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The effect of gravity on inner transport and cell performance in passive micro direct methanol fuel cell

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ABSTRACT

In this paper, the effects of non-isothermal and gravity on inner methanol concentration and thermal distribution of passive micro direct methanol fuel cell (μDMFC) are taken into account to improve the cell performance. A whole two-dimensional model coupled with the mass transfer, the momentum transfer and the heat transfer is established. Simulation results show that both more uniform reactant concentration and higher in reaction temperature are obtained with the gravity effect. Furthermore, a passive μDMFC with the active area of 1.0 cm^2 is designed and fabricated. The detailed experimental validation is conducted to evaluate the inner transport characteristic as well as the corresponding cell performance. Experimental results reveal that when the cell is supplied within a certain concentration range, both the peak power density of cell and cell energy capacity with gravity positive effect is much higher than that without gravity effect. In addition, the anode CO_2 emission and cathode water-flooding of the passive μDMFC are analyzed, and the experimental results are in good agreement with the simulation.

1. Introduction

Conventional batteries have disadvantages of self-discharge and serious environmental impact. Therefore, it is urgent to find a green power source for portable electronic products. Meanwhile, μDMFC attracts more and more attention recently for its immediate response, charging-free, environmentally-friendly and easy storage of fuel. Compared with active DMFCs, which equipped with external devices, such as pumps and fans for delivering reactants and products, fuel delivery in passive methanol fuel cells depends on intrinsic diffusion and natural convection. Therefore, the latter is a better option for portable power applications because of their simple structure, low weight, and limited parasitic power losses [1–5].

The μDMFC is a complex system, whose performance depends on a vast number of parameters, such as cell temperature, reactant concentrations and flow rates, cell temperature, MEA configuration, etc. The performance of fuel cell has been the subject of several research papers [6–8]. Wilberforce et al. [9] explored the effect of cell temperature, humidification and pressure on efficiency of fuel cell. The investigation concluded that the concentration loss and the activation losses increased as temperature increased. Nevertheless, at extremely high temperatures above 55 °C, the performance of the fuel cell began to deteriorate. Sudaroli and Kolar [10] reported that increasing the electrolyte membrane thickness and addition of a microporous layer using polytetrafluoroethylene (PTFE) loading can reduce methanol crossover to enhance the peak power density of fuel cell. Gwak et al. [11] analyzed the effects of anode/cathode stoichiometry, cell temperature and inlet humidification on the transient behavior of DMFCs. Among the DMFC operating parameters under investigation, the anode stoichiometry and cell temperature significantly influenced the DMFC performance.

In view of the complex physical phenomena inside DMFCs, which is difficult to experimentally quantify, a predictive model is essential to investigate the operation of a passive DMFC and explore the key parameters of cell performance. To date, a number of DMFC models have been reported [12–16]. Johan Ko et al. [17] developed a one-dimensional, two-phase model, without taking into account the effects of heat transfer, and validated their model with experimental data. Xue et al. [18] reported a three-dimensional, unsteady-state model coupled with mass transport and momentum transport. They paid attention on the cell cathode side. Yang and Zhao [19] developed a two-dimensional, isothermal two-phase mass transport model for a liquid-feed DMFC. They introduced a micro agglomerate model to describe the cathode catalyst layer.

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Wang et al. [20] also developed a two-dimensional, two-phase, non-isothermal model of a passive DMFC but took into consideration natural convection at the anode. Chippar et al. reported a one-dimensional, transient-thermal DMFC model [21]. Rice and Faghri [22] used a multi-fluid model to simulate the transport of the liquid and gas phases respectively for passive DMFCs which take the effect of continuous phase limitations into account.

In previous studies, only traditional investigations on the mass transport, the heat transfer effect and electrochemical kinetics were engaged briefly without the theoretical analysis and modeling on gravity effect. There is rare investigation to explore the gravity roles in the cell operating process and how it functions in the cell performance. In fact, the fuel delivery in passive μDMFCs is methanol diffusion in anode and oxygen natural convection in cathode. During the transfer process, the gravity effect in the fuel reservoir contributes to the distorted species distribution and the current density distribution. Therefore, mass transport without external driving force exhibits a complex distribution of the whole cell. Moreover, the gravity exhibits an important role in operating temperature and the output performance.

The most effective experimental method to investigate the gravity effects is to put the μDMFC in different operating orientations. Though some researchers have reported the effects of different cell orientations on DMFC performance [23–25], they only simply compared the performance parameters under different conditions by experiments, such as open circuit voltage, fuel efficiency and energy efficiency, without an in-depth exploration of how gravity effects internal mass transport and heat transport by numerical simulation. Based on this understanding, a novel two-dimensional, whole-cell model coupled with non-isothermal and gravity effects were established. In this model, the natural convection, the methanol solution transport, the current density as well as the thermal distribution were numerically defined. The gravity effect on the distributions of reactants and DMFC performance were presented. Then a μDMFC with the effective area of 1.0 cm^2 was fabricated to verify the previous simulation results. The laser-cut technology was applied to fabricate the single-serpentine patterned flow filed in the μDMFC. The cell performance under different operating positions was tested when the μDMFC fed with methanol concentrations of 2.0 M–4.0 M. Finally, effects of different orientations on reactants management as well as cell performance were experimentally examined to further investigate the gravity roles in DMFC operating process. The results of the model were compared to experimental results and shown a good agreement with them.

