Three-dimensional modeling and experimental validation for study of species and charge transport phenomena in a direct methanol fuel cell

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An isothermal three-dimensional computational fluid dynamics model for a liquid-feed Direct Methanol Fuel Cell (DMFC) is presented to investigate the concentration distributions of reactants and resultants in the proton exchange membrane (PEM), fluid channels, gas diffusion layers (GDL) and catalyst layers (CL) under different operating conditions. Semi-empirical relationships based on Tafel equation are introduced to describe the electrochemical behaviors in the anode and cathode electrodes. Coefficients in these semi-empirical relationships are fitted using three-electrode experimental data, and the experimental polarization curve is compared to simulation results obtained from this model with the same temperature and fuel feeding conditions. Besides the operating conditions, this model also takes into account the effects of the physical properties of Membrane Electrode Assembly (MEA), including the porosity and electrical conductivity of GDL and CL, methanol permeability and proton conductivity of PEM, etc.

Figure 1. Fitted and experimental cathodic overpotential—current density curves with ±5% error line.

Figure 2. Fitted and experimental anodic overpotential—current density curves with ±5% error line.

Figure 3. Fitted and Experimental polarization curve of fuel cell with ±5mV error line.

Figure 4. Model calculation value with the cell voltage of 0.1, 0.2, 0.3, 0.4, 0.5 and 0.6V and experimental polarization curve of fuel cell.

Figure 5. Model calculated methanol concentration distribution in catalyst layer and flow field of anode with the cell voltage of 0.4V.

Reference
