NAMS Abstract

Title: Methanol transport through hydrated Nafion examined using multi-scale simulation and experiment.

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Abstract: Polymer electrolyte membranes (PEMs) are an important class of membrane materials for a variety of energy applications. However, a general model for transport through these types of materials under realistic operating conditions has yet to be developed. In particular, the changes in polymer chain conformation and mobility in response to a strongly interacting permeant are often neglected. Herein, a model is developed for the specific case of methanol transport through hydrated Nafion. This system is chosen because of the sizeable amount of data available in the literature and because it is directly relevant to aqueous phase solar fuels devices and direct methanol fuel cells. Theoretical and experimental values are used to inform a fitting-parameter-free reaction-diffusion mechanistic scheme, including swelling, polymer response, and adsorption and desorption at the interfaces. The reaction-diffusion scheme is validated against experimental data on permeation and sorption, which were measured using attenuated total reflectance - Fourier transform infrared (ATR-FTIR) spectroscopy. It is shown that standard analytical models are insufficiently detailed to interpret data on this system. In particular, swelling can create interdependencies between the observed methanol and water data. This work builds towards a general framework for understanding and modeling transport through PEM at the level of fundamental physical chemistry.

Technical Program Topics and Session
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