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Modeling and simulation of the dynamic behavior of a polymer electrolyte membrane fuel cell

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Abstract

The focus of this paper is to develop a mathematical model for investigating the dynamic performance of a polymer electrolyte membrane fuel cell. The model in this work is based on physical laws having clear significance in replicating the fuel cell system and can easily be used to set up different operational strategies. Simulation results display the transient behavior of the voltage within each single cell, and also within a number of such single cells combined into a fuel cell stack system. A linear as well as a nonlinear analysis of the polymer electrolyte membrane fuel cell system has been discussed in order to present a complete and comprehensive view of this kind of modeling. Also, a comparison of the two kinds of analysis has been performed. Finally, the various characteristics of the fuel cell system are plotted in order to help us understand its dynamic behavior. Results indicate that there is a considerable amount of error in the modeling process if we use a linear model of the fuel cell. Thus, the nonlinearities present in the fuel cell system should be taken into account in order to obtain a better understanding of the dynamic behavior of the fuel cell system.

Keywords: Polymer electrolyte membrane fuel cells (PEMFC); Modeling; Simulation

1. Introduction

Recently, there has been a growing concern about acid emissions, CO_2, and other air quality matters which have made renewable technologies an attractive option. Fuel cell technology is expected to play an important role in meeting the growing demand for distributed generation. In an ongoing effort to meet increasing energy demand and also to preserve the global environment, the development of energy systems with readily available fuels, high efficiency and minimal environmental impact is urgently required. A fuel cell system is expected to meet such demands because it is a chemical power generation device which converts the chemical energy of a clean fuel (e.g. Hydrogen) directly into electrical energy. Still a maturing technology, fuel cell technology has already indicated its advantages, such as its high energy conversion efficiency, modular design and very low environmental intrusion, over conventional power generation equipment. A fuel cell system has a net electrical efficiency ranging from 40 to 60% based on the lower heating value of the fuel, which is higher than that of almost all other energy conversion systems.

This paper presents a method for simulating the dynamic behavior of a polymer electrolyte membrane fuel cell (PEMFC) based on a mathematical model. The reason for choosing a PEMFC lies in its easy and safe operational modes, low temperature gradient, low chance of catalyst poisoning and a wide scope of application in power distribution systems [1,2,5,7]. Various attempts are being made to model fuel cell systems. Almost all recent endeavors of modeling [2,3,6], have neglected the effects of inverter load in order to achieve simplicity. In this study, the crucial effects of inverter load are considered, thus providing a vivid and brighter picture of the dynamics of a fuel cell system. A linear as well as a nonlinear model for the polymer electrolyte membrane fuel cell is developed. Simulation results are shown for both the models. The results prove that a considerable amount of error occurs in the modeling process by neglecting the nonlinearities present in the fuel cell. Thus the risk involved with linearizing the PEMFC model is recognized. In fact this study shows that a nonlinear model provides a better and a comprehensive understanding to the dynamics of the PEMFC system.

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This paper is organized as follows. Section 2 presents a brief description of the physical structure and the operating principles of a polymer electrolyte membrane fuel cell. The modeling approach is developed in Section 3 and actual simulation block diagrams are shown in Section 4. Simulation results are given in Section 5. A validation study is given in Section 6. Conclusions are discussed in Section 7.

2. Physical structure and the operating principle of a polymer electrolyte membrane fuel cell

Familiarity with the physical structure and the operating principle of a polymer electrolyte membrane fuel cell is necessary to understand its dynamic behavior [4]. A PEM fuel cell consists of two electrodes with a thin layer of catalyst in contact with a plastic membrane separating gas supply chambers. Hydrogen gas (H_2) which acts as fuel, having its source from methanol (CH_3OH), petroleum products or natural gas, is fed through a narrow channel from one end of the plate (*Anode*). Similarly, oxygen (O_2) enters the fuel cell from the other end of the plate (*Cathode*). Fig. 1 represents a schematic diagram of a polymer electrolyte membrane fuel cell.

H_2 and O_2 have a strong chemical affinity and hence the membrane separating the two gases allows only hydrogen ions (H^+) to pass through it, H_2 oxidation H^+ ions and electrons (e^-). While H^+ ions take the shortest path, i.e. through the membrane, e^- travel all the way round the external circuit creating useful current. The H^+ ions combine with oxygen to produce water and heat energy as a by-product in this case.

The PEMFC uses as its electrolyte a polymer membrane which is an electronic insulator, but an excellent conductor of hydrogen ions. The materials used to date consist of a fluorocarbon polymer backbone, similar to Teflon, to which sulfonic acid groups are attached. The acid molecules are fixed to the polymer and cannot leak out, but the protons on these acid groups are free to migrate through the membrane. With the solid polymer electrolyte, electrolyte loss is not a concern. The anode and the cathode are prepared by applying a small amount of platinum black to the surface of a thin sheet of porous, graphitized paper which has previously been wet-proofed with Teflon. The electrolyte is then sandwiched between the anode and the cathode, and the three components are sealed together under heat and pressure to produce a single membrane-electrode assembly. This assembly is less than a millimeter in thickness.

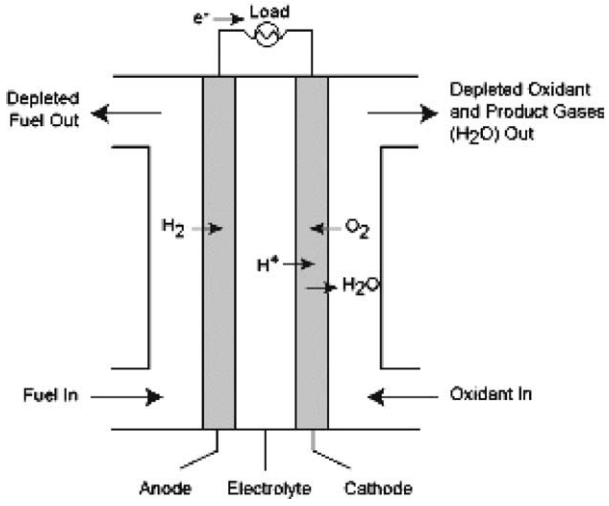

Fig. 1. Schematic diagram of a polymer electrolyte membrane fuel cell [7].

