MICROSTRUCTURAL AND CONTINUUM ELECTROCHEMISTRY MODELS

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In this paper, we presented two levels of electrochemical modeling for solid oxide fuel cells: continuum and microstructural electrochemistry. Continuum electrochemical models to be used for stack design and optimizing material properties have been developed. The stack electrochemistry model calculates the current electrical density, cell voltage, and heat production in solid oxide fuel cell stacks with H_2 or other fuels, taking into account as inputs local values of the gas partial pressures and temperatures. This approach is based on an existing current-voltage (I-V) relation. The model includes the heat generation from both Joule heating and chemical reactions. It also accounts for species production and destruction via mass balance. The model is linked to the finite element analyses code MARC and computational fluid dynamics code Star-CD to allow evaluations of temperatures and stresses during steady state operations. Three-dimensional model geometry, including internal manifolds, was created to simulate a cross-flow stack design. Similar three-dimensional geometries were created for simulation of co-flow and counter flow stack designs. This tool and others are being used to assist in design optimization of cells and stacks for optimum performance. Parameters being optimized include cell performance at high fuel utilization, uniformity of gas flows, and thermal and mechanical stress profiles during stack operation and startup/shutdown. Also a detailed micro-structural electrochemistry models for cell design and optimizing of material properties were developed. The models are capable of simulating the performance of porous electrode materials by based on the microstructure of the material, the distribution of reaction surfaces, and the transport of oxygen ions through the material. We perform lattice Boltzmann simulations on the detailed local micro-structural geometry using the CHEMKIN and SURFACE-CHEMKIN simulation packages to describe the chemical kinetics. We discuss in the paper results based on the continuum electrochemistry and the microstructural models.