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Invasion of Porous Layers for Electrochemical Processes: Experimental Studies and Lattice Boltzmann Simulations

In polymer electrolyte membrane water electrolyzers (PEMWE) and polymer electrolyte membrane fuel cells (PEMFC), efficient electrochemical reactions depend on the optimal flow of water and oxygen within porous electrodes. However, a significant challenge arises due to concentration losses, also known as diffusion overpotential or mass transport overpotential (V_{diff}). This phenomenon is attributed to mass transport limitations caused by the counter-current flow of reactants, such as water in PEMFC and oxygen in PEMWE in the pores of the electrodes. This limitation negatively impacts the voltage output, as the electrochemical reactions are not as efficient as they could be. Understanding and addressing these mass transport challenges is essential for improving the overall efficiency of polymer electrolyte membrane-based devices.

Based on the state of the art, Lattice Boltzmann Modeling (LBM) is used to investigate the two-phase flow in the porous transport layer (PTL) of PEMWE and the cathodic catalyst layer (CL) of PEMFC. For the first case, the invasion of O_2 in a water-saturated anodic PTL structure (drainage invasion process) is delineated with the implementation of the Shan-Chen LBM for PEMWE. The simulation results are discussed with respect to experimental findings and compared to pore network simulation results. For the second case, the model was tailored for the application to two-phase flow inside an initially empty GDL that is invaded by water at constant current density (imbibition invasion process). For this purpose, evaporation of water was additionally implemented in the LBM imbibition algorithm in order to investigate the relationship between water generation and removal by evaporation. For both studies, reconstructed pore structures from 3D tomography image data was used. We aim to present the overall methodology as well as the major outcomes of this study.

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