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A STUDY OF DYNAMIC BEHAVIOUR OF PROTON EXCHANGE MEMBRANE FUEL CELL STACK

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ABSTRACT

The proton exchange membrane fuel cell (PEMFC) stack has shown promise as the leading candidate for use as a non-polluting power source. It discharges water as waste, operates at low temperatures for quick start-up, and uses a solid polymer as an electrolyte which reduces both construction and safety complications. In order to study the dynamic behaviour of PEMFC stack, dynamic model is developed using MATLAB, a high performance technical computing software. The model is based on physical laws having clear significant in replicating the fuel cell system and can easily be used to set up different operational strategies. It consists of several submodels which are integrated to each other. The performances of the fuel cell stack such as thermodynamic efficiency, pressure and humidity profile are also described. As a whole, the output from the modeling technique can be varied to meet the needs of individual investigations as well as for the distribution results.

Keywords: Behaviour Of PEMFC, Dynamic Model, Integration Of Several Submodels, Performance, Individual Investigation And Distribution Results.

1 INTRODUCTION

Fuel cells constitute the most efficient energy transducers known to modern technology; they are twice as efficient as batteries. Fuel cells are electrochemical devices that convert a fuel's energy directly to electrical energy, operating much like continuous batteries when supplied with fuel to the anode (negative electrode) and oxidant (e.g., air) to the cathode (positive electrode). Fortunately, fuel cells do not follow the traditional extraction of energy in the form of combustion heat, conversion of heat energy to mechanical energy, and finally turning mechanical energy into electricity. Instead, they chemically combine the molecules of a fuel and oxidizer without burning, directly producing electricity and dispensing with the inefficiencies and pollution of traditional combustion.

The development of fuel cell technology is catalyzed by the fact that the global energy use is increasing steadily and environmental problems related to energy production and transportation are growing. At the same time, the efficiencies of conventional energy conversion processes are approaching their thermodynamic limits. More efficient solutions are thus needed.

The efficiency of fuel cells is not limited by the Carnot limitations of heat engines. High efficiency makes fuel cells attractive for a large variety of applications, including road vehicles, decentralised power production, residential energy systems and possibly even smaller applications like portable electronics. In many applications, compact size and the lack of local emissions also increase the attractiveness of fuel cells.

2 METHODOLOGY

2.1 DYNAMIC SIMULATION

To study the dynamic performance of fuel cell stack, the modeling methodology incorporates an explicit finite difference scheme. For this purpose, the fuel cell stack is divided into elements whose size is determined by the desired accuracy of the results and the numerical stability of the calculations. The properties of each computational element are assumed be spatially uniform and change with time. The finite difference scheme is used to calculate the temperature only. The remaining properties are calculated using the temperature and various relationships. This requires that the electrochemical kinetics and gas dynamic be treated with steady state formulations. Assumption is made to simplify the resulting equations and reduce the computational requirements of model developed using this methodology.

The stability criterion, an expression used to determine the size range for the elements and time steps needed for numerical stability, is derived using an energy balance on an element. The expression is

(1)

$$\Delta t \leq \frac{(\rho VC)_{ijk}}{[(mC_p)_{H2} + (mC_p)_{Air} + \sum (1/R)]}$$

with Δt is the time step used for the finite difference calculations.p is the average density of the element material, V is the volume of the element while C is the thermal capacitance of the element materials. C_p and m are the specific heat at constant pressure and mass flow rate respectively of the fluids in the element and R represent the thermal resistances of the thermal and surface.s. As seen in equation (1), the stability of the finite difference calculations depends on material properties, fluid properties (if any exists in the element), the resistance of the surrounding elements and time.

2.2 FUEL CELL SYSTEM MODEL

It requires four flow systems (figure 1) which are hydrogen supply system, air supply system, cooling system and humidification system. To simplified the model, it is assumed that the stack temperature is constant. All the variables associated with the lumped anode volume are denoted with a subscript (an). The cathode supply manifold (sm) lumps all the volumes associated with pipes and connection between the compressor and the stack cathode (ca) flow field. The cathode return manifold (rm) represents the lumped volume of pipes downstream of the stack cathode. Another assumption is that the properties of the flow exiting a volume are the same as those of the gas inside the volume. Subscripts (cp) and (cm) denote variables associated with the compressor and compressor motor, respectively.

