

## MODELLING OF A PEM FUEL CELL SYSTEM

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**Abstract:** This paper considers modeling and simulation study of a fuel cell system. A mathematical model of a Polymer Electrolyte Membrane (PEM) Fuel Cell system is presented in this paper. For the convenience of presentation, cathode flow, anode flow, the membrane hydration, and voltage output expressions of the PEM fuel cell system are given in the paper to bridge a generic model to the model of Fuel Cell Test station (FCT). Within the University research facilities, there is a PEM – FCT station available so the PEM-FCT is used for the simulation study. Comparisons are made between the simulation results from the mathematical model which is implemented in MATLAB/Simulink and FCT test data. A general agreement exists but where there are differences and anomalies the paper gave reasons for this. Overall the PEM Fuel Cell (PEMFC) model represents the FCT station. The PEMFC model can be used for controller development to improve FCT system performance.

**Keywords:** Modelling, Mathematical model, Parameter estimation, Parameter optimization, Simulation.

### 1. INTRODUCTION

Recently there is a growing interest in fuel cell systems, since fuel cells are clean and efficient sources of electricity, and have a wide range of vehicle applications (Boccaletti *et al.*, 2006). A fuel cell is an electrochemical energy conversion device which converts the chemicals hydrogen and oxygen into water and in the process produces electricity. Fuel cells are able to provide large amounts of current and hence power, but the only requirement is the constant flow of reactants. It is this supply of reactants which presents one of the several challenges encountered by the fuel cell system investigators. There are several types of fuel cells each using a different chemistry. The PEM fuel cell is commonly used to power a vehicle. In general the fuel cell is considered as a future electrical power source for automotive, portable electronics and stationary applications. To analyse the dynamic problems of controlling a fuel cell system and to develop control schemes for alleviating these problems it is necessary to derive a dynamic model for fuel cell systems.

Modelling of the fuel cell is a complex task since it involves electrostatics, fluid dynamics, heat and electrochemical reactions. In the following sections a mathematical model of PEM-FCT is derived and a simulation study has been conducted. The results are presented in this paper.

### 2. MODEL OF A FUEL CELL SYSTEM

Fuel cell systems are able to deliver electrical power with high efficiency, with low operation noise and little or zero emissions from hydrogen and air (Schell *et al.*, 2005). By-products are water and heat. The generated electrical power can be used in vehicles for propulsion as well as for the operation of electrically powered accessories (Lin *et al.*, 2006). To enhance the long term viability of fuel cell vehicles, it is necessary to introduce a model based and optimization based design approach so that the design process is reusable and systematic, and the final design achieves a guaranteed level of optimality. Such an approach allows the evaluation of the PEMFC dynamic performance

for energy generation systems, reducing cost and time along the design stage and tests. This has been the motivation in the work reported in this paper. Recently, this subject has been addressed by many authors, for example, Amphlett *et al.*, 1995; Haluk, 2006, which describe different aspects of FC systems. Taking these aspects into consideration, in this paper, the overall fuel cell system equations are derived.

To derive this closed form of expressions to the fuel cell system the following assumptions are made; the fuel cell is fed with hydrogen and air only, however some time nitrogen, is also fed to the fuel cell system, but the nitrogen is only used as a purge to clear the system if required, so we ignored the usage of nitrogen in the system modelling. The electrode channels are small enough that the pressure drop across them is negligible, ideal gas law is applicable to all gases, and the fuel cell temperature is stable. The system model contains four interacting sub-systems; cathode and anode flow, the membrane hydration, and stack voltage. The current – voltage relationship is commonly given in the form of a polarization curve, which is the plot of fuel cell voltage,  $v_{fc}$  versus current density  $i$ . The current density,  $i$  is defined as stack current per unit of cell active area,  $i = I_{st} \cdot A_{fc}^{-1}$  since fuel cells are connected in series to form the stack, the total stack voltage can be calculated by multiplying the cell voltage,  $v_{fc}$ , by the number of cells,  $n$  of the stack, i.e.,  $v_{st} = n \times v_{fc}$  and the stack power is  $P_{st} = v_{st} \cdot I_{st}$ . The fuel cell voltage is calculated by subtracting the fuel cell losses or overvoltages from the fuel cell open circuit voltage,  $E$ , and is given by the following equation (Dufour, *et al.*, 2003; Correa *et al.*, 2004; Mueller, *et al.*, 2007)

