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Surface Diffusion Effect on Gas Transport in Nanoporous Materials[1] TAKUMA HORI, YUTA YOSHIMOTO, SHU TAKAGI, IKUYA KINEFUCHI, The University of Tokyo — Polymer electrolyte fuel cells are one of the promising candidates for power sources of electric vehicles. For further improvement of their efficiency in high current density operation, a better understanding of oxygen flow inside the cells, which have micro- or nanoporous structures, is necessary. Molecular simulations such as the direct simulation of Monte Carlo (DSMC) are necessary to elucidate flow phenomena in micro- or nanostructures since the Knudsen number is close to unity. Our previous report showed that the oxygen diffusion resistance in porous structures with a characteristic pore size of ˜100 nm calculated by DSMC agrees well with that measured experimentally. On the other hand, when it comes to the transport in structures with much smaller pore sizes, it is expected that the surface diffusion has a significant impact on gas transport because of their higher specific surface area. Here we present the calculation of gas transport in porous structures with considering surface diffusion. The numerical porous structure models utilized in our simulations are constructed from three-dimensional imaging of materials. The effect of the distance of random walk on the total diffusion resistance in the structures is discussed.

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