Journal of the Taiwan Institute of Chemical Engineers xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Journal of the Taiwan Institute of Chemical Engineers

journal homepage: www.elsevier.com/locate/jtice

Proton exchange membrane fuel cell modeling with diffusion layer-based and sands-based capillary pressure correlations: Comparative study

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ARTICLE INFO

Article history:
Received 12 October 2013
Received in revised form 16 March 2014
Accepted 18 March 2014
Available online xxx

Keywords:
Proton exchange membrane fuel cell
Capillary pressure
Gas diffusion layer
Liquid water saturation
Cell performance

ABSTRACT

Although the Leverett–Udell correlation has been proven inaccurately to describe the capillary pressure-saturation (p_c-s) characteristics of a gas diffusion layer (GDL), this correlation is still extensively applied in the modeling of proton exchange membrane (PEM) fuel cells. The question of how much error is introduced into the determination of the cell current-voltage performance by using Leverett–Udell correlation has not been answered satisfactorily. This study numerically evaluates cell performance using a three-dimensional, two-phase, and non-isothermal fuel cell model, which incorporates the Leverett–Udell correlation and the experimentally measured p_c-s correlation. The performances predicted by the two models were compared for various model parameters – GDL porosity (0.6 and 0.9), GDL tortuosity (1.5 and 2.5), and coefficient of water vapor condensation rate (500 s^{-1} and 5000 s^{-1}). Numerical results indicate that introducing the cosine of the contact angle into the Leverett–Udell correlation inaccurately represents the effect of wettability on the capillary pressure. The Leverett–Udell correlation with a contact angle far larger than the actual contact angle can nevertheless yield a cell performance that is close to that obtained from the experimentally measured p_c-s correlation. Quantitative modeling using the Leverett–Udell correlation is not recommended. However, qualitatively, the comprehensive PEM fuel cell model with the Leverett–Udell correlation can be used for preliminary screening in cell design and performance estimation.

1. Introduction

Proton exchange membrane (PEM) fuel cells convert hydrogen and oxygen into electricity, generating heat and water as byproducts [1–10]. Gas diffusion layers (GDL) are formed from engineered porous material and are critical in water management, and the transport of reactants and electrons. In the pores of GDL, the flow is a capillary dominated two-phase flow behaving like a fingering flow. When liquid water cannot be effectively removed from the GDL, the pores of the GDL become blocked, causing poor reactant transport to the catalyst layer (CL), and therefore poor cell performance [11,12]. Early experimental researches with visualization method [13] and morphology analysis [14] have been carried out to reveal the mechanism of flow behavior in GDL, where simple 1D model has been developed. In the last decade, many two-phase models have been developed to examine water transport and its effect on the performance [12,15–48]. An accurate description of the two-phase transport properties in the GDL is critical to the two-phase modeling of a PEM fuel cell.

The capillary force and the viscous drag of the reactant shear flow govern the liquid water transport process in the GDL. Wang et al. [15,16] developed a capillary pressure-liquid water saturation (p_c-s) correlation to model the two-phase flow in the GDL. The capillary pressure is defined as the difference between the pressures of the gaseous mixture and the liquid water, or $p_c = p_g - p_l$. Since accurate experimentally determined p_c-s correlations for the GDL were lacking, Wang et al. utilized a p_c-s correlation that was proposed by Leverett [49] and Udell [50], based on experimental data obtained

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http://dx.doi.org/10.1016/j.jtice.2014.03.011
1876-1070/

using sand packs, called the Leverett–Udell correlation, in their modeling work. The pore sizes, pore structures and wettabilities of sand packs differ greatly from those of real carbon cloth (or carbon paper) GDLs, and the Leverett–Udell correlation may not be universally applicable to various GDLs of PEM fuel cells. Efforts have been made to measure experimentally p_c-s data for various GDLs that are commonly used in PEM fuel cells [51–68]. The results thus obtained have verified that no universal correlation such as the Leverett–Udell correlation exists for all GDLs, since the p_c-s correlation depends not only on the material of the GDL but also on the capillary pressure hysteresis of water on the GDL.

