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Pore-scale Modeling of Transport Phenomena in a Vanadium Redox Battery using X-ray Tomography and the Lattice Boltzmann Method

ABHIJIT JOSHI, E. CAGLAN KUMBUR, YING SUN, Drexel University — The Vanadium Redox Battery (VRB) promises to be an attractive option for storing electrical energy from renewable energy sources and delivering the stored energy to the grid whenever it is required. In this work, a novel methodology is proposed for modeling the transport mechanisms in the VRB including the flow of electrolyte, chemical species transport through the electrolyte and electrochemical reactions at active sites. The detailed geometry of the electrode is obtained using X-ray computed tomography (XCT) and this geometry is characterized to calculate porosity, pore-size distribution, connectivity and the active surface area. The processed XCT data is then used as geometry input for modeling transport processes in the VRB. The flow of electrolyte through the pore-space within the electrodes and the transport of ionic species in these pores is modelled using the lattice Boltzmann method (LBM). An electrochemical model using the Butler-Volmer equations is used to provide species flux boundary conditions at the surface of the carbon fibers and to provide the necessary coupling to the local concentration of these species present in the pore space. Finally, model predictions for the steady-state discharge of the VRB are then compared with results reported in the literature.

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