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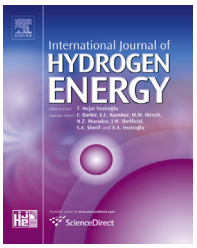

Numerical modeling and simulations of active direct methanol fuel cell (DMFC) systems under various ambient temperatures and operating conditions

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ABSTRACT

Direct methanol fuel cells (DMFCs) are potential candidates for portable backup power generation and auxiliary power units owing to their advantageous features, such as ease of fuel storage and delivery. Optimizing each component of a DMFC system is critical to improving the overall system performance and power density. This paper presents an active DMFC system model, in which a one-dimensional DMFC stack model is combined with major system components, including fuel and water tanks, liquid–gas separator, heat exchangers, pumps, and blowers. The model is implemented using a commercial flow-sheet simulator, ASPEN-HYSYS, and then applied to an active DMFC system to analyze the effects of the DMFC operating parameters and heat management. Special emphasis is placed on establishing active control strategies for the DMFC stack temperature, methanol crossover rate, and water recovery by optimizing the system components and operating conditions. Overall, this study helps identify innovative active DMFC system designs and configurations.

Introduction

The direct methanol fuel cell (DMFC) using a liquid methanol solution as fuel has several advantages in terms of fuel storage and delivery compared to hydrogen fuel cells. This makes DMFC technologies more suitable for small to medium scale power generation up to 1 kW. A passive fuel supply in a DMFC system is based on the direct use of a low concentration methanol feed fuel (<1–2 M) to mitigate methanol crossover. Although the passive design enables the construction of a simple system configuration, the passive DMFC system suffers from a low energy density. On the other hand, pure methanol is stored in an active DMFC system wherein the methanol feed concentration for a DMFC stack is diluted by the water produced during DMFC operation. Therefore, the active system design is more efficient in terms of fuel energy density in the system. The active DMFC system, however, tends to be more complicated and larger, having various additional components for fuel recirculation and phase separation. A high degree of system optimization is needed to achieve high system performance and efficiency.

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Over the past few decades, a number of DMFC models have been developed, focusing on theoretical analysis of the key phenomena in DMFCs. These include electrochemical processes [1], cell polarization [2,3], two-phase transport due to carbon dioxide evolution in the anode and water flooding in the cathode [4,5], methanol crossover and resulting mixed potential effect [6,7], and water and heat management in a DMFC [8–10]. Using these models, the effects of the component materials, cell designs, and operating conditions were elucidated further [11–18]. While considerable efforts have been concentrated on numerical studies at the individual component or full cell level, there are only a few reports related to DMFC system modeling and analysis. Zenith et al. [19] analyzed an active DMFC system in terms of the water recovery capability. Through the water balance of the entire system, they drew the operational range of a DMFC system for successful water recovery as a function of the cathode air flow rate, environmental humidity, and temperatures of the condenser and degasser. On the other hand, the system performance and requirements of the individual components for proper water recovery were not evaluated directly due to the simplicity of their model. None of these studies, however, analyzed an active DMFC system, considering the close interactions between a DMFC stack and the other key auxiliary components, such as liquid–gas separator and heat exchangers.

It should be emphasized that the strong coupling between a cell model and system model is necessary to faithfully analyze active DMFC system operating characteristics. For instance, the amount of methanol and water crossover through the membrane, i.e. predictable via DMFC simulations at the cell level could directly influence system level simulation results, including overall methanol/water/heat balance inside a system, the cooling load of heat exchangers, the amount of water recovery from the cathode to anode, BOP power consumption, etc. Despite the importance of the coupled DMFC modeling approach, to date, no attempt has been made to develop the coupled DMFC model and conduct a comprehensive study of DMFC system behaviors. In this paper, an active DMFC system model was developed, wherein various auxiliary components, such as the pump, blowers, heat exchangers, and gas–liquid separator as well as a DMFC stack were taken into consideration. A one-dimensional (1-D) DMFC model developed in a previous study [6] was coupled with a zero-dimensional (0-D) DMFC system model to simultaneously predict the electrochemical reactions and resulting species/heat transport inside a cell as well as overall system behaviors. Using the coupled DMFC model, numerical simulations were conducted and the DMFC system behavior was analyzed under a range of system operating and external conditions. This study clearly shows that the present DMFC system model is a useful tool for optimizing an active DMFC system configuration and operating conditions.

Numerical model

Model description and assumptions

As shown in Fig. 1, a typical active DMFC system consists of a DMFC stack and fuel recirculation module with several BOP (Balance of Plants) components and anode/cathode heat exchangers. To analyze an active DFMC system, a 1-D DMFC model and 0-D DMFC system model were combined. Fig. 2 describes schematically the 1-D DMFC model, wherein the key electrochemical reaction and transport mechanisms occurring in a DMFC cell are considered along the cell thickness direction. In a previous study [6], the 1-D model was validated successfully against the experimental voltage–current data and methanol crossover data measured experimentally under a range of cell designs and operating conditions. The key performance evaluation factors for a DMFC stack, such as the individual voltage losses and the rate of methanol crossover, etc. are obtainable from 1-D simulations. On the other hand, the 0-D DMFC system model accounts for the other DMFC system modules/components and is used to analyze the overall system behavior and determine the key system design or operating factors. The main assumptions invoked in the DMFC system model are as follows:

(1) The gas phase obeys the ideal gas law because all gases in a DMFC are maintained under low pressure and high temperatures compared to their respective critical pressures and temperatures.
(2) The temperature gradient along the cell thickness is neglected in the 1-D DMFC model due to a thin MEA configuration in a DMFC.
(3) An isotropic and homogeneous porous backing layer (BL) is assumed and characterized by the effective porosity and permeability.
(4) Complete consumption of the methanol crossed over from the anode to cathode is assumed.
(5) The anode and cathode outlet temperatures from a DMFC stack are assumed to be the same.

1-D DMFC model

As shown in Fig. 2, a 1-D DMFC model was applied to a 1-D computational domain of a DMFC comprising a backing layer (BL) and catalyst layer (CL) on both the anode and cathode sides and a membrane. Ko et al. [6] provided a detailed derivation of the conservation equations and source terms. Therefore, only a brief summary of these equations is presented here. First, two-phase methanol diffusion is described using the Maxwell–Stefan's multicomponent diffusion equation. The methanol diffusion equation in the anode and membrane regions is finally expressed as follows:

$$\frac{c^l_{meoh}\left(\frac{I}{6F}+N_{w,mem}\right)-c^l_{tot}D^l_{meoh,eff}\nabla c^l_{meoh}}{c^l_{tot}-c^l_{meoh}} + \frac{c^l_{meoh}\left(-\frac{I}{6F}\right)-c^g_{tot}D^g_{meoh,eff}\nabla c^g_{meoh}}{K_H c^g_{tot}-c^l_{meoh}} = \frac{I}{6F}+N_{meoh,mem} \quad (1)$$

In Eq. (1), $D^g_{meoh,eff}$ and $D^l_{meoh,eff}$ denote the effective diffusivity of methanol in the gas and liquid phases, respectively. Those were modified by Bruggeman factor, n, based on the porosity, ε, and the liquid saturation, s, as follows [25]:

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