

Modeling and Experimental Validation of a PEM Fuel Cell System

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Abstract

This work presents a detailed dynamic model and a model validation study using real data from a Hydrogen Fuel Cell Testing Unit (HFCTU). A parameter estimation technique is employed for the determination of key model parameters and the validation of the overall system behavior is carried out by comparing experimental and simulation results. Data illustrate the transient response of the system during load changes. The model is oriented towards process optimization and control and relies on mass balances and electrochemical equations implemented in the gPROMSTM software environment.

Keywords: PEM Fuel Cell; parameter estimation, dynamic modelling

1. Introduction

Fuel Cells (FC) systems are a potentially good clean energy conversion technology and they can be used in a wide variety of power generation applications. They are categorized mainly on the type of electrolyte used, operating conditions or fuel. The Polymer Electrolyte Membrane fuel cells (PEMFC) are currently considered a good candidate for ground vehicle applications and small portable devices as they have high power density, fast start-up time as well as long cell and stack life. The critical operating parameters are mainly the air and hydrogen feed, flow and pressure regulation, and heat and water management. This work is focused on the validation of a model that incorporates features for these parameters, against a real test bed system. The following section presents a dynamic fuel cell model while the subsequent section introduces a model validation procedure including a comparison of model predictions against experimental results.

2. Modeling

The proposed model rely on first-principle equations combined with equations having experimentally defined parameters thus resulting in a semi-empirical system. The model accounts for mass dynamics in five control volumes: the gas flow channels, the gas diffusion layers and the membrane, as well as thermal dynamics. The mathematical model equations that describe the operation of the FC consist of the voltage-current characteristics and a relationship for the consumption of the reactants as a function of the current drawn from the fuel cell.

2.1. General analysis and modelling assumptions

In order to simplify the modeling and reduce the computation time the following assumptions are drawn. The gases are ideal and uniformly distributed inside anode and cathode. The stack is fed with humidified hydrogen and air because the use of humidified fuel and air improves the efficiency of the FC, thus the model have to take this into account. The temperature is constant and uniform for each experiment. The gas channels along the electrodes have a fixed volume with small lengths, so that it is necessary only to define one single pressure value in their interior. Regarding the operation of the system, during experiments the produced water is continuously removed from the cathode flow and also the condensed water on the anode is dragged by flow of the unreacted hydrogen. The modeling of the gas diffusion layers as well as the modeling of the membrane rely on the same equations as presented in del Real (2007). The physical parameters of these equations are adjusted according to the experimental measurements taken from the real system.

2.2. Electrochemical Equations and Voltage Calculation

Typical characteristics of FC are normally given in the form of polarization curve, which is a plot of cell voltage versus cell current density. To determine the voltage-current relationship of the cell, the cell voltage has to be defined as the difference between an ideal Nernst voltage and a number of voltage losses as it is described in the current section. The main losses are categorized as activation, ohmic and concentration losses. The equation that combines these irreversibilities expresses the actual cell voltage:

$$V_{cell} = E_{nernst} - V_{act} - V_{ohm} - V_{conc} \quad (1)$$

The above equation is able to predict the voltage output of PEM fuel cells of various configurations. Depending on the amount of current drawn the fuel cell generates the output voltage according to (1). The electric power delivered by the system equals the product of the stack voltage V_{cell} and the current drawn I :

$$P = I \cdot V_{cell} \quad (2)$$

This description for the activation overvoltage takes into account the concentration of oxygen at the catalyst layer (Pathapati et al. 2005)

$$V_{act} = \xi_1 + \xi_2 T + \xi_3 T_{st} \ln(I) + \xi_4 T_{st} \ln(c_{O_2}) \quad (3)$$

At a later stage, as current density rises, ohmic losses (V_{ohm}) prevail. They are derived from membrane resistance to transfer protons and from electrical resistance of the electrodes to transfer electrons.

$$V_{ohm} = (\xi_5 + \xi_6 T + \xi_7 I) I \quad (4)$$

Finally the mass transport or concentration losses result from the change in concentration of the reactants at the surface of the electrodes as the fuel is used (Larminie J., 2003):

$$V_{conc} = \xi_8 \exp(\xi_9 I) \quad (5)$$

where ξ represents experimentally defined parametric coefficients whose vary can vary from stack to stack.

