MODELLING, PARAMETER ESTIMATION AND VALIDATION OF A 300W PEM FUEL CELL SYSTEM

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Abstract: In this paper a 300W PEM FC Stack dynamic model is developed and implemented in MATLAB/Simulink. Using semi-empirical equations for modelling a Proton Exchange Membrane (PEM) fuel cell is proposed for providing a tool for the design and analysis of fuel cell stack systems. The modelling results are compared with experimental results. The comparison shows good agreements between the modelling results and experimental data. The model could be used in PEM fuel cell control related studies.

Keywords: Modelling, Parameter optimization, Simulation, Experimental study, Model validation.

NOMENCLATURE

v_{fc}	cell voltage (V)
i_{FC}	cell operating current (A)
v_{st}	stack voltage (V)
I_{st}	stack current (A)
P_{st}	stack power (W)
n	number of cells
E	fuel cell open circuit voltage (V)
v_{act}	activation over-potential (V)
v_{ohm}	ohmic voltage drop (V)
v_{conc}	voltage drop due to mass transport (V)
F	constant of Faraday $(coulombs/mol)$
ΔG	change in the free Gibbs energy (J/mol)
T	cell operation temperature (K)
T_r	reference temperature(K)
R	universal constant of gases $(J/mol.K)$
t_m	thickness of the membrane (cm)
A_{fc}	cell active area (m^2)
v_d	dynamical voltage (V)
V_{an}	fuel cell anode volume (m^3)
V_{ca}	fuel cell cathode volume (m^3)
τ	time constant
R_a	resistance (Ω)
n_d	electro-osmotic coefficient (mol/mol)
M	molar mass (Kg/mol)
W	mass flow $(sccm)$

1. INTRODUCTION

Growing interest in renewable energy has provided motivation for researchers to perform research in the applicable technologies, such as fuel cell etc. Fuel cell technologies are clean and efficient sources of electricity, and have a wide range of vehicle applications (Sedghisigarchi and Feliachi, 2004; 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 usually classified by the

type of electrolyte they use. 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. To enhance the long term viability of fuel cell systems, 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. In the following sections a mathematical model of a 300W PEMFC is presented and a simulation study has been conducted. The model responses obtained are validated by experimental data measured from 300W PEM-FCT station which is available within the University research facility.

2. PEMFC MODEL

In this section, a mathematical modelling approach is presented for building a dynamic model for a PEMFC stack. The overall fuel cell system equations are derived. To derive closed form of equations for the fuel cell system the following assumptions are made; the fuel cell is fed with hydrogen and air only. Note 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 so 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 density, i is defined as stack current per unit of cell active area, $i = I_{st}.A_{fc}^{-1}$ 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 (Mueller, *et al.,* 2007, Thanapalan *et al.,* 2008)

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

where

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

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

$$v_{act} = -\left\{\varsigma_1 + \varsigma_2.T + \varsigma_3.T.\ln\left(\frac{P_{O_2}}{5.1\times10^6.e^{\frac{-498}{T}}}\right) + \varsigma_4.T.\ln(i_{FC})\right\} \qquad (3)$$

where ς 's represent parametric coefficient for the cell model. The ohmic voltage drop v_{ohm} is determined by the following expression:

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

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

$$v_{con} = -B.\ln(1 - \theta) \qquad (5)$$

and

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

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

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

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.

Similarly, the oxygen partial pressure P_{O_2} is modelled by the following expression and P_{O_2} is given by:

$$P_{O_2} = \frac{m_{O_2}.R_{O_2}}{V_{ca}}T \qquad (8)$$

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.

Cathode and anode flow: Applying the principle of conservation of mass the governing equations of cathode and anode flows can be written as follows;

$$\dot{m}_{O_2} = W_{O_2,in} - W_{O_2,out} - W_{O_2,reacted} \quad (9)$$

$$\dot{m}_{w,ca} = W_{v,ca,in} - W_{v,ca,out} + W_{v,gen} + W_{v,mbr} \quad (10)$$

The flow rates of each element in the above equations are determined using thermodynamic and psychometric properties of gas upstream. The rate of oxygen reacted and water generated in the fuel cell reactions are calculated from the cell current, i_{FC} using the electrochemical equations;

$$W_{O_2,reacted} = M_{O_2} \frac{n.i_{FC}}{4F}, \; W_{v,gen} = M_v \frac{n.i_{FC}}{2F} \quad (11)$$

where F is the Faraday number, M_{o_2} and M_v are the molar mass of oxygen and vapour respectively.

$$\dot{m}_{H_2} = W_{H_2,in} - W_{H_2,out} - W_{H_2,reacted} \quad (12)$$

where, $W_{H_2,in}$, $W_{H_2,out}$ and $W_{H_2,reacted}$ are the hydrogen mass flow in, out and reacted respectively.

