A Distributed Electrochemistry Modeling Framework for Investigating Factors Affecting the Performance of Solid Oxide Fuel Cells

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The poster presents a cell-level distributed electrochemistry (DEC) modeling tool that has been developed at PNNL to provide a framework for simulating initial SOFC performance with the long-term goal of investigating electrode damage and performance degradation over the lifetime of the cell. The modeling tool can investigate SOFC performance by considering the coupled and spatially varying multi-physics that occur within the tri-layer. The approach calculates the distributed electrochemistry within the electrodes using a continuum-scale effective properties model, which includes the charge transfer and electric potential fields, ion transport throughout the tri-layer, and gas distributions above and within the composite porous electrodes.

Model validation via comparison of simulation results with experimental data is presented, followed by example applications of the model that explore SOFC performance as affected by electrode microstructural parameters including: pore size and porosity, electrolyte and electrode phase volume fractions, triple-phase-boundary length, and particle size. An example exploring experimental design is also presented, along with initial work on modeling degradation in the SOFC electrodes by considering the effect of chemical mechanisms that mask reaction surfaces, block pores, or alter the electrode microstructures. With this modeling tool we'll be able to examine electrode degradation and performance decay.