Journal of Power Sources 182 (2008) 168–174

Contents lists available at ScienceDirect

Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

Dynamic modeling and simulation of air-breathing proton exchange membrane fuel cell

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ARTICLE INFO

Article history:
Received 4 November 2007
Received in revised form 1 March 2008
Accepted 21 March 2008
Available online 4 April 2008

Keywords:
Air breathing
Proton exchange membrane
Fuel cell
Analytical modeling

ABSTRACT

Small fuel cells have shown excellent potential as alternative energy sources for portable applications. One of the most promising fuel cell technologies for portable applications is air-breathing fuel cells. In this paper, a dynamic model of an air-breathing PEM fuel cell (AB-PEMFC) system is presented. The analytical modeling and simulation of the air-breathing PEM fuel cell system are verified using Matlab, Simulink and SimPowerSystems Blockset. To show the effectiveness of the proposed AB-PEMFC model, two case studies are carried out using the Matlab software package. In the first case study, the dynamic behavior of the proposed AB-PEMFC system is compared with that of a planar air-breathing PEM fuel cell model. In the second case study, the validation of the air-breathing PEM fuel cell-based power source is carried out for the portable application. Test results show that the proposed AB-PEMFC system can be considered as a viable alternative energy sources for portable applications.

1. Introduction

Fuel cells are static energy conversion devices and convert the chemical energy of the input fuel directly into electrical energy. The use of fuel cells can offer significant advantages for many applications, such as improving efficiency, reliability, operating characteristics, zero emission and high energy density [1–21].

Recently small fuel cells have attracted a lot of attention for portable applications [1–9]. Small fuel cells are intended to replace conventional batteries in portable applications [4]. For portable applications, the fuel cell should be small and able to operate at ambient conditions. The most promising fuel cell technologies for portable applications are direct methanol fuel cells, air-breathing fuel cells and proton exchange membrane (PEM) fuel cells [4–9].

The air-breathing PEM fuel cells are being developed to provide power for portable and mobile electronic systems. The air-breathing PEM fuel cells have many unique features when compared to other types of fuel cells, such as relatively, less noise, less volume, light weight, low operating temperature and high energy density and no need for an auxiliary fan or compressor [3]. In this paper, a dynamic model of an air-breathing PEM fuel cell system is presented for portable applications.

The analytical modeling of fuel cells is an important part to simulate the physical behavior of fuel cells. Several fuel cell models are reported in the literature [10–21]. Numerical and experimental studies on modeling of proton exchange membrane fuel cell components and stacks are reviewed [10]. Amphlett et al. [14,15] used a semi-empirical approach to estimate the activation loss and to predict the voltage output of a Ballard Mark V 35-cell stack. A one-dimensional non-isothermal model has been presented in [16], which includes membrane hydration, reacting gases, and phase change of water in the electrodes. El-Sharkh et al. [19] introduced a dynamic model for a stand-alone PEM fuel cell power plant. Then, Uzunoglu and Alam [20] modified the PEM fuel cell model described in [19] in Matlab and Simulink for stand-alone residential applications. Zhang et al. [21] presented the effects of the temperature and the equivalent internal resistance on the output characteristics of the PEM fuel cells.

Some research work involving the modeling and experimental studies on air-breathing PEM fuel cells have been reported in the literature [22–31]. Chu and Jiang [22] presented experimental results of an air-breathing PEM fuel cell stack and simulation results were calculated by empirical equations under different operating conditions. Morner and Klein [23] presented an experimental work of an air-breathing PEM fuel cell stack to investigate steady-state and transient effects of temperature, humidity and air flow on the stack performance. Schmitz et al. [24] developed a planar air-breathing PEM fuel cell using printed circuit boards and then a non-isothermal two-dimensional mathematical model was proposed for a planar air-breathing PEM fuel cell [25]. Ying et al.

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doi:10.1016/j.jpowsour.2008.03.076

[27] performed a three-dimensional mathematical model for an air-breathing PEM fuel cell. Recently, Wang and Ouyang [28] presented a three-dimensional heat and mass transfer analysis for an air-breathing PEM fuel cell. Litster and Djilali [29] developed a semi-analytical model to explain the transport of ions, heat and mass in air-breathing fuel cells. The model includes an empirical correlation for membrane conductivity to improve the accuracy of the modeling for dry membrane condition. Fabian et al. [30] presented experimental studies on the performance of a planar air-breathing PEM fuel cell under different ambient conditions. Most recently, O'Hayre et al. [31] proposed a one-dimensional, non-isothermal, heat and mass transport model of a passive planar air-breathing fuel cell operated on dry-hydrogen in dead-ended mode. A comparison is made against experimental measurements illustrated in [30].

In this paper, we propose a new dynamic model for a planar air-breathing fuel cell that is based on the combination of the one-dimensional model described by O'Hayre et al. [31] and a dynamic model described by Uzunoglu and Alam [20]. The new model is compared against the simulation results presented by O'Hayre et al. [31]. Then, the model is examined for powering a portable device such as a laptop computer. The power requirement of a laptop computer varies significantly under different operating conditions. The dynamic model of air-breathing PEM fuel cells is improved for portable applications. The effectiveness of the proposed model has been verified via extensive simulation using the Matlab software package.

