Topology optimization of porous electrodes for redox flow batteries using the finite element method

Mojtaba Barzegari*, Martin de Waal, Pedro de Carvalho, Antoni Forner-Cuenca
Electrochemical Materials and Systems, Department of Chemical Engineering and Chemistry
Eindhoven University of Technology (TU/e), Eindhoven, The Netherlands
**m.barzegari.shankil@tue.nl*

Redox flow batteries (RFBs) are a class of rechargeable electrochemical systems that are particularly promising for grid-level electricity storage, leveraging electroactive species dissolved or suspended in liquid electrolytes that are pumped to an electrochemical reactor where they undergo electrochemical reactions on the surface of porous electrodes to charge and discharge the battery [1].
To increase the cost-competitiveness of the technology, one strategy is to design electrochemical reactors with higher power density and, in this perspective, the optimization of the cell components (e.g. electrodes, flow fields, membranes) is essential. In RFBs, porous electrodes are performance-defining components affecting the thermodynamics, kinetics, and transport, where the flow distribution, surface area, and transport of species are critical for obtaining high power and electrochemical performance [2]. Traditional and empirical design methodologies are slow and take enormous resources and time. However, computational techniques have the potential to provide a unique perspective to guide the design of porous electrodes, an example of which is predictive inverse design algorithms such as topology optimization (TO). Rather than evaluating the performance of a proposed setup, this method involves setting a performance target and iterating over permissible architectures to meet it [3, 4].
In this project, we have developed a high-performance TO framework for two- and three-dimensional porous electrodes in RFBs integrated with multi-physics computational models of transport processes correlating how reactor design influences RFB performance. This was achieved by numerically solving transport and kinetics equations using the finite element method implemented in the open-source code Firedrake. The macroscale TO problem was formulated to maximize electrochemical performance under a controllable pumping power loss, in which the porous electrode was considered as a macroscopic porosity-variable block in a half-cell of an RFB-like setup (Fig 1-A).
The resulting designs (Fig 1-B) may seem non-intuitive, but their performance is higher than uniform porosity electrodes from the perspective of minimizing the ohmic, kinetics, and pumping power losses of RFBs across various operating conditions. The porosity-variable electrodes can be converted to cellular architectures and triply periodic minimal surface structures to be manufactured using stereolithography 3D printing followed by carbonization, the output of which will be used to assess the performance of the inversely designed electrodes in a real setup.

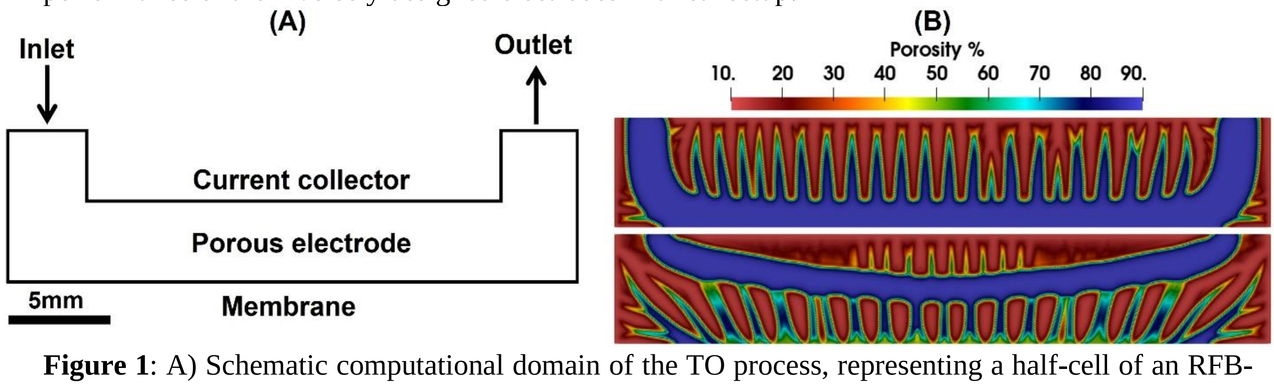

Figure 1: A) Schematic computational domain of the TO process, representing a half-cell of an RFB-like setup, B) Sample results of the TO framework showing the optimized porosity field across the porous electrode. Higher current density and electrolyte conductivity were applied in the top simulation.

References:
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3. Roy et al. *Struct. Multidiscip. Optim.* **65** (2022).
4. Beck et al. *J. Power Sources* **512**, 230453 (2021).