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Electrochemical performance modeling of a proton exchange membrane electrolyzer cell for hydrogen energy

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ABSTRACT

This paper presents a comprehensive computational model for the proton exchange membrane (PEM) electrolyzer cells, which have attracted more attention for renewable energy storage and hydrogen production. A new ohmic loss model of a PEM electrolyzer cell has been developed and the influence of different operating conditions and physical design parameters on its performance has been investigated, including operating temperature, pressure, exchange current density, electrode thickness, membrane thickness and interfacial resistance. The interfacial resistance between the membrane and electrode has been found to play an important part for electrolyzer performance and an overpotential is increased significantly with the interfacial resistance. At a current density of 1.5 A/cm², the performance loss due to the interfacial resistance between the membrane and electrode comprises 31.8% of the total ohmic loss. Thickness changes in either electrode or membrane also have significant impacts on the electrolyzer performance mainly due to their contributions to the diffusion overpotential and ohmic loss. Increasing the operating temperature will result in lower electrolyzer overpotential, while increasing the operating pressure will lead to higher electrolyzer overpotential, which is mainly controlled by the open circuit voltage. Results obtained from the present model will provide a comprehensive understanding of design parameter effects and consequently improve the design/performance in a PEM electrolyzer cell.

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Introduction

An electrolyzer cell taking advantage of a proton exchange membrane (PEM) has attracted more attention for renewable energy storage and pure hydrogen/oxygen production due to their higher energy efficiency/density, faster charging/

discharging, and a more compact design [1,2]. Compared with conventional hydrogen production processes including fossil fuel reforming and alkaline water electrolysis, PEM electrolyzer cells offer a more environmentally friendly approach as well as high hydrogen purity. PEM fuel cells are well known as clean and sustainable energy devices. PEM electrolyzer cells have similar working components to a PEM fuel cell, but

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operate in the reverse direction. There is an abundance of papers detailing PEM fuel cell modeling [3–7] and direct methanol fuel cell modeling [8,9], which will be useful for PEM electrolyzer cell issues. Many physical parameters, including the operating conditions, electrode and membrane characteristics, significantly affect PEM electrolyzer cell system performance and durability. In order to optimize and design a PEM electrolyzer cell system properly, a full performance analysis and modeling of PEM electrolyzer cells is necessary.

In the past years, some experimental studies [10–16] have been conducted to investigate PEM electrolyzer cell performance under different conditions, but there are only a few papers regarding PEM electrolyzer cell modeling.

Choi et al. [17] introduced a simple mathematical model of solid polymer electrolyte water electrolysis. In the model, the cell voltage was calculated by the sum of open circuit voltage, electrode overpotential, ohmic overpotential due to the membrane and interfacial resistances. Gorgun [18] introduced the first dynamic model of PEM electrolyzer cells. This model included water transport phenomenon through the membrane due to electro-osmotic drag and diffusion.

Lebbal et al. [19] conducted a dynamical model including a steady state electrical model and a dynamic thermal model to monitor the PEM electrolysis safety and efficiency. In the model, the total relationship of voltage and current density was expressed as four parts: open circuit voltage, activation overpotential, diffusion overpotential and ohmic overpotential. The diffusion overpotential was related to the values of current due to the effects of gas and water transport and the ohmic loss was given by an empirical relation.

Grigoriev et al. [20,21] developed mathematical models in order to evaluate the electrochemical performance of atmosphere and high pressure (up to 130 bars) PEM electrolyzer cells. To evaluate and optimize electrolyzer efficiency and performance, different operating conditions including pressure, temperature, current density, membrane thickness are discussed.

Marangio et al. [22] also conducted a detailed theoretical model to analyze characteristics of a high pressure PEM electrolyzer cell. In their model, the Gibbs free energy was used to calculate the open circuit voltage under non-standard temperature and pressure conditions. Water flow inside the electrolyzer cell included several parts: water inlet and outlet flow in the anode and cathode, water transport due to concentration difference, water transport due to the electro-osmotic drag, water transport due to pressure difference across the membrane, and water consumed by the electrochemical reaction. The ohmic resistance was calculated by the sum of electrodes, plates, and membrane resistance. A series of modeling polarization curves of PEM electrolyzer cells was obtained and then compared with the experimental results.

Based on the above reviews, since existing models did not fully consider the effects of various operating conditions and design parameters on the cell performance, a comprehensive model for better correlating the effects of both design parameters and operating conditions with PEM electrolyzer cell performance is strongly desired. In this paper, the authors focus on a full mathematical model and electrochemical performance analysis of PEM electrolyzer cells. A new model

with different electrode materials and interface equivalent resistance has been developed. Different operating conditions and physical parameters effects, including operating temperature and pressure, exchange current density, electrode thickness, membrane thickness and interfacial resistance, which may affect and even reduce the electrolysis cell performance, have been investigated. These numerical results help obtain a deeper understanding of PEM electrolyzer cells and improve cell performance.

Mathematical models

A geometric schematic of PEM electrolyzer cells used for the modeling calculations is shown in Fig. 1. Water enters through the flow channel at the anode and then diffuses across the porous gas diffusion layer (GDL). In the catalyst layer (CL) reaction site, water is dissociated into electrons, protons, and oxygen. The protons migrate through PEM and combine with electrons to generate hydrogen at the cathode. In this process, different operating conditions and physical parameters may significantly influence the cell performance.

The performance of PEM electrolyzer cells can be expressed by the voltage and current density relationship. The present model assumes that: (a) the CL is infinitely thin and the electrochemical reaction only occurs at the interface of GDL and PEM; (b) gases transferred inside the electrode and channel are ideal gases; (c) the porous electrode means GDL and CL together and its physical parameters refer to those of GDL. The potential of a single PEM electrolyzer cell is composed by the open circuit voltage, activation overpotential, diffusion overpotential, and ohmic loss overpotential. The total relationship is:

$$V = V_{ocv} + V_{act} + V_{diff} + V_{ohm} \quad (1)$$

where V_{ocv} is the open circuit voltage as well as the theoretical minimum voltage for PEM electrolyzer cells when neglecting other overpotentials, V_{act} is the overpotential due to the electrochemical reaction, V_{diff} is the diffusion overpotential caused by the mass transport in the electrolyzers, and V_{ohm} is the ohmic overpotential caused by the electrolyzer cell resistances. Each of these overpotential models will be determined in the following sections.

Open circuit voltage

The open circuit voltage (OCV) is also called reversible voltage. For PEM electrolyzer cells, OCV can be calculated from the Nernst equation [23].

$$V_{ocv} = V_0 + \frac{RT}{zF} \ln \left(\frac{\alpha_{H_2} \alpha_{O_2}^{0.5}}{\alpha_{H_2O}} \right) \quad (2)$$

Here V_0 is the reversible voltage with standard pressure, which can be calculated by the following relation [23].

$$V_0 = 1.229 - 0.9 \times 10^{-3}(T - 298.0) \quad (3)$$

R is the gas constant, T is the electrolyzer operating temperature, z is the mole number of electrons transferred during the electrolysis reaction, F is the Faraday constant, α_i is the

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