TopeSmash: Topology Optimization of Porous Electrodes in Redox Flow Batteries using Scalable Modeling Approaches

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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. 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. The porous electrodes used in RFBs play a critical role in determining the battery's performance by affecting the thermodynamics, kinetics, and transport phenomena [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]. Project TopeSmash aims to develop novel computational models for accelerating the design of porous electrodes and understanding the role of structure in their performance. The project proposes using topology optimization (TO) to design microarchitected variable porosity 3D porous electrodes for RFBs to decrease power losses across various operating conditions. 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 TopeSmash project, we have developed a high-performance TO framework for 3D porous electrodes in next-generation RFBs. The models were developed across various length scales using finite element/volume/difference methods implemented using the open-source codes Firedrake, OpenFOAM, and PETSc and in-house CUDA codes. The resulting TO designs were transformed into cellular architectures using triply periodic minimal surface (TPMS) structures using open-source codes ASLI and CGAL, the output of which were additively manufactured using stereolithography 3D printing to assess the performance of the inversely designed electrodes in a real setup. We extensively use the CPU and GPU nodes of Snellius for the above computational workflow.

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 framework. Finally, I will show the transformation of the TO results into cellular infills. I will highlight how we employ Snellius in each of the mentioned steps.

References

1. Alotto et al. *Renew. Sustain. Energy Rev.* **29**, 325–335 (2014).
2. B. K. Chakrabarti et al., *Sustainable Energy & Fuels.* **4**, 5433–5468 (2020).