Fiber-size-dependent thermal conductivity of gas diffusion layer of Polymer Electrolyte Membrane Fuel Cell: A Computational Approach

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ABSTRACT – In this study, we present a numerical analysis of the effective thermal conductivity (k_{eff}) of the gas diffusion layer (GDL) of a proton exchange membrane fuel cell (PEMFC) using a two-dimensional lattice Boltzmann method (LBM). GDLs were stochastically generated with a solids fraction of 22% and a fiber diameter variation ranging from 5 µm to 100 µm. A statistical averaging method was applied to eliminate the effect of random fiber placement. The analysis reveals that the average effective thermal conductivity is independent of the fiber diameter with an observed variation of only 1.3% across the entire diameter range studied. This conclusion, consistent with the experimental literature, confirms that the thermal conductivity is dominated by the connectivity and percolation of the solid fiber network. With constant porosity, the fiber size has a negligible impact on the overall thermal performance. This suggests that the fiber diameter can be optimized for other properties such as permeability without thermal penalty.

Keywords: Thermal conductivity, GDL, Fuel cell, Grain size, LBM

1. INTRODUCTION

The transition to renewable energy sources has increased interest in proton exchange membrane fuel cells due to their energy efficiency and emission-free operation [1]. Among the challenges to their large-scale commercialization is thermal management. The electrochemical reaction is exothermic, and inadequate heat dissipation can lead to membrane degradation and a drastic drop in performance [6]. Thermal management plays an important role in the durability of PEMFCs. The gas diffusion layer (GDL), a porous medium composed of interconnected fibers, is necessary for dissipating this heat. Although the effect of porosity on effective thermal conductivity has been extensively studied, the impact of fiber diameter remains poorly quantified. The Gas Diffusion Layer is located between the bipolar plate and the catalytic layer (Figure 1). The GDL is a multifunctional component: it allows the distribution of reactant gases and the removal of the water produced, as well as the conduction of electrons and the conduction of heat from the reaction to the cooling plates [3, 7]. GDL is a composite of highly conductive carbon fibers with a thermal conductivity $k_{\ carbon\ fiber} \approx 150\ W.m^{-1}.K^{-1}$ and air-filled pores considered as an insulator with an approximate thermal conductivity $k_{\ air\text{-}filled\ pores} \approx 0.026\ W.m^{-1}.K^{-1}$. Beyond the microstructural characterization of materials, this work reinforces the central role of PEMFCs in the green hydrogen economy by combining high efficiency and absence of direct emissions; this technology is establishing itself as an essential vector for the decarbonization of transport, thus actively contributing to international carbon neutrality objectives.

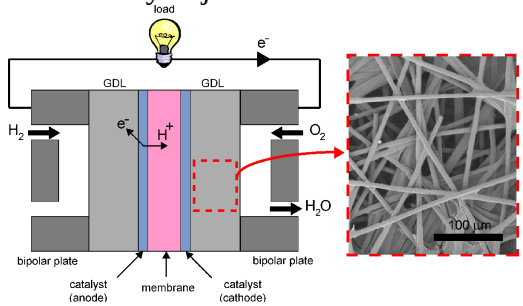

Figure 1: A proton exchange membrane fuel cell (PEMFC). GDL inset outlined by a dashed red line.

Heat transfer by conduction through a GDL requires the contribution of both phases, fluid and solid, constituting the porous matrix, which generally occur in different proportions. Therefore, introducing a conductivity that accounts for the contribution of each phase is important in modeling heat transfer in the GDL. Thus, the concept of effective thermal conductivity emerged to make sense of a heterogeneous porous medium like the GDL. This conductivity is highly dependent on the porosity and thermal conductivities of the solid and fluid phases. Its effective thermal conductivity is therefore critical. While the literature has extensively studied the effect of porosity [2], the impact of the fiber morphology itself, such as their diameter, at constant porosity, remains less clear. Some studies, such as those by Sadeghifar et al. [5], suggest a weak dependence, but this conclusion requires numerical validation. In general, the proposed models are all weighted combinations of series and parallel models based on the electrical analogy. Another possibility for evaluating thermal conductivity is the use of the lattice Boltzmann method. The objective of this work is to quantify the influence of fiber diameter on the k_{eff} of a GDL using direct numerical modeling by the Lattice Boltzmann (LBM) method on virtual microstructures. This research contributes to the understanding of heat transfer in GDLs which enhances the durability and performance of PEMFCs. Optimized thermal management extends the lifespan of these systems and stabilizes their operation. By linking thermal behavior and microstructure, this work supports the development of green hydrogen technologies.