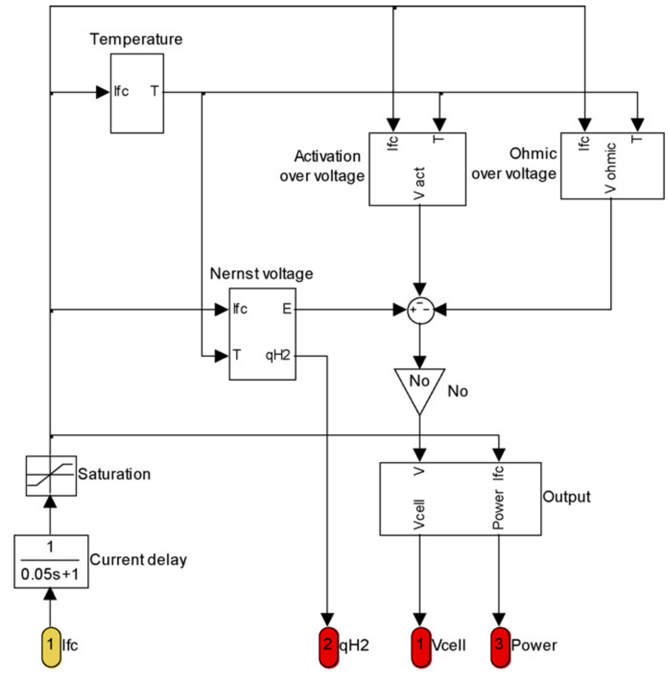

Fig. 1. A simple block diagram of the air-breathing PEM fuel cell.

2. Modeling of the air-breathing fuel cells

Small fuel cell stack provides an alternative solution for small power sources where low weight and simple system configuration are needed. The air-breathing PEM fuel cell technology is one of the most promising fuel cell technologies for portable applications. The mathematical modeling of the air-breathing PEM fuel cells is an important part to simulate the physical behavior of fuel cells. Therefore, some fuel cell models are reported in the literature [22–31]. Recently, the air-breathing fuel cell model, which is a one-dimensional, steady state, non-isothermal, combined heat and mass transport model, was developed by O'Hayre et al. [31].

In the O'Hayre's model [31], the following assumptions are used:

- one-dimensional transport;
- fuel cell operates in the steady state;
- single phase flow;
- effects of liquid water accumulation are not treated;
- dead-ended anode;
- dry hydrogen supply;
- no water accumulation in the anode;
- no net water transport through the membrane;
- water activity is uniform across the membrane and is in equilibrium with the water vapor activity at the cathode catalyst layer;
- cathode catalyst layer is infinitely thin.

In this paper, the dynamic model of the AB-PEMFC is developed based on the O'Hayre's model [31]. The analytical modeling of the AB-PEMFC is verified by developing detailed simulation software using Matlab, Simulink and SimPowerSystems Blockset for portable applications. A simple block diagram of the air-breathing PEM fuel cells is shown in Fig. 1 which involves four main blocks: temperature block, ohmic over voltage block, activation over voltage block, and the Nernst voltage block. The current delay time constant is assumed to be 0.05 s for a small fuel cell. The fuel cell current for the AB-PEMFC is limited by a current limiter according to total fuel cell power. The outputs of the proposed Matlab fuel cell model are the molar flow of hydrogen (qH_2), the output voltage (V_{cell}) and the power output of the AB-PEMFC. This model is used for defining the behavior of the fuel cell stack. In Fig. 1, No represents the number of series fuel cells in the stack.

The output voltage of a single fuel cell can be expressed as

$$V_{cell} = E - \eta_{act} - \eta_{ohm} \quad (1)$$

where E is the Nernst voltage, η_{act} is the activation over voltage and η_{ohm} is the ohmic over voltage. The Nernst voltage may be written as [2]:

$$E = E_0 + \frac{RT}{2F}\left(\ln(P_{H_2}) + \frac{1}{2}\ln(P_{O_2})\right) \quad (2)$$

where E_0 is the standard reversible fuel cell voltage, R is the universal gas constant, T is the fuel cell temperature and F is the Faraday constant. P_{H_2} and P_{O_2} are hydrogen and oxygen partial pressures, respectively. Fig. 2 illustrates the block diagram of the Nernst voltage.

The fuel cell temperature has been assumed to be constant in some previous works [19,20]. But the fuel cell temperature is an important effect on the dynamic behavior of the fuel cell output. The characteristic of the temperature described by Zhang et al. [21] is modified for the proposed dynamic model. The dynamic characteristics of the fuel cell temperature variation may be expressed as

$$T = T_{ic}I_{fc} + T_{rt}\,e^{(tI_{fc}/T_{it})} \quad (3)$$

where T_{ic}, T_{rt} and T_{it} are constant parameters for the fuel cell temperature and I_{fc} is the fuel cell current.

