

MATHEMATICAL MODELING OF MCFC CELLS/STACKS AND NETWORKS

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ABSTRACT

Molten carbonate fuel cell (MCFC) modeling has various uses and involves different degrees of sophistication. In this paper, the various, MCFC cell/stack and network and system models available in the public domain are discussed. Parametric and phenomenological fuel cell mathematical models are being used to simulate individual MCFC cell/stack performance. With the initial demonstration of full-area, full-height 250-kW to 2-MW MCFC power plants, the spatial configuration of the MCFC stacks into networks in the fuel cell power plant takes on new importance. MCFC network and power plant system flowsheet performance is being modeled using the ASPEN system model. ASPEN is a tear and iterate flowsheet simulator in the public domain. ASPEN is suitable for MCFC network simulation since it has strong systems and property database capabilities. With the emergence of larger MCFC power plant system demonstrations, system modeling of MCFC power plants is now essential. The DOE routinely uses MCFC models in making performance comparisons and in decision-making.

INTRODUCTION

The United States Department of Energy (DOE), Morgantown Energy Technology Center (METC) was one of the first organizations to recognize that MCFC systems are promising high-efficiency, power generation systems. Natural gas and gasification MCFC power plant systems with overall system efficiencies from fifty to sixty percent are forecast. Advanced, fully integrated gasification MCFC systems could have cycle efficiencies as high as 60 percent. The high MCFC efficiency makes it attractive for electric utility applications. On-site industrial and commercial applications where the waste heat can be utilized are also attractive. MCFC's are environmentally benign and can be sited in environmentally sensitive areas.

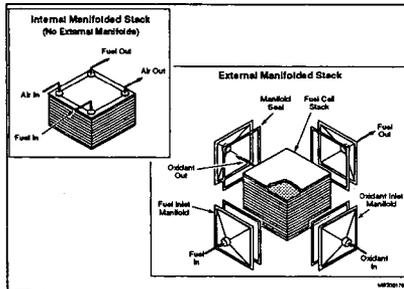
DOE is accelerating the private sector commercialization of multi-fuel, MCFC power plants. To accomplish this, METC is continuing support of power plant development, product development testing or demonstration and product improvement. With the emergence of larger MCFC power plant system demonstrations, system modeling of MCFC power plants is now essential. In addition, with the initial demonstration of full-area, full-height 250-kW to 2-MW MCFC power plants, the spatial configuration of the MCFC stacks in the fuel cell power plant takes on new importance.

The developers of the MCFC have with the aid of the DOE been provided several models of MCFC performance available in the public domain. These models vary in their purpose, degree of complexity, and input requirements. Many have been modified to meet various developers ends. The DOE routinely uses them in making performance comparisons and in decision-making.

MCFC DESCRIPTION

MCFC stack designs incorporate either internal or external manifolding. Internal and external reforming are being considered for both manifolding concepts. All MCFC concepts employ flat cell components in the cell package (i.e., anode, matrix to hold carbonate, cathode, current collector, and separator plate). Operating conditions for MCFC's are projected to be in the ranges of 150 to 250 amperes per ft² at 0.60 to 0.80 volts with 50 to 85 percent fuel utilization (Williams and George, 1990).

Figure 1 illustrates the structure of an MCFC stack. Conductive, bipolar separator plates connect individual cells in a stack both structurally and electrically. Made of stainless steel, each bipolar separator plate physically separates the fuel gas stream of one cell from the oxidant gas stream of the adjacent cell. One side of each separator plate channels a fuel stream so that it flows over a porous anode, while the flip side channels an oxidant stream over a porous cathode. Each bipolar separator plate also collects current, connecting adjacent cells of a stack electrically in series. From the anode, electrons are conducted through the bipolar separator plate and into the cathode of the adjacent cell. There, they react with the oxidant gas stream and carbonate ions are formed. The carbonate ions diffuse through the electrolyte and into the anode, where they react with the fuel gas stream, releasing electrons into the anode. Electrons are conducted in this manner through all the cells, establishing direct current (DC) through the stack. An external circuit connects a load between the two endplates of the stack, completing the circuit.



In conventional fuel cell systems, multiple stacks have been arranged in parallel with regard to the flow of reactant streams. As illustrated in Figure 2, the initial oxidant and fuel feeds are divided into equal streams which flow in parallel through the fuel cell stacks.