The anode and the cathode are contacted on the back side by flow field plates made of graphite in which channels have been formed. The ridges between the channels make electrical contact with the backs of the electrodes and conduct current to the external circuit. These channels simultaneous supply fuel to the anode and oxidant to the cathode.

The PEM fuel cell can operate on air. As is true with all other fuel cells, performance is improved by pressurizing the air. In any application, there will be a trade-off between the energy and financial cost associated with compressing the air to higher pressures and the improved performance.

Because the PEMFC operates at low temperatures and does not contain a liquid electrolyte, catalyst migration and re-crystallization are not problems.

The PEMFC typically operates at 160 F (70 °C) to 185 F (85 °C). About 50% of the maximum power is available immediately at room temperature. Full operating power is available within about 3 min under normal conditions. The low temperature of operation also reduces or eliminates the need for thermal insulation to protect personnel or other equipment.

The fuel cell will operate continuously producing useful current as long as the fuel and oxygen are supplied. However care should be taken not to damage the thin membrane due to the pressure difference created by uneven flow of hydrogen and oxygen gases. We can assemble many single cells into a fuel cell stack system in order to provide the required amount of power.

3. Modeling approach

The mathematical model developed is based on appropriate energy, mass and electrochemical equations as applied to PEM fuel cell [9,10].

There are two methods for modeling the fuel cell system. The first method is to design a one-dimensional fuel cell model, where the fuel input is the only variable through the fuel cell (neglecting the effects of inverter). The second method of modeling is a three-dimensional approach (similar to the one presented in this paper), where besides varying the fuel input, the air supply and the inverter load current, are also varied.

The whole modeling process can be divided into two parts.

3.1. Individual cell modeling aspects

The chemical reactions occurring at the oxidation and reduction electrode of a PEM fuel cell are as follows:

$$\text{Oxidation half reaction}: \ 2H_2 \rightarrow 4H^+ + 4e^- \tag{1}$$

$$\text{Reduction half reaction}: \ O_2 + 4H^+ + 4e^- \rightarrow 2H_2O \tag{2}$$

$$\text{Total cell reaction}: \ 2H_2 + O_2 \rightarrow 2H_2O \tag{3}$$

The various equations necessary for the modeling of an individual cell are presented below.

3.1.1. Nernst model

The result of the chemical reactions inside a fuel cell is the reversible single electrode potential, E_r given by the Nernst equation as

$$E_r = E_r^0 - \left[\left(\frac{RT}{nF}\right) \ln\left(\frac{p_{H_2O}}{p_{H_2} \times \sqrt{p_{O_2}}}\right)\right] \tag{4}$$

where E_r^0 is the standard electrode potential, R represents the gas constant (8.3144 J/mol K), T the temperature in Kelvin scale, n the number of electrons per reacting ion or molecule, F represents Faraday's constant (96,500 C/mol), p_{H_2O} the partial pressure of water, p_{H_2} the partial pressure of hydrogen, and p_{O_2} the partial pressure of oxygen.

3.1.2. Effect of chemical polarization on cell voltage

This is due to the individual chemical reactions occurring at the electrodes of a PEMFC, given by Eq. (5). This equation is more commonly known as Tafel equation.

$$\Delta E_{Chem} = a + b\log(I) \tag{5}$$

where

$$a = \left[\frac{RT}{\alpha nF}\right] \ln(i_o) \tag{5a}$$

$$b = 2.303\left[\frac{RT}{\alpha nF}\right] \tag{5b}$$

where α is the activity coefficient, i_o the exchange current density, and I the applied current density.

3.1.3. Effect of concentration polarization on cell voltage

There is a change in the concentration gradient at the electrodes due to the continuous chemical reactions. The effects of these changes are expressed in the form of concentration polarization as follows:

$$\Delta E_{Conc} = \left[\frac{RT}{nF}\right] \ln\left(\frac{I_L - I}{I_L}\right) \tag{6}$$

where I_L is the limiting current density and I the applied current density.

3.1.4. Effect of resistance polarization on cell voltage

As a result of the electrochemical reactions, there is a certain amount of change in specific conductivity, leading to an additional loss in the potential, given by Eq. (7).

$$\Delta E_{Rest} = \frac{nFD}{\Lambda(1 - t_i)} \ln\left(\frac{I_L - I}{I_L}\right) \tag{7}$$

where Λ represents the equivalent conductance of the reacting ion (cm^2/ohm-equiv), t_i the transference number of the ion, and D the diffusion constant.

So, the sum total of all pertinent components of polarization (ΔE_T) occurring in a single cell is given by

$$\Delta E_T = \Delta E_{Chem} + \Delta E_{Conc} + \Delta E_{Rest} \tag{8}$$

3.1.5. Closed cell voltage

Thus for a closed circuit cell with voltage V, operating at a load current i, the voltage is expressed as follows:

$$\begin{aligned} V &= (E_{r,A} - \Delta E_{T,A}) - (E_{r,C} - \Delta E_{T,C}) - i\sum R_j \\ &= E_{T,r} - \Delta E_{T,A} + \Delta E_{T,C} - i\sum R_j \end{aligned} \tag{9}$$

where $E_{T,r}$ is combined standard electrode potential of anode and cathode obtained from Eq. (4), $\Delta E_{T,A}$ the sum total of all pertinent components of anodic polarization (a positive number), $\Delta E_{T,C}$ the sum total of all pertinent components of cathode polarization (a negative number), 'i' the total current through the cell, and $\sum R_j$ represents the sum of all internal cell resistances including electrolyte, any diaphragms, and resistances in the electrode bodies.

