Dynamic Modeling and Characterization of a Proton Exchange Membrane Fuel Cell

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Abstract - *This paper presents the equivalent dynamic model accounting for the thermodynamic and electrochemical characteristics of Proton Exchange Membrane Fuel Cell (PEMFC). The proposed model was implemented in MATLAB/SIMULINK environment. The effects of temperature variations, fluid flow changes and capacitance due to double layer charging were incorporated in this model. The proposed model responses are in good correspondence with the published experimental results. It also predicts the temperature and pressure response of the PEMFC. The model formulated here would be helpful for the optimal prediction of characteristics and dynamic operation of a fuel cell stack.*

Index Terms — Electrochemical characteristics, Dynamic Model, PEMFC

NOMENCLATURE

A	Area of the fuel cell stack [m^2]
$D_{i,j}$	Binary diffusivity of i - j pair [m_2/s]
E	Reversible potential of each cell [volts]
E_0	Reference voltage [volts]
F	Faraday's constant [96487 C/mole]
I	Current [A]
J	Current density [A/m^2]
k_E	Constant in calculating E_0 [V/K]
k_{RI}	Constant in calculating R_{ohm} [Ω/A]
k_{RT}	Constant in calculating R_{ohm} [Ω/K]
l_a	Width between anode channel to catalyst [m]
l_c	Width between cathode channel to catalyst [m]
m	Constant in calculating V_{trans} [3×10^{-5}V]
n	Constant in calculating V_{trans} [8×10^{-4} m^2/A]
N_{cell}	Number of cells in the fuel cell stack
P	Pressure [pa]
P_i	Pressure of the compartment i [pa]
Pi	Partial pressure of the specie i [pa]
q_{net}	Net heat energy [J]
R	Universal gas constant [8.3143 $Jmol^{-1}K^{-1}$]
R_i	Resistance of type i [Ω]
T	Temperature of the FC stack [K]
$T_{initial}$	Initial temperature of the FC stack [K]
V	FC terminal voltage [V]
V_i	Voltage drop of type i [V]
x_i	Mole fraction of specie i
λ_e	Constant in calculating E_d [0.00333]
τ_e	Overall fuel flow delay [s]
ξ_i	parametric coefficients in calculating V_{trans}

Superscripts and Subscripts

a	Anode
act	Activation
c	Cathode
channel	Conditions at anode or cathode
conc	Concentration
ohm	Ohmic
sat	Saturation condition

I. INTRODUCTION

Fuel cells are static energy conversion devices that produce electrical energy from paired oxidation/ reduction reactions. A schematic diagram of PEMFC is shown in Fig. 1. Fuel cells are classified on the basis of electrolytes. Fuel cells may work under different operating conditions depending upon the fuel cell type. PEMFC can be operated at low temperature (about 80 °K) with high power density product and at same time without impact environment [1] and the only byproduct is pure water. PEM Fuel Cells are gathering much attention in Distributed Generation. Compared with other DG technologies, such as wind and photovoltaic (PV) generation, PEMFC have the advantage that they can be placed at any site without geographic limitations, to achieve the best performance [2].

Performance of a fuel cell is measured by its current-voltage relation (i.e., the polarization curve). At a particular current, the voltage drop is mainly caused by (i) over potentials of electrochemical reactions (mainly on the cathode), (ii) the ohmic drop across the ionomeric membrane, and (iii) the mass transport limitations of reactants and products [3]. PEMFC cannot respond fast to the transients. This dawdling behavior of PEMFC in response to transients is mainly due to their slow internal electrochemical reactions and the corresponding thermodynamic responses.

Modeling and computer simulation of Proton Exchange Membrane Fuel Cell has been attempted by number of researchers in the past fifteen years.