Networking is ducting reactant streams such that they are fed and recycled through fuel cell stacks in series. Figure 2 also illustrates how the reactant streams in a fuel cell network flow in series from stack to stack.

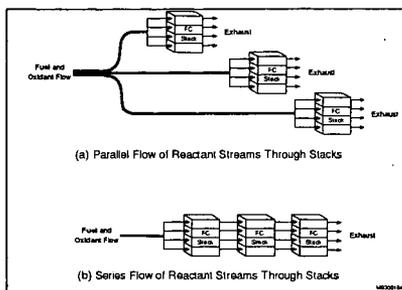
MCFC CELL/STACK MODELING

Lumped Parameter Modeling

Parametric-type models require the least user input information, and are used by some MCFC developers in the US and abroad. One such model is USRMC0 which can be used by itself or as an ASPEN (Advanced System for Process Engineering) user model. It was developed by Gilbert Commonwealth for modeling externally reforming MCFCs. USRMC0 is a lumped parameter and also a statistical, least squares or perturbation model, i.e., it adjusts a "reference" voltage based on deviations in the operating conditions from a set of arbitrary "reference" operating conditions. A separate voltage adjustment is made for deviations in each of the following variables: current density, temperature, pressure, fuel utilization, fuel composition, oxidant utilization, oxidant composition, cell lifetime, production year, and the presence of internal reforming. The user also may specify an additional arbitrary voltage adjustment. The estimated cell voltage is equal to the reference voltage plus the calculated voltage adjustments. After USRMC0 determines the cell voltage, it computes the cell power and heat loss.

Given the feed streams, several fuel cell production parameters (production year, number of stacks, number of cells per stack), and the operating conditions (temperature, pressure, fuel utilization, current density or area, and cell lifetime), the model computes the outlet compositions, cell voltage, power output, heat loss, and either the cell area or current density (whichever is not input).

Stauffer and coworkers (1991) give a discussion of the voltage adjustment correlations and their sources. Briefly, the correlations are simple, piecewise continuous splines that were fit to MCFC operating data culled from the literature. All of the correlations have the following properties: (1) the voltage correction is zero when the operating variable equals the reference state, (2) the greater the deviation of the operating condition from the reference state, the greater is the magnitude of the voltage correction, (3) the greater the deviation from the reference condition, the less accurate is the calculated voltage correction, and (4) the correlations are piecewise continuous but



their derivatives may not be (specifically, the correlations for current density, temperature, pressure, and production year have discontinuous derivatives).

Unfortunately, Stauffer and coworkers (1991) do not give either a comparison of the correlations with the literature data or an estimate of the accuracy of the predictions.

The model assumptions for USRMC0 are as follows: (1) flow through the fuel cell is cocurrent, (2) the anode and cathode are isothermal (although not necessarily at the same temperature), (3) the water gas shift reaction is in equilibrium at the anode outlet, (4) no reforming reactions occur within the fuel cell, (5) transport processes are fast in comparison to the rate of the fuel cell electrochemical reactions, (6) the "fuel" for which the fuel utilization is based consists of H_2 and CO, and (7) no solids are present in the inlet and outlet streams.

The USRMC1 model, which has been recently developed by DOE/METC, is an extension of USRMC0 (White, 1993). USRMC1 is an internally reforming model. This model is being used to compare the performance of various MCFC developers (Ashbaugh 1993).

Phenomenological Modeling

One common and popular phenomenological MCFC model in the public domain is the ICM4X model, referred to as the "PSI model" MCFC model. Unlike the Gilbert-Commonwealth model which is based on macroscopic performance equations, it is a distributed parameter model which attempts to model in detail the microscopic transport processes within the fuel cell (Wilemski and coworkers, 1979, Pigeaud, 1992). The PSI model requires more input and characterization of the MCFC than the Gilbert-Commonwealth model.

Key physical and chemical phenomena modeled include mass transport, ohmic losses, electrode kinetics, fuel and oxidant utilization, gas phase convective heat transfer and inplane conduction through cell hardware. Numerical solution schemes have been developed to calculate overpotential versus current density curves for electrodes, current-voltage performance curves, and current and temperature distributions. The solution involves solving a set of heat and mass balance equations.

DOE/METC (Gardener 1993) has recently compared the performance data of the major MCFC manufacturer's including Ansaldo Ricerche, Energy Research Corp., Hitachi Corp., International Fuel Cells Corp., Ishikawajima-Harima Heavy Industries Co., Kansai Electric Corp., MC-Power Corp. and Mitsubishi Electric Corp.

