



Analytical modeling of liquid saturation jump effect for hydrogen alkaline anion exchange membrane fuel cell



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ABSTRACT

Alkaline anion exchange membrane fuel cell (AEMFC) has been recognized as a promising zero-emission power source for portable, mobile and stationary application in recent years. To ensure high ionic conductivity and efficient reactants delivery, water management is regarded as one of the most critical issues for AEMFC. In this study, an analytical model is formulated to investigate the effect of electrode wettability on the water transport and resultant AEMFC performance. The pressure continuity method is considered to simulate liquid saturation jump on the interfaces of adjacent electrode layers. The results show that decreasing the cathode catalyst layer (CL) contact angle improves the performance because more water can be kept in the cathode CL decreasing polarization losses. The anode micro porous layer (MPL) is generally helpful, by forcing the liquid water to back-diffuse to the cathode. However, cathode MPL hinders the water transport to the cathode CL, leading to a lower reaction rate and membrane conductivity. The liquid water injection into the cathode has great potential to further improve the performance of AEMFC, however it may cause flooding in the flow channel and GDL. The cathode reaction kinetics should be considered as one of the most significant factors dragging the cell performance.

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1. Introduction

Along with the rapid development of the proton exchange membrane fuel cell (PEMFC) technology [1,2], alkaline anion exchange membrane fuel cell (AEMFC) has also attracted considerable attention over last few decades [3]. AEMFCs, which directly convert chemical energy of fuel and oxidant to electricity in the alkaline environment, have been regarded as clean and efficient power sources for various applications including power plants, zero/low emission vehicles [4], combined heat and power (CHP) systems [5] and aerospace power systems [6].

Although PEMFC exhibits remarkable thermal and mechanical stability, as well as high ionic conductivity, several prominent disadvantages have been presented which preclude its commercialization, including slow electrochemical kinetics, carbon monoxide poisoning of precious Pt-based catalysts, and the high cost of polymer membranes. Compared with PEMFC, AEMFC has several advantages, such as environmentally friendly alkaline chemistry with fast electrochemical reaction and potential uses of non-precious-metals-based catalysts which is critically important for the cost reduction and commercial development. Since the

development of the AEMFC is still in its early stage, the researches mainly focus on two aspects, preparation of high performance ionic membrane and non-precious electrode catalysts.

In recent years, several high performance alkaline membranes have been developed for AEMFCs. Li and Zhao measured the water uptake and transport properties of an alkaline membrane (A201 membrane from Tokuyama Corporation, Japan) [7]. The water uptake, ionic conductivity (hydroxide ions (OH⁻)) and swelling properties were also measured for the same membrane by Duan et al. [8]. The membranes developed by Tuan et al. [9] aminated with the trimethylamine (PAEK-TMA), triethylamine (PAEK-TEA), tripropylamine (PAEK-TPA) has ionic conductivities up to 0.014, 0.003, and 0.0008 S cm⁻¹ at 40 °C and 0.021, 0.006, and 0.0014 S cm⁻¹ at 80 °C, respectively. Lin et al. [10] synthesized an imidazolium-based cross-linked AEM that has ionic conductivity up to 0.02 S cm⁻¹ with long-term chemical stability in 1 M KOH solution. The studies for alkaline membrane greatly facilitate the rising of the AEMFC.

On the other hand, a wider variety of catalysts utilizing non-precious metals and metal-free materials have been developed and demonstrated in the alkaline environment. Krusenberget al. developed a catalyst using Co and Fe phthalocyanine and reported that the performance was slightly inferior to the commercial Pt/C catalysts [11]. Li et al. carried out cell performance tests

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using non-precious catalysts synthesized from precursors of carbon, nitrogen, and transition metals. They reported a maximum power density of 177 mW cm^{-2} at 50°C [12]. Other catalysts, such as carbon-supported non-platinum materials, were also developed for hydrogen and methanol AEMFCs exhibiting excellent performances [13,14].

Similar to PEMFC, water management is also an important issue which is definitely worth exploring [15,16]. However, in the most of the previous researches in the literature, the water management, which actually plays a pivotal role in maintaining and promoting AEMFC performance, has been generally ignored. So far, only a small number of numerical modeling and experimental works have been conducted to investigate the characteristics of water transport in AEMFC [17–26]. It should be noticed that the heat and mass transfer characteristics, such as the liquid water saturation jump effect at the interfaces of the cell components, still need further investigation. Therefore, this study can be viewed as an important supplement to the literature, which mainly focuses on the development of a complete analytical model for AEMFC with consideration of the saturation jump effect. Fig. 1a illustrates the operation of a hydrogen AEMFC with micro-porous layer (MPL). Water is produced in the anode catalyst layer (CL) and consumed in the cathode CL. Water should be removed from the anode while humidification is necessary for the cathode. It should be noticed that liquid saturation jump on the interfaces of different layers (CL/MPL, MPL/GDL) should be taken into consideration due to the different porosity, permeability and wettability on the neighboring layers. To optimize the water transport between anode and cathode, the MPL has been widely used in PEMFCs, and approved to be an effective way to improve the performance [27–31], by affecting mass transport and water removal. Liquid water breakthrough was observed in the MPL of a PEMFC using synchrotron X-ray radiography [27]. The electrical and thermal conductivity of MPL was calculated through a phase-differentiated model [28]. Two main functions of MPL in PEMFC, reducing the water droplet size and blocking the liquid water breakthrough toward GDL, were discussed [29]. Chen et al. also pointed out that MPL could prevent water flooding at low operating temperature and high inlet humidification, and also enhance the membrane thermal and electrical performance under dry condition [30]. Tabe et al. also proposed that MPL could help mitigate the water flooding problem under normal operation, and even improve the cold start performance [31]. The similar mechanisms can be applied to AEMFCs however the effect of MPL and electrode wettability has been generally ignored in previous studies. In addition, most of the previous modeling studies assumed continuous liquid concentration at the interfaces between the neighboring layers and the liquid concentration jump caused by the different physical properties of both sides are neglected.

