Title: A versatile optimization framework for porous electrode design: Coupling a genetic algorithm and a pore network model

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Porous electrodes are performance- and cost-defining components in modern electrochemical systems as they determine the hydraulic resistance, facilitate mass transport, conduct electrons and heat, and provide surfaces for electrochemical reactions [1]. Thus, electrode engineering is an effective approach to improve cost competitiveness by increasing power density. In convection-enhanced technologies, currently used porous electrodes are fibrous substrates developed for low-temperature fuel cells, but their microstructure and surface chemistry limit the performance of emerging electrochemical systems. Microstructure-informed multiphysics simulations can be leveraged to aid the theoretical design of advanced electrode architectures [2]. However, they have only recently been deployed for the bottom-up design of electrode microstructures [3]. The combination of microstructure-informed multiphysics with evolutionary algorithms could accelerate progress in the optimization of porous electrodes for a given application. In this work, we combine three-dimensional simulations with a genetic algorithm for the bottom-up design of porous electrodes for redox flow batteries.

In the first part of the talk, I will describe a methodology to couple an experimentally validated pore network modeling framework that is microstructure-informed and electrolyte-agnostic [4], with an evolutionary algorithm [5]. This genetic algorithm is used to optimize electrode microstructures by evolving the structure 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 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. The fitness improved by 75% driven by a reduction in the pumping requirements by 73% and an enhanced electrochemical performance of 42%. The evolutionary design resulted in a bimodal pore size distribution containing longitudinal electrolyte flow pathways of large pores and an increased surface area at the membrane-electrode interface.

In the second part, I will discuss our latest progress including the introduction of geometrical versatility by adding a pore merging and splitting function, the impact of various optimization parameters, geometrical definitions, and objective functions, and the incorporation of electrode structures and flow fields with well-defined geometries [6]. Moreover, I will show the need for optimizing electrodes for specific reactor architectures and operating conditions to design next-generation electrodes by analyzing the optimization for initial starting geometries with diverse flow field designs (flow-through and interdigitated), morphologies (cubic and a tomography-extracted commercial electrodes), and redox chemistries (VO^{2+}/VO_2^+ and TEMPO/$TEMPO^+$). The presented genetic algorithm offers potential for the predictive design of high-performance electrode microstructures for a broad range of operating conditions, electrolyte chemistries, reactor designs, and electrochemical technologies. While applied to flow batteries in this study, this methodology can be leveraged to advance electrode microstructures in other electrochemical systems by adapting the relevant physics.

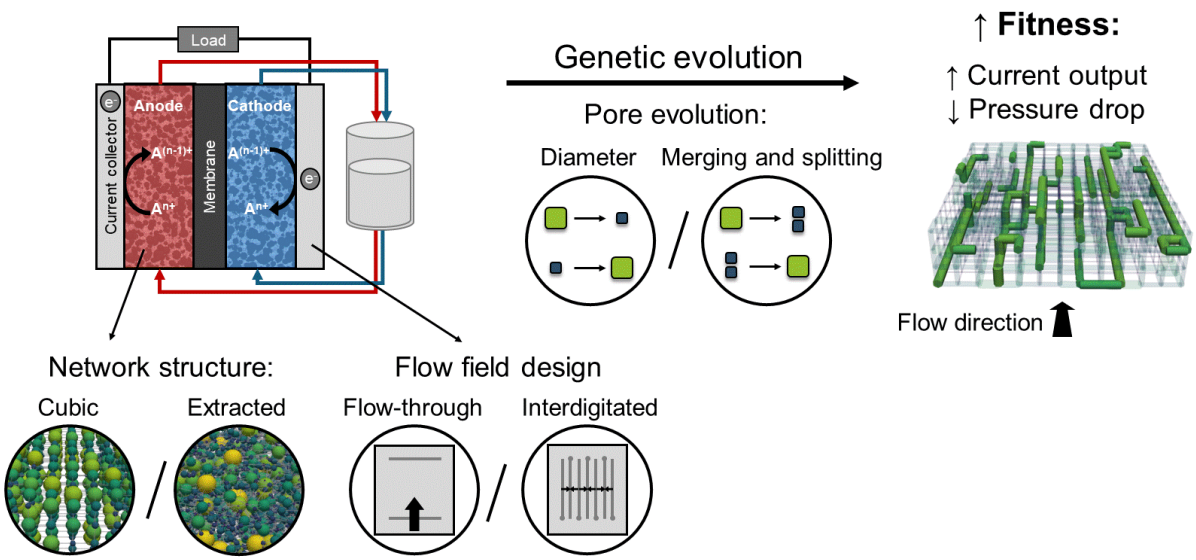

Figure 1: An optimization tool is presented by coupling a genetic algorithm with a pore network modeling framework for the bottom-up design of porous electrodes for a broad range of operating conditions, electrolyte chemistries, and reactor designs.

Acknowledgments

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References

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