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# Mesoscale modeling of electrochemical reactive transport in Unitized Reversible Fuel Cells

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Global climate change is a pressing issue that has prompted humankind to reduce the overutilization of fossil fuels to fulfill their energy demands. Accordingly, renewable energy sources, such as wind, solar, and geothermal have gained significant attention in recent years, catering to an ever-increasing proportion of the overall energy supply chain. However, the intermittent nature of these renewable sources precludes their continuous application, thereby leading to the introduction of secondary batteries or reversible fuel cells (RFCs) in the energy mix for long-duration storage [1]. Polymer Electrolyte Membrane Unitized Reversible Fuel Cells (PEM-URFCs) is an environmentally benign electrochemical device that offers round-trip energy conversion by integrating a fuel cell (FC) mode with an electrolysis cell (EC) mode. Owing to its distinct advantages, such as high specific energy density, compact design, and zero tailpipe emissions, PEM-URFCs are used in a gamut of applications such as spacecraft, solar rechargeable aircraft, and residential power sources [2]. As the pursuit to develop next-generation PEM-URFCs continues, optimizing the porous catalyst layer (CL) design –primarily the oxygen electrode, which hosts the sluggish oxygen reduction reaction (FC mode), and oxygen evolution reaction (EC mode) is essential. Particularly important is controlling the microfluidics of fluid flow at the interfaces (water drainage for FC vs supplement for EC mode), which depends on a detailed mechanistic understanding of the multiphase reactive transport interactions occurring within the CLs. In this work, we present a mesoscale modeling framework to probe the electrochemical landscape of the PEM-URFC. The input to this workflow is stochastically generated realistic CL structures with various microstructural attributes such as pore size, ionomer content, and electrode thickness. Reactive transport simulations employing pore-network modeling [3] are subsequently performed on these structures to analyze the underlying electrochemical signatures. We further reveal the influence of CL structural parameters on the resulting ohmic overpotentials and mass transport limitations within a wide range of operating conditions. A mesoscale optimization study demonstrated in this work aims at unraveling the intricate structure-transport-process-performance relationships in the catalyst layers of PEM-URFCs.

## Country

United States

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## References

[1] Wang, Yifei, et al. "A review on unitized regenerative fuel cell technologies, part-A: Unitized regenerative proton exchange membrane fuel cells." Renewable and Sustainable Energy Reviews 65 (2016): 961-977. [2] Sadhasivam, Thangarasu, et al. "A comprehensive review on unitized regenerative fuel cells: Crucial challenges and developments." International Journal of Hydrogen Energy 42.7 (2017): 4415-4433. [3] Gostick, Jeff, et al. "OpenPNM: a pore network modeling package." Computing in Science & Engineering 18.4 (2016): 60-74.

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