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Simulation of mass transfer in a passive direct methanol fuel cell cathode with perforated current collector

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The current collector offers passages for mass transport and is one of the key components of the passive direct methanol fuel cell (DMFC). The effect of perforated current collector design on mass transport is studied based on a three-dimensional (3D), unsteady-state, two-phase mass transport model of a passive DMFC cathode. The model is implemented via the mixture multiphase model, which solves the continuity and momentum equations for the mixture and the volume fraction equation for the secondary phases. Numerical results indicate that the distributions of oxygen in both cathode catalyst layer (CCL) and cathode diffusion layer (CDL) are non-uniform because of the effect of the perforated current collector plate (CCP) structure. Liquid water produced by an electrochemical reaction in the CCL accumulates significantly at the bottom. Clearly, the distribution of liquid water in the cathode catalyst and diffusion layers is affected by gravity. The size of the circular holes and the distance between them are taken into account to investigate the effect of the CCP structure. Small uniformly arrayed circular holes in the entire active area of CCP are advantageous to the transfer of gas and liquid water in the cathode side of a passive DMFC.

1. Introduction

Direct methanol fuel cells (DMFCs) directly use methanol as fuel to convert chemical energy into electrical energy, which is considered a possible alternative power supply for modern portable electronic products [1,2]. It is well known that the performance of a passive DMFC (direct methanol fuel cell) is lower than that of an active DMFC. However, compared with active DMFCs, passive DMFCs do not involve the use of methanol peristaltic pumps and air fans. Thus, the power consumption of the fuel cells is reduced significantly and energy efficiency is improved. Many parameters have to be considered when optimizing a fuel cell [3]. The main parameters that affect the performance of DMFCs are temperature, species concentration such as methanol concentration, and channel geometry [2]. A certain species concentration is required to maintain high electrochemical reaction rate in the catalyst layer. Species concentration in the catalyst layer is influenced by the structure of a passive DMFC, especially by the current collector structure. The current collector is one of the key components of passive DMFCs; it not only collects electric current but also offers passages to reactants and production inside the cell [4]. Since the current collector offers passages for reactants, the types of channel e.g. circular or parallel may influence the mass transport. The ratio of the total area of channels to the whole active area is normally called open ratio, which has important effect on the structure of current collector and is important for reactant transport.

1.1. Experimental investigations on the current collector

The material and structure of the current collector have been investigated by many researchers. Takahiro [5] fabricated and tested two perforated current collectors; one was made of a stainless steel (SUS mesh) sheet, and the other was made of gold-plated SUS mesh (SUS/Au). They simply compared the performances of fuel cells with these two current collectors. Chen et al. [6,7] compared a porous current collector made of an Ni–Cr alloy metal foam plate with the conventional perforated-plate current collector made of a 316L stainless steel plate. The results showed that the former provides a higher oxygen transfer rate and a more effective water removal rate than the latter. Conventional current

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collectors usually have a perforated structure with circular and parallel flow channels. Yang [8] and Ye [9] discussed the effect of current collector structure on the performance of an air-breathing DMFC. The parallel current collector improved the removal and mass transfer of reactants at both the anode and cathode. However, a micro DMFC with a parallel flow-field at the anode and a perforated flow-field at the cathode performed better. Gholami [10] tested and compared the performance of a passive DMFC with two arrangements of current collectors. The two arrangements of current collectors had different flow fields with different open ratios to allow the authors to investigate the effect of current collector structure on performance. Zhang et al. [11] employed a shutter structure as the cathode current collector; the structure combines the benefits of flow fields and air-breathing holes. Compared with a conventional planar one, the shutter structure not only supplies a larger active area but also benefits fabrication during production. Esquivel et al. [12] also evaluated the influence of current collector open ratio on the performance of a passive DMFC by changing the distance between consecutive channels. The open ratio was found to affect the performance and stability of fuel cell. The authors demonstrated that the performance of cell with different anode and cathode open ratios was better than that with the same anode and cathode open ratio.