$$v_{fc} = E - v_{act} - v_{ohm} - v_{conc} \quad (1)$$

where

$$E = \frac{1}{2F} \left\{ \Delta G + \Delta S(T - T_r) + RT \left( \ln(P_{H_2}) + \frac{1}{2} \ln(P_{O_2}) \right) \right\} \quad (2)$$

where  $E$  is the potential of the cell obtained in an open circuit.  $F$  is the constant of Faraday;  $\Delta G$  is the change in the free Gibbs energy;  $\Delta S$  is the change of the entropy;  $R$  is the universal constant of the gases; while  $P_{H_2}$  and  $P_{O_2}$  are the partial pressures of hydrogen and oxygen respectively. Variable  $T$  denotes the cell operation temperature and  $T_r$  is the reference temperature.

The activation overpotential  $v_{act}$ , including anode and cathode can be calculated as follows:

$$v_{act} = - \left\{ \zeta_1 + \zeta_2 T + \zeta_3 T \ln \left( \frac{P_{O_2}}{5.1 \times 10^8 e^{-\frac{498}{T}}} \right) + \zeta_4 T \ln(i_{FC}) \right\} \quad (3)$$

where  $\zeta$ 's represent parametric coefficient for the cell model.  $i_{FC}$  is the cell operating current.

The ohmic voltage drop  $v_{ohm}$  is determined by the following expression:

$$v_{ohm} = i_{FC} (\rho_m t_m A_{fc}^{-1} + c) \quad (4)$$

In this model a general expression for resistance is defined to include all the important parameters of the membrane. The resistance to the transfer of protons through the membrane is assumed to be a constant ( $c$ ) and included in the equation as an additional term.  $\rho_m$  is the specific resistivity of the membrane for the electron flow.  $t_m$  is the thickness of the membrane,  $A_{fc}$  is the cell active area.

The voltage drop due to the mass transport can be determined by

$$v_{con} = -B \cdot \ln(1 - \theta) \quad (5)$$

and

$$\theta = (i_{FC} \cdot A_{fc}^{-1}) \left( (i_{FC} \cdot A_{fc}^{-1})_{\max} \right)^{-1} \quad (6)$$

where  $B$  is a parametric coefficient, that depends on the cell and its operation state.

The hydrogen partial pressure  $P_{H_2}$  is modeled by the following expression

$$P_{H_2} = \frac{m_{H_2} \cdot R_{H_2}}{V_{an}} T \quad (7)$$

where  $m_{H_2}$  is the mass of hydrogen in the anode,  $R_{H_2}$  hydrogen gas constant and  $V_{an}$  fuel cell anode volume. The principle of conservation of mass is applied to obtain governing equation for hydrogen mass inside the anode volume and is given by:

$$\dot{m}_{H_2} = W_{H_2,in} - W_{H_2,out} - W_{H_2,reacted} \quad (8)$$

where,  $W_{H_2,in}$ ,  $W_{H_2,out}$  and  $W_{H_2,reacted}$  are the hydrogen mass flow in, out and reacted respectively. Each of these terms are modelled as follows:

$$W_{H_2,in} = \phi^{-1} \cdot W_{H_2,an,in} \quad (9)$$

and

$$\phi = 1 + k_t \cdot T M_v M_{H_2}^{-1} (P - k_t \cdot T)^{-1} \quad (10)$$

$W_{H_2,an,in}$  is the anode inlet flow (system input).  $P$  pressure and  $k_t$  is the linking function of the fuel cell temperature and saturation pressure and is given by,  $k_t = \exp(a - b/T)$ ,  $a$ ,  $b$  are constants.  $M_v$  and  $M_{H_2}$  are the vapor molar mass and hydrogen molar mass respectively. Similarly, the hydrogen flow out  $W_{H_2,out}$  is given by:

$$W_{H_2,out} = \phi^{-1} \cdot W_{H_2,an,out} \quad (11)$$

The rate of hydrogen reacted;  $W_{H_2,reacted}$  in the fuel cell reaction is calculated by using the electrochemical equations.