3.2. Fuel cell stack model

In this section, we will present the various equations necessary for the modeling of the overall fuel cell system.

For 'N' single cells connected in a fuel cell stack system, the total stack voltage (ΔV_T) is calculated using the following nonlinear equation

$$\Delta V_T = N\left[V_r - \Delta E_{T,A} + \Delta E_{T,C} - i\sum R_j\right] \tag{10}$$

$$\begin{aligned} \Delta V_T = N &\left[E_r^0 - \left(\left(\frac{RT}{nF}\right) \ln\left(\frac{p_{H_2O}}{p_{H_2} \times \sqrt{p_{O_2}}}\right)\right)\right] \\ &- N\left[\left(\frac{RT}{\alpha nF}\right) \ln(i_o I) + \left(\frac{RT}{nF}\right) \ln\left(\frac{I_L - I}{I_L}\right) \right. \\ &\left. + \frac{nFD}{\Lambda(1 - t_i)} \ln\left(\frac{I_L - I}{I_L}\right)\right] - N\left[i\sum R_j\right] \end{aligned}$$

A pressure difference is generated by the fuel and oxidant gases passing through the anode and cathode gas compartments. The partial pressures of the reactants in the anode and cathode are given by

$$\frac{dP_i}{dt} = \frac{RT_s}{V_s}\left(m_{i_i} X_i - m_{o_i} X_i - \frac{I_s N}{n_i F}\right) \tag{11}$$

where P_i is the partial pressure of the reactant species i inside the fuel cell stack, T_s represents the average stack temperature, V_s the volume of the channel for gas flow inside the stack, m_i and m_o are the net instantaneous input and output flow rates of gases, X_i represents the mole fraction of the species i in the stack, N the number of single cells connected in the stack, I_s the stack current, and n_i the number of electrons transferred during the reaction of species i.

Continuous operation of the fuel cell requires removal of the water produced by the chemical reaction. Since the electrolyte is stationary, the most convenient way to remove the water is by evaporation through the porous electrode into a gas stream. The model developed in this work has indicated that for current densities around 100 A/ft^2, moisture control is facilitated by the removal of water at the hydrogen electrode.

The pressures inside the humidifier is given by

$$\frac{dP_h}{dt} = \frac{RT}{V}(n_i - n_o) \tag{12}$$

where n_i is the input mol/s, n_o the output mol/s, P_h the pressure in the humidifier, and V the volume within the humidifier.

The molar output flow rate is given by the pressure–flow relationship,

$$n = K(P_h - P_s) \tag{13}$$

where K is known as the flow constant, determined by the laminar flow relationship, and P_s the stack pressure.

The rate of water formation is directly proportional to the current drain, whereas the rate of water removal depends upon the temperature and pressure of operation, electrolyte composition, and pore structure of the electrodes.

In this study, all the variables that affect the rate of moisture removal are held relatively constant with the exception of the gas flow rate and the partial pressures of the gases.

While designing the overall fuel cell model, it is very important to consider the leakage currents between single cells via the common electrolyte supply.

This leakage current I_l is given by

$$I_l = \frac{(N-1)V}{2r_p + (N-1)r_a} \tag{14}$$

where V is the terminal voltage per cell in a stack of N cells, r_a the resistance of a pair of radial ports, and r_p the resistance of a pair of axial ports.

4. Model simulation

The whole modeling process is divided into two parts which are:

(i) nonlinear modeling of the fuel cell system, and
(ii) linear modeling of the fuel cell system.

4.1. Nonlinear model of PEM fuel cell system

Fig. 2 shows the simulation block diagram of a PEMFC plant. This model is developed on the basis of the equations

