A Two-Dimensional Model of a Single-Chamber SOFC with Hydrocarbon Fuels

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The single chamber fuel cell (SCFC) is a novel simplification of the conventional solid oxide fuel cell (SOFC) into which a premixed fuel/air mixture is introduced. It relies on the selectivity of the anode and cathode catalysts to generate a chemical potential gradient across the cell. For SCFC running on hydrocarbon fuels, the anode catalyst promotes in-situ internal reforming of the hydrocarbon and electrochemical oxidation of the syngas, while the cathode catalyst reduces oxygen simultaneously. Laboratory tests of small designs of such fuel cells have demonstrated excellent electrical performance (1, 2).

Although the power output is typically less than that of conventional dual-chamber designs, the much lower operational temperature range, higher thermal and mechanical shock resistivity, and lack of seals, make it an ideal solution to a variety of applications (3). However, many issues need to be resolved before the benefits of SCFCs can be realized. For SCFC systems, a major question is the optimum fuel to air ratio. The achievable efficiency is also of great interest. The optimization of SCFC stacks and scale-up also requires understanding of such questions as how to minize the oxidation of electrochemical fuels at the cathode, how to deploy the MEAs (membrane-electrolyte-assembly) ideally in the gas channel, what the best electrode and electrolyte parameters are, etc.

To answer these questions, we have developed a computational model that accounts for the coupled effects of gas channel fluid flow, heat transfer, porous media transport and chemistry in the electrodes, and electrochemistry at the electrode-electrolyte interfaces. In the gas channel, the set of partial differential equations describing the transport of momentum, species and energy is integrated with the SIMPLEC algorithm, and isothermal computation can handle the interaction of multiple MEAs in the channel.

For the anode, an elementary heterogeneous reaction mechanism of methane partial oxidation over Ni is used, consisting of 46 heterogeneous reactions between 6 gaseous species and 13 adsorbed surface species (4). The cathode mechanism accounts for oxidation of the fuel and its partial oxidation products over the surface of $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_3$ (BSCF) catalyst using an empirical formulation (5). Electrochemistry is represented by the Butler-Volmer formalism, assuming hydrogen produced by partial oxidation within the anode and oxygen within the cathode are the electrochemically active species.

When applied to simulate laboratory tests, the trends predicted by the model are in good agreement with experiment results reported in Ref. 1. Figure 1 and 2 show typical simulated polarization curves and 2D gaseous species distribution. In this paper, we will describe the model and its use for parameter exploration with methane as the fuel. The model can also be used for other hydrocarbon fuels and catalysts as long as corresponding mechanisms are provided.

References
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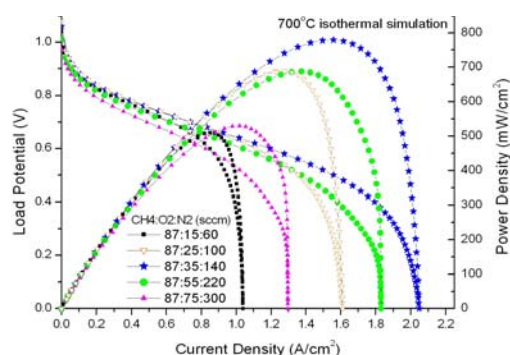5. J. Mederos, Caltech thesis, 2004

Figure 1: Simulated polarization curves at different flow rates
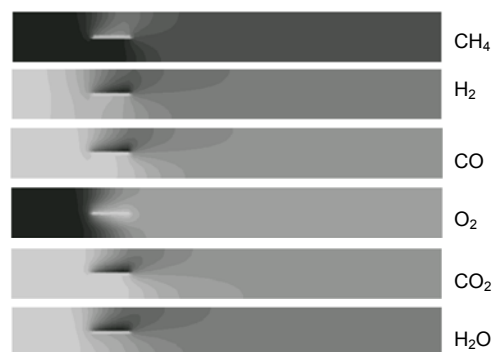

Figure 2: Computed species distribution with anode on the top of the cell; darker shades correspond to higher concentrations