Starting from the bottom: Coupling a genetic algorithm and a pore network model for redox flow battery porous electrode optimization

Maxime van der Heijden[1*], Rik van Gorp[1], Gabor Szendrei[1], Victor de Haas[1], Mohammad Amin Sadeghi[2], Jeffrey Gostick[2], and Antoni Forner-Cuenca[1]

[1]Eindhoven University of Technology, (Chemical Engineering and Chemistry), (Membrane Materials and Processes), 5600 MB Eindhoven, Netherlands
[2]University of Waterloo, (Chemical Engineering), Waterloo, ON, Canada
m.v.d.heijden@tue.nl

Porous electrodes are performance- and cost-defining components in modern electrochemical systems as they facilitate mass transport, conduct electrons and heat, determine the hydraulic resistance, and provide surfaces for electrochemical reactions [1]. Combining microstructure-informed multiphysics simulations with evolutionary algorithms can accelerate progress in the optimization of porous electrodes as a pathway to system cost reduction. In this work, we deploy pore network modeling in combination with a genetic algorithm for the bottom-up design of porous electrodes for redox flow batteries.

In the first part, the coupling of an experimentally validated microstructure-informed, electrolyte-agnostic pore network modeling framework [2] with an evolutionary algorithm [3] is described. This genetic algorithm is used to optimize electrode microstructures by evolving the structure driven by a fitness function that maximizes electrochemical power output and minimizes pumping power requirements. The analyzed proof-of-concept flow-through cubic lattice structure with fixed pore positions shows significant improvement in the networks' fitness 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%, resulting in a bimodal pore size distribution with large-pore longitudinal electrolyte flow pathways.

In the second part, I will discuss our latest progress on the genetic algorithm by implementing commercial fibrous electrodes as offspring networks, integrated flow field geometries, and extended evolutionary freedom during the optimization (i.e., merging and splitting of pores outside fixed coordinates). Coupling the genetic optimization to the desired flow field geometry affects the evolution of the fitness function, shifting the balance between hydraulic and electrochemical performance. By including more evolutionary freedom, existing electrodes can be enhanced. This algorithm offers great potential for the predictive design of electrode microstructures for specific electrochemical systems. Hence, this framework will accelerate and broaden the design and fabrication of advanced electrode structures.

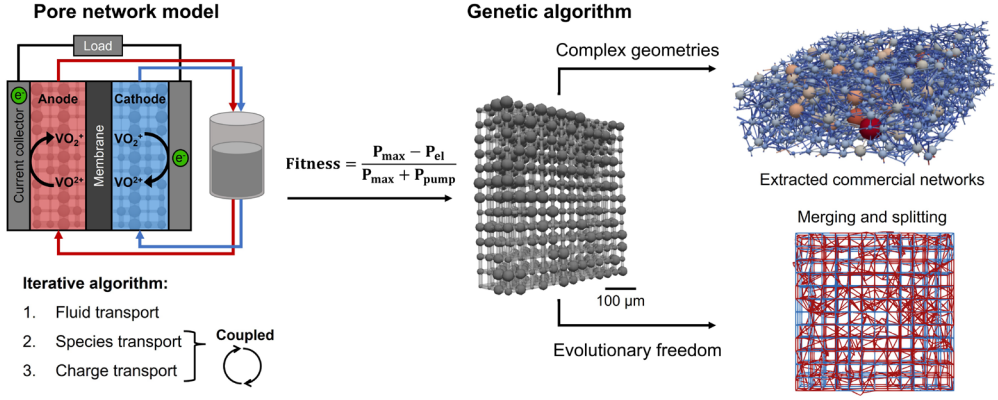

Figure 1: Schematic representation of the pore network model and genetic algorithm framework. The pore network model is coupled to a genetic algorithm that evolves the porous electrode microstructure driven by a fitness function. By implementing complex geometries and evolutionary freedom, the genetic algorithm offers great potential for the predictive design of electrode microstructures tailored for specific reactor architectures and redox chemistries.

[1] M. van der Heijden, A. Forner-Cuenca, *Encyclopedia of Energy Storage*, 480-499 (2022)
[2] M. van der Heijden & R. van Gorp *et al.*, *J. Electrochem. Soc.*, **169** 040505 (2022)
[3] R. van Gorp & M. van der Heijden *et al.*, *Chem. Eng. J.*, 139947 (2022)