In the block diagram of Fig. 2, the hydrogen partial pressure P_{H_2} can be written as [18–20]:

$$P_{H_2} = \frac{1/k_{H_2}}{1+\tau_{H_2}s}\left(q_{H_2}^{in} - \frac{2I_{fc}}{4F}\right) \quad (4)$$

where τ_{H_2} is hydrogen time constant (s), k_{H_2} is hydrogen valve molar constant (mol/atm s), I_{fc} is the stack current (A) and $q_{H_2}^{in}$ is

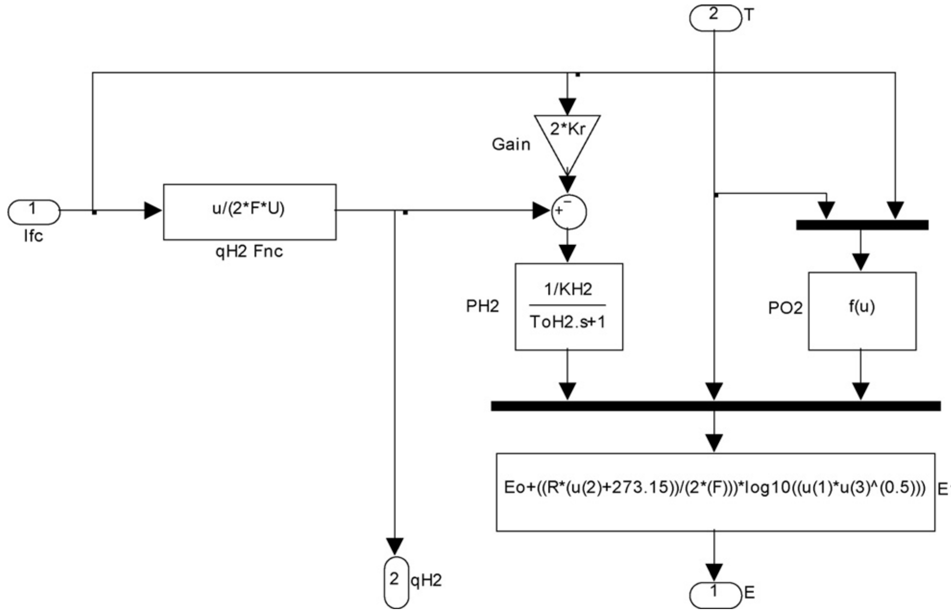

Fig. 2. The block diagram of the Nernst voltage.

hydrogen molar flow (mol/s). The relationship of the molar gas flow through the valve with its partial pressure is expressed as [19]:

$$\frac{q_{H_2}}{P_{H_2}} = \frac{k_{an}}{\sqrt{M_{H_2}}} = k_{H_2} \tag{5}$$

where k_{an} is anode valve constant and M_{H_2} represents molar mass of hydrogen. The hydrogen time constant can be defined as [19]:

$$\tau_{H_2} = \frac{V_{an}}{k_{H_2}RT} \tag{6}$$

where V_{an} is volume of the anode. The hydrogen molar flow can be written as [19]:

$$q_{H_2} = \frac{I}{2F} = 2K_r I \tag{7}$$

where K_r represents a modeling constant. The oxygen concentration is written by [2]:

$$x_{O_2} = x_{O_2}^0 - \delta_{GDL}\frac{jRT}{4FPD_{O_2}^{eff}} \tag{8}$$

where j is the current density, P is the total pressure, δ_{GDL} represents the cathode gas diffusion layer (GDL) thickness and $D_{O_2}^{eff}$ is the effective diffusivity which is described by

$$D_{O_2}^{eff} = D_{O_2,air}\frac{\varepsilon}{\tau} \tag{9}$$

where $D_{O_2,air}$ is the binary diffusivity of O_2 in air, ε represents the GDL porosity and τ is the GDL tortuosity. We can calculate the oxygen partial pressure, P_{O_2} by using the relation between the oxygen concentration and the oxygen partial pressure [2]. The activation over potential is obtained by

$$\eta_{act} = \frac{RT}{\alpha nF}\ln\left(\frac{j}{j_0}\right) \tag{10}$$

where α is charge transfer coefficient and j_0 is the reference exchange current density. The ohmic over potential is calculated as [31]:

$$\eta_{iR} = jA_{cell}(R_{elec} + R_{mem}) \tag{11}$$

where A_{cell} is the cell active area, R_{elec} is the electrical resistance of the cell and R_{mem} represents the resistance of the cell membrane. Fig. 3 illustrates the block diagram of the ohmic over potential. The resistance of the cell membrane is defined as