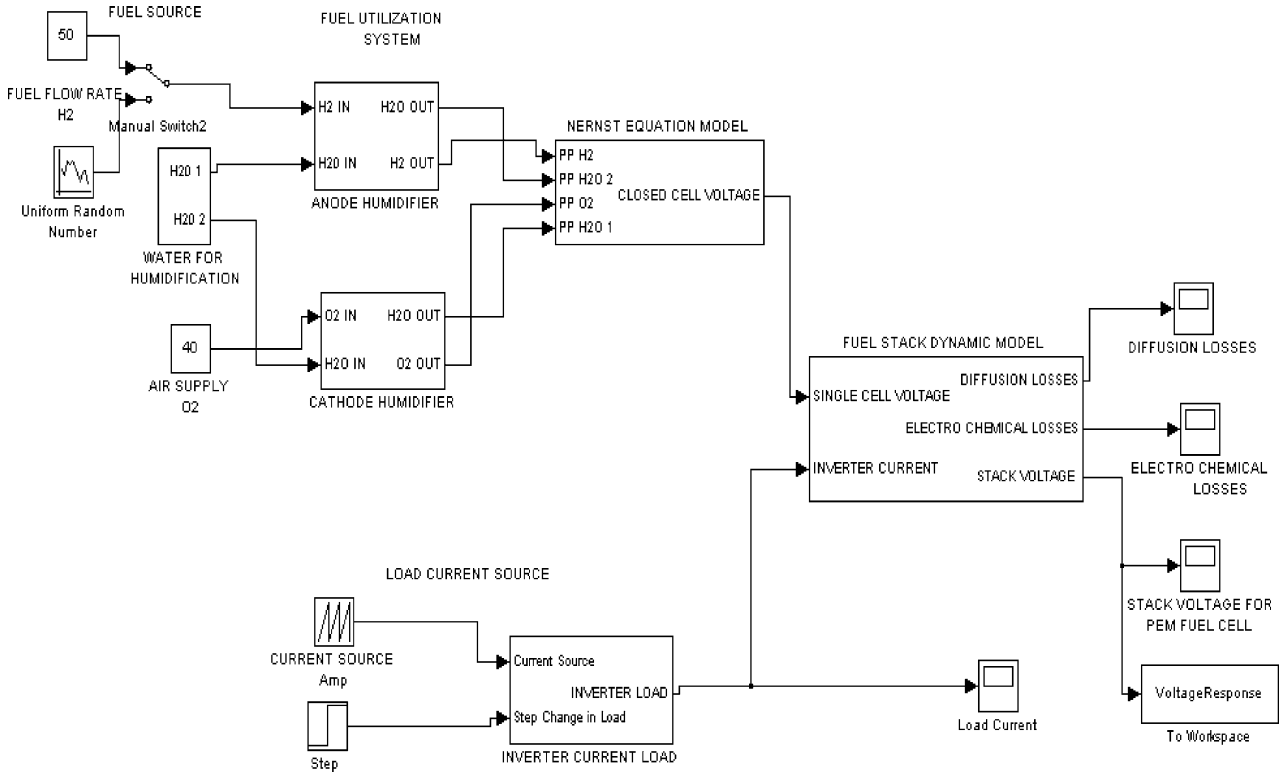

Fig. 2. Simulation block diagram for the PEMFC model including nonlinearities.

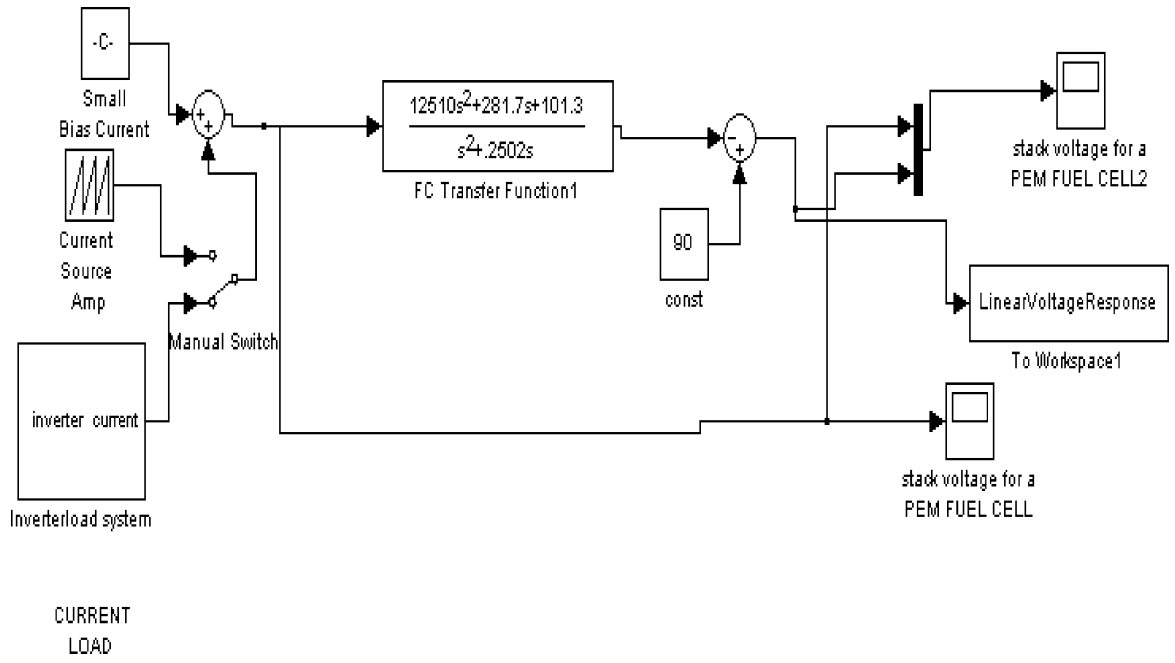

Fig. 3. Simulation block diagram for the linear model of the PEMFC system.

given in the previous section. Using a manual switch located at the top left corner of the block diagram, the fuel flow rate is set to a constant level (which is practically feasible), or switched to a uniform random flow.

The fuel and the air enter anode and cathode humidifiers respectively where water is added to the gases and they are subjected to humidification. These humidified gases are the inputs for the Nernst model block, where the open circuit