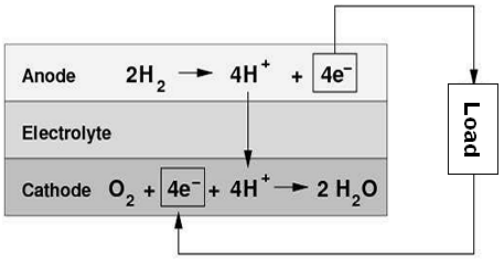

Fig. 1. A Schematic Diagram of PEMFC

Notable work, on one dimensional model of fuel cell, includes that of Bernardi and Verbrugge [4,5] and Springer-et al [6,7]. Some work on dynamic modeling of fuel cell has also been reported [8-10]. These studies are mostly based on electrochemical reactions and empirical equations of the fuel cell.
In this paper, a dynamic model of a Proton Exchange Membrane Fuel Cell is presented. The voltage drops due to activation losses, ohmic losses and concentration losses are modeled. The double layer charging is also considered by adding the effect of an equivalent capacitor. Thermodynamic characteristics of the fuel cell are also incorporated in the model. The model is formulated using MATLAB/ SIMULINK tools.

II. Dynamic Model Formulation

This section covers a mathematical approach for dynamic modeling a PEMFC. Following assumptions are made to simplify the methodology [11]-[15].

1- One-dimensional treatment.
2- Ideal and uniformly distributed gases.
3- Constant pressures in the fuel-cell gas flow channels.
4- The fuel is humidified H_2 and the oxidant is humidified air. Assume the effective anode water vapor pressure is 50% of the saturated vapor pressure while the effective cathode water pressure is 100%.
5- The fuel cell works under 100°C and the reaction product is in liquid phase.
6- Thermodynamic properties are evaluated at the average stack temperature, temperature variations across the stack are neglected, and the overall specific heat capacity of the stack is assumed to be a constant.
7- Parameters for individual cells can be lumped together to represent a fuel-cell stack.

A. Reactant Gases Diffusion in the Electrodes

To calculate the PEMFC output voltage, the effective partial pressures of O_2 and H_2 should be determined. In a gas mixture consisting of *N* species, the diffusion of component *i* through the porous electrodes can be described by using Stefan-Maxwell equations as written to be [12]

$$\nabla x_i = \frac{RT}{P}\sum_{j=1}^{N}\frac{x_i N_j - x_j N_i}{D_{i,j}} \qquad (1)$$

At anode, the input gas stream is a mixture of H_2 and $H_2O_{(g)}$. In the one-dimensional (1-D) transport process along the x-axis the effective mole fraction of water at the anode catalyst interface is calculated by modifying the above equation as

$$x_{H_20} = x_{H_2O}^{channel}\exp\left(\frac{RTjl_a}{2FP_aD_{H_2O},H_2}\right) \qquad (2)$$

As at anode the input is the mixture of water vapors and hydrogen, so

$$x_{H_20} + x_{H_2} = 1 \qquad (3)$$

The partial pressure of hydrogen at anode can be calculated as

$$p_{H_2} = \frac{p_{H_2O}}{x_{H_2O}}(1 - x_{H_2O}) \qquad (4)$$

According to the assumption (4) mentioned above, p_{H_2O} at anode is taken to be $0.5p_{H_2O}^{sat}$. Therefore, the partial pressure of hydrogen at anode can be found by combining equations (2) and (4) as

$$p_{H_2} = 0.5p_{H_2O}^{sat}\left[\frac{1}{x_{H_2O}^{channel}\exp\left(\frac{RTjl_a}{2FP_aD_{H_2o,H_2}}\right)} - 1\right] \qquad (5)$$

