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Mesoscopic modeling of porous media with application to electrochemical energy conversion and storage devices: the case of gas diffusion layers and proton-exchange membranes

Tuesday, 1 June 2021 11:15 (15 minutes)

Porous media are an integral part of energy conversion and storage electrochemical devices. Among them, we have gas diffusion layers (GDLs) and catalyst layers used in polymer electrolyte membrane fuel cells (PEMFCs), as well as fibrous electrodes used in redox flow batteries (RFBs) [1-10]. These porous media must fulfill several critical functions, such as providing a transport pathway for reactants/products through its pore volume and ensuring charge and heat conduction through its solid structure. Catalyst layers and active electrodes have the added functionality of providing a reactive surface area. Conduction in proton-exchange membranes (PEM) through water-filled ionic channels can also be modeled using percolation theory [11].

In this talk, an overview of mesoscopic modeling approaches applied to transport in GDLs and PEMs is presented. A composite continuum-pore network formulation is used to model two-phase transport in GDLs [9,10]. The composite model incorporates a control volume mesh at the layer scale, which embeds a structured cubic pore network. Capillary transport is simulated using the discrete pore network, considering the Purcell toroid model to determine the local entry capillary pressures of the fibrous material. The pore-network model is also used to determine analytically local anisotropic effective transport properties (local effective diffusivity and permeability), which are mapped onto the CV mesh to simulate transport within the porous layer using a continuum formulation. As a second example, proton conduction in multiblock copolymer membranes is modeled based on percolation theory [11]. The mesoscopic model solves simplified Nernst-Planck and charge conservation equations on a random cubic network. To mimic experimental conditions, hydrated sulfonated sites not connected to the edges of the domain are excluded from the network.

A comparison with experimental data is presented in terms of capillary pressure curves, water distribution and effective diffusivity in carbon-paper GDLs, as well as proton conductivity and water uptake in multiblock copolymer membranes of sulfonated polysulfone and polyphenylsulfone.

Time Block Preference

Time Block B (14:00-17:00 CET)

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