Pore-scale simulation of water vapor generation, condensation, and transport in the cathode of a proton exchange membrane fuel cell

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Fundamental understanding of water transport in proton exchange membrane fuel cell (PEMFC) is of great importance for achieving high cell performance [1-4]. In this study, we propose a new lattice Boltzmann (LB) framework for pore-scale investigation of multi-component multiphase reactive transport in the porous media of PEMFC. Unlike most existing pore-scale simulations [3, 5-8] that relied on the assumption of equal density between liquid water and air/water vapor, the current LB framework can handle large density ratios between liquid and gas phases. Moreover, it can predict vapor to liquid condensation, as well as oxygen and water vapor transfer and heterogeneous surface chemical reactions. The LB framework is adopted to study the multiple coupled transport and interfacial processes taking place in the entire cathode of a PEMFC, including a heterogeneous catalyst layer (CL), a gas diffusion layer (GDL) and a gas channel (GC). The simulation results show that as the oxygen is consumed, water vapor is gradually generated in the catalyst layer. Once the concentration of the water vapor exceeds the local saturation level, the vapor condenses into liquid water and thus the initial single gas phase system becomes gas-liquid water two-phase. In the catalyst layer, liquid water is initially presented as micro droplets which then agglomerate into large droplets. As the solubility of oxygen in the liquid water is extremely low and electrochemical reaction mainly occurs at sites not covered by the liquid water, the liquid droplets tend to gradually grow towards regions with high vapor concentration, namely the regions free of liquid water. The liquid water gradually fills the pore space of the CL. When the entire CL is fully filled, the electrochemical reaction stops and no water is further generated. Under such circumstances, a continuous capillary flow of liquid water is unlikely to take place in a PEMFC, contrary to the assumption in previous pore-scale studies [4, 5, 7]. It is also found that liquid water will not only condense in the CL, but also in the GDL and even in the GC because water vapor diffuses into the GDL and GC and its concentration there may exceed the local saturation level due to reduced temperature from CL to GC, leading to continuous liquid flow. Thus, temperature plays an important role in the liquid water transport processes in the PEMFC, whose effect needs to be considered to form continuous capillary liquid flow in the PEMFC.

Keywords: proton exchange membrane fuel cell; multi-component multiphase reactive transport process; water; condensation; pore-scale; lattice Boltzmann method

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