The gasses assumed to be flowing in the cathode chamber are oxygen, water vapors and nitrogen. Using the similar analysis for anode, the effective molar fraction of water and nitrogen at the cathode catalyst interface is formulated as

$$x_{H_20} = x_{H_2O}^{channel}\exp\left(\frac{RTjl_c}{4FP_cD_{H_2O},O_2}\right) \qquad (6)$$

$$x_{N_2} = x_{N_2}^{channel} \exp(\frac{RTjl_c}{4FP_c D_{N_2},O_2}) \quad (7)$$

The effective molar fraction of oxygen at cathode channel is determined as

$$x_{O_2} = 1 - x_{H_2 0} - x_{N_2} \quad (8)$$

According to assumption (4), the partial pressure of water vapor in the cathode is fixed at the saturation level, the partial pressure of O_2 at the cathode channel is

$$p_{H_2} = \frac{p_{H_2O}^{sat}}{x_{H_2O}}(1 - x_{H_2O} - x_{N_2}) \quad (9)$$

Effective partial pressures calculated from the equation (5) and (9), are used in finding the Nernst equation for finding Fuel Cell output voltage.

B. Output Voltage Calculations

This section covers the mathematical modeling for the output voltage of PEMFC. According to the assumption (5), the product in the fuel cell is water in liquid form. The corresponding Nernst equation [2] used to calculate the reversible potential is

$$E_{cell} = E_0 + \frac{RT}{2F}\ln(p_{H_2}.p_{O_2}^{1/2}) - E_d \quad (10)$$

Where E_0 and E_d are expressed as

$$E_0 = E_0^* - k_E(T - 298) \quad (11)$$

$$E_d = \lambda_e I_{(s)}\left(\frac{\tau_e s}{\tau_e s + 1}\right) \quad (12)$$

Where, E_0^* is the standard voltage at 1-atm pressure and temperature of 298-K.

Equation (10) shows the open circuit voltage for the fuel cell where as under normal operating conditions fuel cell voltage is less than the open circuit voltage due to certain voltage drops across the fuel cell. These voltage drops will be modeled in the following subsection.

1) Ohmic Voltage Drop

Ohmic voltage drop in PEMFC is due to the resistances of electrodes, the conducting resistance between the membrane and electrodes, and resistance of polymer membrane. The overall ohmic voltage drop is determined as

$$V_{ohm} = IR_{ohm} \quad (13)$$

Where, R_{ohm} is given as

$$R_{ohm} = R_{ohm0} + R_{ohm1} + R_{ohm2} \quad (14)$$

Where, R_{ohm0} is the constant part, R_{ohm1} is the current dependant part and R_{ohm2} is temperature dependant part of the resistance [11]. Above equation is redefined in terms of temperature and current as

$$R_{ohm} = R_{ohm0} + k_{RI} I - k_{RT} T \quad (15)$$

2) Activation Voltage Drop

This is caused by the slowness of the reactions taking place on the surface of the electrodes. This loss is integrated in the system [16] by the following equation

$$V_{act} = -[\xi_1 + \xi_2 T + \xi_3 T \ln(c_{O_2}^*) + \xi_4 T \ln(I)] \quad (16)$$

Where, ξ_i are the parametric coefficients and $c_{O_2}^*$ is the oxygen concentration, on the cathode catalytic interface, given by

$$c_{O_2}^* = \frac{p_{O_2}^*}{5.08 \times 10^6 \exp\left(\frac{-498}{T}\right)} \quad (17)$$

3) Concentration Voltage Drop

This drop is due to the change in concentration of the reactants at the surface of the electrodes as the fuel is used. This voltage drop is modeled [14] as

$$\Delta V_{conc} = m\exp(nI) \quad (18)$$

Where, m and n are constants whose values taken are $3x10^{-5}$ V and $8x10^{-3}$ mA^{-1} respectively.