2.3. Mass Balance Equations

The model equations consist of the standard material balance of each component. Every individual gas follows the ideal gas equation. Therefore mass is described through partial pressures of each gas in the material balances. Applying mass balance to the cathode channel volume, assessing the inlet and outlet flows of the channel and the exchange flow between it and the gas diffusion layer, the following equations are derived:

$$\frac{dm_{O_2,cach}}{dt} = \dot{m}_{O_2,cach,in} - \dot{m}_{O_2,cach,out} - \dot{m}_{O_2,caGDL2cach} \quad (6)$$

$$\frac{dm_{N_2,cach}}{dt} = \dot{m}_{N_2,cach,in} - \dot{m}_{N_2,cach,out} \quad (7)$$

$$\frac{dm_{v,cach}}{dt} = \dot{m}_{v,cach,in} - \dot{m}_{v,cach,out} + \dot{m}_{v,caGDL2cach} + \dot{m}_{evap,cach} \quad (8)$$

$$\dot{m}_{l,cach,in} - \dot{m}_{l,cach,out} - \dot{m}_{evap,cach} = 0 \quad (9)$$

$$m_{ma,cach} = m_{O_2,cach} + m_{N_2,cach} + m_{v,cach} \quad (10)$$

$$\dot{m}_{O_2,caGDL2cach} = \frac{N_{fc} M_{O_2} I}{4F} \quad (11)$$

The amount of water vapor in the fuel and air is calculated from the value of relative humidity ($\phi_{[an,ca]ch,in}$), the saturation pressure (p_{sat}) and the temperature ($T_{[an,ca]ac,in}$):

$$w_{v,[an,ca]ch,in} = \frac{M_{H_2O}}{M_{air}} \frac{\phi_{[an,ca]ch,in} p_{sat}(T_{[an,ca]ch,in})}{P_{[an,ca]ch,in} - \phi_{[an,ca]ch,in} p_{sat}(T_{[an,ca]ch,in})} \quad (12)$$

The equations that give the amount of each species going into the channels which will be useful for the determination of the pressure inside the channels are presented at Pukrushpan et al. (2005). In order to describe the evaporation and condensation dynamics inside the channel, the proposed equations refer to those used by Golbert & Lewin (2007). In conjunction with these equations the inlet mass flow rate of the nitrogen, oxygen and vapor going into the anode channel can be determined:

$$\dot{m}_{k,cach,in} = w_{k,cach,in} \frac{1}{1 + w_{v,cach,in}} \dot{m}_{cach,in} \quad ,k=[O_2, N_2, v] \quad (13)$$

At the cathode the liquid water condensed is dragged by the air, so the outlet flows are:

$$\dot{m}_{cach,out} = K_{cach,out} (p_{cach} - p_{out}) \quad (14)$$

$$\dot{m}_{k,cach,out} = \frac{m_{k,cach}}{m_{ma,cach}} \dot{m}_{cach,out} \quad ,k=[O_2, N_2, v] \quad (15)$$

The equations that describe the anode channel are analogous to the ones that describe the cathode flow channel.

3. Experimental Validation

In order to assess the validity of the developed model a real Polymer Electrolyte Membrane (PEM) fuel cell system has been used to generate experimental data under various conditions. The effect of operational conditions such as temperature, pressure and humidity in the performance of the system was investigated, as the underlying operating conditions significantly affect profitability, effectiveness and safety aspects. Thus the validation procedure relies on experiments under steady state and dynamic conditions. The optimally defined values of the parameters were then used to validate the model under other experiments at different operational conditions.