Although Leverett–Udell correlation has been demonstrated inaccurately to describe the capillary pressure-saturation (p_c-s) characteristics of the GDL, the correlation is still extensively utilized in modeling proton exchange membrane (PEM) fuel cells [12,15–48]. The question of how much error is introduced into the determined liquid water distribution and resulting cell current–voltage performance by using of Leverett–Udell correlation should be answered. Recently, some efforts [69,70] have been made to answer it. Mench et al. [69] were the first to study the applicability of the Leverett function to the prediction of one-dimensional capillary flow in a fuel cell GDL. They derived a p_c-s correlation from the experimental data that were presented by Gostick et al. [55]. They integrated this empirically derived into a one-dimensional analytic model to compare the liquid water saturation profiles in the GDL that were predicted by the Leverett–Udell correlation and the empirically derived correlation. Their results showed that use of the Leverett–Udell correlation can produce significant errors concerning liquid water saturation, so an extension of Leverett–Udell correlation to a fuel cell GDL with mixed wettability was required for reliable model predictions. Subsequently, Ye and Nguyen [70] studied the distribution of liquid water in the GDL and its effect on oxygen transport by incorporating an experimentally measured p_c-s correlation into a three-dimensional full-cell model. In their work, the GDL was made of Toray TGP-H-060 carbon paper and the measured water withdrawal p_c-s data were fitted using $p_c = (e^{-a_1(s-c)} - e^{a_2(s-c)})d + b$, where a_1, a_2, b, c and d are fitting parameters. Ye and Nguyen showed that the three-dimensional two-phase model with the experimentally determined p_c-s correlation reasonably described the distribution of liquid water without any artificially imposed boundary conditions at the cathode GDL–channel interface. However, they did not compare the predictions made using the model with the p_c-s correlation with those made using the model with the Leverett–Udell correlation. Lately, Wood et al. [71] presented a fundamental investigation of the surface phenomena of liquid water wettability of PEMFC porous media. Single-fiber contact angle and surface energy data of a wide range of GDL types were analyzed. As a result, advancement to the Young-Laplace capillary pressure equation was proposed for the porous media in PEMFC, where combined effects of capillary pressure, pore structure and surface heterogeneity in GDL and MPL composite structures were taken into account.

Following the pioneering work of Mench et al. [51–54,69], this work develops a three-dimensional, two-phase PEM fuel cell model by refining similar models in the literature [30,31,36–38,42] and numerically evaluates the model using the experimentally measured p_c-s correlation from the work of [66] and the Leverett–Udell correlation. The goal is to answer the question, "Can the Leverett–Udell capillary pressure correlation describe two-phase transport properties and predict the performance of a proton exchange membrane fuel cell?"

2. Model development

2.1. Model geometry

The parallel flow field design was utilized to study the effects of the p_c-s correlation on the transport of liquid water in, and the

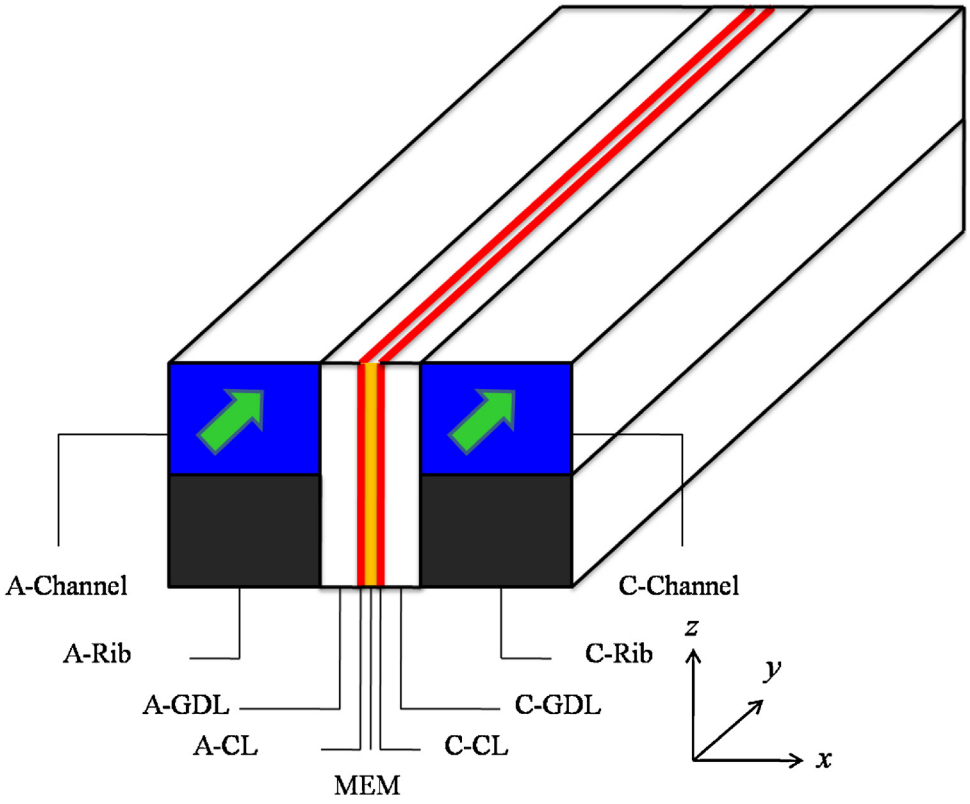

Fig. 1. Schematic of symmetric unit of PEMFC with parallel flow field design, where GDL is short for gas diffusion layer, CL is short for catalyst layer, MEM is short for membrane, "A" represents in the anode side, "C" represents in the cathode side.

Please cite this article in press as: Wang X-D, et al. Proton exchange membrane fuel cell modeling with diffusion layer-based and sands-based capillary pressure correlations: Comparative study. J Taiwan Inst Chem Eng (2014), http://dx.doi.org/10.1016/j.jtice.2014.03.011