

## **A MATHEMATICAL MODEL FOR A DIRECT HYDROCARBON FUEL CELL**

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Most fuel cells currently being developed use either hydrogen or methanol as the fuel. If the fuel cells oxidized hydrocarbons directly, then theoretically they could operate at much greater energy efficiencies than is possible with either hydrogen or methanol. The reason why direct hydrocarbon fuel cells receive little attention is that they produce small current/power densities. In this work, numerical simulation techniques have been employed to investigate the performance of direct hydrocarbon fuel cells, in an attempt to understand the cause of their limitations. A one-dimensional mathematical model for the entire cell has been developed.

The fuel cell unit is composed of several distinct layers: gas channels, gas diffusion layers and catalyst layers for the anode and cathode as well as the electrolyte compartment. A gaseous hydrocarbon, such as methane or propane is oxidised at the anode, while oxygen in air is reduced at the cathode. Platinum dispersed on carbon is assumed as the electrocatalyst. The model considers porous three-phase electrodes in accordance with current engineering practice. The catalyst layers are modelled using the concept of agglomerated particles. The smaller pores within the agglomerated Pt/C particles are completely filled with electrolyte. The larger pores around the agglomerates provide gas channels for the reactants and products. The agglomerates are assumed to be spherical in shape and the reactant gas concentration profile within them is obtained by a radial diffusion and reaction equation. The phenomena described in the model include multi-component gas phase diffusion in the electrode gas-filled pores (Hydrocarbon/CO<sub>2</sub>/H<sub>2</sub>O at the anode and O<sub>2</sub>/N<sub>2</sub>/H<sub>2</sub>O at the cathode), gas dissolution in the electrolyte, adsorption and electrochemical reaction of the reactant gases on the electrocatalyst surface and ionic transport in the electrolyte. Gas phase diffusion is described using the Stefan-Maxwell equations and both molecular diffusion and Knudsen diffusion are considered. The electrochemical reactions are modelled using the Butler-Volmer equations.

Modelling of the relevant phenomena in the unit cell results in a different differential-algebraic system of equations for each fuel cell layer. The iterative solution uses the shooting method to satisfy global conditions. Within each iteration, the systems of equations are solved sequentially for each fuel cell layer using the Runge-Kutta method. After convergence the cell terminal voltage is reset, so that the whole polarization curve is obtained. The solution of the system results in the concentration profiles of all gaseous and liquid species across all layers of the cell. In addition the model can provide the anodic and cathodic overvoltages and the effect of several operating and design variables on the power density delivered by the unit cell. The variables include the gas composition in the gas channels, the thickness of the (electrolyte, catalyst and gas diffusion) layers, the catalyst loading, the temperature and the liquid electrolyte concentration. The effects of parameters related to the electrolyte, such as the concentration of phosphoric acid for a phosphoric acid

fuel cell, and of using different fuels such as propane, are investigated. Some electrocatalytic aspects of hydrocarbon oxidation are also discussed. The results predicted by this model are in good qualitative agreement with experimental data found in the literature.