$$R_{mem} = \left(\frac{\delta_{mem}}{A_{cell}\sigma_{a,T}}\right) \tag{12}$$

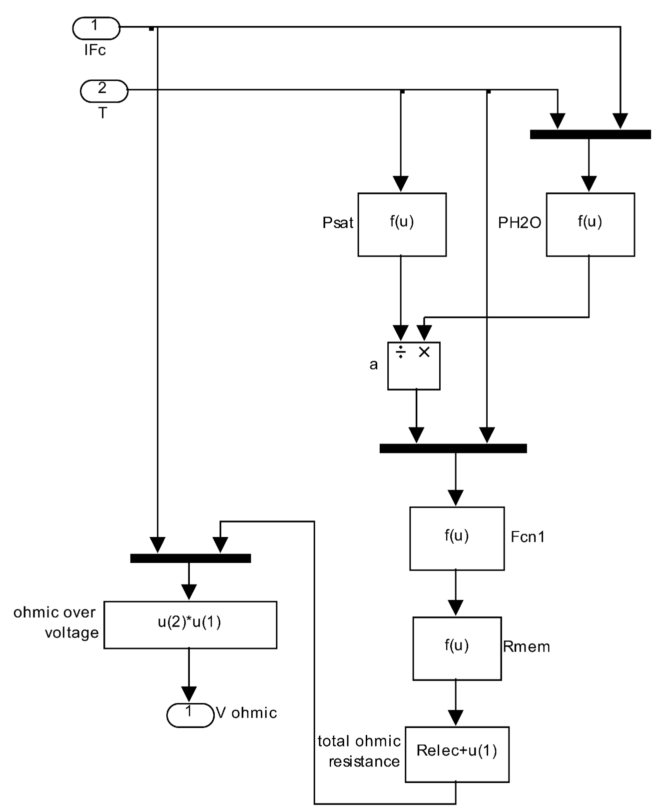

Fig. 3. The block diagram of the ohmic over potential.

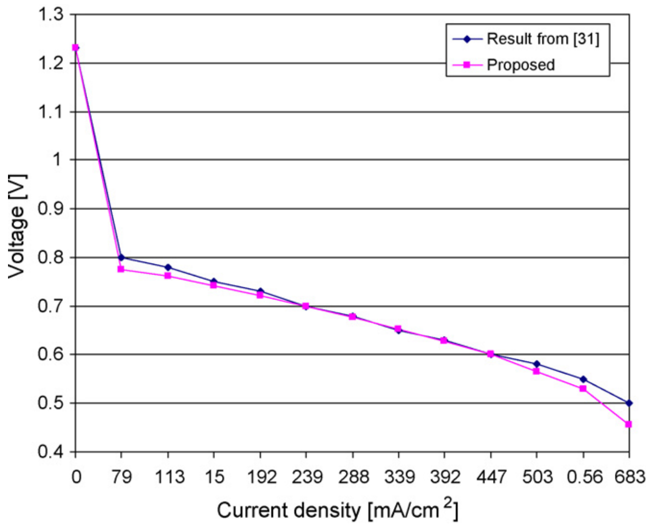

Fig. 4. Polarization curves for proposed AB-PEMFC system and O'Hayre model [31].

where δ_{mem} is Nafion thickness and $\sigma_{a,T}$ represents the conductivity of Nafion, given by

$$\sigma_{a,T} = (3.46a^3 + 0.0161a^2 + 1.45a - 0.175) \times (e^{1268((1/303)-(1/T))}) \tag{13}$$

In Eq. (13), the water vapor activity a in the system can be defined as [2]:

$$a = \frac{P_{H_2O}}{P_{sat}} \tag{14}$$

where p_{H_2O} is the partial pressure of water vapor and P_{sat} is the saturation water vapor pressure for the fuel cell system at the operated temperature. The saturated water vapor pressure can be expressed as

$$\log(P_{sat}) = (-2.1794 + 0.02953T - 9.1837 \times 10^{-5}T^2 + 1.4454 \times 10^{-7}T^3) \tag{15}$$

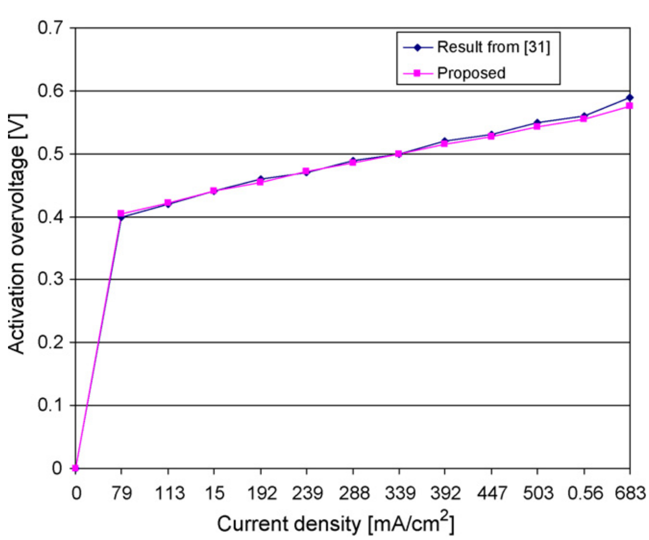

Fig. 5. Activation over voltages of proposed AB-PEMFC system and O'Hayre model [31].