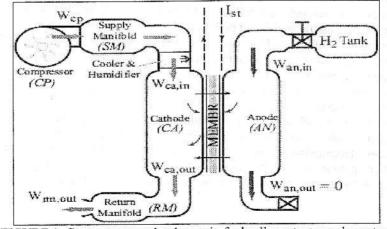


FIGURE 1. Components and volumes in fuel cell reactant supply system

The power of the fuel cell stack depends on current drawn from the stack and stack voltage. The fuel cell voltage is a function of current, reactant partial pressure,

temperature and membrane humidity. As the current is drawn from the fuel cell, oxygen and hydrogen are used in the reaction. Water and heat are also generated.

2.3 FUEL CELL STACK MODEL

The fuel cell stack model contains four interacting sub-models which are stack voltage model, anode flow model, cathode flow model and membrane hydration model. It is assumed that the stack temperature is constant at 80°C (353.15 K). The voltage model contains an equation to calculate stack voltage based on fuel cell pressure, temperature, reactant gas partial pressure and membrane humidity. The dynamically varying pressure and relative humidity of the reactant gas flow inside the stack flow channels are calculated in the cathode and the anode flow models.

2.3.1 Stack Voltage Model

The stack voltage is calculated as a function of stack current, cathode pressure, reactant partial pressures, fuel cell temperature and membrane humidity. Fuel cell voltage is

Vfc = E - Vact - Vohm - Vconc

with E is the open circuit circuit while Vact, Vohm and Vconc are activation, ohmic and concentration overvoltages, which represent losses due to various physical or chemical factors.

2.3.1.1 Activation Overvoltage

It arises from the need to move electrons, to break, and to form chemical bond at the cathode and anode. The relation between the activation overvoltage and the current density is described by the Tafel equation which is however not valid for small current density. Therefore, the Tafel equation is approximated by expression

 $Vact = Vo - Va (1 - e^{-Cli})$

The calculation for Vo and Va is based on electrochemical, kinetics and thermodynamic laws.

2.3.1.2 Ohmic Overvoltage

It arises from the resistance of the polymer membrane to the 'transfer of protons' and the resistance of the electrodes and controller plates to the 'transfer of electrons'. The voltage drop that corresponds to the ohmic resistance is proportional to the current density

 $V_{ohm} = i. R_{ohm}$

with i is current and R_{ohm} is ohmic resistance

2.3.1.3 Concentration Overvoltage

It results from the increased loss at high current density) e.g., a significant drop in reactant concentration due to both high reactant consumption and head loss at high flow rate. An equation that approximates the voltage drop from concentration losses is given by

 $V conc = i (c2 x i/i_{max})^{c3}$

This term is ignored is some models, because it is not desirable to operate the stack at regions where Vconc is high. However, this term needs to be included, if the stack will operate at high current density. c2, c3 and i_{max} are constants that depend on temperature and reactant partial pressure.

(4)

(5)

(2)

(3)

2.3.2 Cathode Flow Model

This model captures the cathode air flow behavior, and is developed using the mass conversation principle and the thermodynamic and psychometric properties of air. Several assumptions are made. First, all gases obey ideal gas law and the temperature of the air inside the cathode is equal to the stack temperature which is 80oC. It should be noted that the properties of the flow exiting the cathode such as temperature, pressure and humidity are assumed to be the same as those inside the cathode. Furthermore, when the relative humidity of the gas exceeds 100%, vapor condenses into the liquid form. The liquid water does not leave the stack and will either evaporate when the humidity drops below 100% or accumulate in the cathode.