$$W_{H_2,reacted} = M_{H_2} \frac{n i_{FC}}{2F} \quad (12)$$

Due to the electrochemical reaction the system also produces water and heat as a byproduct, and the water mass flow inside the anode volume  $\dot{m}_{w,an}$  is expressed as follows:

$$\dot{m}_{w,an} = W_{v,an,in} - W_{v,an,out} - W_{v,mbr} \quad (13)$$

each of the elements in this equation is determined by the following equations:

where  $W_{v,an,in}$  water mass flow in to the anode is given by:

$$W_{v,an,in} = (1 - \phi^{-1}) W_{H_2,an,in} \quad (14)$$

similarly,  $W_{v,an,out}$  water mass flow out from the anode is expressed as:

$$W_{v,an,out} = (1 - \phi^{-1}) W_{H_2,an,out} \quad (15)$$

The mass flow of vapor across the membrane  $W_{v,mbr}$  is calculated using mass transport principles and membrane properties (Pukrushpan *et al.*, 2002)

$$W_{v,mbr} = M_v A_{fc} n \cdot \left( \frac{n_d \cdot i_{FC}}{F} \right) \quad (16)$$

where  $n$  is the number of cells,  $n_d$  is the electro-osmotic coefficient. It is assumed that the relative humidity in the anode can be controlled at 100%. The supplied hydrogen is regulated by a valve that uses proportional control to maintain a minimum pressure difference across the membrane.

The oxygen partial pressure  $P_{O_2}$  is calculated by using process used to obtain the  $P_{H_2}$ , and  $P_{O_2}$  is given by:

$$P_{O_2} = \frac{m_{O_2} \cdot R_{O_2}}{V_{ca}} T \quad (17)$$

where,  $m_{O_2}$  is the mass of oxygen in the cathode,  $R_{O_2}$  oxygen gas constant, and  $V_{ca}$  fuel cell cathode volume. The principle of conservation of mass is used to obtain governing equation for oxygen mass inside the cathode volume and is given by:

$$\dot{m}_{O_2} = W_{O_2,in} - W_{O_2,out} - W_{O_2,reacted} \quad (18)$$

where  $W_{O_2,in}$ ,  $W_{O_2,out}$  and  $W_{O_2,reacted}$  are the oxygen mass flow in, out and reacted respectively. Each of these components is expressed as follows:

$$W_{O_2,in} = \gamma \psi^{-1} W_{a,in} \quad (19)$$

and

$$\psi = 1 + k_t T M_v M_{O_2}^{-1} (P - k_t T)^{-1} \quad (20)$$

where,  $W_{a,in}$  is the inlet air flow (system input),  $\gamma$  oxygen molar fraction parameter in air,  $M_{O_2}$  oxygen molar mass, Similarly, the oxygen flow out  $W_{O_2,out}$  is given by:

$$W_{O_2,out} = \gamma \psi^{-1} W_{a,out} \quad (21)$$

The rate of oxygen reacted;  $W_{O_2,reacted}$  in the fuel cell reaction is calculated by using the electrochemical equations.

