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Numerical Modeling and Prediction of Nanoscale Transport Phenomena in Vertically Aligned Carbon Nanotube Catalyst Layers by the Lattice Boltzmann Simulation

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Abstract : In this study, the nanoscale transport properties and catalyst utilization of vertically aligned carbon nanotube (VACNT) catalyst layers are computationally predicted by the three-dimensional lattice Boltzmann simulation based on the quasi-random nanostructural model in pursuance of fuel cell catalyst performance improvement. A series of catalyst layers are randomly generated with statistical significance at the 95% confidence level to reflect the heterogeneity of the catalyst layer nanostructures. The nanoscale gas transport phenomena inside the catalyst layers are simulated by the D3Q19 (i.e., three-dimensional, 19 velocities) lattice Boltzmann method, and the corresponding mass transport characteristics are mathematically modeled in terms of structural properties. Considering the nanoscale reactant transport phenomena, a transport-based effective catalyst utilization factor is defined and statistically analyzed to determine the structure-transport influence on catalyst utilization. The tortuosity of the reactant mass transport path of VACNT catalyst layers is directly calculated from the streaklines. Subsequently, the corresponding effective mass diffusion coefficient is statistically predicted by applying the pre-estimated tortuosity factors to the Knudsen diffusion coefficient in the VACNT catalyst layers. The statistical estimation results clearly indicate that the morphological structures of VACNT catalyst layers reduce the tortuosity of reactant mass transport path when compared to conventional catalyst layer and significantly improve consequential effective mass diffusion coefficient of VACNT catalyst layer. Furthermore, catalyst utilization of the VACNT catalyst layer is substantially improved by enhanced mass diffusion and electric current paths despite the relatively poor interconnections of the ion transport paths.

Keywords : Lattice Boltzmann method, nano transport phenomena, polymer electrolyte fuel cells, vertically aligned carbon nanotube
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