2.3.3 Anode Flow Model

This model is quite similar to the cathode flow model. First assumption is pure hydrogen gas is assumed to be supplied to the anode from a hydrogen tank. Next, the inlet hydrogen flow is assumed to have 100% relative humidity. Hydrogen flowrate can be instantaneously adjusted by a valve while maintaining a minimum pressure difference across the membrane.

2,3,4 Membrane Hydration Model

The water transport across membrane is achived through two distinct phenomena. First, the electro-osmotic drag phenomenon is responsible for the water molecules dragged across the membrane from anode to cathode by the hydrogen proton. Second, the gradient of water concentration across the membrane due to difference in humidity in anode and cathode gases causes "back-diffusion" of water from the cathode to anode.

2.4 PERFORMANCE

The calculation for thermodynamic efficiency of the fuel cell is accomplished by dividing the net electrical energy produced by the energy value of the fuel used to produce the electricity. The net electrical energy is calculated by numerically integrating the net power with respect with time. The modeling allows for either the higher or lower haeting value of the fuel to be used for this calculation.

$$\eta = \underbrace{\int \mathbf{P}}_{\mathrm{HV}_{\mathrm{fuel}} \, \mathrm{m}_{\mathrm{fuel}}} \, \mathrm{dt} \tag{6}$$

with η is the thermodynamic efficiency of the stack, P is the net power produced by the stack, HV is the heating value of the fuel and m is the mass of the fuel used to produce the power.

2.5 PROPERTIES

Pressure and humidity profiles are computed using the design of the bipolar plates, output from the air flow, the ideal gas equation and psychometric relationship. The bipolar plate design, output from the air flow and the ideal gas equation are used to calculate the density and velocity of the gases in the flow channel; both of which are required to calculate the pressure drop.

2.6 CONTROL SYSTEM

The purpose of control system is to regulates the entire stack system. It determines the amount of process gas required to meet particular load as well as calculates the amount of energy used to deliver the gas to the fuel cells. It is also calculates the amount of cooling flow required by the stack to maintain the desired temperature. If the stack is pressurized, the energy required to pressurize the system will be calculated. The amount of the process gas required and the amount of the water produced by the fuel cell stack is calculated using the electrochemical equations

3 RESULT

Single value results are most often being used for parameter investigation because they are the main variables of interest when designing a fuel cell power system. These variables can indicate the size, mass and range capability of a vehicle or the construction and operating costs of an electrical generating plant. The main function of distribution results is to identify potential problems that could make a particular combination of parameters undesirable. Combinations of parameters that result in fuel cell stacks with excessive cell temperatures, pressure drops or water accumulations should be avoided because these combinations could result in reduced performance and/or lifetime of the stack. Table 1 shows an example of single value result for fuel cell model while Figure 2 shows an example of distribution result.

TABLE 1. Single value result from the m	Value
Result	1.6381 L/s
Maximum H ₂ consumption	0.40631 L/s
Maximum O ₂ consumption	47.2 %
Fuel cell thermal efficiency	7.468 kW
Maximum power	155.99 Amp
Maximum current	155.99 Allip

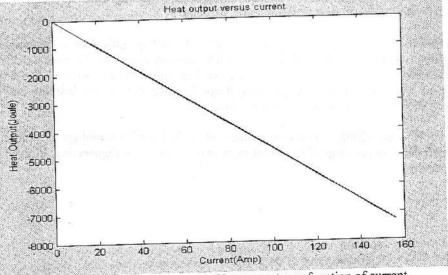


FIGURE 2. Distribution result - Heat output as a function of current

4 CONCLUSION

The mathematical model developed is based on appropriate energy, mass and electrochemical equations as applied to PEMFC. Familiarity with the physical structure and the operating principle of a PEMFC is necessary to understand its dynamic behaviour. The model is used to predict the load following capability of the fuel cell system subject to various control strategies. It can also perform a detailed analysis of the effects of the PEMFC on the power distribution system. This will eventually determine the necessary specifications of a fuel cell system which can be operated as a distributed generator in power system. Since it may not be cost efficient to use real fuel cell for preliminary research work, the fuel cell model will prove to be very useful.

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