

Multi-Physics Numerical Analysis of PEMFC for Automobile Application

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ABSTRACT

Polymer Electrolyte Membrane Fuel Cell (PEMFC) is regarded as a potential alternative clean energy source for automobile applications. Key challenges to the acceptance of PEMFC for automobiles are the cost reduction, improvement in power density for its compactness, and cold-start capability. High current density operation is a promising solution for them. However, high current density operation under normal and sub-zero temperature requires more oxygen flux for the electrochemical reaction in the catalyst layer, and it causes more heat and water flux, resulting in the significant voltage losses. So, the theoretical investigation is very helpful for the fundamental understanding of complex transport phenomena in high current density operation under normal and sub-zero temperature. In this study, the numerical model was established to elucidate the impacts of mass transport phenomena on the cell performance through the numerical validation with experimental and visualization results. The results indicated that the higher current density operation causes non-uniform reaction distribution, resulting in lower cell performance under normal temperature and less accumulated produced water under sub-zero temperature. They also quantitatively indicated the limiting factors for this non-uniform reaction distribution such as heat and water transport in rib/channel direction, oxygen transport resistance near Pt area, and the water transport through the membrane.

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INTRODUCTION

Polymer Electrolyte Membrane Fuel Cell (PEMFC) is regarded as an alternative clean energy source for automobile applications. Key challenges to the acceptance of PEMFC for automobiles are the cost reduction and improvement in power density for its compactness. In particular, higher current density operation is one of the promising solutions to realize the cost reduction due to the reduction of Pt amount and compactness of the stack for wide applicability to vehicle types.

However, higher current density operation produces more heat and water and requires more proton and oxygen flux for electrochemical reaction in the catalyst layer. Phase change of water has to be considered because water condenses into the liquid water and the liquid water prevents oxygen and hydrogen gas transfer from the gas channel to the catalyst layer. So, transport phenomena are known to have great impact on the stack performance. In addition, the stack performance is also affected by fuel cell system operation.

Cold-start capability is one of the biggest issues to be affected by fuel cell system operation. Produced water is frozen inside the stack under sub-zero conditions, causing the significant voltage drop and material/structure degradation. Higher current density operation contributes to a rapid start-up from sub-zero temperatures because of rapid temperature increase of the fuel cell stack due to more heat generation.

Regardless of its importance, the transport phenomena under both normal and sub-zero temperatures is not yet fully understood because of its complexities. So, the objective of this research is to establish a numerical model to solve the water and heat transport processes under various operating conditions, i.e. both normal and sub-zero temperatures, and to elucidate the dominant factors through the validation against experimental studies.

NUMERICAL MODEL

A steady-state PEMFC model involves five principles of conservation, namely mass, momentum, energy, species, and



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charge. These can be presented, within the multiphase mixture model framework, as equations (1, 2, 3, 4, 5, 6).

Continuity conservation

$$\nabla \cdot (\rho \vec{u}) = 0 \quad (1)$$

Momentum conservation

$$\frac{1}{\varepsilon^2} \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla P + \nabla \cdot \tau + S_u \quad (2)$$

Species conservation

$$\nabla \cdot (\gamma_c \vec{u} C^k) = \nabla \cdot (D_g^{k,eff} \nabla C_g^k) - \nabla \cdot \left[\left(\frac{mf_l^k}{M^k} - \frac{C_g^k}{\rho_g} \right) \vec{j}_l \right] + S_k \quad (3)$$

Energy conservation

$$\nabla \cdot (\rho C_p \vec{u} T) = \nabla \cdot (\kappa^{eff} \nabla T) + S_T \quad (4)$$

Charge conservation (proton)

$$0 = \nabla \cdot (\kappa_{proton} \nabla \phi_e) + S_{\phi_e} \quad (5)$$

Charge conservation (electron)

$$0 = \nabla \cdot (\sigma^{eff} \nabla \phi_s) + S_{\phi_s} \quad (6)$$

Electrochemical reaction is implemented as source terms based on Butler-Volmer equation in conservation equations (2, 3, 4, 5, 6). Two-phase transport is also implemented based on the mixture model developed by Wang et al. [1] The detail procedure of numerical study is described in the reference [2,3]. In this study, catalyst layer model and cold-start model were implemented to understand the influence of high current density operation with lower platinum loading on both of cell performance and cold-start issue for obtaining key factor for realizing it without worsening in cold-start capability. Detail of those two models is following.

