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Virtual Analysis of Gas-Diffusion-Electrode O₂ Electrolyzers

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Abstract

The electrochemical reduction of CO₂ (CO₂R) to value-added products is an attractive technology for tackling the rising atmospheric CO₂ levels and storing intermittent renewable energy into chemical bonds. Fundamental understanding of CO₂R has progressed significantly in recent years and is critical in the development of CO₂R to liquid-fuel electrolyzers, where gas-diffusion electrodes (GDEs) have been shown to be key enabling architectures. Various designs have been proposed and studied in the literature to enhance overall selectivity, rates, and maximize the conversion of CO₂, the latter of which is only now being recognized as a critical issue. In this respect, there is a need to explore the governing phenomena inherent in these architectures to enable optimization. Mathematical modeling is ideally suited to tackle and explore these multiphysics interactions and provide virtual design analysis.

In this talk, we discuss modeling methodologies and physics inherent in these devices and present our recent modeling of GDEs for CO₂ reduction. We specifically examine the impacts of multiphase flow and related phenomena on overall cell performance. We then explore the performance and limitations of various cell designs guided by simulation results and examine potential methods for improving water management and tuning catalyst selectivity including the use of different anion-exchange and bipolar membranes. Finally, we discuss the disparities in local environments between aqueous and GDE devices and propose strategies to reduce the gap in knowledge between the two systems.

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