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Bridging Micro and Nano Scales in Fuel Cell Electrodes Using Multi-modal Imaging and Scale-Bridging Modeling

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Polymer-electrolyte fuel cell (PEFC) is a promising energy conversion technology with high thermodynamic efficiency, power density and zero-emission. Due to their low cost and material abundancy, PGM-free electrodes are promising candidates for meeting 2020 cost targets set by U.S. Department of Energy (DOE) [1]. However, to compensate the lower volume-specific activity, these catalyst layers are about an order of magnitude thicker compared to conventional Pt-based electrodes. Due to larger thickness, mass-transport and Ohmic losses can be significant within these PGM-free electrodes. Previous modeling efforts, which treat catalyst layer as a porous media with effective properties obtained with imaging methods (FIB-SEM, X-ray tomography), lack in capturing through-thickness morphology inhomogeneity. To better understand the influence of the electrode microstructure on the transport processes, we bridge micro and nano-scales obtained with X-ray computed tomography (CT) to model the transport processes in the PGM-free electrodes.

Two iteration algorithms for modeling scale-bridging between imaged morphology with micro X-ray CT and nano X-ray CT are presented. Micro X-ray CT can capture larger cracks and morphological inhomogeneity. Nano X-ray CT with higher resolution serves as a powerful tool to characterize the meso and nano-scale, which cannot be captured by micro X-ray CT due to imaging resolution limits. In both algorithms, the micro-scale domain is discretized in z-direction into a finite grid, where the effective properties of each grid cell are computed with nano-scale model at each iteration step. Furthermore, the micro- and nano-scale models are linked through boundary conditions. The algorithms work for Poisson's equations, where two boundary conditions are needed to solve the ODEs. In algorithm 1, micro-scale model generates Dirichlet boundary condition on node i and Neumann boundary condition on node i+1 for nano-scale model to compute the Dirichlet boundary condition for node i+1. Then this Dirichlet boundary condition is fed back to micro-scale model to renew the Neumann boundary condition on node i+1 until solution convergence is reached. In algorithm 2, micro-scale model generates Dirichlet boundary conditions on both sides of the element and passes them to nano-scale model to compute the Neumann boundary condition for node i+1. Then this information is fed back into micro-scale model to update the Dirichlet boundary condition on node i+1. The procedure repeats until the solution converges.

Transport processes in idealized geometries are calculated to assess the algorithms'effectiveness and to study the convergence rate. Then the two algorithms are applied to study the transport processes in the PGM-free electrodes of the PEFCs. A case study with the reaction rate as a function of local concentration has been studied. The spatial variations of the effective transport coefficient and reaction rate have been shown through the numerical results. The effective diffusivity and tortuosity are proved to be not only determined by the geometry of the material, but also influenced by the reaction rate and boundary conditions in the material. The new algorithms fully consider the influence of microstructure and spatial variations.

References:

[1] A. Kongkanand, M.F. Mathias, The Journal of Physical Chemistry Letters, 7 (2016) 1127-1137.

References

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