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Optimization of Platinum Utilization by Using Stochastic Modeling of Carbon-Supported Platinum Catalyst Layer of Proton Exchange Membrane Fuel Cells

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Abstract : The composition of catalyst layers (CLs) plays an important role in the overall performance and cost of the proton exchange membrane fuel cells (PEMFCs). Low platinum loading, high utilization, and more durable catalyst still remain as critical challenges for PEMFCs. In this study, a three-dimensional material network model is developed to visualize the nanostructure of carbon supported platinum Pt/C and Pt/VACNT catalysts in pursuance of maximizing the catalyst utilization. The quadruple-phase randomly generated CLs domain is formulated using quasi-random stochastic Monte Carlo-based method. This unique statistical approach of four-phase (i.e., pore, ionomer, carbon, and platinum) model is closely mimic of manufacturing process of CLs. Various CLs compositions are simulated to elucidate the effect of electrons, ions, and mass transport paths on the catalyst utilization factor. Based on simulation results, the effect of key factors such as porosity, ionomer contents and Pt weight percentage in Pt/C catalyst have been investigated at the represented elementary volume (REV) scale. The results show that the relationship between ionomer content and Pt utilization is in good agreement with existing experimental calculations. Furthermore, this model is implemented on the state-of-the-art Pt/VACNT CLs. The simulation results on Pt/VACNT based CLs show exceptionally high catalyst utilization as compared to Pt/C with different composition ratios. More importantly, this study reveals that the maximum catalyst utilization depends on the distance spacing between the carbon nanotubes for Pt/VACNT. The current simulation results are expected to be utilized in the optimization of nano-structural construction and composition of Pt/C and Pt/VACNT CLs.

Keywords : catalyst layer, platinum utilization, proton exchange membrane fuel cell, stochastic modeling
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