3.1. Experimental Setup

The fuel cell unit is integrated with several auxiliary components to form a complete fuel cell system. The setup is comprised of a PEM Fuel Cell working at a constant pressure and a Power Conversion Device capable of controlling the current drawn from the FC. All experiments were conducted on a Fuel Cell Testing Unit (FCTU) composed of a humidification system, two mass flows for the regulation of the hydrogen and the air flow and two PID controllers for the anode and cathode pressure regulation. Also the temperature control subsystem includes an air cooling system and a heat up system. A simplified process and instrumentation diagram of the unit is presented in Fig 1.

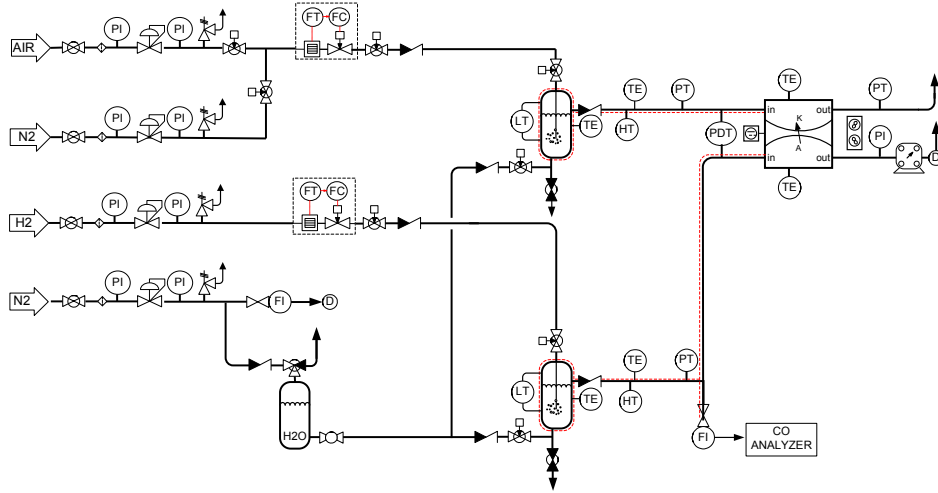


Figure 1 Fuel Cell Testing Unit

3.2. Experimental Procedure

The experimental procedure consists of reading the dynamic response of the cell voltage and cell power after the occurrence of small changes in the load demand. This experimental procedure intended to derive the fuel cell polarization curve and acquire

data from the overall operational range. The overall experiment is conducted using constant pressure and temperature and fixed intervals for the load demand. More specifically the load varies from 0A to 20A with a step change of 2A every two minutes. Two sets of experiments were used for the generation of data for the parameter estimation procedure. The varying condition between the set of experiments was the pressure, 0Barg and 1Barg. Regarding the operational settings of the system: a) the FC temperature was stable at 65°C and the humidification temperature was 75°C, b) the air flow was 2000cc/m and the hydrogen flow 500cc/m. At each condition four identical experiments were conducted.

3.3. Parameter Estimation

The developed model has been implemented in the gPROMS modelling environment. Simulation runs indicated the sensitivity of the system concerning the most critical parameters to be selected for the estimation. Once the model is constructed, estimation is performed to define a set of selected parameters in activation and ohmic losses. A nonlinear regression technique with a constant variance model defining a maximum likelihood estimation problem was employed to determine the optimum values for the selected parameters, including the parametric coefficients in activation losses (ξ_1) and in ohmic losses (ξ_7). The characteristic cell voltage and the applied current density were measured through an on-line supervisory control and data acquisition system. The bounds for the parameters and the estimated values are presented in Table 1.

Table 1. Parameters for estimation

Parameter	Est. Value	Up Bound	Low Bound	Std. Dev	95% Conf Int
ξ_1	1.3205	1.4	0.954	$1.04 \cdot 10^{-3}$	$2.04 \cdot 10^{-3}$
ξ_7	$7.85 \cdot 10^{-4}$	$4.3 \cdot 10^{-4}$	$1.1 \cdot 10^{-6}$	$4.12 \cdot 10^{-6}$	$8.1 \cdot 10^{-6}$

Model predictions are in a very good agreement with the experimental data as indicated in Fig 2. As it can be observed both experimental and simulation results show that a pressure increase raises cell voltage and consequently the power output.