Catalyst Layer Model

In previous multiphase mixture model [2,3], oxygen transport phenomena in catalyst layer treated in same manner with gas diffusion media, in other words it is described as only a diffusion phenomena in porous media. However, according to the reference [4], there were two types of oxygen transport resistance in catalyst layer. One was oxygen transport resistance through the pores in the through plane direction, the other is oxygen transport resistance from secondary pore in catalyst layer to Pt surface. Figure 1 shows a schematic of transport phenomena in catalyst layer. Here, the Knudsen diffusion resistance in the secondary pore of catalyst layer is called macro transport resistance, which is

expressed by $R_{O_2, CCL-macro}$ as represented in the references [5]. Furthermore, the local transport resistance near Pt through the ionomer and/or water is defined as micro transport resistance, which is referred to as $R_{O_2, CCL-micro}$. In this work, 3-D numerical model was elaborated based on multiphase mixture model to implement $R_{O_2, CCL-macro}$ and $R_{O_2, CCL-micro}$ in catalyst layer. The effect of $R_{O_2, CCL-macro}$ was expressed in the diffusion coefficient as pressure independent effective diffusivity. Thus, the diffusion coefficient is constant under various pressure conditions. The effect of $R_{O_2, CCL-micro}$ was implemented to modify the source term of oxygen in species conservation as following manner. With the value of $R_{O_2, CCL-micro}$ the oxygen flux towards Pt surface is given by

$$\frac{j}{4F \cdot vrf} = \frac{1}{R_{O_2, CCL-micro}} \Delta C_{O_2} \quad (7)$$

where volumetric roughness factor, vrf converts geometric Pt surface area to realistic Pt surface area and j denotes volumetric transfer current density. ΔC_{O_2} shows the difference between oxygen concentration in secondary pores of catalyst layer, $C_{O_2, bulk}$ and that at platinum surface, $C_{O_2, Pt}$ and defined as equation (8)

$$\Delta C_{O_2} = C_{O_2, bulk} - C_{O_2, Pt} \quad (8)$$

Based on the oxygen concentration on platinum surface, the volumetric transfer current density can be obtained with Butler-Volmer equation and then the source term in equation (3) was modified as equations (9, 10).

$$S_{O_2} = \frac{j}{4F} = \frac{A \cdot C_{O_2, bulk}}{4F \cdot C_{O_2, ref}} \left(\frac{4 C_{O_2, ref} \cdot F \cdot vrf}{4 C_{O_2, ref} \cdot F \cdot vrf + A \cdot R_{O_2, CCL-micro}} \right) \quad (9)$$

$$A = -a i_0 \exp \left(-\frac{\alpha_c F}{RT} \eta \right) \quad (10)$$

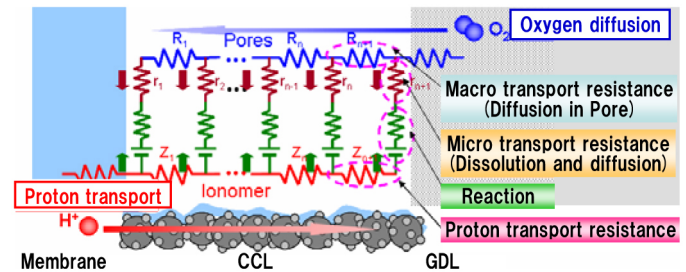


Figure 1. Schematic image of electric circuit model of transport phenomena in the catalyst layer [3]