$$W_{O_2,reacted} = M_{O_2} \frac{n i_{FC}}{4F} \quad (22)$$

$\dot{m}_{w,ca}$  water mass flow inside the cathode volume is expressed as follow:

$$\dot{m}_{w,ca} = W_{v,ca,in} - W_{v,ca,out} + W_{v,gen} + W_{v,mbr} \quad (23)$$

where  $W_{v,ca,in}$  water mass flow in is expressed by the following equation:

$$W_{v,ca,in} = (1 - \psi^{-1}) W_{a,in} \quad (24)$$

Similarly,  $W_{v,ca,out}$  water mass flow out is given by:

$$W_{v,ca,out} = (1 - \psi^{-1}) W_{a,out} \quad (25)$$

and,  $W_{v,gen} = M_v \frac{n I_{st}}{2F}$  is the water generated in the fuel cell reaction, also heat  $H$  produced during the reaction is given by :

$$H = i_{FC} \cdot n \cdot \left( 1 - \frac{v_{fc}}{n} \right) \quad (26)$$

### 3. PARAMETER ESTIMATION OF THE FUEL CELL MODEL

It is important to realise that no matter how comprehensive the model there will be some errors between the model and the actual performance of the real PEMFC system, because of the assumptions and approximations made in the modelling. In order to improve the accuracy of the model and make the model reflect the real system performance better, it is necessary to optimize the parameters of the model. Since it is difficult to optimize the partial differential equations of the

mechanistic and high-dimension models, a simplified PEMFC model suitable for engineering application and optimization is presented here. Among the parameters in this model some are only available in empirical values or only the ranges of these values can be estimated. Thus, the key problem is to determine these parameters for the optimal implementation.

Parameters of this PEMFC model is determined and optimized by means of optimizations algorithms, by using FC output-voltage, power demand, anode flow and cathode flow as input-output data. We used the traditional optimization search method, so-called simplex search algorithm, because in general, this algorithm works faster than many other optimization methods. Since it's a direct search optimization method, therefore it can exploit all local information in an effective way.

The PEM Fuel Cell Test station (PEM-FCT), shown in Fig.1 was tested to obtain a set of data. The parameters and operating conditions are shown in Table 3.1. Successive measurements of the PEM-FCT current, voltage and power were recorded for different cases. In order to fit the experimental data to match with the PEMFC model output data, it is necessary to optimize the values of the following parameters:  $\zeta_1, \zeta_2, \zeta_3, \zeta_4, B, c$ . The upper and lower bounds of these parameters (Jeferson, *et al.*, 2004) are given in Table 3.2

Table 3.1: PEM-FCT parameters and operation conditions

Parameters	Values	Units
$A$	25	$cm^2$
$t_m$	178	$\mu m$
$P$	1	$atm$
$T$	343.15	$K$

The following objective function is used for optimization to determine the model parameters.

$$\min_{(\zeta_1, \zeta_2, \zeta_3, \zeta_4, B, c)} f \quad (27)$$

and

$$f = \frac{1}{\delta} \sum_{t=0}^{t=t_s} \left( (v_{fct} - v_{sim})^2 + (p_{fct} - p_{sim})^2 \right) \quad (28)$$

where  $f$  is the objective function,  $v_{fct}, p_{fct}$  are the experimental data of voltage and power of the PEM-FCT test station respectively. Likewise,  $v_{sim}, p_{sim}$  are the PEMFC model data of voltage and power respectively.

The PEM-FCT parameters and operational range are described in Table 3.1. In its operational range, many different sets of experimental data are used for parameter optimization. The parameters of the PEMFC model were

optimized by simplex search method (SSM) and pattern search method (PSM). The contrast results are shown in Table 3.3. As mentioned above, the simplex search method found the optimal solution much quicker than the PSM. It is clear from the results shown in Table 3.3 there was not much improvement in the accuracy of the optimal solution found by the PSM. After parameter optimization, the model parameters are determined and the model now reflects the performance of the PEM-FCT.

