

TOPOLOGY OPTIMIZATION FOR ENGINEERED FLOW BATTERY ELECTRODES

Victor Beck, Todd Weisgraber, Anna Ivanovskaya, Swetha Chandrasekaran, Bryan Moran, Seth Watts, Daniel Tortorelli, Eric Duoss, Juergen Biener

Lawrence Livermore National Laboratory, United States

beck33@llnl.gov, weisgraber2@llnl.gov, ivanovskaya1@llnl.gov, chandrasekar2@llnl.gov, moran5@llnl.gov, watts24@llnl.gov, tortorelli2@llnl.gov, duoss1@llnl.gov, biener2@llnl.gov

Keywords: Topology optimization, flow batteries, electrochemistry, multidisciplinary optimization

Abstract: Flow batteries are a promising technology for large scale energy storage and load balancing from intermittent power sources, but their viability hinges on our ability to attain high-power outputs while minimizing costs and meeting performance constraints. Effective engineering of these systems is further complicated both by limitations on the control of the electrochemical cell component morphologies across scales and accurate modeling of the multiple, simultaneous physical processes. At Lawrence Livermore National Lab, we have pioneered a potential solution to this problem using additive manufacturing techniques which enable hierarchical structures controlled from the sub-micron through the centimeter length scales. Yet, even with this expanded design space, the complexity and tight coupling of the underlying physical processes remains as an obstacle to effective design: Apparently obvious choices can nevertheless lead to an unexpected adverse performance impact. To address this challenge, we present an automatic design methodology to optimize the electrode topology over precisely defined performance criteria. We combine forward physics solvers for the full, multidisciplinary electrochemical problem, including fluid flow, electrochemistry and mass transfer, with adjoint solvers to determine topological sensitivities. Our algorithms compute optimal electrochemical cell geometries which are then physically created using additive manufacturing techniques and post-processed to create carbon electrodes. Our work provides a systematic path toward rational design of cost-effective, high-power flow batteries.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.