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

The rate of hydrogen reacted in the fuel cell reaction is calculated from the cell current is given by

$$W_{H_2,reacted} = M_{H_2} \frac{n.i_{FC}}{2F} \quad (14)$$

Membrane hydration: it captures the effect of water transport across the membrane. Both water content and mass flow are assumed to be uniform over the surface area of the membrane, and are functions of cell current and relative humidity of the gas in the anode and cathode. The mass flow of vapour across the membrane $W_{v,mbr}$ is calculated using mass transport principles and membrane properties (Thanapalan *et al,* 2008, Pukrushpan, *et al,* 2002).

$$W_{v,mbr} = M_v A_{fc} n. \left(\frac{n_d . i_{FC}}{F} \right) \quad (15)$$

where 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 dynamic properties of the fuel cell depend mainly on the so-called charge double-layer effect (Wang *et al.,* 2005). Such phenomenon normally exists on every contact between two different materials due to charge accumulation on the opposite surfaces or a load transfer from one to the other. The charge layer on both electrode/electrolyte interfaces is storage of electrical charges and energy; in this way, it behaves as an electrical capacitor. This effect causes retardation in the dissipation of the electrical charges near the electrolyte/electrode interface. Then, when there is a change in the FC current, there is a delay until the FC voltage change. The ohmic voltage drop is not affected by the charge double-layer effect as it is directly related to the current. In this way, it can be considered that there is a first-order delay associated to activation and concentration voltages. The time constant associated with this delay is the product given by;

$$\tau = R_a . C_{fc} \quad (16)$$

where

$$R_a = \frac{v_{act} + v_{conc}}{i_{FC}} \quad (17)$$

where C_{fc} represents the electrical capacitance of the system and the resistance R_a is determined from the cell output current and the activation and concentration voltage drop described as above in equations [3] and [5]. Then the dynamic equation including the dynamic behaviour can be written as follow;

$$\frac{dv_d}{dt} = \frac{1}{C_{fc}} i_{FC} - \frac{1}{\tau} v_d \quad (18)$$

Thus, the resulting FC voltage including the charge double-layer effect is then defined by;

$$v_{fc} = E - v_{ohm} - v_d \quad (19)$$

where v_d represents the dynamical voltage across the capacitor.

3. PARAMETER OPTIMISATION OF PEMFC MODEL

It is important to realise that no matter how complete the model; there must be some errors between the model and the actual performance of the real PEMFC system, because assumptions and approximations are made in modeling. 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 as 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. Simulation optimisation is an area that has attracted the attention of many researchers, see for example, Akbay, 1996; Azadivar, 1992. There are many different simulation optimisation methods described in the literature. Carson and Maria, 1997 provide a review of optimisation algorithms, with an extensive reference list pointing to detailed treatment of specific techniques.

Simulation optimisation entails finding optimal values of the parameters of interest, which optimise the output responses.

In this work we used the Genetic Algorithms (GA) optimisation and traditional optimization search method, so-called simplex search algorithm (SSM). In general, SSM 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 simplex optimisation method is basically a hill climbing strategy. Given that n variables are defined, then in the simplex method, geometrical figure simplex with $n+1$ vertices randomly placed in search space. Then step by step the vertex with worst quality is replaced by mirroring along the centre of gravity of all other vertices. The quality of the new vertex is tested and eventually an expansion or shrinking of the simplex figure is performed, especially when the simplex approaches the optimum. The disadvantage of this method is that it may detect the next best optimum, thus it may not find the global optimum.

By contrast heuristic optimisation methods, such as Genetic Algorithms (GA) are frequently used for simulation optimisation. These heuristic techniques balance exploration with exploitation thereby resulting in efficient global search strategies (Mohamed and Jenkins, 2004). GA are computational procedures, which use ideas borrowed from evolution genetics in that they solve problems by maintaining populations, which survive and evolve through chance and the rule "Survival of the fittest". GA's are search algorithms based on mechanics of natural selection and natural genetics. They start with a group of knowledge structures, which are usually coded into binary strings (chromosomes). These structures are evaluated with in some environment and the strength (fitness) of a structure is defined. The fitness of each chromosome is calculated and a new set of chromosomes is then formulated by random selection and reproduction. Each chromosome with the higher fitness values will tend to survive and those with lower fitness values will tend to become extinct. The selected chromosomes then undergo certain operations such as crossover, where chromosomes are paired and randomly exchange information, and mutation, where individual chromosomes are altered. The resulting chromosomes are re-evaluated and the process is repeated until no further improvement in overall fitness is achieved. In addition, there is often a mechanism to preserve the current best chromosome (elitism). In general any task to be accomplished can be thought of as solving a problem, which in turn can be perceived as a search through a space of potential solutions, and since we are after the best solution, we can view this task as an optimisation process (Thanapalan, 1999). A flowchart of the steps of the genetic code used to get the optimal parameters is shown in Fig. 1.

