11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

Numerical Analysis of Gas Transport in Micro-porous Material by DSMC Method

Ikuya Kinefuch[1] and Yoichiro Matsumoto[2,*]

[1] Department of Mechanical Engineering, The University of Tokyo
Hongo, Bunkyo-ku, Tokyo 113-8656, Japan, kine@fel.t.u-tokyo.ac.jp
[2] Department of Mechanical Engineering, The University of Tokyo
Hongo, Bunkyo-ku, Tokyo 113-8656, Japan, ymats@fel.t.u-uokyo.ac.jp

Key Words: *Fuel cell, Multi-scale Problems, Gas-surface Interaction, DSMC Methods.*

Downsizing of polymer electrolyte fuel cell (PEFC) systems, which is important especially for automotive use, requires the increase of the current density. As the current density increases, the loss due to oxygen transport has a significant impact on the overall cell performance. Therefore, the improvement of gas transport characteristics in porous materials is of great importance to realize the high current density. While the structure and the gas transport phenomena in a gas diffusion layers, a porous structure with a characteristic length scale of a few μm, were investigated, those fluid-structure interaction of multi-scale have not been well understood. It is important to develop simulation method for the fuel cell design. We employ multi-scale analysis of fluid-structure phenomena in the fuel cell, multi-scale gas, liquid and surface interaction.

This paper describes the analysis of gas transport in MPLs based on the three-dimensional structure obtained from X-ray nano computed tomography (CT). We employ the direct simulation Monte Carlo method [1] in order to accurately analyze the gas transport phenomena where the characteristic length scale of the structure is comparable to the mean free path of gas molecules. Counter diffusion of gas molecules in the porous structures is simulated. The left and right boundaries of the simulation domain have contact with gas reservoirs of pure N_2 and O_2 at 22 °C. The pressure of the reservoirs is set at between 10 - 300 kPa. Since the pressure of both sides is the same, macroscopic flow velocity remains zero throughout the system. However, some of N_2 and O_2 molecules reach the opposite side of the porous layer because of the counter diffusion.

The computational domain is divided into 64 × 64 × 72 cells for DSMC calculations. Each DSMC cell is a cube 90 nm on each side. The variable hard sphere (VHS) model is employed for gas collisions. The velocities of gas molecules after colliding with the surface are determined by the cosine scattering with perfect energy accommodation. The subsequent 5×10^4 - 1×10^5 steps are used for sampling the flow field. The simulation system at the steady state contains approximately 3.6×10^6 sample particles. The simulations were performed using a parallel computation code developed for the present analysis. The simulation system is decomposed into sub domains, each of which is simulated by an independent process. Sample particles going into the adjacent domains are handled using message passing interface (MPI). We employed 384 MPI processes (24 nodes) in most of the current study.

The Knudsen diffusion resistance is observed at the zero pressure, where gas molecules collide only with solid surface. As the pressure increases, the diffusion resistance increases linearly because of the more frequent collisions between gas molecules and finally the molecular diffusion mechanism becomes dominant in the gas transport. The numerical simulation well reproduces the experimentally observed pressure dependence of diffusion resistance [2] originating from the coexistence of the Knudsen and molecular diffusion mechanisms.

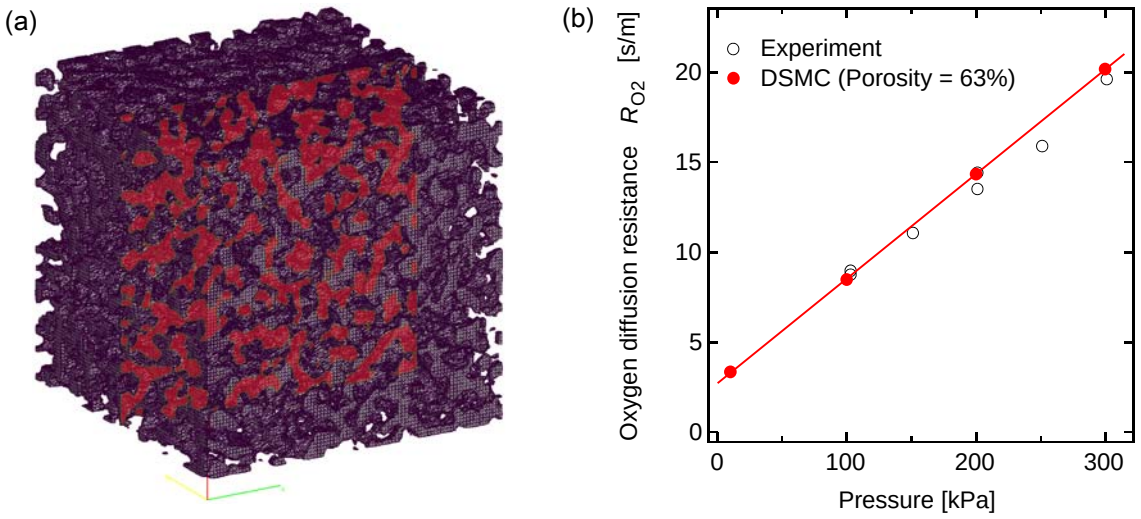

Figure 1. Three-dimensional structure data of the MPL sample and the oxygen diffusion resistance through the porous layer as a function of pressure. (a) Polygonal representation generated from the X-ray CT image using the marching tetrahedrons algorithm [3]. The red regions illustrate the sliced cross section of the solid. (b) Comparison between the experimental and simulation results. The experimental values [2] are for the MPL sample with a thickness of 45.8 μm. The diffusion resistance obtained from DSMC calculations are scaled for the same thickness as in the experiment. The temperature is 22 °C both in the experiments and the simulations. The porosity of the porous structure used in the simulation agrees with the experimentally determined value (63%).

REFERENCES

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford University Press, (1994).
[2] A. Aoki, Y. Tabuchi, S. Kuwata, K. Yamaguchi, J. Oyama, K. Yokoyama, N. Kubo, The 25nd Battery Symposium in Japan, (2011).
[3] A. Doi and A. Koide, *IEICE Trans.*, **E74-D**, 214 (1991).