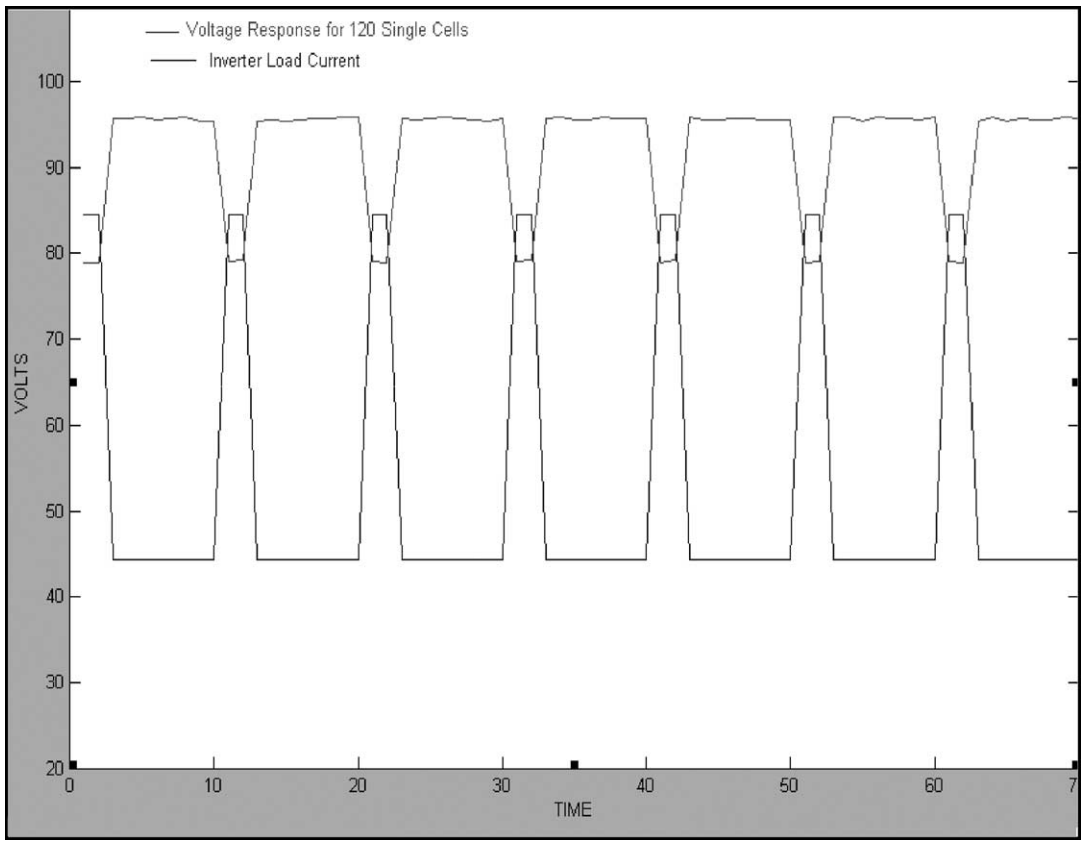

Fig. 4. Voltage output of a PEMFC stack system containing 120 single cells.

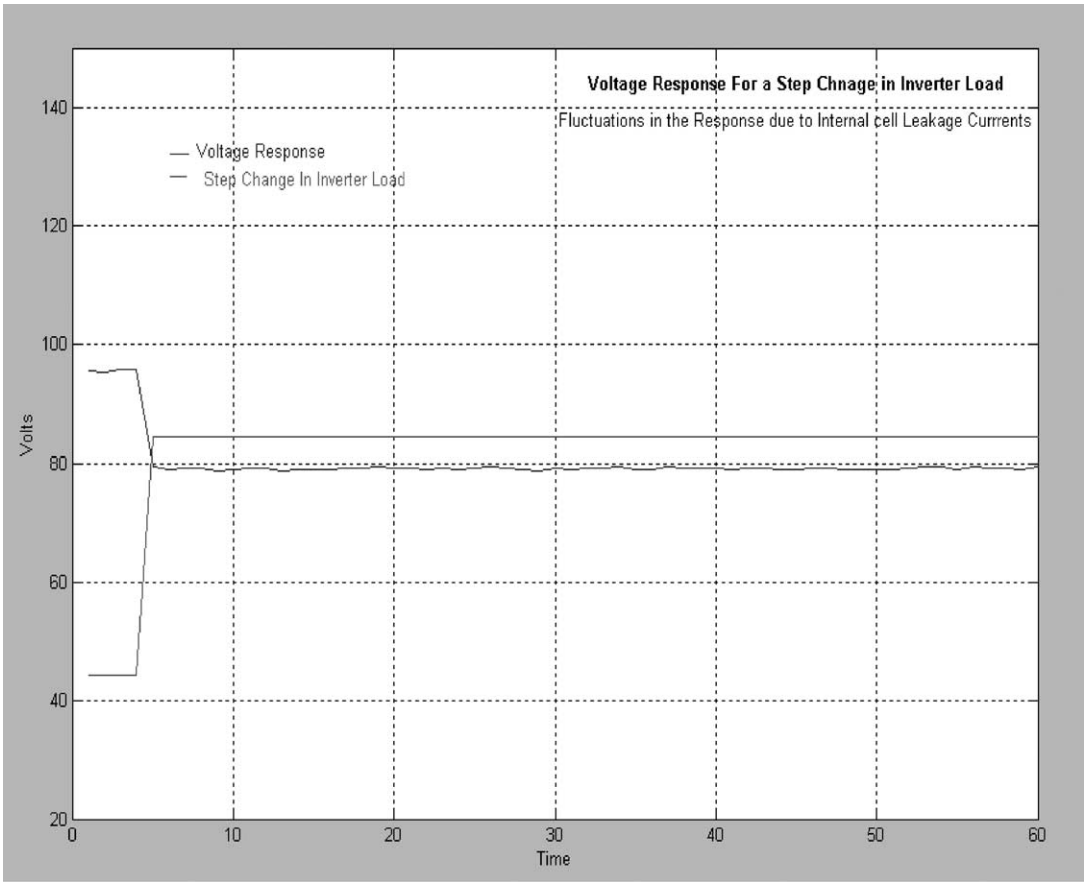

Fig. 5. Voltage response of the fuel cell for a step change in the inverter load current.

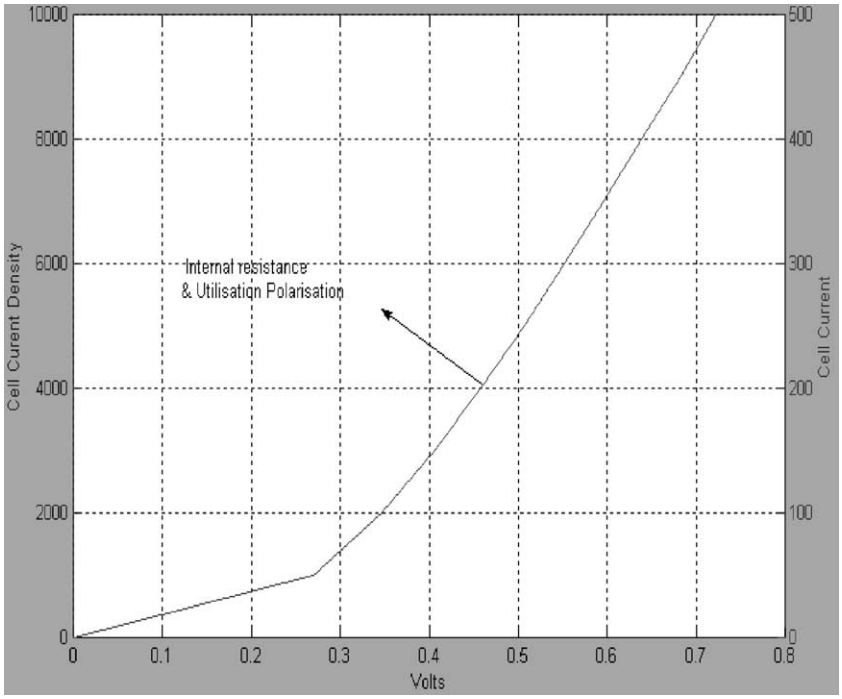

Fig. 6. Internal resistance and utilization polarization for varying load currents (A) and current densities (A/m^2).

voltage is calculated. The accumulator maintains the pressure balance between the oxygen and the fuel cell coolant. If the oxygen or the hydrogen pressure decrease, the coolant pressure is also decreased in order to prevent damage to the stack.

