Inverse design of porous electrodes in redox flow batteries: a computational approach integrating topology optimization and multi-physics modeling

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ABSTRACT

The increasing effects of global climate change urge a global energy transition, in which large-scale storage of renewable energy technologies is expected to play a primary role. Redox flow batteries (RFBs) have emerged as a promising technology for grid-scale energy storage with appealing features such as higher durability and power-energy decoupling. During the RFB operation, the liquid electrolytes, stored in external tanks, are actively circulated through the electrochemical stack consisting of flow fields, porous electrodes, and membranes, where electrochemical reactions take place on the surface of the porous electrodes, which are performance-defining components [1]. Despite its advantages, RFB technology has seen limited adoption due to economic and technical challenges. Aiming to boost cost-effectiveness, one effective strategy is to increase the stack power density by increasing the efficiency of the electrodes leading to an increase in the overall system performance [2]. Optimizing reactor performance is challenging due to seemingly contradictory requirements such as providing high surface area for reactions, reducing ohmic drop across the cell, facilitating mass transport in porous media, and reducing pumping power requirements.

Parallel to experimental research, computational techniques have the potential to accelerate and guide the design of porous electrodes. An emerging approach in this regard is to use predictive design algorithms that invert the design process and enable the exploration of a broader design space. Topology optimization (TO) is a powerful inverse design technique combining numerical simulations with mathematical optimization algorithms, which involves setting a performance target of minimizing the pumping power and overpotential losses and iterating mathematically over various electrode structures to satisfy the target [3, 4]. This approach requires integrating two different types of models: 1) multi-physics models to build a theoretical framework to adequately relate the local electrode properties to the overall RFB performance, and 2) TO models to inversely design microarchitected variable porosity 3D porous electrodes.

In this research, we have developed a high-performance TO framework for three-dimensional porous electrodes in next-generation RFBs integrated with multi-physics computational models of mass, momentum, and charge transport processes using the porous electrode theory, in which the electrode was considered as a macroscopic porosity-variable block. The model was developed using finite element/volume methods implemented using the open-source codes Firedrake, OpenFOAM, and PETSc. The macroscale TO problem was formulated to maximize electrochemical performance under a controllable pumping power loss in a half-cell redox flow cell. The resulting designs were transformed into cellular architectures using triply periodic minimal surface (TPMS) structures and additively manufactured using stereolithography 3D printing followed by carbonization, the output of which can be used to assess the performance of the inversely designed electrodes in a real setup.

In this presentation, I will first discuss the structure of the multi-physics modeling approach. Second, I will present the integration of these models into the TO algorithms. Finally, I will show the transformation of the TO results into cellular infills and will highlight some technical aspects of the manufactured TPMS structures.

References

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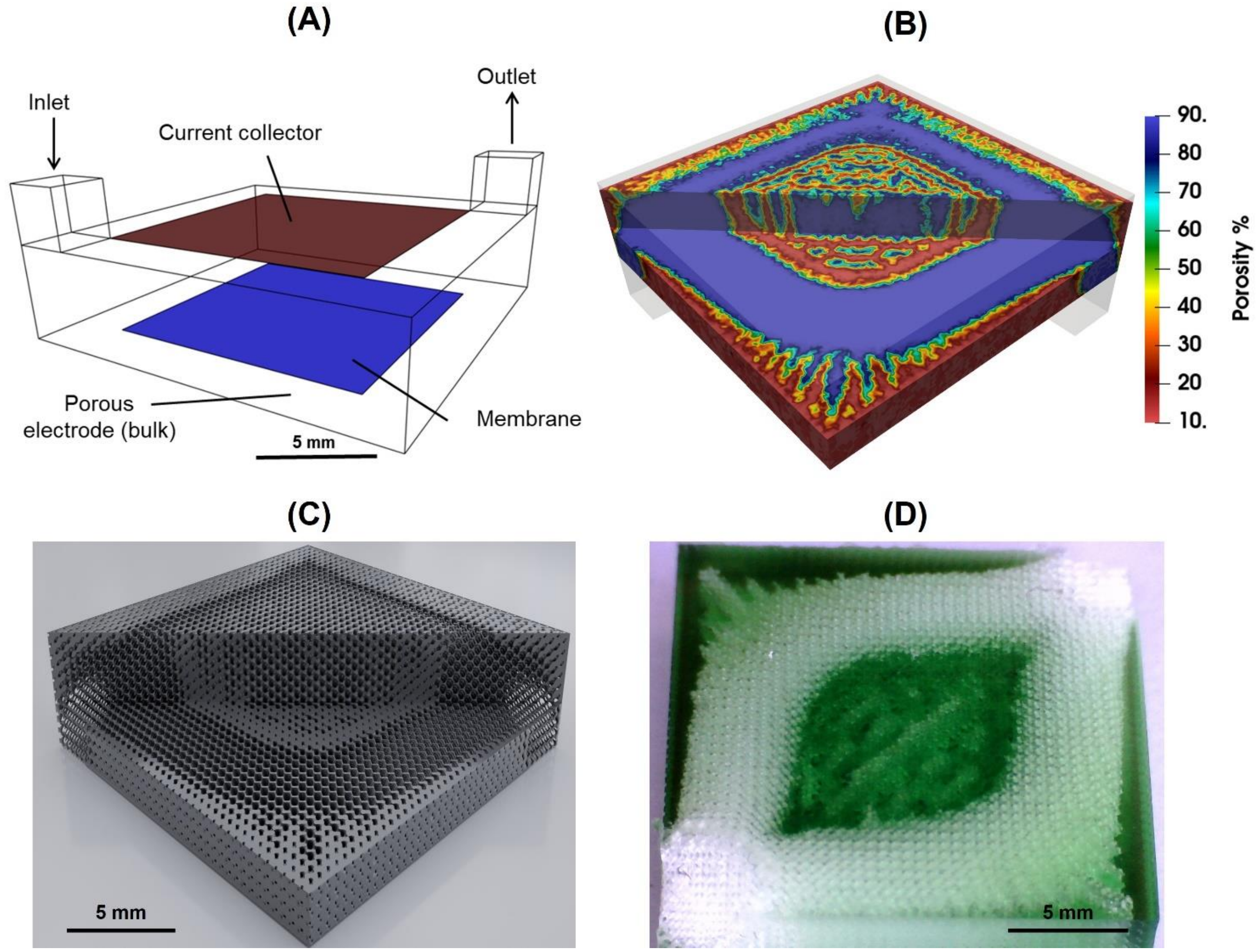

Figure 1: A) Considered geometry of the half-cell of an RFB with the labeled boundaries, B) Topology optimization result of the 3D geometry for a certain applied current density and solution conductivity, visualized as cross-section cuts on the porosity field mapped into the range of [0.1, 0.9], C) Converted TPMS geometry using Gyroid unit cells, demonstrating how the volume fraction of the cells changes to reflect the porosity field, D) 3D printed sample from the TPMS infills showing the surface that faces the current collector.