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Pore network modeling to explore the effects of compression on multiphase transport in polymer electrolyte membrane fuel cell gas diffusion layers

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HIGHLIGHTS

- High resolution synchrotron X-ray tomography of compressed GDLs.
- Direct pore space extraction from computed tomography of compressed GDLs.
- Pore network modeling used to predict liquid water distributions in GDLs.
- Mass transport losses induced by GDL compression is material/condition dependent.

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ABSTRACT

Understanding how compression affects the distribution of liquid water and gaseous oxygen in the polymer electrolyte membrane fuel cell gas diffusion layer (GDL) is vital for informing the design of improved porous materials for effective water management strategies. Pore networks extracted from synchrotron-based micro-computed tomography images of compressed GDLs were employed to simulate liquid water transport in GDL materials over a range of compression pressures. The oxygen transport resistance was predicted for each sample under dry and partially saturated conditions. A favorable GDL compression value for a preferred liquid water distribution and oxygen diffusion was found for Toray TGP-H-090 (10%), yet an optimum compression value was not recognized for SGL Sigracet 25BC. SGL Sigracet 25BC exhibited lower transport resistance values compared to Toray TGP-H-090, and this is attributed to the additional diffusion pathways provided by the microporous layer (MPL), an effect that is particularly significant under partially saturated conditions.

1. Introduction

Polymer electrolyte membrane fuel cells (PEMFCs) have several advantages compared to conventional power sources, including high efficiencies, zero-local emissions, low operating temperatures, and rapid startup capabilities. However, the accumulation and transport of liquid water in the cathode gas diffusion layer (GDL) remains a significant issue that influences the operation and performance of the PEMFC.

The GDL is a porous layer in the PEMFC that plays a critical role in fuel cell performance. This porous medium is responsible for maintaining open diffusion pathways for reactants between the gas channels and the reaction sites. It also provides pathways for conducting the heat and electrical current produced at the catalyst layer (CL) to the current collector plates while providing sufficient

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mechanical strength for protecting the membrane electrode assembly. In addition, the GDL is mainly responsible for removing the excess liquid water produced during the cathode half-cell reaction while maintaining sufficient membrane hydration for effective proton conductivity [1].

In a fuel cell stack, cell components are assembled under high compression loads to ensure contact quality and minimize transport contact resistance between the fuel cell materials. However, over-compressing the GDL can negatively affect cell performance [2]. The non-uniform compression of the GDL due to its contact with the rib and channel structured flow fields alters the microstructure of the material, the dynamics of liquid water transport through the GDL, and the reactant diffusion pathways and consequently the performance of the PEMFC [2].

Several authors have explored the use of analytical [3,4], experimental [5] and numerical [6] methods for investigating the effects of compression on the performance of the PEMFC. Numerical methods have been used extensively for analyzing PEMFC performance. In particular, commercial computational fluid dynamics (CFD) software packages have been utilized frequently to develop multidimensional models of the PEMFC for studying the performance of the cell under compression loads [7]. In these models, the non-uniform distribution of transport properties of compressed and uncompressed GDLs, such as porosity and permeability are generally measured experimentally and used as model inputs [7].

Experimental and numerical measurements of the effective transport properties, e.g. oxygen diffusivity and thermal conductivity, of compressed GDLs have been the concentration of a number of studies [8]. Imaging techniques such as X-ray computed tomography [9–11] and synchrotron X-ray imaging [12–19] have been utilized to provide new insight into the porous microstructure and liquid water accumulation in PEMFCs. These methods have also been used to analyze the effects of uniform and non-uniform compression on the microstructure and transport properties of commercial GDL materials, such as porosity, tortuosity, and permeability [20–22]. Some studies have used X-ray computed tomography to study the effect of compression on the distribution of PTFE in the GDL [23]. Finally, capillary pressure – saturation relations and liquid water breakthrough pressures were measured for commercial GDL materials at various compression states [24].

