Title: Starting from the bottom: Coupling a genetic algorithm and a pore network model for porous electrode design

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Porous electrodes are performance- and cost-defining components in modern electrochemical systems as they provide surfaces for electrochemical reactions, facilitate mass transport, conduct electrons and heat, and determine the hydraulic resistance [1]. Hence, electrode engineering is a valid approach to increase power density and improve const competitiveness. In convection-enhanced technologies, currently used porous materials are fibrous carbonaceous electrodes developed for low temperature fuel cells; yet their microstructure and surface chemistry limits the performance of emerging electrochemical systems such as redox flow batteries. Moreover, the empirical design of these electrodes is time- and resource-intensive which limits exploration of the wider design space. Microstructure-informed multiphysics simulations can be leveraged to aid the theoretical understanding and design of advanced electrode architectures [2]. However, while these simulations have improved our understanding, they have only recently [3] been deployed to realize the bottom-up design of electrode microstructures. The combination of microstructure-informed multiphysics with evolutionary algorithms could accelerate progress in the optimization of porous electrodes for specific applications. In this work, we deploy three-dimensional simulations in combination with a genetic algorithm for the bottom-up design of porous electrodes for redox flow batteries.

In the first part of the talk, the coupling of a pore network modeling framework [4] with an evolutionary algorithm [5] is described. The pore network model is a microstructure-informed, electrolyte-agnostic simulation framework for flow batteries utilizing a network-in-series approach to account for species depletion over the entire length of the electrode, developed using an open-access platform (OpenPNM) [6]. The electrochemical model is solved for the electrolyte fluid transport and couples both half-cells by iteratively solving the species and charge transport at a low computational cost. In the genetic algorithm, the electrode microstructure evolves driven by a fitness function that minimizes pumping power requirements and maximizes electrochemical power output, where the optimization only relies on the electrolyte chemistry and initial electrode morphology and flow field geometries as inputs. The analyzed proof-of-concept employs a flow-through cubic lattice structure with fixed pore positions and shows significant improvement of the fitness function over 1000 generations, where the fitness improved by 75% predominantly driven by reducing the pumping requirements by 73%. The evolutionary design resulted in a bimodal pore size distribution containing longitudinal electrolyte flow pathways of larges pores. Additionally, we found an increase in surface area at the membrane-electrode interface resulting in a 42% enhancement of the electrochemical performance.

In the second part of the talk, I will discuss our latest progress in the development of the topology optimization by implementing commercial fibrous electrodes as offspring networks, integrated flow field geometries, and extended evolutionary freedom during the optimization. Coupling the genetic optimization to the desired flow field geometry affects the evolution of the fitness function, shifting the balance between electrochemical and hydraulic performance,

highlighting the importance of the coupled optimization of flow fields and electrodes. By including more evolutionary freedom in the algorithm (i.e., by allowing merging and splitting of pores outside fixed coordinates), existing fibrous electrodes can be enhanced by for example reducing their pumping losses. The presented genetic algorithm offers great potential for the predictive design of electrode microstructures tailored for specific reactor architectures and redox chemistries. Hence, this framework can be used to accelerate and broaden the design and fabrication process of advanced electrode structures. Although applied to flow batteries in this study, the methodology can be leveraged to advance electrode microstructures in other electrochemical systems by adapting the relevant physics.

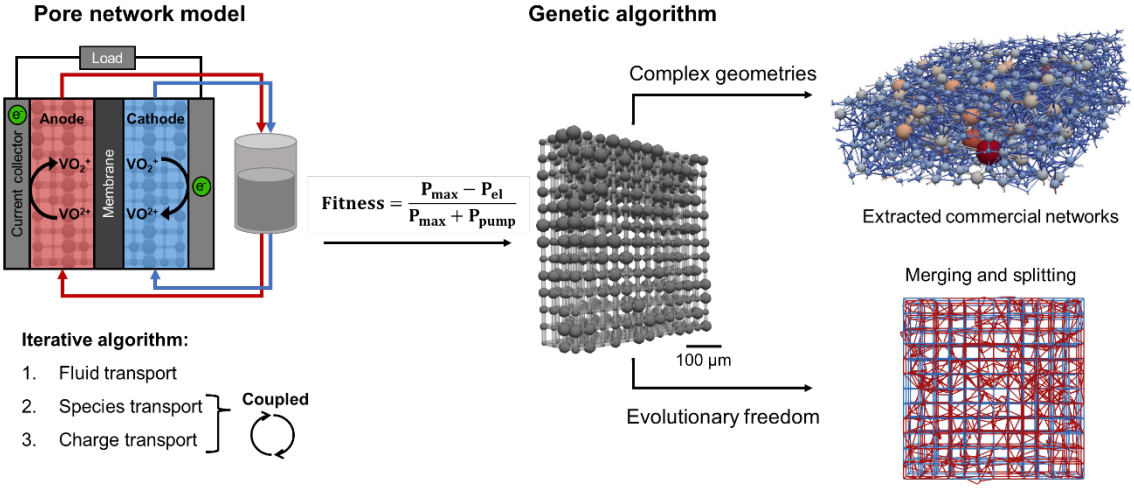

Figure 1: Schematic representation of the pore network model and genetic algorithm framework. The pore network model is solved for the electrolyte fluid transport and couples both half-cells by iteratively solving the species and charge transfer. This model is coupled to a genetic algorithm that evolves the porous electrode microstructure driven by a fitness function that minimizes pumping power requirements and maximizes electrochemical power output. By implementing complex geometries and evolutionary freedom, the genetic algorithm offers great potential for the predictive design of electrode microstructures tailored for specific reactor architectures and redox chemistries

References

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