2. METHODOLOGY

Since our interest in this article is solely to evaluate the value of the effective thermal conductivity of a GDL, heat transfer by pure conduction is considered and the following assumptions are made: there is no convection or radiation in the system under study and no phase change occurs. The virtual 2D GDLs were generated using a stochastic placement algorithm. A target solid fraction (carbon fibers) of 22% (corresponding to 78% porosity) was kept constant for all simulations. The variable parameter was the average fiber diameter, ranging from 5 µm to 100 µm, with zero diameter variance. The lattice Boltzmann method is an efficient numerical method for simulating fluid flows. Several lattice models [4] have been developed, including the D2Q9 model (Figure 2) used in this article in which, the computational domain is discretized into a square grid, and each node has its eight surrounding nodes as neighbors (Figure 2). At each time step, each node has particles whose state is described by the density distribution function, and which move towards its neighbors. Simultaneously, the neighboring nodes also have particles moving towards that node. At the next time step, they simultaneously reach their respective target nodes, collide, and, after this interaction, evolve towards a new particle distribution.

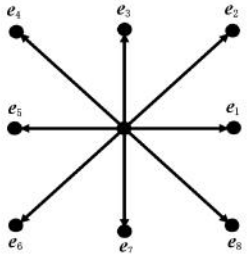

Figure 2: D2Q9 model of the LBM employed

$f_i(x.t)$is the density distribution function of a single particle. The the Boltzmann equation governing the density distribution function is:$f_i(x + e_i, t + 1) - f_i(x, t) = \frac{1}{\tau}\left(f_i^{eq}(x.t) - f_i(x.t)\right), i = 0,1,..8$ where x is the coordinate of the spatially discrete node, t represents the discrete time step, τ is the relaxation time, and $f_i^{eq}(x.t)$ is the local equilibrium distribution function of node x at time step t. Various macroscopic quantities can be deduced from the distribution function. The macroscopic temperature and thermal flux are defined from the internal energy as: $T = \sum_i f_i$ and $(q = \sum_i e_i f_i)\frac{\tau - 0.5}{\tau}$; τ is the thermal relaxation time and the equilibrium distribution function is only related to the local density and velocity, and can be

chosen as $f_i^{eq} = \rho w_i T$ Where $w_0 = \frac{4}{9}, w_1 = w_3 = w_5 = \frac{1}{9}, w_2 = w_4 = w_6 = w_8 = \frac{1}{36}$. Finally, the effective thermal conductivity is estimated as follows: $\boldsymbol{k_{eff}} = \frac{\boldsymbol{q \times L_x}}{\boldsymbol{L_y(Th - Tc)}}$.

3. Results and discussion

The simulation domain is a 2D grid of 200x200 nodes in lattice units. This grid represents a physical cross-section of a GDL of 500 µm x 500 µm. The GDLs are generated by a stochastic placement algorithm. The solid fraction of carbon fibers is fixed at 22%, (i.e., 78% porosity), for all simulations. The variable parameter is the fiber diameter. (Figure.3)

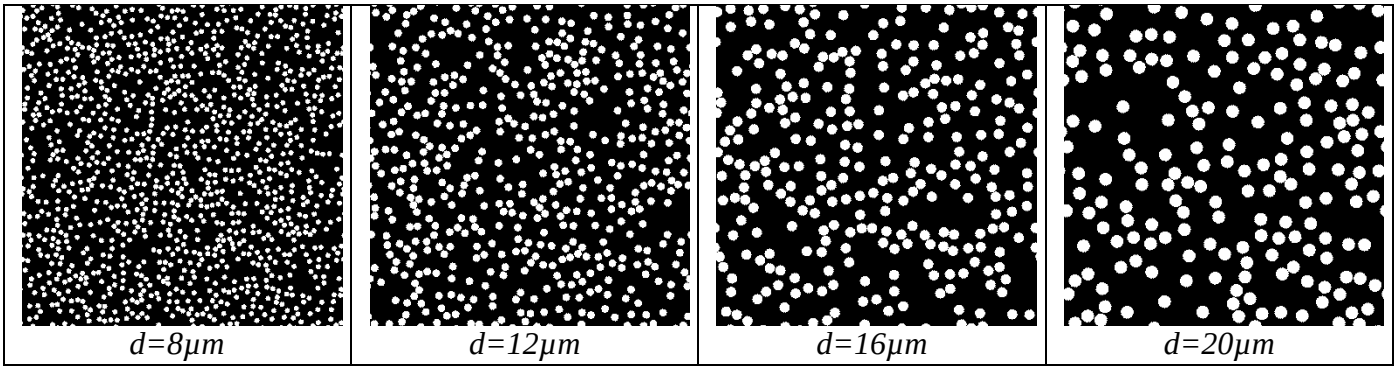

Figure 3 GDL with 78% porosity and different fiber diameters d.