The inverter load current is the main input for the PEMFC system, since the fuel flow is set to constant. The inverter load current along with the open circuit voltage provides the basis for the dynamic analyses of the PEMFC stack system.

Reactant consumption is directly related to the current produced, i.e. if there are no internal or external loads on the fuel cell, no reactants will be used. Because of this direct proportion, leaks may be detected by comparing reactant consumption and the current produced. An appreciable amount of excess reactants indicates a probable leak.

4.2. Linear model of PEM fuel cell system

Fig. 3 depicts the simulation block diagram for the linear PEMFC model. This approach to the modeling is based on a set of practical assumptions and justifications which are given as follows:

(i) The reactant and the product gases obey Ideal Gas law. The justification behind this assumption is that while the operating pressures of the gases are relatively low compared to their critical pressure, the operating temperatures are significantly higher than the critical temperatures of the gases. This is a valid assumption according to Boyle's law.
(ii) Fuel cell stack temperature gradient in the flow direction is negligible. This is because the temperature gradients are measured in the direction of the air flow and the heat capacity of the fuel stream is only a few percent of the heat capacity of the air stream.

Applying the above approximations to the nonlinear equations given in the previous section, we obtain the linear model for the fuel cell system.

5. Simulation results

5.1. Stack voltage

The simulation of the output voltage of a PEMFC stack system as obtained from the nonlinear model is shown in Fig. 4. We have considered a PEMFC stack system having 120 single cells connected in series. This simulation output can be used for analyzing the dynamic behavior of the fuel

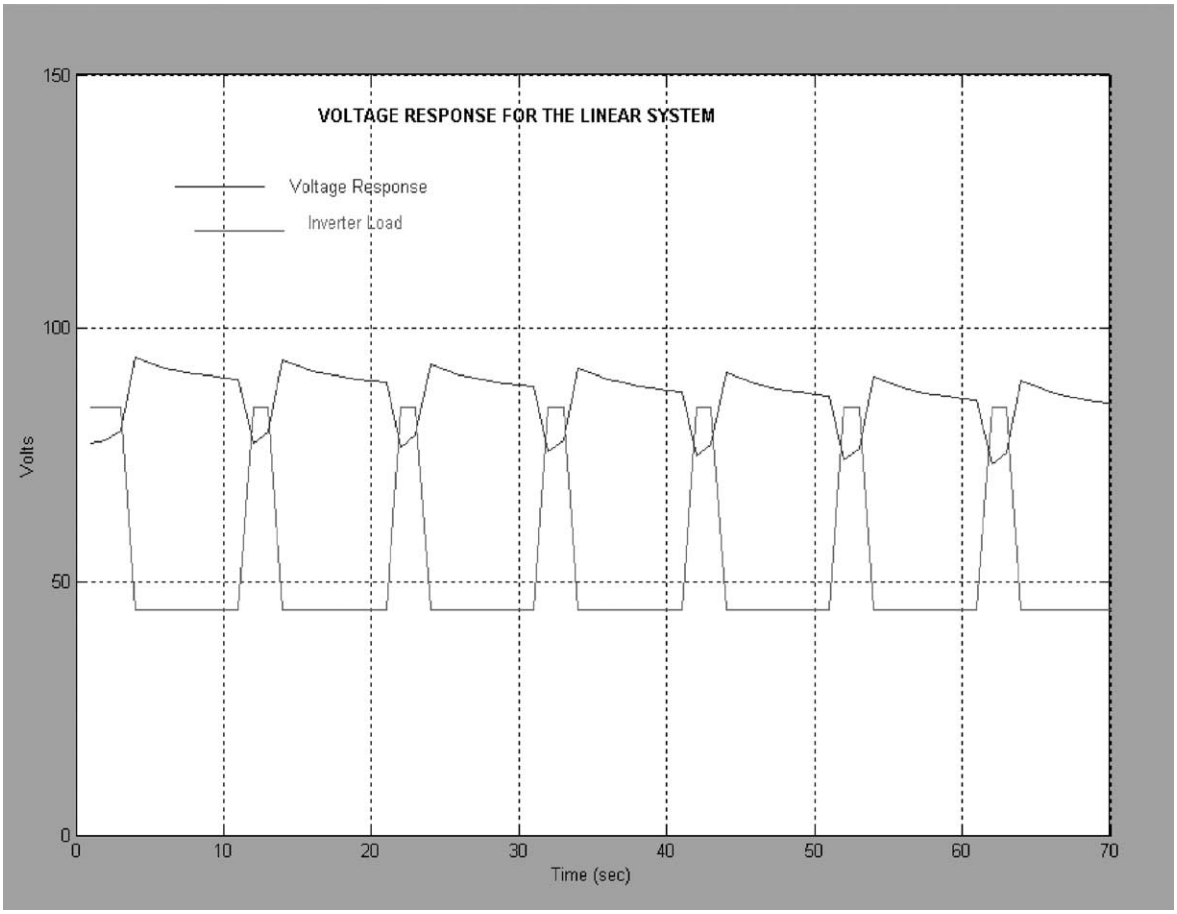

Fig. 7. Voltage response of the linearized PEMFC model.

cell system. The voltage is observed to follow the inverter load in the form of a ripple.

