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Multi-Scale Modeling of Hydrogen Transport in a Porous Fuel Cell Anode

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Abstract

Proton-exchange-membrane fuel cells (PEMFC) are a clean energy conversion alternative to traditional fossil-fuel combustion; however, transport resistances in the electrode pose a lower-limit to catalyst loading and commercialization of PEMFCs. PEMFCs consist of simultaneous hydrogen (H_2) oxidation and oxygen (O_2) reduction at the anode and cathode, respectively. While oxygen transport resistances in PEMFCs have been widely studied both experimentally and analytically, hydrogen transport resistances are less understood. Herein, we present a physics-based model that encompasses multi-scale transport within the anode side of the PEMFC. The O_2 in the cathode here is omitted and replaced with H_2 to deconvolute O_2 transport resistance contributions, similar to that of a hydrogen pump. Replication of the hydrogen pump setup allows for comparison of the model against experimental analysis of H_2 gas-transport resistance in H_2 limiting-current experiments, which can also inform gas transport (including oxygen) in general. Herein, we present a multi-scale analytical model of the porous anode catalyst layers and individual catalyst agglomerates that enables determination of the effects of electrode morphology such as agglomerate size, catalyst loading, *etc*. on H_2 transport resistance through the porous electrode to complement and better understand H_2 limiting current experiments and deconvolute local H_2 transport resistances.

Electrodes within PEMFCs are heterogeneous porous structures formed by agglomerates of carbon particles containing Pt nanoparticles, held together by an ion-conducting polymer (ionomer). The gas transport hence involves transport through multiple phases and length-scales: (i) gas-phase transport through electrode pores at the length scale of electrode thickness (micrometer) and (ii) diffusion into the agglomerate through an ionomer film at the length scale of agglomerate radius (nanometer). Based on previous modeling efforts of varying length-scales of the catalyst layer, our analytical model adequately and simultaneously captures reaction-diffusion at all of the aforementioned scales (*i.e.*, the electrode thickness and agglomerate radius) to better describe porous anode performance. A sensitivity analysis is subsequently performed to compare current generated against transport parameters for both scales. This work ultimately

provides insight that will guide the design and engineering of future porous anodes for applications in hydrogen pumping and PEMFCs.