Table 1
Parameters in the air-breathing PEM fuel cell model

Parameter	Representation	Value
No	Number of cells in series in the stack	25
E_0	Standard reversible fuel cell voltage at 303 K and 1 atm pressure	1.23 V
R	Universal gas constant	8.315 J/(mol K)
T_{ic}, T_{rt} and T_{it}	Constant parameters for fuel cell temperature	8.5, 11.2 and 1500
F	Faraday's constant	96,500 C/mol
P	Ambient pressure	101,000
$D_{O_2,air}$	Binary diffusivity of O_2 in air	2.1×10^{-5} m^2/s
$D_{H_2O,air}r$	Binary diffusivity of H_2O in air	2.6×10^{-5} m^2/s
L	Characteristic dimension of fuel cell device (square)	0.07 m
L_a	Length of active cell side (square)	0.03 m
A_{cell}	Cell active area	0.0009 m^2
δ_{mem}	Nafion thickness	5.2×10^{-5} m
δ_{GDL}	GDL thickness	3.0×10^{-4} m
ε	GDL porosity	0.40
τ	GDL tortuosity	3.0
k_{GDL}	GDL thermal conductivity	10 W/m K
R_{elec}	Cell electrical resistance	0.012 Ω
J_0	Reference exchange current density	1.0×10^{-5} A/cm^2
α	Charge transfer coefficient	0.28
U	Utilization factor	0.7
τ_{H_2}	Hydrogen time constant	0.3096 s
k_{H_2}	Hydrogen valve constant	3.62694×10^{-5} kmol/(s atm)

Using Eq. (8), a similar equation for the water concentration can be derived as [2]:

$$x_{H_2O} = x^0_{H_2O} + \delta_{GDL}\frac{jRT}{2FPD^{eff}_{H_2O}} \tag{16}$$

where $D^{eff}_{H_2O}$ is the effective diffusivity of H_2O which is described by

$$D^{eff}_{H_2O} = D_{H_2O,air}\frac{\varepsilon}{\tau} \tag{17}$$

where $D_{H_2O,air}$ is the binary diffusivity of H_2O in air. We can calculate the partial pressure of water vapor to use the relation between the water concentration and the water partial pressure [2].

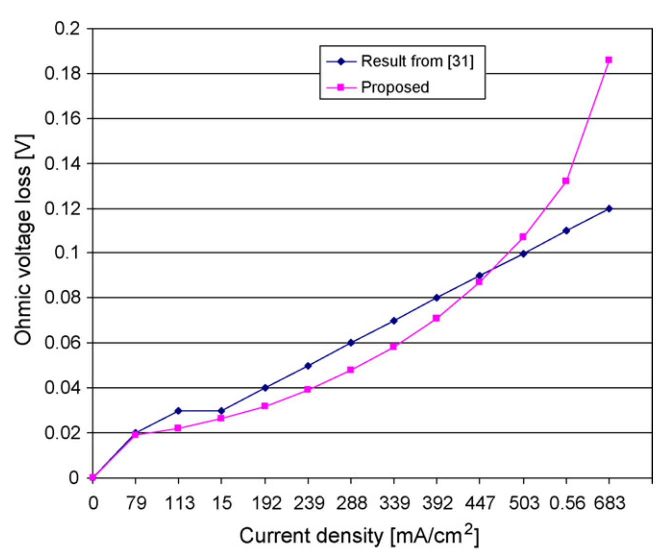

Fig. 6. Ohmic voltage loss of proposed AB-PEMFC system and O'Hayre model [31].

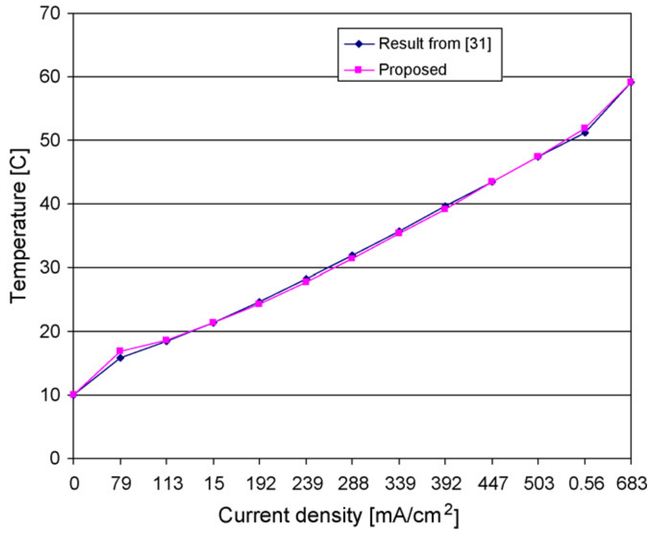

Fig. 7. The fuel cell temperature of proposed AB-PEMFC system and O'Hayre model [31].

One of the most important values to affect the fuel cell output voltage is the fuel cell temperature. The Nernst voltage, the oxygen concentration, the activation over potential, the water concentration and the resistance of the cell membrane (Eqs. (2), (8), (10)–(16)) are related to temperature. Therefore, we calculated the dynamic characteristic of the fuel cell temperature variation using Eq. (3) to determine precisely the fuel cell output voltage.