C. Practical Output Voltage

Including all the voltage drops calculated above, the practical output voltage for fuel cell becomes

$$V_{cell} = E_{cell} - V_{ohm} - V_{act} - \Delta V_{conc} \quad (19)$$

According to the assumption (7), the output stack voltage of fuel cell can be determined as

$$V_{stack} = N_{cell} V_{cell} \quad (20)$$

D. Capacitance due to Double Layer Charging

The membrane between the electrodes of a PEMFC only allow H^+ ions to flow and block the electrons flow. After passing through the load, electrons gather at the cathode surface and attract the H^+ ions. This forms two charged layers which are known as double layer. This double layer acts a capacitor and can store electrical energy. The effect of capacitance (C) due to double layer charging is modeled [2] as

$$V_c = \left(I - C\frac{dV_c}{dt} \right)(R_{act} + R_{conc}) \qquad (21)$$

Where R_{act} and $R_{conc.}$ can be calculated using equation (15), (17) and output current. The effect of this capacitance is integrated in the model by using V_c instead of V_{act} and ΔV_{conc}. The output voltage for the PEMFC becomes

$$V_{cell} = E_{cell} - V_{ohm} - V_c \qquad (22)$$

E. PEMFC Temperature Calculations

The net heat generated in the fuel cell is calculated in terms of the fuel cell output voltage and output current [14], formulated as

$$q_{net} = nI(1.485 - V_{cell}) \qquad (23)$$

This heat generated is used to calculate the change in temperature, given as

$$\Delta T = \frac{q_{net}}{MC} \qquad (24)$$

Where, *M* is the mass and *C* is the specific heat energy of fuel cell stack. This change in temperature is further used to find the temperature of the fuel cell stack.

$$T = T_{initial} + \Delta T \qquad (25)$$

III. PEMFC Dynamic Model in MATLAB/SIMULINK

MATALAB/SIMULINK environment was used for developing a dynamic model of the PEMFC, based on thermodynamic, electrical and chemical characteristics of the PEMFC discussed in the above section. Block diagram of the proposed dynamic model of a PEMFC is shown in Fig. 2. The model developed, gives the output voltage, which is determined by the respective equations mentioned above. The input parameters to the model are anode pressure, cathode pressure and initial temperature of the fuel cell. The temperature of the fuel cell stack is calculated at the given load current, output voltage and initial temperature of the fuel cell. This temperature, load current and voltage are then fed back to the different blocks for calculating the output voltage for the fuel cell.

The equations, formulated in previous section, are used to calculate the partial pressures of H_2 and O_2, temperature of the fuel cell stack, open circuit voltage of fuel cell, ohmic voltage drop, concentration voltage drop, activation voltage drop and finally output voltage of the fuel cell.

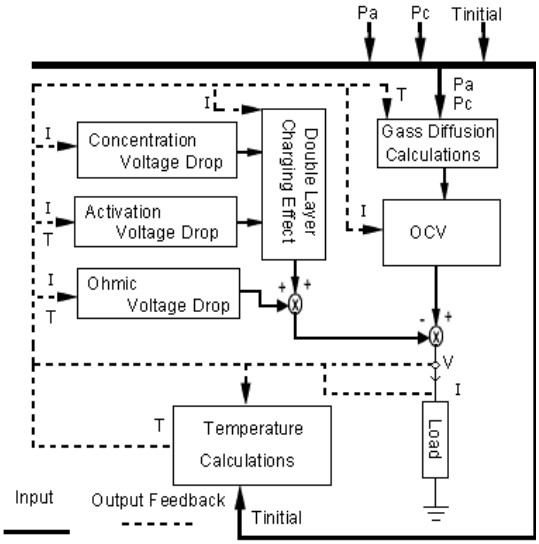

Fig. 2. Block Diagram of the Proposed Dynamic Model of a PEMFC

IV. Simulation Results

Simulation results for the dynamic model of PEMFC presented in this paper are shown in this section. The results are in good agreement with the published experimental results. The result includes V-I characteristics, Power versus Current (P-I) curves at different temperature and pressures.