1.2. Numerical studies on the current collector

The aforementioned studies on the current collector were performed through experiments. They showed that the performance of passive DMFCs is influenced by the design of the structure of the current collector, which is dominated by the mass transport process. Considering that the investigation of mass transfer is experimentally intractable, numerical simulations should be applied to better understand the mass transfer inside passive DMFCs. Several models for passive DMFCs have been developed. However, the current collectors were disregarded in most of the one-dimensional (1D) and two-dimensional (2D) models because of the dimension limitation [13–24]. Several 2D models had a current collector with constant channel and rib widths [25–27]. Chen et al. [28] developed a 2D two-phase passive DMFC model and investigated the effects of the open ratio (fixing the sum of channel and rib widths at 2.0 mm) and channel and rib widths of the current collectors (maintaining the ratio of channel width to rib width at 1:1) on cell performance. The researchers found that the mass transfer rate in both the anode and cathode increases with the increase in open ratio and decrease in rib width. A 2D model has also been developed in Ref. [11] to further evaluate the mass transport in the cathode of air-breathing DMFCs.

A three-dimensional (3D) model provides more comprehensive view to study the effect of current collector structure on species distribution in the catalyst layer. Several 3D models have been developed for flow field research in DMFCs. Krewer et al. [29] investigated the hydrodynamic behavior of different anode flow field designs of liquid-fed DMFCs, including parallel channel, spot, and rhomboidal designs. They paid attention on the cell anode side. Hsieh et al. [30] developed a 3D mathematical model to investigate the flow and heat transfer in a micro DMFC with serpentine flow fields. Ghayor et al. [31] simulated the dropping pressure, velocity, and heat transfer of a cell with a cross strip and parallel flow field by 3D modeling in Fluent software. Their simulation was based on a steady flow, single-phase transport model. Wang et al. [32] presented the anodic flow velocity and temperature distributions based on four different designs, namely, double serpentine, parallel, helix, and single serpentine, with a 3D model. Zhang et al. designed a spoke cathode structure [33] and a perforated structure with parallel flow channels [34] for passive DMFCs by using a steady, 3D, two-phase model. The simulation results showed that the improved structure enhances cell performance and water removal because of the increase in oxygen mass transport. Hwang et al. [35] developed a single-phase, 3D, air-breathing cathode model with a unit cell of 1.5 mm × 1.5 mm in the active area. Circular holes current collectors were used in their model. The open ratio and radius of the hole were different for each current collector design. The thickness of the porous cathode and the electrolyte layer was similar. With this model, the effect of the air-breathing cathode current collector was investigated and optimized by maintaining the distance between holes at 1.5 mm. These 3D numerical simulation studies have been implemented with steady or single-phase model. Besides, several of these studies have paid attention to the DMFCs anode.

1.3. Present research

From the literature mentioned above, it can be seen that the current collector design influences the performance of DMFCs. It is necessary to investigate the current collector for better fuel cell design. Since the investigation of mass transfer in DMFC is experimentally intractable, numerical simulation approach seems to be a good method. No work has been done on the investigation of the effect of current collector design on mass transfer in a passive DMFC cathode with a 3D, transient, two-phase model. A 3D, transient, two-phase mixture model for a passive DMFC cathode was developed in our previous work [36]. Based on this model, the water and oxygen transport characteristics in a passive DMFC cathode with a traditional perforated current collector plate is analyzed in the current study. The effect of current collector design on mass transport is investigated with a constant open ratio. In the present work, the open ratio is defined as the ratio of the total area of holes to the whole active area. The results presented in this study can provide guidance to enhance mass transfer in the cathode of passive DMFCs, which further promotes the performance of fuel cells. Moreover, it is helpful to optimize the structure of passive DMFCs.

2. Model formulation

2.1. Computational domain and assumptions

The schematic of the modeling domain for a passive DMFC cathode is illustrated in Fig. 1. The domain is divided into the

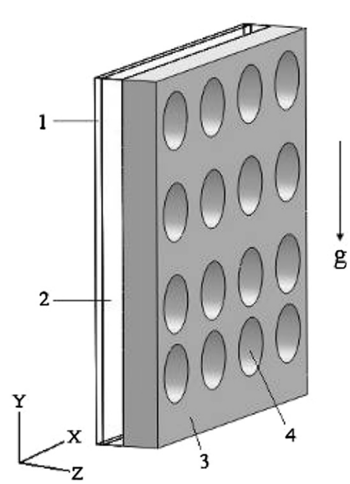

Fig. 1. Computational domain of a passive DMFC cathode system: 1-CCL, 2-CDL, 3-CCP, 4-flow channels.