3. Simulation results

The analytical modeling and simulation of the air-breathing PEM fuel cell system are verified using Matlab, Simulink and SimPowerSystems Blockset. In this section, we will present two case studies: the dynamic behavior of the proposed AB-PEMFC system is compared with that of the O'Hayre model [31] in the first case study; and the validation of the air-breathing PEM fuel cell-based power source is carried out for portable applications in the second case study.

3.1. Case study 1

O'Hayre et al. [31] compared their simulation results against experimental measurements of a 3 cm × 3 cm air-breathing fuel cell device [30]. In this paper, we compared the behaviors of the proposed AB-PEMFC model and O'Hayre model [31]. A simple block diagram of the air-breathing PEM fuel cell system is given in Fig. 1. Table 1 shows the model parameters of the air-breathing PEM fuel cell which are taken from [31]. The hydrogen valve constant and the hydrogen time constant are determined using Eqs. (5) and (6) for the air-breathing PEM fuel cell system assuming the temperature parameters T_{ic}, T_{rt} and T_{it} remain constant.

The polarization curves of the proposed AB-PEMFC system and O'Hayre model [31] are shown in Fig. 4. The proposed model nicely predicts the behavior of the air-breathing fuel cell. The fuel cell output voltages obtained using the proposed model are very similar to those of the O'Hayre model as depicted in Fig. 4.

The activation over voltages of the proposed AB-PEMFC model and O'Hayre model [31] are illustrated in Fig. 5. A good agreement between simulated activation over voltages of the proposed model and O'Hayre model [31] is clearly seen from Fig. 5. The ohmic voltage losses of the proposed AB-PEMFC model and O'Hayre model [31] are shown in Fig. 6. The proposed model nearly predicts the behavior of the ohmic voltage loss of the air-breathing fuel cell as seen in Fig. 6. The ohmic voltage loss of the model is calculated by Eq. (11) which includes R_{mem} the resistance of the cell membrane and R_{elec} the electrical resistance of the cell. The resistance of the