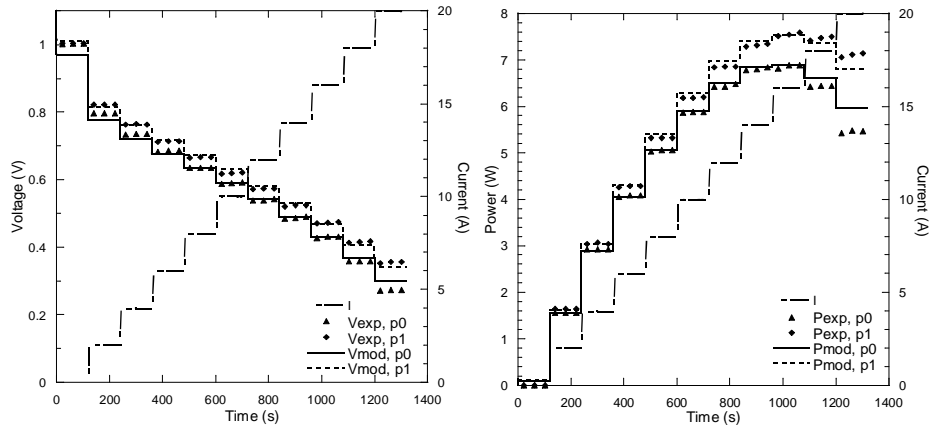


Figure 2 Voltage and power output to current changes (0Barg, 1Barg)

The validated model demonstrated an excellent behaviour both at steady and transient conditions and therefore it can be used both in system startup and during variable load changes.

3.4. Model Validation

A new set of experiments were conducted to assess the accuracy of the validated model. The varying condition was pressure of 0.5Barg and 1.5Barg. Fig 3 that the model predictions are in good agreement with the experimental results. It is clear that under different pressure conditions the model response is similar to the experimental behaviour for the whole range of current variation.

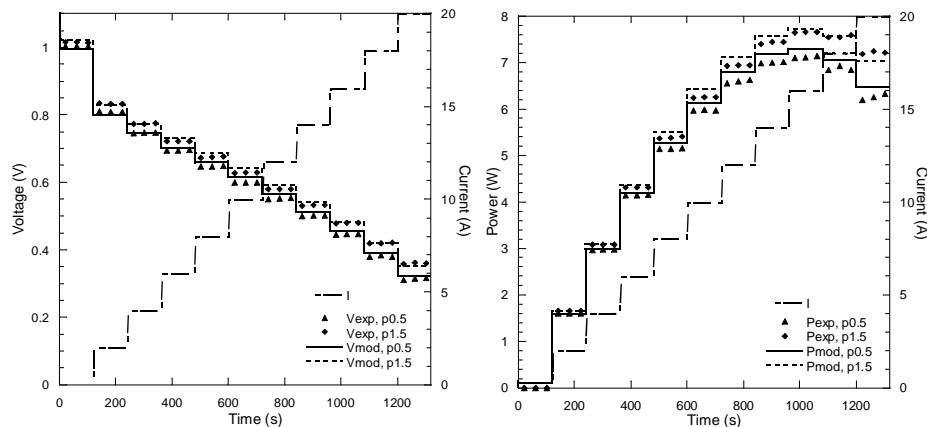


Figure 3 Voltage and power output to load changes using the validated model (0.5Barg, 1.5Barg)

4. Results and Future Work

A dynamic model of a PEM fuel Cell system has been presented followed by a validation procedure relying on the optimal determination of selected model parameters. The predictions of the model are in good agreement with experimental data under various operating conditions. Therefore the validated model can provide the basis for deriving flexible design options and real-time control policies which are the subject of future work.

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