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# Lattice Boltzmann Simulations of Water Transport from the Gas Diffusion Layer to the Gas Channel in PEFC

Koji Moriyama[1,2,*] and Takaji Inamuro[2,3]

[1] *Fundamental Research Center, Honda R&D Co. Ltd., Saitama 351-0193, Japan.*
[2] *Department of Aeronautics and Astronautics, Graduate School of Engineering, Kyoto University, Kyoto 606-8501, Japan.*
[3] *Advanced Research Institute of Fluid Science and Engineering, Graduate School of Engineering, Kyoto University, Kyoto 606-8501, Japan.*

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**Abstract.** Water management is a key to ensuring high performance and durability of polymer electrolyte fuel cell (PEFC), and it is important to understand the behavior of liquid water in PEFC. In this study, the two-phase lattice Boltzmann method is applied to the simulations of water discharge from gas diffusion layers (GDL) to gas channels. The GDL is porous media composed of carbon fibers with hydrophobic treatment, and the gas channels are hydrophilic micro-scale ducts. In the simulations, arbitrarily generated porous materials are used as the structures of the GDL. We investigate the effects of solid surface wettabilities on water distribution in the gas channels and the GDL. Moreover, the results of $X$-ray computed tomography images in the operating PEFC are compared with the numerical simulations, and the mechanism of the water transport in PEFC is considered.

**AMS subject classifications**: 76M28, 76T10, 76S05, 65D18

**Key words**: Two-phase lattice Boltzmann method, polymer electrolyte fuel cell, $X$-ray CT imaging, gas diffusion layer.

## 1 Introduction

Polymer electrolyte fuel cell (PEFC) is expected to be the future driving power of vehicles because of its low emission and high efficient conversion into energy. The PEFC is composed of an electrolyte membrane, a catalyst layer, a gas diffusion layer (GDL), bipolar plates, etc. Water management in the PEFC is one of the inevitable and difficult issues to

*Corresponding author. *Email addresses:* koji_moriyama@n.t.rd.honda.co.jp (K. Moriyama), inamuro@kuaero.kyoto-u.ac.jp (T. Inamuro)

 

realize high performance and durability. While the electrolyte membrane has to be kept humid to facilitate proton conductivity, the liquid water in the catalyst layer, GDL and gas channels has to be continually discharged to ensure oxygen or hydrogen transport to catalyst surfaces [1].

Recently, various investigations of water transport in the GDL and the gas channels have been performed [2–5]. However, they are elementary evaluations of the GDL and the gas channels, and there are few pore-scale analyses on water transport in the GDL and the gas channels at the same time. Furthermore, there are few studies which compare in-situ measurements in the operating PEFC to numerical simulations with the complex GDL geometries.

In this study, in order to obtain fundamental knowledge of water transport in the PEFC, two-phase lattice Boltzmann simulations are performed and compared with $X$-ray computed tomography images in the operating PEFC. In the simulations, the surface tension of liquid water, the wettability of the GDL and the gas channel, and the high density and viscosity ratios of water and air are taken into account.

The paper is organized as follows. In Section 2, we describe the numerical method and the computational setup. Comparison with $X$-ray computed tomography images and numerical results are shown in Section 3. Finally, conclusions are given in Section 4.

## 2 Numerical method and calculation conditions

### 2.1 Two-phase lattice Boltzmann method

Recently, the lattice Boltzmann method has been developed into an alternative and promising numerical scheme for simulating viscous fluid flows and multi-phase fluid flows. The advantages of the lattice Boltzmann method are the simplicity of the algorithm, the accuracy of the mass and momentum conservations, the straightforward resolution of complex boundaries, and the suitability for parallel computing. These features are quite suitable for simulating multiphase flows in the complex GDL.

In this study, the two-phase lattice Boltzmann method proposed by Inamuro et al. [6], which can simulate two-phase flows with a large density ratio, is used. The fifteen-velocity model ($N=15$) is used in the present paper. The velocity vectors in this model are given by

$$\begin{aligned}&\left[\boldsymbol{c}_1,\boldsymbol{c}_2,\boldsymbol{c}_3,\boldsymbol{c}_4,\boldsymbol{c}_5,\boldsymbol{c}_6,\boldsymbol{c}_7,\boldsymbol{c}_8,\boldsymbol{c}_9,\boldsymbol{c}_{10},\boldsymbol{c}_{11},\boldsymbol{c}_{12},\boldsymbol{c}_{13},\boldsymbol{c}_{14},\boldsymbol{c}_{15}\right]\\ &=\begin{bmatrix} 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1\\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1\\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \end{bmatrix}.\end{aligned} \tag{2.1}$$

Two particle velocity distribution functions, $f_i$ and $g_i$ are used. The function $f_i$ is used for the calculation of an order parameter which represents two phases, and the function $g_i$ is used for the calculation of a predicted velocity of the two-phase fluid without a