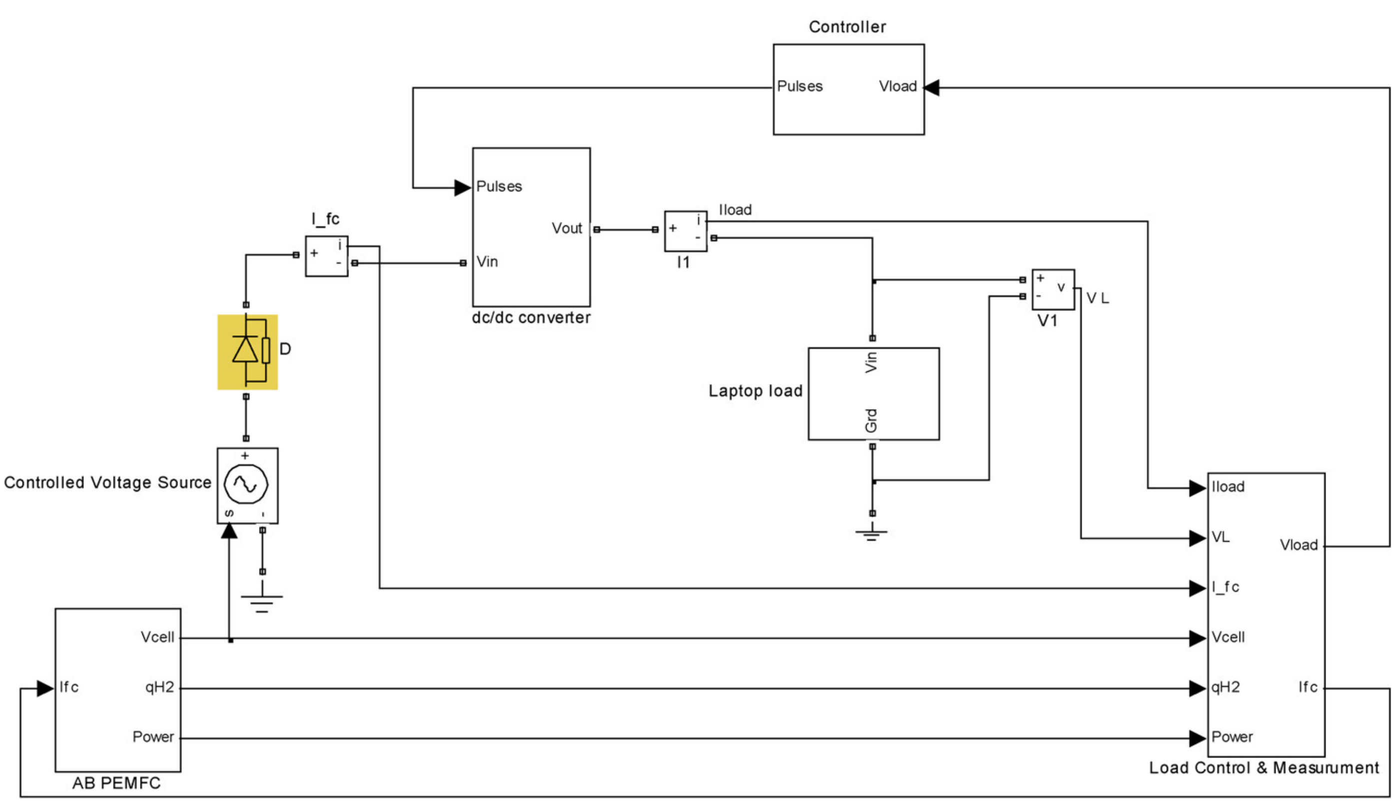

Fig. 8. General diagram of the AB-PEMFC system for a Laptop computer.

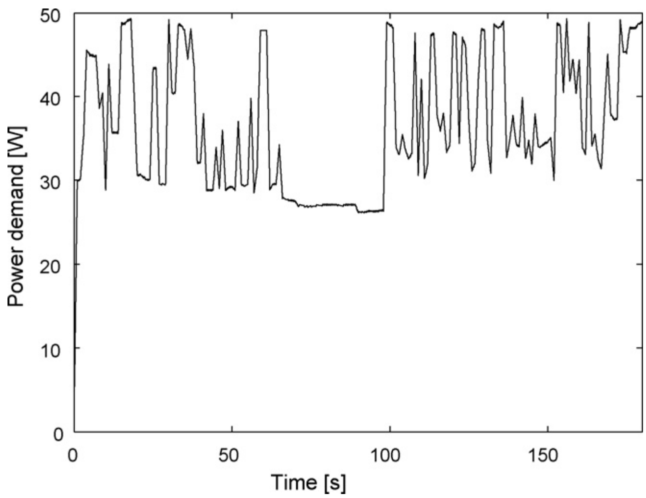

Fig. 9. Power demand.

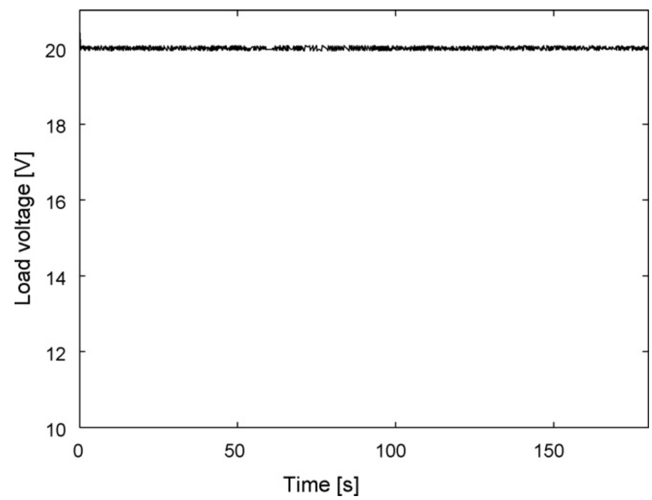

Fig. 11. Load voltage under different operation conditions.

cell membrane is strongly related to the conductivity of Nafion, the membrane water content and membrane temperature as described by Eqs. (12)–(16). The membrane conductivity is not linear with the current density shown in [29,30]. Therefore at higher current density, the proposed model has higher ohmic voltage loss than the result of the O'Hayre model [31].

The fuel cell temperature is an important parameter for calculating the fuel cell output voltage as indicated earlier. Therefore, the characteristic of the fuel cell temperature is predicted by Eq. (3) in the proposed AB-PEMFC system. Fig. 7 shows the comparison of the fuel cell temperature of the proposed AB-PEMFC system and O'Hayre model [31]. The fuel cell temperatures obtained using the proposed AB-PEMFC system are similar to that of the O'Hayre model as shown in Fig. 7.

3.2. Case study 2

In the second case study, the dynamic performance of the air-breathing PEM fuel cell-based power source was tested under various load conditions of a laptop computer, which is a Dell Inspiron 8000. Assume that the rated power of the AB-PEMFC system is 70 W. The fuel cell stack consists of 25 cells. The model parameters of the air-breathing PEM fuel cell system are shown in Table 1. The hydrogen valve constant and the hydrogen time constant are determined using Eq. (5) and (6) for the 70 W air-breathing PEM fuel cell system.

Fig. 8 shows the general diagram of the air-breathing PEM fuel cell system for a Laptop computer. The proposed system consists of the AB-PEMFC model, a boost dc/dc converter, a feedback controller, a laptop load and a load control and measurement unit. The modeling and simulation of the air-breathing PEM fuel cell-based power source are verified using Matlab, Simulink and SimPowerSystems Blockset for a simulation time of 180 s.

The output voltage and current of the ac adapter of Dell Inspiron 8000 are 20 V and 3.5 A, respectively. The dc power consumptions of Dell Inspiron 8000 have been measured using a power quality analyzer. The laptop load is modeled in Matlab using the experiment results obtained from the power quality analyzer for dc power consumption.

