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Towards bottom-up design of porous electrode microstructures - coupling genetic algorithms with pore network modeling of redox flow battery electrodes

Tuesday, 1 June 2021 10:00 (1 hour)

Integrating renewable energy technologies into the grid is necessary to enable a sustainable energy economy but is currently challenged by their intrinsic intermittency. 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 RFB systems remain too costly for widespread deployment [1]. Porous electrodes are performance-defining components as they must facilitate mass transport, provide surfaces for electrochemical reactions, and conduct electrons and heat. Thus, optimizing the porous electrode microstructure offers a promising pathway to cost reduction by increasing power density [2], [3]. Traditional, empirical design of electrodes is time- and resource-intensive and does not enable exploration of the wider design space but is currently limited to carbonaceous fibrous structures. To accelerate progress, microstructure-informed multiphysics simulations (e.g. pore network modeling, lattice Boltzmann) can be leveraged to aid the theoretical understanding and design of advanced electrode architectures but has been limited to exploration of existing, carbon-fiber based electrodes [4]–[6]. In this work, we explore the following scientific question: *Can we deploy three-dimensional simulations in combination with evolutionary algorithms to enable artificial generation of electrodes from the bottom-up?*

In the first part of this talk, the modeling framework will be introduced. We developed a microstructure-informed, electrolyte-agnostic electrochemical pore network model (PNM) integrated in an open access platform (OpenPNM) [6], [7]. The model was validated using a symmetric flow cell for two distinct electrolytes (an aqueous Fe2+/Fe3+ and a non-aqueous TEMPO./TEMPO+) and two types of porous electrodes (a carbon paper -Freudenberg H23- and a carbon cloth -ELAT Cloth-). The dry electrode microstructure was obtained with x-ray computed tomography and converted into a network of spherical pores and cylindrical throats using the SNOW algorithm [8]. The electrochemical model is solved for the electrolyte fluid transport, species transport, and charge transport with low computational cost (123,335 pores, 60-120 min on an Intel® Core(TM) i7-8750H CPU). For the non-aqueous electrolyte, the model accurately predicts the electrochemical performance without fitting parameters, allowing rapid benchmarking of porous electrode microstructures in a time-efficient manner. For the aqueous electrolyte, we find that incomplete wetting of the electrode results in overprediction of the electrochemical model that assumes one-phase flow and employ thermal pretreatment to demonstrate the importance of complete wetting on the modeling validation [9]. Fitting of the near-surface mass transfer coefficient enables accurate representation of the experimental data. Finally, the PNM framework was coupled with a genetic algorithm based on Darwin's evolutionary theory that is used to perform artificial generation of porous electrodes for RFBs from the bottom-up. With this method, chemistry-specific electrode architectures can be optimized based on the electrolyte properties alone.

Time Block Preference

Time Block A (09:00-12:00 CET)

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