Several attempts have been made in the visualization and quantification of liquid water distribution in compressed GDLs. These include experimental methods, such as fluorescence microscopy [2,25], X-ray computed tomography [26], and synchrotron radiography [27], among others [28]. In addition, continuum models have been employed to numerically investigate liquid water flooding in deformed GDLs [29]. Commercial CFD software packages have been frequently used to investigate water transport in compressed GDLs [30]. Chippar et al. investigated the effects of non-uniform GDL compression on liquid water transport in the GDL as well as its effect on the performance of the cell [30], and they reported that in a compressed GDL, more water tends to accumulate near the ribs due to the reduced porosity and permeability in that region. Olesen et al. developed and utilized a 3D model to investigate the effect of GDL compression on the distribution of liquid water and oxygen in the cathode side of a PEMFC [31], and they observed a decrease in the oxygen transport rate near the rib with the compression of the GDL, which led to decreasing liquid water production in the CL under the rib. Wan and Chen studied the distribution of liquid water in a fuel cell with a compressed GDL [32] and found that land compression can substantially lower the liquid water saturation in this region. While traditional continuum-based models are widely used for simulating water transport in the GDL, pore-scale liquid water transport has not been fully resolved. In addition, these models require a priori knowledge of multiphase transport properties as the constitutive relationships.

While traditional continuum models cannot be used to describe the observed capillary fingering regime in the GDL [33], pore network modeling provides this capability and has become widely popular for studying multiphase transport in the GDL [34–39]. In a pore network, the pore space is represented with a network of pores and throats, where pores are the locations of large void spaces, and throats are the local constrictions that connect adjacent pores. Rebai and Prat [33] used a cubic pore network model to calculate liquid water saturation at breakthrough under land and channel regions at various compression values. Pore network modeling provides a tremendous opportunity for accurately simulating the distribution of liquid water and calculating the corresponding wet oxygen transport resistance in actual GDL materials under compression, which should aid the evaluation of cell performance under compression.

Various techniques have been developed and employed for specifically modeling the compression of the GDL. Traditionally, finite element methods were used to simulate the deformation of the GDL under compression [40], which were then coupled with a continuum model for analyzing species transport. Schulz et al. [41] simulated the compression of the GDL using a reduced model of compression. In this model the macroscopic behavior of the GDL structure under compression was transferred into the unidirectional morphological displacement of solid voxels with the assumption of negligible transverse strain. By applying this compression model to reconstructed images of commercial GDL materials, the pore size distribution, through-plane permeability and the capillary pressure – saturation curves were reported for various compression levels. The same compression model was used to determine the effect of GDL compression and water saturation on the effective diffusion coefficient of the material [42]. Mukherjee et al. [43] applied this compression model to stochastically generated non-woven carbon paper GDLs and investigated liquid water distribution in the GDL at various compression states using a two-phase Lattice Boltzmann model. A single-phase Lattice Boltzmann model was also used to study the effect of compression on the permeability of numerically reconstructed Toray TGP-H-090 and SGL Sigracet 10BA GDL materials [44]. In another study, Froning et al. [45] simulated compression in a stochastically generated fibrous GDL and used Lattice Boltzmann modeling to simulate mass transport. In this model, adjacent layers of the materials were merged to simulate GDL compression. Recently, Gaiselmann et al. [46] introduced a parameterized model that virtually generates the microstructure of compressed fibrous materials. In their model, fibers are translated with a vector field that depended on the locations of fibers and the rate of compression.

Previous work has provided valuable insight into the effect of compression on fuel cell performance and multiphase transport in the GDL. Various studies have reported differences in local liquid water saturation under land and channel in a compressed GDL [2,26,30–32]. However, a common conclusion has not been drawn concerning the effect of compression on multiphase transport in the GDL and fuel cell performance. While some studies conclude that GDL compression improves mass transport in the GDL and fuel cell performance [6,7,29], other studies confirm that GDL compression can negatively impact GDL mass transport [24,30,31,40]. Moreover, there is a scarcity of modeling work to provide a pore-scale understanding of liquid water transport and oxygen diffusion in realistically compressed GDLs as previous studies have mainly focused on using continuum models [7,29–32] or numerically compressed GDL models [42–45] to study multiphase transport in compressed GDLs. While other studies [20,21] have used realistic 3D images of compressed GDLs to study the