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Modeling heat transfer through phase-differentiated nano-scale constructions of polymer electrolyte membrane fuel cell microporous layers

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ABSTRACT

In this work, we investigated the influence of nano-particle orientation in polymer electrolyte membrane (PEM) fuel cell microporous layer (MPLs) on heat transfer behavior. In practical applications, polytetrafluoroethylene (PTFE) is added as binding and hydrophobic agents to the MPL. However, the thermal conductivity of PTFE is significantly lower than that of carbon, and the impact of PTFE content on the thermal conductivity of the MPL has not been reported. In this work, we considered a phase-differentiated model with carbon, PTFE, and air as separate phases, and heat transfer was modeled through the nano-particles using Fourier's law of heat conduction. Particle separation was found to have the strongest impact on the thermal conductivity of the MPL. The thermal conductivity decreased by over 50% when the particles were separated by 10 nm. The thermal conductivity was not largely impacted by particle radii, but the thermal conductivity increased by 8% when the PTFE filling radius increased from 10 nm to 30 nm. The same methodology was also used to calculate the electrical conductivity of the MPL. The increase in particle separation resulted in a linear decrease in the electrical conductivity, with a decrease of 16.4% when the particle separation increased from 0 nm to 10 nm. Introducing a fluid phase has an insignificant effect (less than 1%) on the electrical conductivity, and the impact of changing the filling radii was also significantly less than for the case of thermal conductivity.

1. Introduction

Polymer electrolyte membrane (PEM) fuel cells are electrochemical devices that produce electricity through the conversion of hydrogen and oxygen into water and heat. Heat is generated during the exothermic reactions at the cathode catalyst layer and during operation through resistive heating [1–3], and as a result most fuel cells (especially fuel cell stacks) are actively cooled to prevent overheating [2]. Since the heat distribution in the PEM fuel cell influences the distribution of water and the overall performance [1,3,4], a detailed understanding of how the material characteristics influence the thermal gradients within the fuel cell layers is vital for designing new materials for effective thermal management. Although a variety of authors have investigated the thermal conductivity of the gas diffusion layer (GDL) [5–19], there is still a pressing need to understand the thermal transport mechanisms in the micro-porous layer (MPL).

In 2008, Sadeghi et al. [5] incorporated the geometrical features and the mechanical strength of the GDL into their thermal resistance modeling work to predict the effective thermal conductivity of the GDL. Karimi et al. [9] experimentally measured the through-plane thermal conductivity of GDL materials with varying degrees of PTFE content. They reported that increasing the PTFE content leads to increases in the effective thermal conductivity, and this increase can be attributed to the increase in heat transport pathways for thermal conduction. Yablecki et al. [12–14] determined the thermal conductivity of the GDL using a point to point contact model, showing how the thermal conductivity changed with compression pressure. Their resistance model incorporated solid carbon fibers and the PTFE as distinct phases, and their thermal resistance predictions were based on fiber to fiber contacts. The authors also studied the effect of liquid water saturation on thermal conductivity and found that increasing liquid water saturation

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led to increases in the through-plane thermal conductivity. They attributed this outcome to the additional pathways for thermal transport provided by the presence of liquid water.

In 2010, Karimi et al. [9] experimentally measured the thermal conductivity of GDLs with and without an MPL coating. They showed that introducing the MPL led to a decrease in the overall thermal conductivity of the GDL. Their work further motivates the need to understand the contribution of the MPL to thermal resistance in order to enable the informed design of materials for efficient water and thermal management.

In 2012, Zamel et al. [7] used an approximation for the effective thermal conductivity of the MPL to include in their model of the GDL. They applied Fourier's law of thermal conduction to study the macroscopic region of the GDL. For the MPL, they used effective properties and employed the Bruggeman approximation. The authors noted that their numerical results were higher than experimental measurements and attributed this difference to the penetration of the MPL into the GDL substrate region (that was not included in their model). In the same year, Unsworth et al. [20] also experimentally measured the thermal conductivity of the bi-layer GDL and showed that the thermal conductivity of the MPL was 0.3 W/m-K. The application of the MPL resulted in a decrease in the overall thermal contact resistance of the fuel cell, and this led to a reduction in thermal gradients across the GDL (between catalyst layer and the reactant gas channels). The thermal conductivity of the MPL did not change significantly with changes in compression pressure.