The PEM Fuel Cell Test station (PEM-FCT), shown in Fig.2 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: $\varsigma_1, \varsigma_2, \varsigma_3, \varsigma_4, B, c$. The upper and lower bounds of these parameters are given in Thanapalan, *et al* 2008.

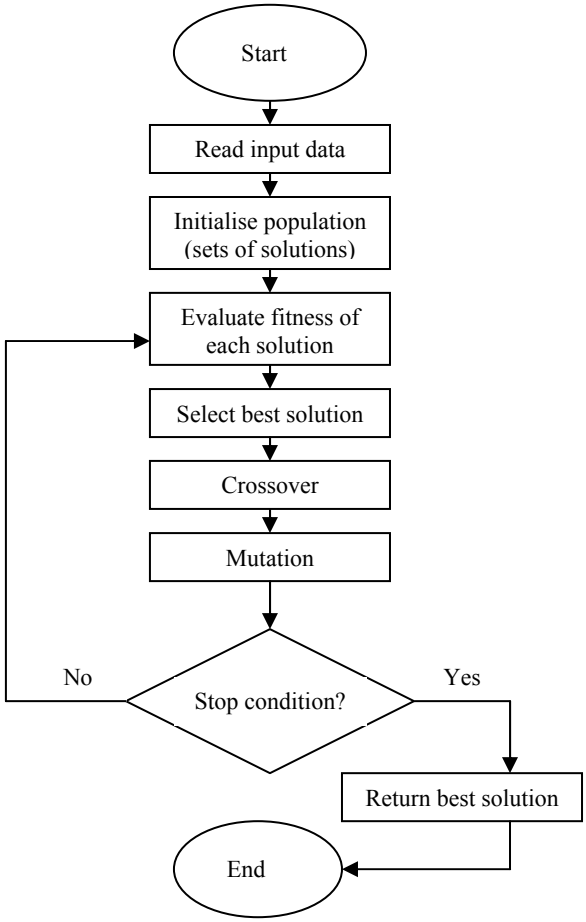

Fig.1. Top level description of GA to obtain the PEMFC optimal parameters

Table 3.1: PEM-FCT parameters and operation conditions

Parameters	Values	Units
A_{fc}	20	cm^2
t_m	178	μm
P	1	atm
T	343.15	K

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

$$\min_{(\varsigma_1,\varsigma_2,\varsigma_3,\varsigma_4,B,c)} f \tag{20}$$

and

$$f = \frac{1}{\delta}\int_0^{t_s}\left(\left(v_{fct}-v_{sim}\right)^2+\left(p_{fct}-p_{sim}\right)^2\right)dt \tag{21}$$

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 GA optimisation method. The results are shown in Table 3.2. As mentioned above, the simplex search method found the optimal solution much quicker then the GA. It is clear from the results shown in Table 3.2 there was not much improvement in the accuracy of the optimal solution found by the GA. After parameter optimization, the model parameters are determined and the model now reflects the performance of the PEM-FCT.

Table 3.2: Optimized parameters of PEMFC model

Parameters	SSM	GA
ς_1	-0.948	-0.945
ς_2	0.0047	0.0049
ς_3	7.45×10^{-5}	7.76×10^{-5}
ς_4	-1.88×10^{-4}	-1.96×10^{-4}
B	0.0182	0.0180
c	0.00062	0.00061

4. VALIDATION OF 300-W PEMFC STACK MODEL

The Fuel Cell Test station (FCT) available within the University research facilities consists of five subsystems (see Fig.3). The gas delivery subsystem, 300W FC Stack subsystem, humidification subsystem, load subsystem and control subsystem. Fig.2 gives an overview of the present setup which utilizes a 300W FC Stack. The 300W FC Stack 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 (Williams, *et al* 2007).

