

Integrating renewable energy technologies into the grid is necessary to enable a sustainable energy economy. Redox flow batteries (RFBs) are rechargeable electrochemical reactors that are promising for grid-level energy storage due to their ability to decouple energy and power. However, current flow battery designs are too expensive and must be optimized for widespread deployment. Porous electrodes are performance-defining components, as they must facilitate mass transport, provide surfaces for electrochemical reactions, and conduct electrons and heat. Therefore, optimizing porous electrodes offers a promising approach to decrease the cost. To accelerate progress, Multiphysics simulations can be leveraged to understand the influence of the electrode microstructure with increasing level of detail.

In this work, we developed a three-dimensional, electrolyte-agnostic electrochemical pore network model (PNM) integrated in an open access platform (OpenPNM). The model was validated using a symmetric cell for three distinct chemistries ($\text{Fe}^{2+}/\text{Fe}^{3+}$, $\text{VO}^{2+}/\text{VO}_2^+$, and $\text{TEMPO}/\text{TEMPO}^+$). The electrode geometry was reconstructed over a dry x-ray computer tomograph and solved for the electrolyte fluid transport, species transport, and charge transport with low computational cost. The model accurately predicts the electrochemical performance, allowing rapid benchmarking of porous electrode microstructures in a time-efficient manner.