5.2. Step response

In a practical fuel cell serving a variety of load, it is quite common for the overall load to increase or decrease rapidly. This is because of the switching of various electrical appliances drawing power from the fuel cell system. In order to analyze the performance of a fuel cell system during such a step change in its load, we subject the inverter load current to a step change. The voltage response of the PEMFC stack system due to this change in its load is shown in Fig. 5.

5.3. Cell utilization

Fig. 6 depicts the variation of the cell Utilization Polarization inside a PEM fuel cell system. The maximum voltage response of the fuel cell system is found to occur at a utilization range of around 80%. Cell utilization is an important aspect of the fuel cell performance. Care should be taken while varying the cell utilization range, as higher or lower ranges of utilization will decrease the performance of the fuel cell system.

5.4. Voltage response of linearized PEMFC model

Fig. 7 shows the output voltage of the linear model of a PEMFC stack system using the same value of the system parameters used for simulating the nonlinear model. The nature of this response should be taken into consideration while designing a damping controller for the PEMFC system operating as a distributed resource in a power system. It is also used for comparing the voltage response of a linear and a nonlinear model operating under similar conditions.

5.5. Linear step response

A similar kind of step change in the inverter load, as discussed in Section 5.2 is applied to the linear PEMFC model. Fig. 8 depicts the behavior of the voltage response for such a load change. A comparison of this output with the one from Section 5.2 indicates that the linear model stabilizes its voltage faster than the nonlinear model.

5.6. PEMFC linear versus nonlinear model

Plots of the voltage versus current inside a single cell of the fuel cell system are shown for a linear as well as a nonlinear PEMFC model. From Fig. 9, one can conclude that

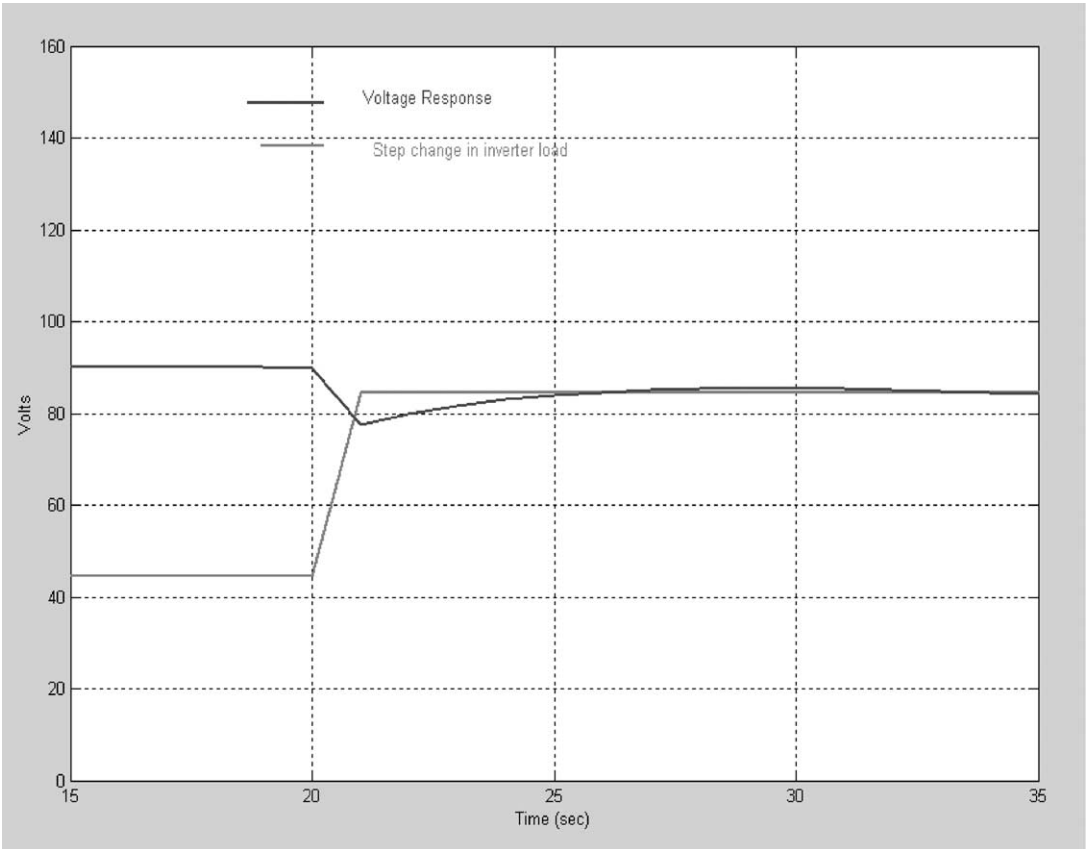

Fig. 8. Step response of the linearized PEMFC model.