A. V-I Curve

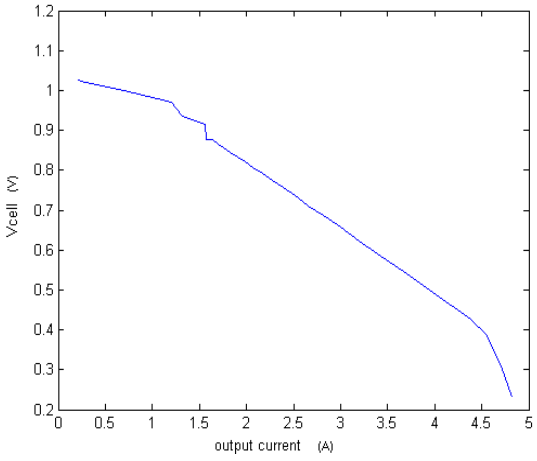

Fig. 3. V-I characteristics of the model

Fig. 3 shows the V-I curve of the PEMFC, from the MATLAB/SIMULINK. Simulation result for V-I curve shows some variations as compared to the published results but it predicts the V-I characteristics of the PEMFC. The voltage drop at the beginning is due to the activation loss, the voltage drop in the middle of the curve, which is approximately linear, is due to ohmic loss and the voltage drop at the end of the curve is due to the mass transportation (concentration) loss.

B. P-I Curve

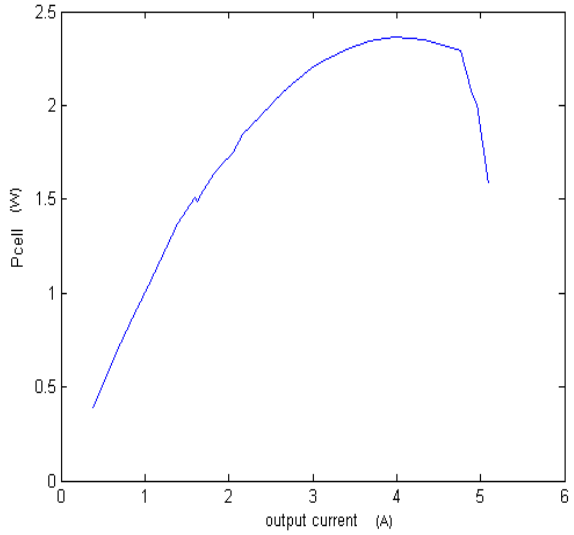

Fig. 4. P-I characteristics of the model

Fig. 4 shows the power versus current (P-I) curve of the PEMFC, obtained from the model response. The model response in this case matches well with the published experimental results. Fig. 3 also shows that the peak output power occurs at the rated output of the PEMFC. After which the fuel cell goes into concentration region, in which the fuel cell output power will decrease with increase in load current due to the sharp terminal voltage drop.

C. Temperature Response of the Model

Fig. 5 and 6 shows the impact of temperature on the fuel cell voltage and output power. The proposed dynamic model temperature response of the PEMFC shows that the temperature of the fuel cell is increased from 333.15 K to 353.15 K, the output voltage and output power also increases. The temperature responses of the model (Voltage-Current curves and Power-Current curves) are in good agreement with the published results.

