperature in the 3-D space are obtained by resolving the seepage control equation system coupled with electrochemical equations. The induced methods and results can guide the optimal design of PEMFC.

Introduction

The fuel cell is an electrochemical power generator with the potential for obtaining very high electrical energy conversion efficiencies while operating quietly with minimal polluting emissions. Particularly, the proton exchange membrane fuel cell (PEMFC) which can be classed as low temperature fuel cell is considered a contender for next-generation portable and micropower sources, offering a combination of simplicity, robustness, short start-up time, little impact on the environment and high energy density due to the use of hydrogen. In the cell, the development of PEMFC was restricted by the performance of the porous electrode which is characterized as the power converter, thus the modeling and simulation study on the complex seepage mechanism of porous electrode not only is used to guide the optimal design of fuel cell, but also contribute to reduce the cost and experimental expenses. so far, considerable simulation research of the PEMFC has been carried out on the one- dimension, two- dimension and three- dimension[1,2,3,4,5,6], however, to get a good understanding of these complex transport phenomena as well as the effect on the cell performance, reasonable numerical simulation is thus essential[7,8,9,10,11,12,13,14,15] and this study remains challenge.

Our goal in this paper is to explore and develop such a comprehensive, three-dimensional numerical model on the PEMFC for the sake of studying the distributions of temperature and chemical components to research effect on cell performance as well as optimize the cell design.

Mathematical Model and Solution

To support the design process, the need for computational tools has resulted in the development of a number of proton exchange membrane fuel cell models. In this paper, modeling efforts focus on special parts of the PEMFC which consists of the anode bipolar plate(ABP), anode gas channel (AGC), anode porous diffusion layer(anode backing layer, ABL), anode catalyst layer(ACL),proton exchange membrane(MEM), cathode catalyst layer(CCL), cathode porous diffusion layer(cathode backing layer ,CBL), cathode gas channel (CGC) and cathode bipolar plate(CBP), As schematically
shown in Figs. 1a and 1b, the cell output voltage and power of unit-fuel cell is small so that we have to form cell stack to external discharge by a number of cell in series or in parallel manner. However, our computational domain is one of the flow channels engraved to make reactant supply and product removal. Finite element method [12, 15] which is used in modeling process has strong applicability, the range of application is very wide and can solve many problems such as conduction of heat and hydrodynamics fields. The mathematical model of the PEMFC to be simulated is applied with several assumptions: The flow in PEMFC is considered to be laminar; The water in the channel is in the form of gas, ignoring the volume occupied by liquid water; Assuming the channel is long enough, namely, the fluid in the outlet is full development; Electrochemical kinetics is controlled by the Butler-Volmer equation [4].

![Fig.1 (a) the cross section(xz plane) of the 3D model and the location of each layer (b) computational domain for 3D model.](image)

**Model Equation.** The governing equation of the proton exchange membrane fuel cell (PEMFC) consists of the following five categories: mass conservation equation, momentum conservation equation, material conservation equation, heat transfer equation, potential control equation:

\[
\nabla \cdot (\rho \phi \mathbf{u}) = S_m .
\]

\[
\nabla \cdot (\rho \phi \mathbf{u}) = -\phi \nabla p + \nabla \cdot (\rho \mu_{\text{eff}} \nabla \mathbf{u}) + S_u .
\]

\[
\nabla \cdot (\phi \mathbf{u} C_k) = \nabla \cdot (D_{k,\text{eff}} \nabla C_k) + S_k .
\]

\[
\nabla \cdot (\lambda_{\text{eff}} \nabla T) = \nabla \cdot (\phi \rho C_T u T) + S_T .
\]

\[
\nabla \cdot (\sigma_{e,\text{eff}} \Phi_e) + S_{\Phi_e} = 0 .
\]

\[
\nabla \cdot (\sigma_{s,\text{eff}} \Phi_s) + S_{\Phi_s} = 0 .
\]

Here \( \phi \) is the porosity; \( \rho \) and \( \mathbf{u} \) denote the density and intrinsic velocity vector of the fluid respectively; \( S_m \) names the mass source term, which is the sum of variable quantity of the reactants and resultants in the catalyst layer, and is zero in the other layers; \( p \) and \( \mu_{\text{eff}} \) separately are the pressure and effective viscosity of the fluid; \( S_u \) in Eq.2 represents the source term of the momentum equation; \( \lambda_{\text{eff}} \) names the effective thermal conductivity; \( D_{k,\text{eff}} \) is the effective diffusion coefficient of species \( k \); \( C_k \) stands for the density of species \( k \); \( S_k \) denotes the velocity of production or consumption of each species (source or sink), caused by electrochemical reaction in the catalyst layer; \( T \) is temperature; \( \rho C_T \) denotes isobaric specific heat capacity; \( S_T \) names quantity of heat in the electrochemical reaction, caused by ohmic heat effect, reversible thermal effect and activation
polarization thermal effect; $\sigma_{s,eff}$ and $\sigma_{s,eff}$ are the effective conductivity of carbon phase and membrane phase respectively; $\Phi_\sigma$ and $\Phi_\sigma$ stand for membrane phase potential and carbon phase potential respectively; $S_{\phi_e}$ and $S_{\phi_e}$ represent the increasing or decreasing speed of proton and electron in the electrochemical reaction respectively, specific expression and instruction can be found in these documents[4,15].