Fig.2. Fuel cell Test bench with 300-W fuel cell stack

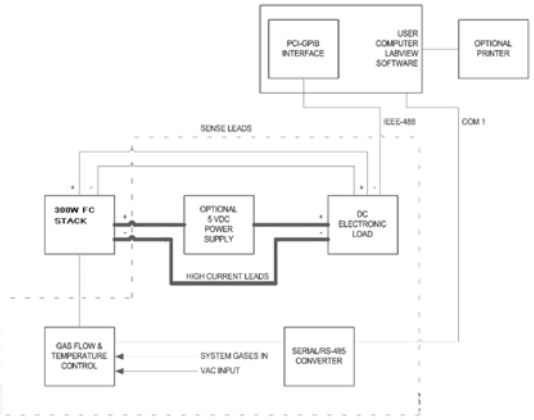

Fig.3. Block diagram of FCT system

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 current-voltage relationship is commonly given in the form of a polarization curve, which is the plot of fuel cell stack voltage against current density i. The current density is defined as stack current per unit of cell active area, i.e, $i = I_{st}.A_{fc}^{-1}$. Here the current –voltage relationship for the 300-W FC stack model and the real system were plotted to the same scale for the comparison of the characteristics. The comparison shows good agreements between the model results and experimental data, see Fig.4. The figure shows the ability of the PEMFC model's prediction in the steady state condition for the real system.

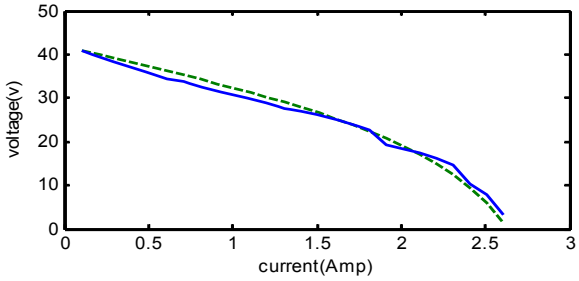

Fig.4. $I-V$ curve of 300-W FC Stack
(model ------ FCT ——)

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 Figures 5 and 6). 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), were the dashed lines and solid lines are indicating the simulation model and FCT test station responses respectively. The anode flow and current (disturbance) inputs were used to drive the model. In this case the real data were obtained for the constant current (I=0.1A) mode setup. 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.

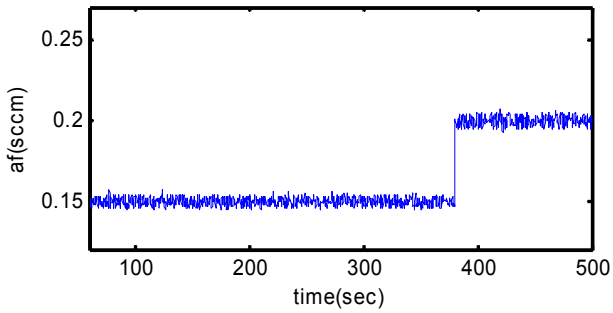

Fig. 5. Fuel cell system input: anode flow

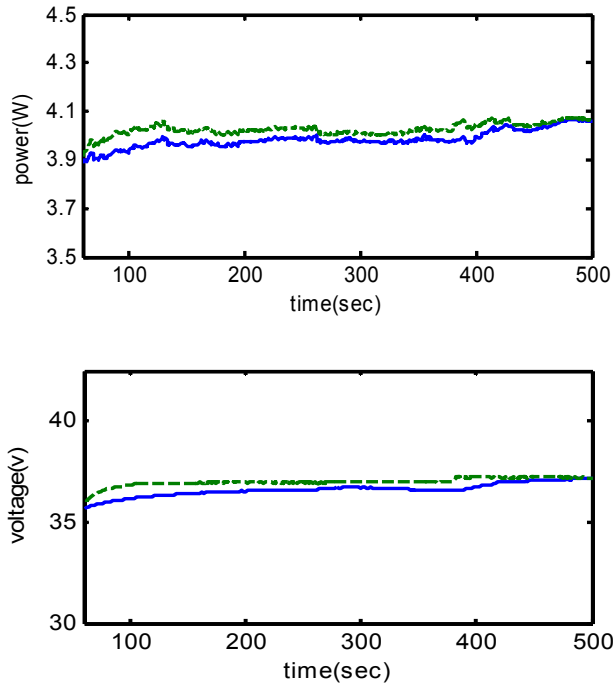

Fig. 6. Comparison of simulation model and FCT responses (model ------ FCT ——)

5. CONCLUSIONS

This paper presents the dynamic model development for 300W PEM FC Stack in MATLAB/Simulink environments. The double-layer charging effects are taken into account in the modelling process. Validation of the model has been carried out through experiments on a 300W PEM FC Stack. Form the results we can say that, overall the 300W PEM FC Stack model represents the FCT station. The model could be useful in controller design applications for PEM FC Stack.

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