Table 3.2: Bounds of PEMFC model parameters

Parameters	Lower bound	Upper bound
$\zeta_1$	-0.952	-0.944
$\zeta_2$	0.001	0.005
$\zeta_3$	$7.4 \times 10^{-5}$	$7.8 \times 10^{-5}$
$\zeta_4$	$-1.98 \times 10^{-4}$	$-1.88 \times 10^{-4}$
$B$	0.016	0.5
$c$	0.0001	0.0008

Table 3.3: Optimized parameters of PEMFC model

Parameters	SSM	PSM
$\zeta_1$	-0.948	-0.947
$\zeta_2$	0.0047	0.0047
$\zeta_3$	$7.45 \times 10^{-5}$	$7.74 \times 10^{-5}$
$\zeta_4$	$-1.88 \times 10^{-4}$	$-1.93 \times 10^{-4}$
$B$	0.0182	0.0175
$c$	0.00062	0.00063

#### 4. MODEL VALIDATION OF FUEL CELL SYSTEM USING FCT STATION

The Fuel Cell Test station (FCT) available within the University research facilities was designed and manufactured in partnership with Fuel cell Technologies Inc (see Fig.1). The test station consists of five subsystems. The gas delivery subsystem, fuel cell subsystem, humidification subsystem, load subsystem and control subsystem. The block diagram shown in Fig.2 gives an overview of the present setup which utilizes a single fuel cell membrane electrode assembly. The gas delivery subsystem delivers the reactants (gases) of hydrogen to the anode and oxygen to the cathode. It consists of hydrogen and compressed air tank along with inlet filters, pressure regulators and flow meters and controllers. The fuel cell subsystem is the heart of the FCT. Here within the fuel cell membrane electrode assembly the chemical process occurs, which produces electricity to power end users. It

consists of the typical fuel cell structure of anode and cathode plates separated by a PEM material.



Fig.1 Fuel cell Test station

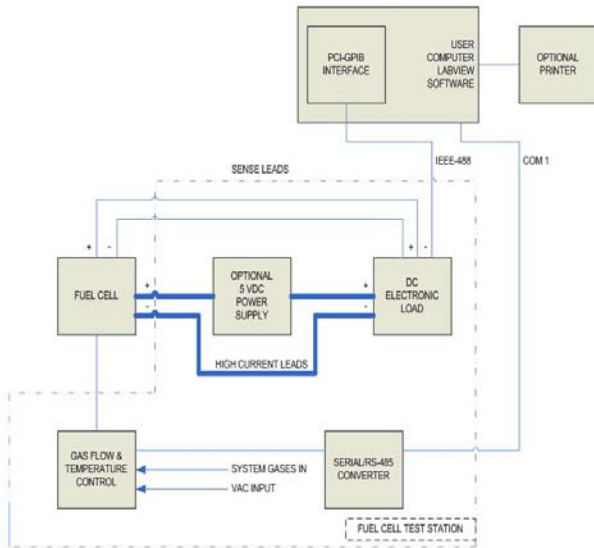


Fig.2 Block diagram of FCT system

Now, using the optimal parameters, the PEMFC model presented in the previous section is tuned to represent the FCT test station and it is implemented in MATLAB/Simulink. The optimal parameters for the PEMFC model used in the simulation studies are presented in the Tables 4.1 ~ 4.3. The inputs used to drive the model are presented in Fig.3. Comparison results show that there is a general agreement between the FCT data and the simulation model results. FCT data were generated from the tests conducted for the specific conditions at the University research laboratory. An extensive simulation is carried out and a simulation result for a typical case is presented in this paper as an example (see Fig.4). The simulation model response was computed using the actual measured control inputs. Both the FCT data and the simulation data were plotted to the same scale, which enables an easier comparison of the variables of interest, such as voltage ( $v$ )

and power ( $P$ ), where the dashed lines and solid lines are indicating the simulation model and FCT test station responses respectively. The anode flow, cathode flow and current (disturbance) inputs were used to drive the model. There exists reasonably good correlation with the FCT data response; however some discrepancies are evident, which might be an indication that some unstable factors in the real FCT have not been included into the model.