The boost dc/dc converter is used to adjust output voltage of the AB-PEMFC system to 20 V. The gate pulses of the boost dc/dc converter are produced by a feedback controller based on a discrete PID controller. The most appropriate parameters of the discrete PID controller are determined as: 1 for proportional gain constant, 10 for integral gain constant, and 0.0002 for derivative gain constant. In the PID controller, the output voltage is compared with the refer-

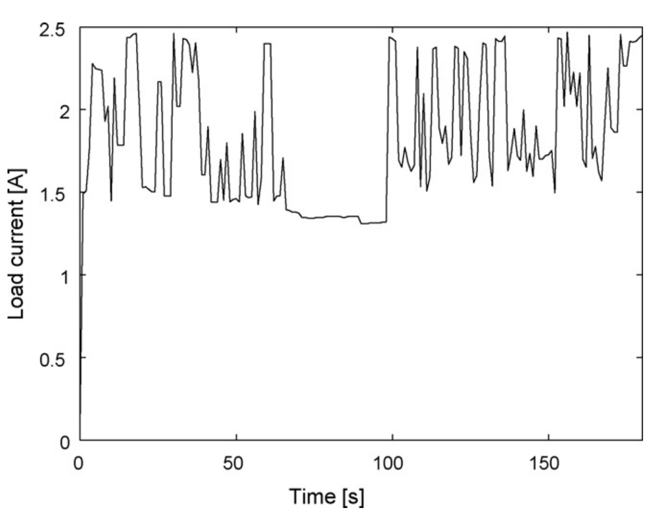

Fig. 10. Load current.

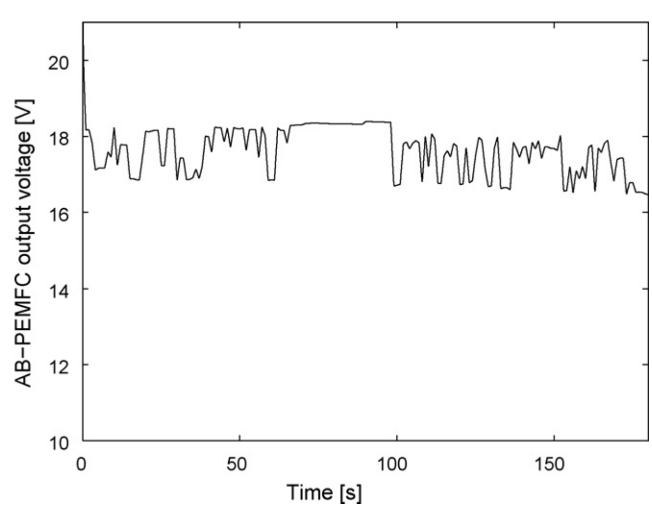

Fig. 12. Fuel cell output voltage under different operation conditions.

ence voltage and the difference between them is used as the input of the discrete PID controller.

The load control and measurement unit is employed for measuring load currents and load voltages. The measured data is used to supply the appropriate feedback current to the AB-PEMFC and the load voltage is provided to the PID controller to produce the trigger signal for the dc–dc converter thyristor. The power demands of the laptop computer may vary significantly under different operational conditions. Fig. 9 shows the change of dc power demand and the dc power consumption of the laptop may vary from 25.2 to 49.6 W. Fig. 10 illustrates the change of the load current of the laptop and the current may vary from 1.31 to 2.46 A. It is clear from Figs. 9 and 10 that the power consumption of the laptop computer varies significantly when the laptop is operated at different operational conditions.

From Fig. 11, we observe that the feedback control system keeps the load voltage at 20 ± 0.2 V under various operational conditions. The errors in power output of the model versus what the laptop requires depend on the load voltage variations. The output voltage of the AB-PEMFC system is illustrated in Fig. 12 and it is obvious that the FC stack voltage is changed slightly under various operation conditions. The AB-PEMFC produces output powers and voltages according to the feedback currents.

4. Conclusion

In this paper, an air-breathing PEM fuel cell-based system is proposed for portable applications. The dynamic modeling and simulation of the AB-PEMFC system were verified using Matlab, Simulink and SimPowerSystems Blockset. In the first case study, the comparison of dynamic behavior of the proposed AB-PEMFC system and O'Hayre model has been carried out. The results obtained from the proposed AB-PEMFC system are similar to those of O'Hayre model. The fuel cell temperature is an important role for calculating the fuel cell output voltage and is predicted in the proposed model. In the second case study, the validation of the air-breathing PEM fuel cell-based power source was performed for portable applications. The simulation results demonstrate that the power consumption of a laptop varies significantly depending on various operational conditions. The feedback control system keeps the load voltage at a desirable level, i.e., 20 V under various operational conditions of the laptop computer. The proposed system supplies adequate power at constant voltage for the laptop computer. The proposed AB-PEMFC system can be considered as a viable alternative energy sources for portable applications.

Acknowledgment

This work was supported in part by the U.S. Department of Energy under Grant DE-FG02-05CH11295.

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