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Gas Transport Properties in Gas Diffusion Layers: A Lattice Boltzmann Study

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Abstract. The lattice Boltzmann method is applied to the investigations of the diffusivity and the permeability in the gas diffusion layer (GDL) of the polymer electrolyte fuel cell (PEFC). The effects of the configuration of water droplets, the porosity of the GDL, the viscosity ratio of water to air, and the surface wettability of the GDL are investigated. From the simulations under the PEFC operating conditions, it is found that the heterogeneous water network and the high porosity improve the diffusivity and the permeability, and the hydrophobic surface decreases the permeability.

AMS subject classifications: 76S05, 76R50, 76R05, 76M28

Key words: Diffusivity, permeability, lattice Boltzmann method, gas diffusion layer.

1 Introduction

Polymer electrolyte fuel cells (PEFCs) are expected as one of the alternative energy sources. The management of generated water in the PEFC is important especially at the cathode side, since the generated water prevents oxygen from reaching a catalyst layer. In order to remove the generated water from the catalyst layer and provide the continuous transport of oxygen, gas diffusion layers (GDLs) are bound with the catalyst layer. Therefore, the understanding and the improvement of drainage and gas transport properties in the GDL are important issues to realize the high performance of the PEFC [1].

In this study, we focus on the gas transport in the GDL. Among the gas transport properties, we consider the diffusivity (Fick's law) [2] and the permeability (Darcy's

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law) [3]. These properties have been roughly estimated by simple models or by empirical rules [4], but in those works the PEFC operating conditions such as the water network, the viscosity ratio of water to air, and the surface wettability of the GDL are neglected. However, these conditions may affect the gas transport properties. So, we investigate the effects of the PEFC operating conditions on the diffusivity and the permeability of the GDL by using the lattice Boltzmann method (LBM). In recent years, the LBM has succeeded in simulating flows in porous media, because of the simple algorithm without convergent calculations and the easy handling of local boundary conditions.

The outline of this paper is the following. In Section 2, the problem is described. In Section 3, the numerical method is presented. In Section 4, the numerical simulations are carried out to investigate the effects of droplet configuration, structure porosity, viscosity ratio of water to air, and surface wettability. Conclusions are given in Section 5.

2 Problem setting

The whole calculation process is divided into two steps. First, the equilibrium configuration of water droplets in the gas diffusion layer (GDL) is made up. Next, the diffusivity and the permeability in the GDL containing water droplets are examined.

2.1 GDL structure and water configuration

In this study, a GDL structure is constructed by randomly laminated fibers as shown in Fig. 1. The whole domain is discretized into 101^3 grid points, and its resolution is 4×10^{-6}m. The diameter of the fiber is 3 grids, and 700 fibers are placed in the structure.

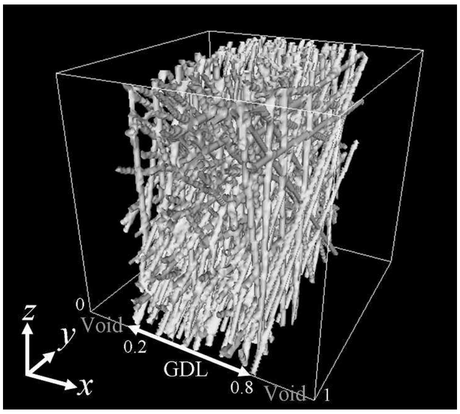

Figure 1: A GDL used in the simulations. Gray and transparent area are for solid and fluid spaces, respectively.

In the operating PEFC, the GDL pores are partly filled with the generated water. So the water configuration is modelled by droplets. The water droplets are placed randomly in the GDL as the initial configuration (Fig. 2(a)). The size of droplets is also chosen at