Results and Conclusions

The basic characteristic parameters and operating condition solving mathematical model are listed in Table 1, other definitions of various physical parameters and coefficients are all referred to the documents of Bernardi[6].

<table>
<thead>
<tr>
<th>Table 1. Basic physic parameters of fuel cell</th>
</tr>
</thead>
<tbody>
<tr>
<td>the length of the cell [cm]</td>
</tr>
<tr>
<td>the width of the cell [cm]</td>
</tr>
<tr>
<td>the width of the ABL [cm]</td>
</tr>
<tr>
<td>the width of the AGC [cm]</td>
</tr>
<tr>
<td>the width of the ABL [cm]</td>
</tr>
<tr>
<td>the width of the ACL [cm]</td>
</tr>
<tr>
<td>the width of the MEM [cm]</td>
</tr>
<tr>
<td>the width of the CCL [cm]</td>
</tr>
<tr>
<td>the width of the CBL [cm]</td>
</tr>
<tr>
<td>the width of the CGC [cm]</td>
</tr>
<tr>
<td>the width of the CBL [cm]</td>
</tr>
<tr>
<td>cell voltage [V]</td>
</tr>
<tr>
<td>anode inlet pressures [kPa]</td>
</tr>
<tr>
<td>cathode inlet pressures [kPa]</td>
</tr>
<tr>
<td>H2 percentages at anode inlet /Molar fraction</td>
</tr>
<tr>
<td>O2 percentages in cathode inlet /Molar fraction</td>
</tr>
<tr>
<td>cell temperature [K]</td>
</tr>
<tr>
<td>anode water saturation temperatures [K]</td>
</tr>
<tr>
<td>cathode water saturation temperatures [K]</td>
</tr>
<tr>
<td>cathode inlet relative humidity</td>
</tr>
<tr>
<td>Stoichiometry number of anode</td>
</tr>
<tr>
<td>Stoichiometry number of cathode</td>
</tr>
<tr>
<td>constant current density applied [$A/m^2$]</td>
</tr>
</tbody>
</table>

Distributions of component concentration. It is essential to understand the distributions of reactant concentration on the interface between catalyst layer and diffusion layer in the porous electrode, due to the distributions determines the reaction rate and local current density of fuel cell, which will eventually have an immense impact on the cell performance. The concentration distributions of hydrogen and oxygen at a voltage of 0.6V are shown in Figs.2a and 2b respectively, meanwhile, the results shown in Figure. 2 indicate that the distributions of reactant concentration is symmetrical in the direction of the z axis. According to the reaction kinetics, the concentration of the hydrogen and oxygen near the gas channel inlet is larger, the rate of reaction is faster as well as the trend of concentration decreased along the flow direction. However, when it reaches to the middle position, the reactant concentration decreased along the flow channel is larger, the speed of the reaction kinetics is slower, thus the variation of concentration is not obvious in the later stage.
Fig. 2(a) 0.6V, the distributions of hydrogen concentration on the interface between catalyst layer and diffusion layer in the porous electrode.

Fig. 2(b) 0.6V, the distributions of oxygen concentration on the interface between catalyst layer and diffusion layer in the porous electrode.

Figs. 3a and 3b represent the distributions of hydrogen and oxygen concentration in the direction of the z axis (z=0.001m), xy plane and at a voltage of 0.6V. As shown in Figs. 3a and 3b, the variation trend of them is similar, the electrochemical reaction that happened in the catalyst layer leads to the concentration of the reactants gradually decrease along the gas channel, because the conditions discussed are the moderate current density, the concentration of the reactants decreased along the gas channel is not obvious, which does not reach to the condition that happened in the limiting current density.

Fig. 3(a) the distributions of hydrogen concentration in the direction of the z axis (z=0.001m), xy plane.

Fig. 3(a) the distributions of hydrogen concentration in the direction of the z axis (z=0.001m), xy plane.
The distributions of temperature. The distributions of temperature in the direction of the y axis (y = 0.001m), xz plane and at a voltage of 0.6 is shown in Fig. 4. As shown in it, the temperature of the proton exchange membrane is the highest in various layers, at this time the polarization mainly is ohmic polarization due to the quantity of heat which is generated by ohmic resistance account for the main part, in the fuel cell, although the high temperature contributes to the dynamics, does not contribute to the hydration of the proton exchange membrane, which will result in the increase of membrane resistance and the deterioration of membrane, this phenomenon is firmly prohibited.

Conclusions

A three-dimensional mathematical model is described, the distributions of temperature field and component concentration field are getted by numerical simulation in the proton exchange membrane fuel cell. The electrochemical reaction in the catalyst layer of porous electrode leads to the reaction concentration decrease along the fluid flow direction, the larger joule heat which generated by the ohmic resistance leads to the temperature of the membrane become higher, in conclusion, this study will contribute to optimize the device of PEMFC.

Acknowledgment

This work is supported by National Nature Science Foundation of China under Grant Nos 10932010, 11072220 are gratefully acknowledged.

References