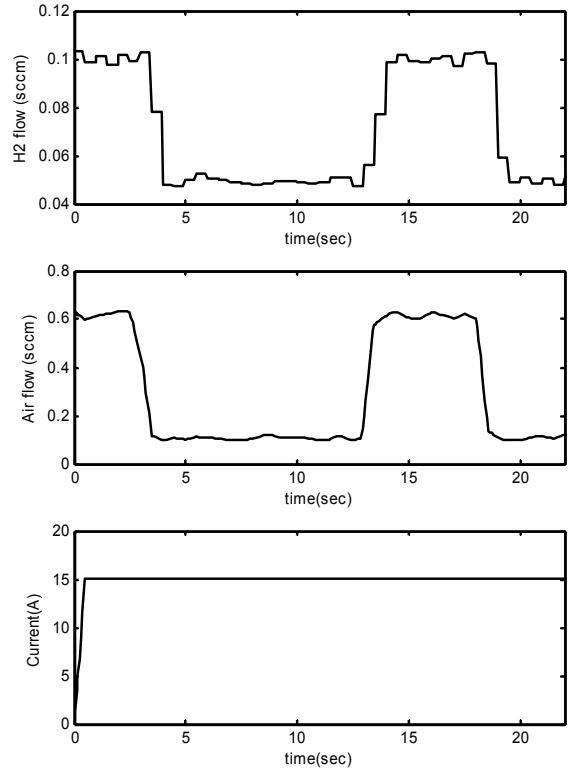


Fig. 3 Fuel cell system inputs

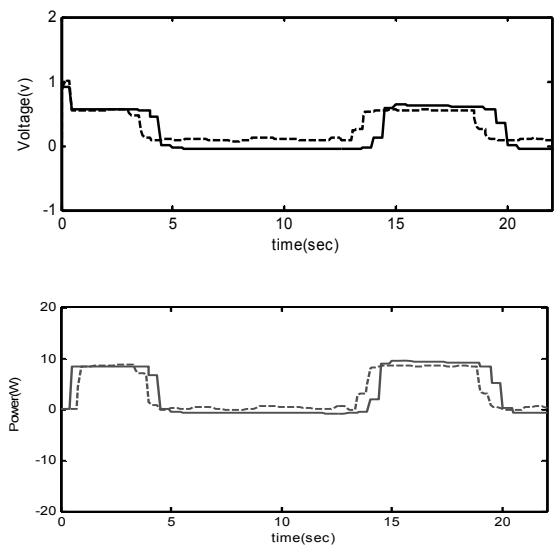


Fig. 4 Comparison of simulation model and FCT responses (model ----- FCT ——)

## 5. CONCLUDING REMARKS

The paper describes modeling and simulation study of a fuel cell system. A mathematical model for a fuel cell system has been developed for simulation study and control analysis. For the simulation study in this paper a Fuel Cell Test station is used. The model responses are compared with FCT data. Correlation in the main is satisfactory but anomalies are present. Possible reasons for those anomalies are suggested. Overall satisfactory results are achieved. Simulation analysis for the flow changes with the mathematical model itself are currently being undertaken and the results will be investigated for the analysis of system stability and control.

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## PARAMETERS OF FCT

PEM fuel cells data are gathered from various sources are presented below (Sedghisigarchi and Feliachi, 2004; Schell, *et al*, 2005; Fuel cell Technologies manual, 2005). These parameters were used to run the simulation model, which represent the FCT station.

Table 4.1: Membrane water transport group

Parameter	FCT value	Units
$M_v$	$18.02 \times 10^{-3}$	kg / mol
$A_{fc}$	25	cm <sup>2</sup>
$n$	1	-
$n_d$	0.27	mol / mol
$F$	96485	C / mol

Table 4.2: Anode mass flow group

Parameter	FCT value	Units
$M_{H_2}$	$2.016 \times 10^{-3}$	kg / mol
$P$	1	atm
$R_{H_2}$	$4.1243 \times 10^3$	J / kgK
$V_{an}$	0.005	m <sup>3</sup>

Table 4.3: Cathode mass flow group

Parameter	FCT value	Units
$M_{O_2}$	$32 \times 10^{-3}$	kg / mol
$R_{O_2}$	259.8	J / kgK
$V_{ca}$	0.01	m <sup>3</sup>
$T$	333.15	K
$t_m$	$178 \times 10^9$	cm