In 2015, Botelho and Bazylak [21] presented a novel method for modeling the thermal transport through the nano-scale features of the MPL by determining the thermal resistance between individual particles. They used Atomic Force Microscopy (AFM) images to obtain the particle contact morphology of their model. They performed a parametric study of the thermal resistance due to the particle to particle contacts. Although Botelho and Bazylak [21] presented a fundamental method to model the thermal transport between the MPL particles, they did not account for the thermal conductivity of polytetrafluoroethylene (PTFE) that is a key component of the MPL. Botelho and Bazylak's model considered a weighted average thermal conductivity of 114 W/m^2-K for the solid material, which was composed of 5% PTFE and 95% carbon. However, the PTFE should be spatially resolved in order to understand the impact of PTFE on heat transfer behavior through the MPL.

In this current work, a phase differentiated approach was used to model heat transfer through the carbon, PTFE and the fluid phases of the MPL. The fluid phase can be modeled as air in the case of an unsaturated MPL, liquid water in the case of a fully saturated MPL, or as water vapor which presents another likely case of the MPL where the water transport through the MPL is assumed to be entirely in the vapor phase [22]. A model was developed that advances the work reported by Botelho and Bazylak [21] by utilizing a phase differentiated approach for modeling the thermal transport through the particle to particle contacts of the MPL. This paper investigates the effects of particle separation, particle overlap, and surrounding fluid on the thermal transport behavior. In addition to studying the thermal transport, this work also investigated the analogous electrical conductivity through the MPL particle to particle contact, utilizing the phase differentiated approach.

2. Methodology

In this work, the thermal conductivity of an MPL consisting of carbon black and PTFE binder was calculated. Fig. 1 is a schematic showing the interaction of the three phases considered in this work: carbon black (Phase 1), PTFE (Phase 2), and air (Phase 3).

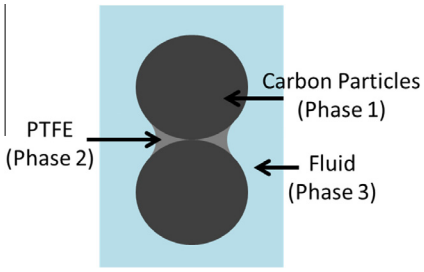

Fig. 1. Phase-differentiated representation of the three-phase MPL model.

The PTFE acts as the binder for the carbon particles. The PTFE is mixed with the carbon to form a slurry, which is sintered to form the MPL [23–27]. The PTFE acts as a wetting fluid and accumulates in the gaps between the carbon particles. In this work, PTFE was assumed to be the binding agent between the carbon particles. In an unsaturated condition, air behaves as the wetting fluid surrounding the MPL particles. For a fully saturated condition two cases are considered here: liquid water transport and water vapor transport. A benchmark case for validation and comparison purposes was also modeled, whereby the solid MPL particles were surrounded by a vacuum with a thermal conductivity of zero. This benchmark case was used to ensure that thermal leakage from the particle to particle contacts did not occur. Table 1 contains the values of thermal conductivities and the associated references for materials considered in our study. In comparison to graphitized carbon, the thermal conductivity of PTFE is several orders of magnitude lower. This indicates that the largest thermal resistance is provided by the presence of PTFE in the MPL.

Fig. 2 illustrates the four distinct particle contact parameters explored in this work: carbon particle overlapping distance, PTFE filling radii, carbon particle diameter, and carbon particle separation distance. The carbon particles often fuse together during the sintering process, which is simulated in the overlapping particle case. The overlapping case was also used to successfully benchmark the results of Botelho and Bazylak [21]. A range of filling radii and particle separation distances were considered as parameters for controlling PTFE content. For the overlapping, filling radii, and separation distance simulations, particles were assumed to be 50 nm in diameter, in agreement with literature [21,28–30]. However, since a range of particle diameters have also been observed during the AFM study by Botelho and Bazylak [21], we also studied the impact of particle diameter on thermal conductivity.

Fig. 3 provides a schematic of the modeling domain and employed boundary conditions. Three planes of symmetry were assumed, as described in Fig. 3. Fig. 3(a) shows several connected MPL particles, while the region of interest (Fig. 3(b)) was a single particle to particle contact. Future work may incorporate a full MPL model that utilizes the information of particle contacts and the associated thermal conductivities. Fig. 3(b) shows the particle to particle contact in three dimensional form. The plane of symmetry is used three times to reduce the size of the modeling domain as shown in steps 3(b)–(e). Fig. 3(e) is the repeating structure that

Table 1
Thermal conductivity of the materials and fluids considered in the thermal modeling study.

Material name	Thermal conductivity (W/m-K)	Refs.
Carbon (black)	120	[21]
PTFE	0.649	[21]
Air (gas)	0.03	[20]
Water (liquid)	0.58	[20]
Water vapor (gas)	0.016	webbook.nist.gov