The temperature contours across the domain are shown in Figure 4.

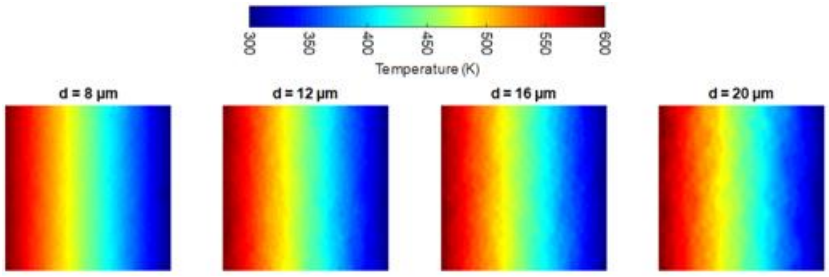

Figure 4. Distribution of the thermal field through the GDLs for different fiber diameters

The isotherms clearly indicate the heterogeneous nature of the transfer within the GDL.
A single simulation for a given diameter produces variable results due to the random generation of microstructures and the random formation of conductive paths. To mitigate these fluctuations, we averaged N = 15 simulations for each diameter. The averaged results (Figure 5) show that the effective thermal conductivity is practically independent of the fiber diameter, stabilizing around 0.305 $W.m^{-1} \cdot K^{-1}$, with a total variation of only 1.3%.

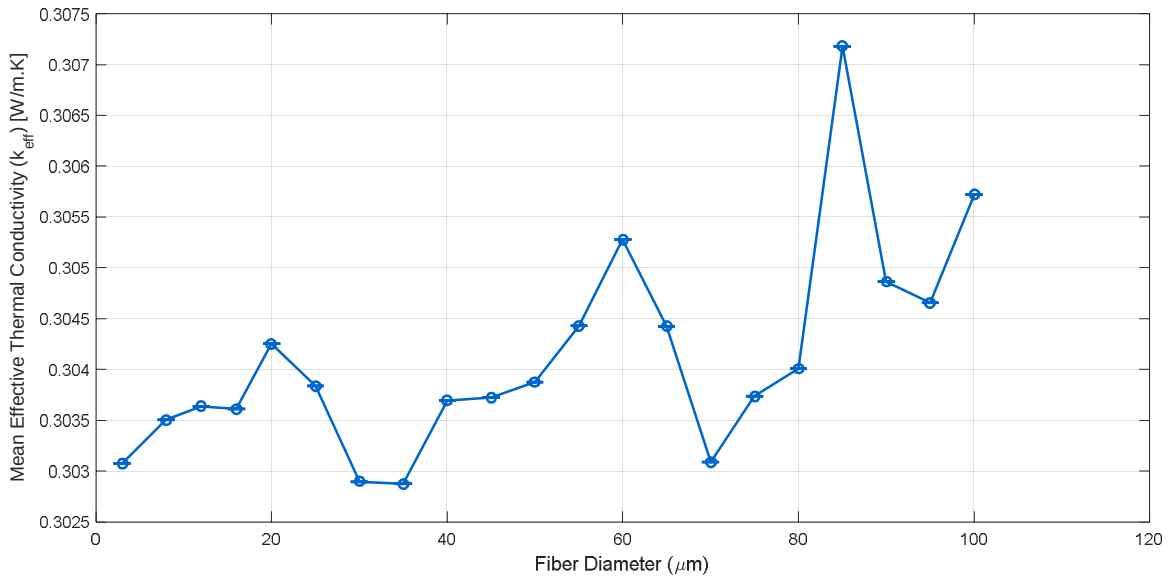

Figure 5: Influence of Fiber Diameter d on $\boldsymbol{k_{eff}}$ *(Solid Fraction = 22%, N=15 runs/pt)*

These observations confirm that, for a solid fraction of 22%, a continuous network of conductive fibers is already established, and that the overall thermal resistance does not depend on the fiber size. This result is consistent with the work of Sadeghifar et al. [5]

CONCLUSION

A numerical model based on the Lattice Boltzmann Method (LBM) was developed to estimate the effective thermal conductivity of gaseous diffusion layers (GDLs). The study was performed on randomly generated 2D microstructures, varying the fiber diameter while maintaining constant porosity. The results show that statistical processing of several independent realizations is essential to mitigate the fluctuations associated with random microstructures. Once these variations are controlled, it becomes clear that, for a solid fraction of 22%, the effective thermal conductivity is practically independent of the fiber diameter. This conclusion is of major importance. The choice of fiber diameter in the GDL can be directed towards optimizing other essential properties such as permeability without compromising the thermal conductivity performance of the material.

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