Journal of Power Sources 378 (2018) 53–65

Contents lists available at ScienceDirect

Journal of Power Sources

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

The effects of gas diffusion layers structure on water transportation using X-ray computed tomography based Lattice Boltzmann method

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HIGHLIGHTS

- X-ray computed tomography used to reconstruct three different types of GDL.
- Models of GDLs analysed using Lattice Boltzmann method.
- Invasion pattern and saturation of water in the GDLs is controlled by wettability.
- Liquid water travelled with a stable displacement under hydrophilic angles.
- Conversely, at hydrophobic contact angles it travelled with capillary fingering.

ARTICLE INFO

Keywords:
PEM fuel cells
X-ray computed tomography
Gas diffusion layers
Lattice Boltzmann method
On water transportation
Hydrophilic contact angles

ABSTRACT

The Gas Diffusion Layer (GDL) of a Polymer Electrolyte Membrane Fuel Cell (PEMFC) plays a crucial role in overall cell performance. It is responsible for the dissemination of reactant gasses from the gas supply channels to the reactant sites at the Catalyst Layer (CL), and the adequate removal of product water from reactant sites back to the gas channels.

Existing research into water transport in GDLs has been simplified to 2D estimations of GDL structures or use virtual stochastic models. This work uses X-ray computed tomography (XCT) to reconstruct three types of GDL in a model. These models are then analysed via Lattice Boltzmann methods to understand the water transport behaviours under differing contact angles and pressure differences.

In this study, the three GDL samples were tested over the contact angles of 60°, 80°, 90°, 100°, 120° and 140° under applied pressure differences of 5 kPa, 10 kPa and 15 kPa. By varying the contact angle and pressure difference, it was found that the transition between stable displacement and capillary fingering is not a gradual process. Hydrophilic contact angles in the region of $60^\circ < \theta < 90^\circ$ showed stable displacement properties, whereas contact angles in the region of $100^\circ < \theta < 140^\circ$ displayed capillary fingering characteristics.

1. Introduction

With the recent proliferation of environmentally friendly consciousness regarding energy use, various sustainable energy conversion technologies have been explored to mitigate anthropogenic climate change concerns. One such technology is the hydrogen fuel cell. When sustainably sourced H_2 is used as an input fuel, Polymer Electrolyte Membrane Fuel Cells (PEMFC) are considered to be zero-emissions energy conversion devices. Already used in commercial applications such as consumer electronics and automotive traction power units, the PEMFC has shown great promise. However, there are still areas that require improvement as to advance this promising technology; one of which is the performance of the cell.

The Gas Diffusion Layer (GDL) of a PEMFC plays a crucial role in overall performance in the form of providing unrestricted pathways for the reactant gases to be adequately transported from a gas channel in the separating plates to the Catalyst Layer (CL), allowing the initiation of the reaction. The GDL is also responsible for the removal of product water from the CL to the gas channels, and ultimately out of the cell. The excessive presence of liquid water in the GDL drastically diminishes the performance of the cell by blocking reactant gas access to active sites in the CL. To this end, GDLs are normally treated with a hydrophobic coating (Polytetrafluoroethylene (PTFE)) to ease the removal of product water from the cell.

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https://doi.org/10.1016/j.jpowsour.2017.12.016
Received 13 October 2017; Received in revised form 28 November 2017; Accepted 7 December 2017

1.1. Existing work in the literature

A wide range of studies have investigated water transport within a PEMFC in recent years, however the behaviour of liquid water in the GDL at a pore-level is currently inadequately understood. Experimental methods including Nuclear Magnetic Resonance (NMR) imaging, neutron imaging, X-ray imaging, and direct optical visualisation remain difficult to fully understand at a microscopic level due to the limitations of spatial and temporal resolutions involved in such techniques [1].

Fluorescence microscopy techniques combined with conventional optical photography were used by Lister et al. [2] to visualize through-plane liquid water transport in the GDL. Bazylak et al. [3] from the same research group examined the influence of cell compression on the behaviour of liquid water transport in GDL materials using the same technique, finding that certain compressed regions of the GDL provided preferential pathways for liquid water transport, leading to a breakthrough in the test apparatus. Both works showed good advancements in visualisation of liquid water behaviour in a PEMFC GDL, however their technique was limited to the visualization of liquid water transport in the upper layers of the GDL due to the opacity of the material.

1.1.1. Macro-scale modelling

Prediction of the saturation distribution of liquid water has been modelled on a macroscopic level by numerous previous studies [4–10]. These models are based on volume averaging theory and make the assumption of homogeneous GDL material. Due to this, they fail to incorporate the influence of pore morphology of the GDL material on the transportation of liquid water [11]. Furthermore, these existing models depend upon empirical relationships of capillary pressure-saturation and relative permeability-saturation in order to predict liquid water behaviour within the GDL. Capillary pressure is normally expressed as a function of saturation using the Leverett function, and therefore is more likely to harbour inaccuracies as it was based upon experimental data of homogenous soil or sand with uniform wettability. These media differ significantly when compared to a GDL structure in a PEMFC [11–13].