In this work, an analytical model has been developed for a hydrogen AEMFC to investigate the effect of the MPL and the electrode wettability on water transport. The liquid saturation jump is all considered using pressure continuous method. Experimental testing was also carried out for results comparison. The model formulation and experimental conditions are described in the following sections.

2. Model formulation

As shown in Fig. 1, humidified hydrogen (H_2) and air are supplied for the AEMFC operation. Water back diffusion, electro-osmotic drag and water production all occur during operation, which is similar to PEMFC. However, the direction of electro-osmotic drag of AEMFC is opposite to PEMFC; the water production is in anode for AEMFC but cathode for PEMFC; and water is even

consumed in AEMFC cathode. These differences may also result in different water back diffusion directions. The oxygen (O_2) and water is consumed in the cathode generating OH^- , and OH^- move through the ionomer membrane to the anode where the H_2 reacts with OH^- to generate water and electrons (e^-). The e^- transfers through the external circuit to the cathode. Specifically, water is produced at the anode and consumed at the cathode. The electro-osmosis drag effect moves water from the cathode to the anode, and due to the concentration gradient, water can also diffuse back from the anode to the cathode through the membrane.

In this model, the cell output voltage is calculated from reversible voltage, activation overpotentials of anode and cathode, and ohmic overpotentials of the cell components. Reactants are assumed to be ideal gases and their transports are analyzed to calculate the overpotentials. The modeling parameters are listed in Table 1. The mass balance equations of liquid water and gas species are listed in Tables 2 and 3, respectively.

2.1. Modeling assumptions

- (1) Due to the low Reynolds number, the flow is assumed to be laminar and in steady state.
- (2) The gases follow the ideal gas law.
- (3) The model is assumed to be isothermal due to the small cell size and low reaction rate (low current density).
- (4) To simplify the calculation in water phase change, it is assumed that if the local water vapor is saturated, the product water is in liquid form, and otherwise, it is in vapor form.
- (5) The gas pressure is assumed to be 1 atm and evenly distributed in the fuel cell.
- (6) The membrane is assumed to be impermeable to the gas phase.

2.2. Output voltage

The cell output voltage, E_{out} (V), is calculated as

$$E_{out} = E_{rev} - \eta_{ohm} - \eta_{act} \quad (1)$$

where E_{rev} (V) is the reversible cell potential, η_{ohm} (V) is the ohmic overpotential, and η_{act} (V) is the activation overpotential. Based on the Nernst equation [32], the reversible cell potential can be expressed as

$$E_{rev} = 1.229 - 0.846 \times 10^{-3}(T - T_{ref}) + \frac{RT}{2F} \left(\ln p_{\text{H}_2, \text{ano}} + \frac{1}{2} \ln p_{\text{O}_2, \text{cat}} \right) \quad (2)$$

where T is the operating temperature (K), T_{ref} is the reference temperature (298.15 K). F is the Faraday's constant ($96,487 \text{ C mol}^{-1}$), R is the universal gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$), and $p_{\text{H}_2, \text{ano}}$ and $p_{\text{O}_2, \text{cat}}$ (atm) are the partial pressures of the H_2 and O_2 at the inlets. Note that this equation is for water production in liquid form, and the partial pressures are divided by a standard pressure of 1 atm.

2.3. Ohmic overpotential

Ohmic resistances are taken into consideration in the membrane, porous media, and flow field plate. The ohmic overpotential, η_{ohm} (V), is expressed as follows:

$$\eta_{ohm} = \eta_{ohm, p} + \eta_{ohm, por} + \eta_{ohm, m} = (R_{e^- - p} + R_{e^- - por} + R_{\text{OH}^- - por} + R_{\text{OH}^- - m}) \times I \quad (3)$$

where I (A m^{-2}) is the current density. $\eta_{ohm, p}$, $\eta_{ohm, por}$ and $\eta_{ohm, m}$ (V) denote the ohmic overpotential of the bipolar plate, porous media

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