A computational study to investigate the effects of the bipolar plate and gas diffusion layer interface in polymer electrolyte fuel cells

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ABSTRACT

In this study, a multi-phase, two-dimensional model that integrates the bipolar plate (BP) and gas diffusion layer (GDL) interfacial morphology was developed to understand the effects of this interface on mass, charge and heat transport and performance of polymer electrolyte fuel cells (PEFCs). Two different case studies were performed. The first case assumes a perfect contact interface between the BP and GDL, whereas in the second case, the BP|GDL interfacial layer was incorporated as a separate domain based on the measured BP|GDL morphology. In the BP|GDL interface case, the interfacial voids were assumed to be filled with liquid water to investigate the role of the interfacial voids. For both cases, the effects of different current densities on the in-plane temperature, saturation, and oxygen concentration distribution in the GDL were investigated. Simulations indicate that the Ohmic and concentration losses are increased due to the inclusion of the realistic BP|GDL interface. The electrical contact resistance contribution of the BP|GDL interface was predicted to be 3.8 mΩcm^2. The saturation in the GDL was found to be higher for the BP|GDL interface case, which results in higher concentration losses. The temperature was predicted to be slightly higher for the BP|GDL interface case, which could be attributed to the higher thermal contact resistance due to the fewer contact regions at the interface.

Introduction

Polymer electrolyte fuel cells (PEFCs) are of great importance as a clean alternative to conventional heat engines. However, PEFCs still need to be further improved for utilization in stationary and transport applications [1]. Two important limitations to PEFC performance and durability are water and thermal management [1–3]. Hydration is vital for proton transport through the membrane, whereas excess water may cause flooding in the catalyst layer (CL) and hinder mass transport [4]. Electrochemical reactivity and water transport are strongly dependent on the temperature distribution [5]. In addition, the temperature distribution has a profound impact on liquid water transport in PEFC components [6]. Improper temperature distribution may lead to hot spots in PEFCs which

may cause degradation of the cell components and decrease the cell lifetime.

Recent studies have shown that the interfaces between the PEFC components have a significant effect on water and thermal management [7–19]. Among the interfaces, the bipolar plate (BP) and gas diffusion layer (GDL) interface is critical because this interface plays a key role in the contact resistance for electron and heat transport. There have been several experimental studies to determine the electrical contact resistance at the BP|GDL interface [20–26] for different compression pressures and for different materials [27,28]. To date, majority of the PEFC modeling studies considers the BP|GDL interface as an infinitely thin layer that has certain bulk properties, or simply as a boundary condition. In particular, some studies include this interface into their models by introducing an electrical contact resistance as a boundary condition [23,29–31] to account for this interface and related effects on PEFC performance. While this approach provides a useful starting point to account for this critical interface, these models unfortunately cannot sufficiently explain the effects of the morphological features of the BP and GDL surfaces on water/heat management and PEFC performance.

The water distribution and removal in the cell are closely linked to the thermal management of PEFCs. In that regard, the BP plays an important role since it serves as a heat removal component in the cell, and therefore more condensation of water is expected to occur in the parts of GDL located under the BPs due to the cooling effects. Turhan et al. [32]. showed in their neutron imaging study that more water accumulates under the BPs than under the channel for the same BP-channel width, suggesting that the BP|GDL interface could affect the water distribution in the GDL due to high heat removal rate through this interface, therefore careful consideration of thermal contact resistance of this interface is needed to better understand the water distribution inside the cell.

The thermal contact resistance at the BP|GDL interface depends on the thermal conductivities of the neighboring domains, contact pressure, surface roughness and asperities [33]. There have been several studies to determine the thermal conductivity of the GDL and the thermal contact resistance of the BP|GDL interface [33–36]. In these studies, the thermal contact resistance is mostly incorporated into the thermal conductivity of the GDL. However, Sadeghi et al. [37]. has shown that the thermal contact resistance could contribute up to 90% of the total GDL thermal resistance, suggesting that the thermal contact resistance at the BP|GDL interface and effective thermal conductivity of the GDL should be evaluated separately. Furthermore, these studies have measured the thermal contact resistance ex-situ under different compression pressures; however the effects of partially or fully filled interfacial voids at the BP|GDL interface have not been considered in the calculations of the thermal contact resistance of this critical interface.

In addition to the electric and thermal contact resistance, this interface can also act as a pooling location for liquid water due to the existence of large interfacial voids resulting from imperfect contact of the BPs with the GDL surface. This water pooling can affect the water distribution in the GDL and may cause significant mass transport losses. There have been several neutron imaging and X-ray radiography studies [32,38–40], which suggest that the BP|GDL interface can store considerable amount of water. In a recent study, Swamy et al. [9] estimated that 5–16% of the total water can be stored at the BP|GDL interface, which is significant considering the overall water balance in a PEFC.

Here, the objective of this study is to investigate the effects of BP|GDL interface on the mass/charge/heat transport and the performance of PEFCs. Previously, we developed a two-dimensional, multi-phase, non-isothermal model to investigate the effects of the microporous layer (MPL)|CL interface which governs the mass and Ohmic losses on the PEFC performance [15]. In this study, with a similar approach in our previous model, we developed a rib-channel configuration model including the BP|GDL interface as a separate domain (while assuming perfect contact at MPL|CL interface) to investigate the role of this interface on the system performance. Two case studies were conducted to study the effects of the BP|GDL interfacial morphology. In the first case study, the interface between BP and GDL was assumed to be in a perfect contact. In the second one, the measured BP|GDL interfacial morphology (measured by Swamy et al. [9]) was incorporated into the model as a separate domain, where the interfacial voids were simulated as filled with liquid water. Several simulations have been performed for both cases and compared to each other to investigate the role of BP|GDL interface morphology on the water, current, reactant and temperature distribution in a PEFC.

Method of approach

Model development

In this study, a two-dimensional, multi-phase and non-isothermal model was developed with a multi-fluid modeling approach. The model has a rib-channel configuration and particularly simulated for the cathode side. The computational domain consists of two BPs, GDL, MPL, CL and membrane. The BP|GDL interfacial domain measured by Swamy et al. [9] was incorporated into the model as a separate domain. In the study by Swamy et al. [9], the optical profilometry images of graphite BP and SGL 10BB GDL were obtained and the BP|GDL interface was virtually constructed under homogeneous compression of 1.5 MPa. The modeling domain and virtually constructed BP|GDL interfacial morphology are schematically shown in Fig. 1.

The following assumptions were made for the model development:

1. The model is two-dimensional and runs at steady state operating conditions.
2. The water produced during electrochemical reaction is in liquid phase.
3. Gas mixture is assumed to be ideal gas mixture.
4. Membrane is assumed to have constant ionic conductivity, and is impermeable to gas and electron transport.
5. The interfacial voids between BP and GDL are modeled as the two-dimensional cross section.
6. Convective heat transfer effects are considered negligible.