Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2016-0231

Vol. **23**, No. 4, pp. 1078-1093
April 2018

Using Orthorhombic Lattice Boltzmann Model to Research the Liquid Transport in Gas Diffusion Layer with Different Micro Porous Layer Coated

Peng Xu, Sichuan Xu and Yuan Gao*

Clean Energy of Automotive Engineering Center & School of Automotive Studies, Tongji Unversity, China.

Received 2 December 2016; Accepted (in revised version) 7 March 2017

Abstract. Water management in gas diffusion layer (GDL) and micro porous layer (MPL) poses a great impact on performance of proton exchange membrane fuel cells (PEMFCs). And enhancement of the performance of fuel cells requires an appropriate water balance between the conservation of membrane humidity and the discharge of excess water produced in the cell. The Lattice Boltzmann method (LBM) can enable more straight simulation of fluid flow with complex solid structures, compared with conventional computational fluid dynamics (CFD) method based on Navier-Stokes equations. In this study, the orthorhombic pseudo-potential multiphase lattice Boltzmann method (LBM) is used to investigate liquid water transport in the MPL and GDL of polymer electrolyte membrane fuel cells (PEMFC). And the GDL and MPL structure image are all acquired by the stochastic generation method. We compared the GDL coated by the MPL with different thickness and different porosity. Numerical results confirm that influence of porosity is much greater than the thickness, which can help to improve the GDL and MPL design.

AMS subject classifications: 76P05, 76S05

Key words: Proton exchange membrane fuel cell, lattice Boltzmann method, stochastic generation method, water management, gas diffusion layer, micro porous layer.

1 Introduction

Proton exchange membrane fuel cell (PEMFC) has been considered as one of the most promising power sources for practical applications such as automotive and backup power station due to its zero emission, low operating temperature, high efficiency, high power density. One of the key technologies in PEMFC is the water management. Enhancement

*Corresponding author. *Email addresses:* `xpxp1991@tongji.edu.cn` (P. Xu), `scxu@tongji.edu.cn` (S. C. Xu), `rays_chien@hotmail.com` (Y. Gao)

of the performance of fuel cells requires an appropriate water balance between the conservation of membrane humidity and the discharge of excess water produced in the cell. Excessive amount of water floods porous media in high current or low temperature situations, thus blocking the reactant gas channel from flow field to catalyst layer (CL); Loss of water leads to dehydration of membrane and poses a threat to performance and durability of cell. Therefore, the optimization of water management is of vital importance to improve fuel cell performance.

There is much potential for material design to optimize fuel cell performance such as hydrophilic and hydrophobic treatment of porous media, refinement of carbon substrate, application of novel flow filed. In the typical MEA design, an MPL between CL and MPL is basically made from a mixture of carbon black power and hydrophobic agent. The hydrophobic agent is usually composed of polytetrafluoroethylene (PTFE), yielding a finer pore geometry and highly hydrophobic characteristic than GDLs [1]. The design parameters for the gas diffusion layer (GDL) in the PEMFC are pore size, thickness, hydrophobic/hydrophilic properties, porosity, which impact the water management characteristics during PEMFC operation [2]. One of the beneficial effects of an MPL is the achievement of better water management because it results in a more favorable water profile in cell [3]. Several investigations have been demonstrated that MPL coated on the GDL substrate can effectively improve the water management characteristic and then enhances the performance. T. Kitahara et al. [2] clarified that optimized MPL design parameters depend on humidification of supplied gas significantly and GDL coated by MPL not only prevent the deterioration of MEA in low humidity condition but also reduce the flooding phenomenon under high humidity condition. Decreasing the MPL pore diameter and PTFE content is effective in preventing the dry of MEA in low humidity condition, whereas downsizing the MPL mean flow pore diameter to 3μm leads to flooding. The authors also developed a novel triple MPL coated GDL, in which a hydrophilic layer was coated on a hydrophobic double MPL with a gradient of hydrophobicity inside [4]. And the results showed that the thin hydrophilic layer in the triple MPL is good to maintain the hydration of MEA in low humidity while the hydrophobic double MPL prevents the removal of water from hydrophilic layer. T. Kitahara then developed a new hydrophilic and hydrophobic double MPL coated GDL to enhance PEMFC performance under no-humidification condition at the cathode and the influences of the pore diameter, thickness, and hydrophilic and hydrophobic properties for the double MPL on PEMFC are investigated [5]. An MPL is not only effective for water management in normal temperature but also in subfreezing temperature. Extending ice storage of electrode into MPL region is useful for fuel cell to start in cold environment. J. Ko [6] carried out three-dimensional simulations with and without the dual-functional MPL for a numerical comparison and found that the dual-functional MPL kept cell operational, even after CL was completely filled with ice, extending the cold start time before failure. To summarize, there is a great potential to optimize the water management thus improving the cell performance when focusing on optimizing the design parameters of the porous media.

Much attention has been paid to the investigation of fluid flow in porous media by