When comparing the performance data, it was necessary to normalize the data. Ideally, when the engineering performance comparison is made, all fuel cells should be operating at the same

constant fuel and oxidant utilizations on the same anode fuel and cathode oxidant. The fuel cells should also be operating at the same pressure. During a performance comparison test when the fuel cells are operating in the manner just prescribed, the current (load) is varied and the change in voltage is measured. As the current is increased, the voltage decreases and the fuel cell oxidant flows must increase to keep utilizations constant. As the current is increased from zero, the power output (the product of current and voltage) goes through a maximum, whereas the fuel cell efficiency decreases with increasing voltage. There are three engineering performance test curves which resulted from the DOE's performance test: 1) the plot of current density versus voltage, 2) the plot of current density versus power density, and 3) the plot of current density or voltage versus fuel cell efficiency.

MCFC NETWORK AND POWER SYSTEMS MODELING

With the initial demonstration of full-area, full-height 250-kW to 2-MW molten carbonate fuel cell (MCFC) power plants, the spatial configuration of the MCFC stacks into networks in the fuel cell power plant takes on new importance. METC has recently completed computer simulations were done to evaluate the performance of various internal reforming (IRMCFC) networks and to compare conventional IRMCFC power systems to networked ones (Wimer et. al 1993). The simulated performance of MCFC networks was found to be superior to the performance of unnetworked cells/stacks.

These important simulations were accomplished with the public version of ASPEN. ASPEN is an extremely powerful and complex tool. ASPEN is an iterative, flowsheet solver which tears recycles streams and iterates until convergence. ASPEN is a state-of-the-art process simulator and economic evaluation package which was designed for use in engineering fossil energy conversion processes. ASPEN can represent multiphase streams, including solids, and handle complex substances such as coal. The system can perform steady-state material and energy balances, determine equipment size and cost, and carry out preliminary economic evaluations. It is supported by a comprehensive physical property system for computation of major properties such as enthalpy, entropy, free energy, molar volume, equilibrium ratio, fugacity coefficient, viscosity, thermal conductivity, diffusion coefficient, and thermal conductivity for specified phase conditions -- vapor, liquid, or solid. The properties may be computed for pure components, mixtures, or components in a mixture, as appropriate. The ASPEN input language is oriented towards process engineers.

The DOE ASPEN IRMCFC stack model gives the user great freedom in defining the process he wishes to simulate. However, some details of the internal operation of the stack are not as flexible as others. For instance, the internal flow geometry of the stack is always assumed to be co-current. In addition, the internal voltage losses, ohmic, activation and concentration polarizations,

are not individually calculated by ASPEN. Instead, the user is required to specify the total voltage polarization at the stack outlet.

While a modest MCFC data input is required for the use of ASPEN, the system information input required can be extensive. Training in the use of ASPEN is required. ASPEN must have the composition and flowrate of the IRMCFC stack's inlet fuel and oxidant streams as well as a sufficient definition of their thermodynamic state (e.g. temperature and pressure). This information can be directly defined by the user, or ASPEN can calculate it from upstream process data.

Once the inlet reactant streams are known, the IRMCFC stack must be described. The number of cells in the stack must be given. Either the stack current or single-pass fuel utilization must be defined. The total outlet voltage polarization must be provided. The ASPEN model assumes that there is sufficient heat transfer between the fuel and oxidant streams such that they exit the stack at a common outlet temperature. Specification of this outlet temperature is optional. If left unspecified, ASPEN assumes that the stack is adiabatic. If the outlet temperature is provided, ASPEN equilibrates the exhaust gases at this temperature and calculates the corresponding heat duty.

The stack power output is computed by ASPEN as the product of stack current and stack voltage. Finally, by subtracting the stack power output from the total enthalpy change in the reactant streams, ASPEN calculates the heat duty of the stack (Shah 1988).

For a given total outlet voltage polarization, the performance predicted by the ASPEN IRMCFC model is generally conservative. The outlet Nernst potential which is calculated is the minimum possible for a given fuel utilization. Since the model assumes a co-current internal flow geometry, the conditions at the outlet of the stack generate the smallest local Nernst potential of anywhere within the stack. For a given fuel utilization, the Nernst potential which ASPEN calculates is the smallest possible for any internal flow geometry.

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