1.1.2. Pore-scale modelling

To model on a pore-scale rather than macro-scale, techniques such as Pore Network (PN) and Lattice Boltzmann (LB) modelling have emerged as favourable methods for simulating fluid flow through porous media. In opposition to macro-scale techniques, PN and LB methods can uncover the underlying influence of microscopic features on liquid water transportation in the GDL structure.

1.1.2.1. Pore Network modelling. Numerous PN models have been used to analyse water transportation in porous media, using 2D [14–18] and 3D [19–23] domains. In such works, however, the complex structure of the GDL material is often simplified to a regular sphere [23] or cubic pores [22] that are then connected via columnar throats for 3D PNs. 2D PNs are connected via an array of randomly distributed, equal-sized disks with random diameters [14,15].

1.1.2.2. Lattice Boltzmann modelling. The Lattice Boltzmann method has increased in popularity in recent years, due to its capability to incorporate complex boundaries of an actual GDL material as manufactured [11,24]. To date however, the majority of existing studies on fluid transport in GDL materials integrate artificial structures that are generated by stochastic simulation techniques [25–27]. The stochastic method uses a set of structural inputs obtained from design specifications or measured data to then reconstruct a porous medium [27]. However, this method is inadequate to fully reconstruct a GDL material sample. Another potential drawback to the use of stochastic methods is that it struggles to model the binding material that holds a GDL material together sufficiently. Many works therefore ignore the binder material altogether, resulting in an over-simplification and possibly altering the pore size and shape within the model.

For these reasons, XCT techniques have been increasingly used in this field to more accurately reconstruct the GDL material in a digital domain [28–31]. Rama et al. [24] undertook a study on the feasibility of using the combined methods of XCT and LB modelling to simulate liquid flow, at a pore scale, through PEMFC GDL materials. Their simulated results were compared to experimental results using a Frazier air tester, and their correlation error was found to be 3% greater than the measured one. This breakthrough, alongside numerous other studies [28–30], showed that XCT and LB are well suited for combination to accurately model liquid water flow through a PEMFC GDL.

1.2. Literature review conclusions

Existing work by various authors shows that PEMFC GDLs have been heavily simulated using a variety of techniques to discover a wide range of results. The emerging methodology has been shown to be the use of XCT in combination with the LB method to simulate GDL water transport properties. Although existing work has looked into water flow through GDLs under differing operating conditions, there is little work in the area of differing wettability of XCT reconstructed GDLs, and this effect on water transport.

To this end, this work looks at the water transport behaviour under varying wettability conditions by using XCT reconstructed GDL models of three types of commercial GDL material. These models are then analysed using the LB method.

The GDL wettability parameters are then altered so that the effect of this change can be analysed. The wettability of a GDL sample is defined by the contact angle (θ) of liquid water with the solid surface structure of the GDL sample. Hydrophilic wettability is considered to exist between $0^\circ < \theta < 90^\circ$, and hydrophobic wettability is considered to exist between contact angles of $90^\circ < \theta < 180^\circ$. The GDL samples were simulated between the full range of contact angles and at pressure difference of 5 kPa, 10 kPa, and finally 15 kPa.

2. X-ray reconstructed GDL models

Three types of commercially available GDL materials were used in this study; Freudenberg H2315 felt, Toray TGP-H-120 paper and SGL 24AA paper. The GDL samples were untreated and contained no PTFE or Micro-Porous Layer (MPL) additions. All samples are similar in that they are all non-woven and are composed of multiple layers. Their inherent structure however, differs between samples. The Freudenberg felt has curved fibres travelling in both the in-plane and through-plane directions. Both the Toray and SGL papers have straight fibres which are mainly orientated in the in-plane direction. Both paper GDL fibres are held together by a carbonized binder, which differ in construction. The SGL binder has a rougher texture binder than the Toray paper, and it lies within the in-plane and through-plane directions, whereas the Toray binder is only located between layers in the in-plane direction.

Each sample was analysed through XCT processes at a resolution of 2.5μm/pixel, and reconstructed in digital form. A General Electric Phoenix nanotom® system was used, equipped with an X-ray source of 160 kV (max) and 250 μA (max), with an X-ray spot size of around 1 μm.

The detector was a 5-megapixel flat panel CMOS (complementary metal-oxide semiconductor) with a GOS (gadolinium oxysulfide) scintillator deposited on a fibre optic plate.

The results of the scans are presented in Fig. 1 alongside their 3D digital reconstructions.

3. Two-phase Lattice Boltzmann modelling

As discussed in Section 1, the LB method is widely used to model fluid particle flow through porous media. In this work, multiple