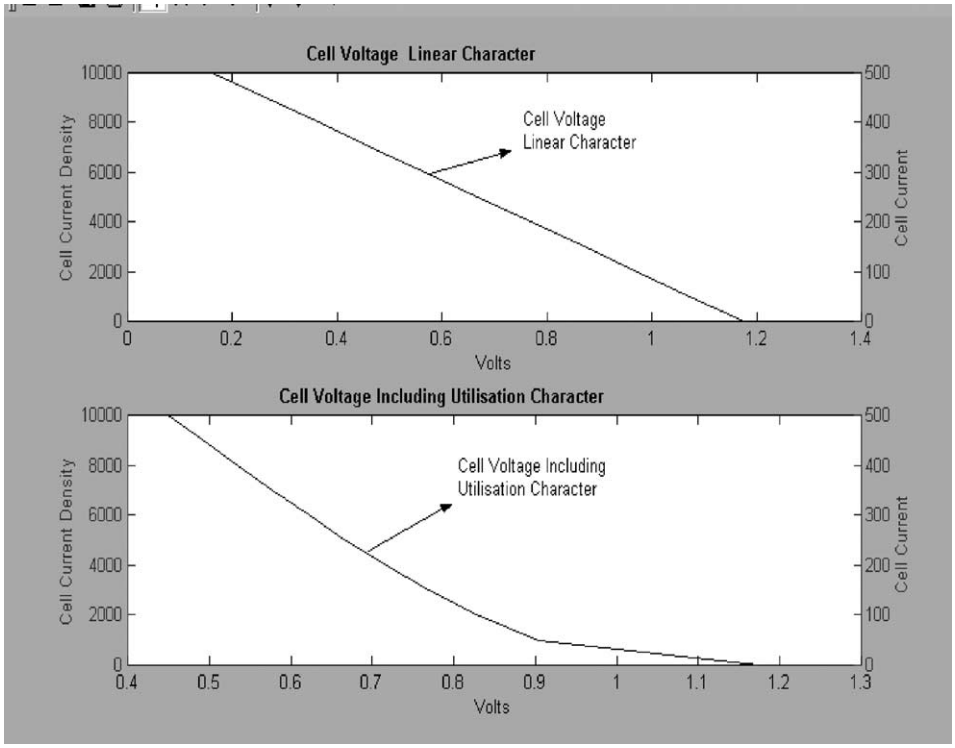

Fig. 9. Comparison of voltage response for the linear and the nonlinear PEMFC models.

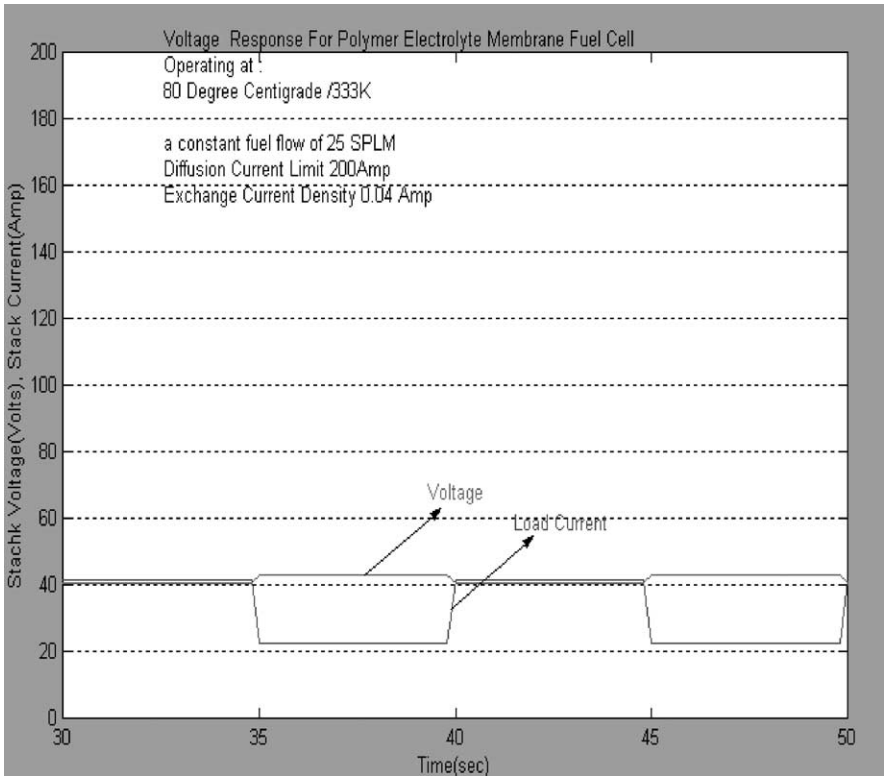

Fig. 10. Voltage response of the PEMFC model based upon the specifications of a real fuel cell.

the nonlinear model (including utilization characteristics), provides a better insight to the behavior of the fuel cell system. However, for preliminary transient stability analysis and damping controller design, the linear model developed in Section 5.5 may be used.

6. Validation of the developed PEMFC model

This section presents a validation study of the fuel cell model by comparing the simulation results with a practical test result [8]. A test was carried out on a 1.5 kW PEMFC plant located at the National Energy Technology Laboratory, Morgantown, WV, USA. We performed a simulation of our model using the specifications of the above mentioned PEMFC plant. During the test, the load from the inverter was set to a frequency range between 45 and 1150 Hz. The same frequency range was maintained during the simulation process. The simulation of the voltage response is shown in Fig. 10 which was found to be similar to the practical test result. This justifies the modeling approach as applied to practical test systems.

7. Conclusions

A mathematical model for the polymer electrolyte membrane fuel cell was derived and the model was simulated using Simulink®. The results from the simulation illustrate the effects of load changes on the fuel cell system. The rapid drop in the voltage during the initial stages of a step change in the fuel cell load is due to the fact that the chemical kinetics involved with the fuel cell system has a very fast response, commonly not observed in conventional forms of energy sources.

We find that for varying currents from the inverter load, the voltage response appears in the form of a ripple. This fluctuation might cause a problem, especially when the fuel cell is working as a major power source delivering high voltages. So, proper control action should be taken whenever there is a rapid fluctuation in the load. The PEM fuel cell system by itself (without a proper controller), will not be able to withstand the load fluctuations.

We also notice that the output voltage curves are not smooth. This is due to the fact that the internal leakage currents between the individual cells play a prominent role in the fuel cell performance. Thus, one of the objectives of designing an efficient PEM fuel cell system is to reduce its leakage currents.

The model developed in this paper can be used for the design of a controller necessary to integrate the fuel cell into a power distribution system. This model will be used to predict the load following capability of the fuel cell system subject to various control strategies. We can also perform a detailed analysis of the effects of the PEM fuel cell on the power distribution system using the developed model. This will eventually help us to determine the necessary specifications of a fuel cell system which can be operated as a distributed generator in a power system. A real fuel cell may not always be available for such design purposes or it might not be cost efficient to use a real fuel cell for preliminary research work. In such situations the fuel cell model will prove to be very useful.

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