2. The model analysis

A 2D whole-cell model was established to investigate the temperature distribution inside the passive μDMFC. The calculation region is shown in Fig. 1. From left to right, the cell consists of fuel tank, current collector (ACC), flow channel (AC), diffusion layer (ADL) and catalyst layer (AC) at the anode side; catalyst layer (CC), diffusion layer (CDL), flow channel (CC), current collector (CCC) at the cathode side; and a polymer electrolyte membrane (MEA) in between.

In order to simplify the processes in a DMFC the following simplifications and assumptions are defined:

(1) The fuel cell operates at the steady state condition.
(2) The ACL and CCL are idealized as linear boundaries.
(3) The concentration of methanol in the anode fuel tank is assumed to be constant.
(4) The membrane is fully hydrated and is impermeable to gases.

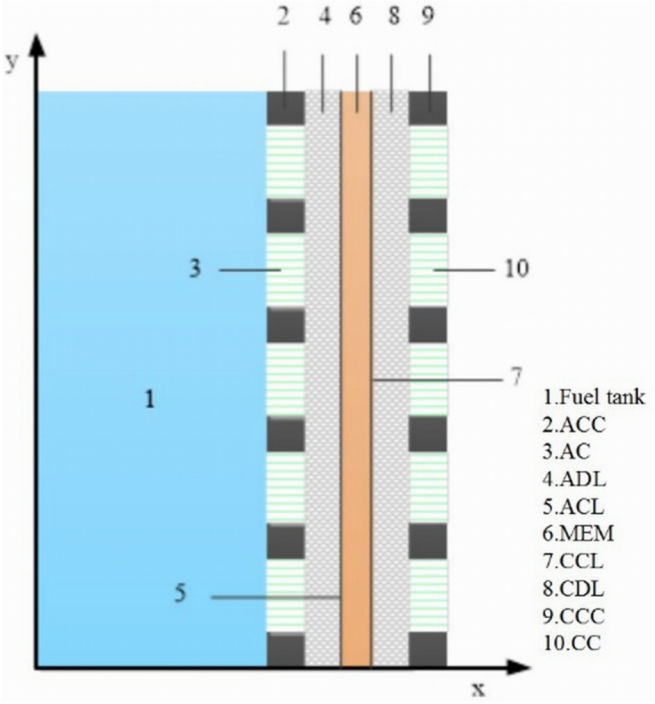

Fig. 1. Schematic of simulation domains.

2.1. Anode/cathode flow channel

The Navier-Stokes and continuity equations governing the steady motion of an incompressible fluid of constant density and viscosity, so the momentum of methanol can be written as:

$$\rho_l(\boldsymbol{u_l}\cdot\nabla)\boldsymbol{u_l} = -\nabla P_{ca} + \nabla\cdot\left[\mu_l\left(\nabla\boldsymbol{u_l} + (\nabla\boldsymbol{u_l})^T\right]\right] \quad (1)$$

$$\rho_l\nabla\cdot(\boldsymbol{u_l}) = 0 \quad (2)$$

where ρ_l is the density of methanol, $\boldsymbol{u_l}$ is the liquid phase velocity, P_{ca} is the liquid pressure in the anode flow field, μ_l represents the dynamic viscosity coefficient of the liquid, T represents the temperature of operation.

Due to the diffusion and convection effect, methanol transport into the anode diffusion layer through the fuel channel from anode fuel tank. The transport equation in the fuel channel is given as:

$$\nabla\cdot(-D_m\nabla c_m) + \boldsymbol{u_l}\cdot\nabla c_m = 0 \quad (3)$$

D_m denotes the diffusion coefficient of methanol, c_m is the concentration of methanol.

Similarly, the momentum and mass transport of oxygen in cathode flow channel can be described as:

$$\rho_g\left(\boldsymbol{u_g}\cdot\nabla\right)\boldsymbol{u_g} = -\nabla P_{cc} + \nabla\cdot\left[\mu_g\left(\nabla\boldsymbol{u_g} + \left(\nabla\boldsymbol{u_g}\right)^T\right)\right] \quad (4)$$

$$\rho_g\nabla\cdot\left(\boldsymbol{u_g}\right) = 0 \quad (5)$$

$$\nabla\cdot\left(-D_{O_2}\nabla c_{O_2}\right) + \boldsymbol{u_g}\cdot\nabla c_{O_2} = 0 \quad (6)$$

where ρ_g is the density of oxygen, $\boldsymbol{u_g}$ is the gas phase velocity, P_{cc} is gas pressure in the anode flow field, μ_g represents the dynamic viscosity coefficient of the gas, T represents the temperature of