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Mathematical modeling of an anion-exchange membrane water electrolyzer for hydrogen production

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ABSTRACT

A mathematical model that considers coupled mass transport, charge transport, and electrochemical reactions in an anion-exchange membrane (AEM) water electrolyzer is developed. Validations against the literature experimental data show that the present model can accurately predict the performance of the water electrolyzer. Numerical results show that the voltage loss in the electrolyzer is majorly due to the activation polarizations of hydrogen and oxygen evolution reactions. The effects of the exchange current density, the membrane thickness, and the liquid saturation on the performance are also studied; it is shown that the performance of the water electrolyzer improves with an increase in the exchange current density and liquid saturation, but with a decrease in the membrane thickness.

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Introduction

Alkaline water electrolyzers that use the liquid electrolyte (typically 10 M KOH) are a promising water electrolysis technology for hydrogen production, primarily because both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in alkaline media do not require precious metals as electro-catalysts [1,2]. However, an issue with conventional alkaline water electrolyzers is that the alkaline liquid electrolyte reacts with carbon dioxide from the air to produce carbonate, which can easily precipitate in the porous

electrodes, physically blocking the access of water to the active sites and of gaseous hydrogen and oxygen from the active sites and thus negatively affecting the water electrolyzer performance and durability [3]. Another issue with conventional alkaline water electrolyzers is associated with the use of diaphragms (porous separators) in the system, which are typically permeable to hydrogen and oxygen gases and lead to hydrogen and oxygen crossover problems [4]. Oxygen permitted from the anode to the cathode will be catalyzed back to water, reducing the efficiency of the hydrogen production. In the meantime, hydrogen crossover can cause even more serious safety problem. In addition, the

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use of the concentrated liquid electrolyte and thick diaphragms in conventional alkaline liquid electrolyte water electrolyzers may cause a high ohmic loss, reducing the maximum current density, i.e.: maximum hydrogen production rate [4].

Recently, the use of the solid-state anion-exchange membrane (AEM) in the alkaline water electrolyzers, which has been extensively used in fuel cells [5–10], has received ever-increasing attention, primarily because of its several unique characteristics as opposed to conventional liquid electrolytes [3]: i) the use of the AEM avoids the carbonate precipitation problem due to the absence of metal cations; ii) the gas permeability of the AEM is much smaller than that of the diaphragm, alleviating the gas crossover; and iii) the AEM thickness is much thinner than the diaphragm, thereby lowering the ohmic loss and making the system more compact. For these reasons, efforts have been recently devoted to the development of the AEM water electrolysis [3,11–15]. Xiao et al. [15] proposed an alkaline water electrolyzer by using an AEM and non-precious metal catalysts, and working only with pure water. Their preliminary results showed that the developed AEM water electrolyzer yielded comparable performance with the conventional alkaline water electrolyzer. Leng et al. [3] developed a high-performance, durable alkaline membrane water electrolyzer by using an AEM. The experimental results demonstrated that the developed AEM water electrolyzer had a lifetime around 535 h.

As a series of physicochemical processes simultaneously take place in an AEM water electrolyzer, including mass transport, charge transport, and electrochemical reactions, it is difficult to shed light on the physicochemical processes through experimental investigations. On the other hand, the mathematical modeling, as a powerful and economical tool, may play an important role in quantifying the complicated physicochemical processes. To our best knowledge, there is no attempt to mathematically investigate the AEM water electrolyzer. In this work, we develop a mathematical model for the AEM water electrolyzer by considering the complicated physicochemical processes, including mass/charge transport and electrochemical reactions. With this model, the voltage loss is specified and the effects of the exchange current density, the membrane thickness, and the liquid saturation, on the performance are also studied.

Formulation

Consider an AEM water electrolyzer, as shown in Fig. 1, which consists of an anode flow field (FF), an anode diffusion layer (DL), an anode catalyst layer (CL), an AEM, a cathode CL, a cathode DL and a cathode FF. On the anode, the hydroxide ions migrated from the cathode will be oxidized to release electrons, water, and oxygen:



The generated water and oxygen are removed by the anode flow stream, while the produced electrons pass through an external electrical load to the cathode for the HER. On the

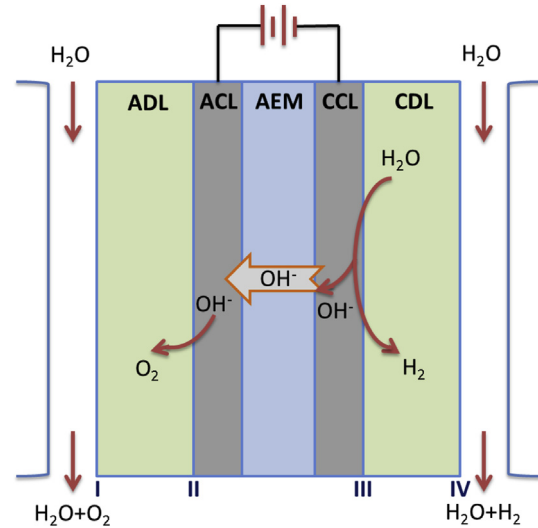


Fig. 1 – Schematic of an anion-exchange membrane water electrolyzer.

cathode, the water is transported through the cathode DL to the cathode CL, where water combines with electrons from the anode to form hydrogen and hydroxide ions according to:



Subsequently, the generated hydroxide ions are conducted through the membrane to the anode for the OER. Therefore, combining Eqs. (1) and (2) results in an overall reaction for an AEM water electrolyzer:



It is clear from the above description that operating the AEM water electrolyzer involves rather complex two-phase transport processes coupled with electrochemical reactions, including the OER on the anode and the HER on the cathode. To make the complicated process tractable, we develop a one-dimensional model (x axis: through-plane direction) with the following simplifications and assumptions:

- (1) The AEM water electrolyzer is assumed to operate under steady-state and isothermal conditions.
- (2) Each CL is treated as an interface since it is much thinner than the DL and AEM.

Mass transport in the DL

Based on unsaturated flow theory in porous media, the liquid pressure in the DL is assumed to be constant [16]. The produced gas transfers back to the FF by the capillary force. The two-phase mass transport in the DL can be modeled by Ref. [16]:

$$\vec{\nabla} \cdot \left(\frac{\rho_g}{M_g} u_g \right) = 0 \quad (4)$$

where ρ_g and M_g present the density and molar weight of gas, respectively. In Eq. (4), u_g is the superficial velocity vector, which can be obtained from Darcy's law [17]:

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