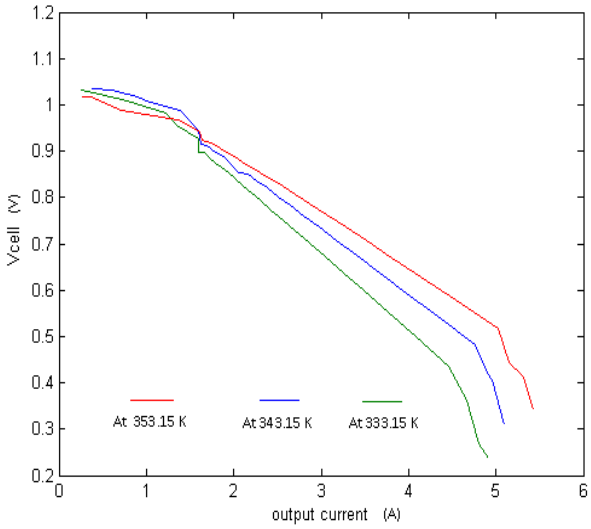

Fig. 5. V-I characteristics of the model at different

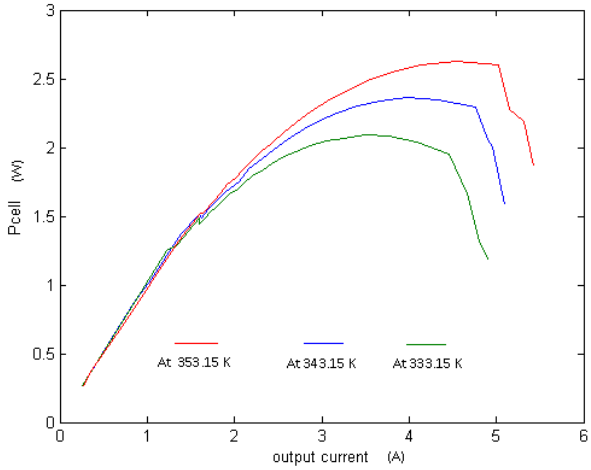

Fig. 6. P-I characteristics of the model at different temperatures

D. Pressure Response of the Model

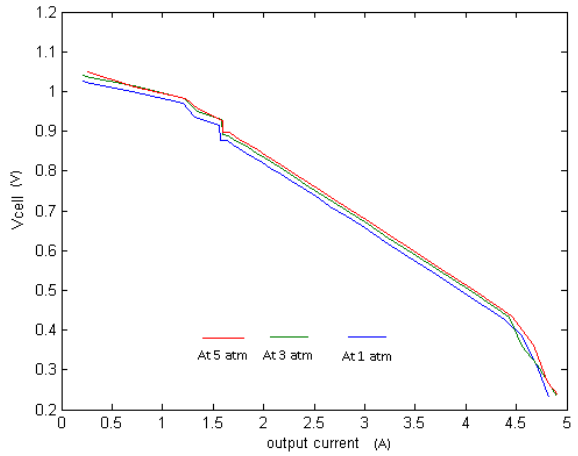

Fig. 7. V-I characteristics of the model at different pressures

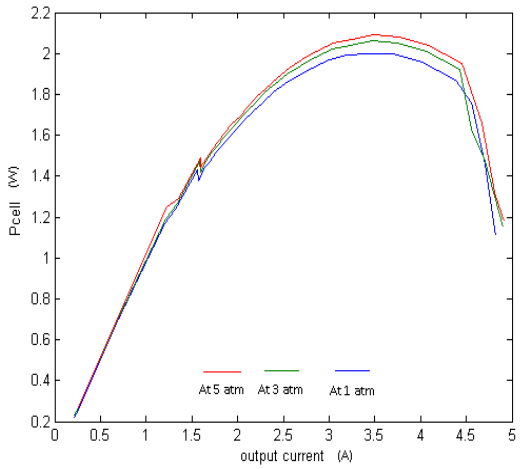

Fig. 8. P-I characteristics of the model at different pressures

Fig. 7 and 8 shows the effect of varying hydrogen pressure on the output voltage and output power of the fuel cell. Pressure response of the proposed dynamic model is in good correspondence with the published experimental results. As, Hydrogen pressure is increased from 1 atm to 5 atm, the output voltage and power of the fuel cell increases.

V. CONCLUSION

The paper presents the dynamic model for the PEMFC in MATLAB/SIMULINK environment. The effects of temperature and pressure variations along with double layer charging property of the fuel cell are taken into account. Activation, ohmic and mass transport (concentration) losses are also integrated in the model. The model predicts the temperature and pressure response of the PEMFC. Although the proposed model is not validated on a practical system but a good agreement has been obtained between the proposed dynamic model and published experimental result. It is observed that, the voltage and power of the fuel cell increases by increasing the input temperature of fuel cell and increasing the pressure of hydrogen leads to increase of the voltage and power of cell. The proposed model can also be useful in prediction of dynamic behavior of the fuel cell stack and can be used for the fuel cell power plants behavioral studies.

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