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Analyses of mass and heat transport interactions in a direct methanol fuel cell



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ABSTRACT

In this paper, a two-dimensional, two-phase, non-isothermal model is presented to predict the electrochemical, mass transfer and heat transfer behaviors in a direct methanol fuel cell (DMFC). Governing equations including the momentum, continuity, heat transfer, proton and electron transport, species transport for water, methanol, and all the gas species (carbon dioxide, methanol vapor, water vapor, oxygen, and nitrogen) and the auxiliary equations are coupled to studying the various phenomena in DMFC. The modeling results agree well with the four different experimental data in an extensive range of operation conditions. A parametric study is also performed to examine the effects of the cell voltage on the different variables, such as cell temperature, liquid methanol concentration distribution, oxygen concentration distribution, and anode gas pressure distribution. The results show that the cell temperature is highly sensitive to the change in the cell voltage as well as methanol concentration distribution. Moreover, it is found that the cell voltage significantly influences the oxygen concentration distribution and the anode gas pressure distribution.

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Introduction

A direct methanol fuel cell (DMFC) directly converts the chemical energy of cell reactions to electricity. It has been regarded as one of the most promising contenders to compete with other non-conventional power sources because of its high efficiency, simple structure, low-temperature operating, easy handling and environmentally friendly nature, which has received tremendous attention recently. Despite these advantages of DMFCs, fundamental technological improvements are still one of the main prerequisites for the DMFC to be able to contend with existing power sources [1].

To improve DMFC components and long term durability, a precise understanding of the couplings of mass, momentum and species with an emphasis on electrochemical kinetics and thermal issues is indispensable. In the last decade with the progress in computing technology, numerical simulation is playing an increasingly important role in understanding the performance of DMFC.

Recently, significant research effort has been focused by researchers all over the world on DMFC modeling. One of the first attempts was made by Baxter et al. [2], who presented an isothermal, steady-state model for the porous anode of a liquid fed DMFC. A simple model of the flow with gaseous bubbles in the anode channel developed by Kulikovskiy [3], which is based on the experimental findings of Yang et al. [4]. His model

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showed that the bubbles effects on cell performance by lowering the stoichiometry of anode flow. Murgia et al. [5] presented a one-dimensional model based on phenomenological transport equations for DMFCs. In order to consider the two-phase flow interaction in the diffusion layer (DL), they introduced a Gaussian function to approximately account for the influence of the capillary pressure on the effective gas porosity. Schultz and Sundmacher [6] developed another one-dimensional dynamic model, validated also on water transport experimental measurements, neglecting the two-phase behavior in both diffusion layers and flooding effects.

Recent models of the DMFC have commonly developed in two dimensions because of its ability to predict transport phenomena. Wang and Wang [7] developed a two-dimensional, two-phase model for DMFCs. In their model, the gas phase at the anode was assumed to be saturated with water and methanol, and the liquid phase was assumed to be saturated with carbon dioxide. Rice and Faghri [8] developed a transient, multiphase model for a passive fuel feed DMFC. These models examined the evaporative effects. Yang and Zhao [9,10] developed a two-phase mass transport model for DMFCs, which was formulated based on classical multiphase flow theory in porous medium and with the effect of non-equilibrium evaporation and condensation of methanol and water taken account. Liu and Wang [11] developed a liquid–gas two-phase transport model for the DMFC, in which different water crossover mechanisms, including diffusion, electro-osmotic drag, and convection, were analyzed. Xu and Faghri [12] presented two-dimensional, two-phase, non-isothermal model for the DMFC, which was developed based on multiphase flow theory in porous media. Most recently, Li et al. [13] developed a two-dimensional, isothermal, two-phase mass transport model for the DMFC. These models examined influences of the structural properties of the anode micro-porous layer (MPL) on water and methanol crossover through the membrane.

Our literature review indicates that little experimental work about DMFC, especially on the water transport characteristics in the DMFC, have been reported and none of the previous works compare their simulation results with actual experimental results, especially results of saturation distributions. Furthermore, this review shows that a general model to study the effect of cell voltage on different variables in DMFC is still missing.

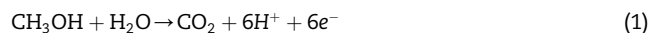
In this work, a two-dimensional, two-phase, non-isothermal model for the DMFC using the multi-fluid approach is developed. The water and methanol crossover through the membrane are considered with the effect of diffusion, electro-osmotic drag, and convection. With this model, the effects of cell voltage on the different variables, such as cell temperature, liquid methanol concentration distribution, oxygen concentration distribution, and anode gas pressure distribution are studied. The results of model are validated with the experimental data.

Model development

Fig. 1 shows the schematic of the cross section of the modeled domain for the base case. The dimension parallel to gas

channel width (x direction) and the dimension normal to the reactive surface (y direction) are modeled here. The model domain consists of half the width of the anode channel, half the width of the anode current collector (CC), an anode diffusion layer (ADL), an anode catalyst layer (ACL), a polymer-electrolyte membrane (PEM), a cathode catalyst layer (CCL), a cathode diffusion layer (CDL), half the width of the cathode CC, and half the width of the cathode channel. Electrochemical reactions in a DMFC included the methanol oxidation reaction (MOR) in the anodic catalyst layer and the oxygen reduction reaction (ORR) in the cathodic catalyst layer. Methanol solution and air are supplied to the inlet channels of the anode and cathode, respectively.

Methanol and water are transported from anode channel to the ACL, where part of methanol is oxidized according to Eq. (1) to generate electrons, protons, and CO_2 , while the remainder is directly transported to the cathode through the membrane [13].



In the cathode side, oxygen is transported from air channel to the CCL, where reacts with the protons and electrons to generate the liquid water according to Eq. (2). The liquid water generated in the CCL removes through the CDL by the capillary pressure coupled with evaporation. On the other hand some of the water electrochemically reacts with the permeated methanol similar to anodic reaction.



The governing equations are divided to four main parts (1. Anode porous region equations, 2. Cathode porous region equations, 3. Membrane region equations, and 4. Public equations).

Anode porous region

In the anode porous region concluding the gas diffusion and catalyst layer, three types of equations consisting of gas species concentrations, liquid methanol concentration ($C_{M,l}$) and liquid saturation ($S_{l,a}$) are pivotal for the modeling. The ADL is composed of inactive carbon, and no any electrochemical reaction occurs within this region, hence the phase change is only term for generation and consumption, whereas the ACL provides catalytic sites for methanol oxidation. Therefore, in addition to the phase change the term of generation and consumption by MOR are taken into account in this region. The major equations are, respectively, given.

Gas species

For the gas species, mass conservation by taking the divergence of mass flux through diffusion, convection, and thermal mass diffusion (Soret effect) can be written as (Maxwell–Stefan equation):

$$\nabla \cdot \left(-\rho\omega_{i,ga} \sum_{j=1}^n D_{ij}^{\text{eff}} \left(\nabla x_j + (x_j - \omega_j) \frac{\nabla P_{g,a}}{P_{g,a}} \right) + D_i^T \cdot \frac{\nabla T}{T} \right) + (\rho u \nabla \omega_{i,ga}) = R_{i,ga} \quad (3)$$

Here, D_{ij}^{eff} is the effective binary diffusion coefficient and is related to the ordinary binary diffusivities as follows:

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