PEM Fuel Cell model in the Simulation of a Distributed Generation Network

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ABSTRACT: This paper presents a Proton Exchange Membrane (PEM) Fuel Cell model. Mass balance and semi-empirical equations are used in the modelling process. The model has been implemented in Matlab/Simulink and tested using various scenarios in order to study the transient behaviour of a PEM fuel cell. The need for a Power Conditioning Unit (PCU) connecting the fuel cell to a Distributed Generation (DG) network has also been investigated.

Keywords: Fuel cells, distributed energy resources, modelling, power distribution, islanding operation

I. INTRODUCTION

Fuel cells are electrochemical devices which convert the chemical energy contained in a fuel directly into electricity and heat. Fuel cells are considered to be suitable for both small and large scale Distributed Generation (DG) applications ranging from a few kW to a few MW.

The most common types of fuel cells used in DG are Solid Oxide Fuel Cells (SOFC), Molten Carbonate Fuel Cells (MCFC) and Proton Exchange Membrane or Polymer Electrolyte Fuel Cells (PEMFC). The main advantages of fuel cells are high efficiency, low or zero emissions when hydrogen is used as a fuel, low noise during operation and high modularity. From the above mentioned types of fuel cells the PEMFC are the most common and widely used. Some of their advantages over other types are the low operating temperature, fast start-up and high current density.

There have been many studies concerning modelling of PEM fuel cells [1]-[8]. Most of the models are based on the electrochemical description of the phenomena inside the fuel cell. The use of empirical equations is common in order to compute the voltage drop due to various losses [4]. Mass balance equations are used to compute the species changes inside the fuel cell [1], [8]. Energy balance equations are also used especially in high temperature fuel cells [8], [10]. Finally, the interaction of fuel cells with the grid is studied in various papers using simple inverter models [1], [5].

In this paper a dynamic PEM fuel cell model is proposed in order to investigate the behaviour of a PEMFC connected into a distributed generation network. Various simulations are carried out for different scenarios usually encountered in distributed generation networks, such as partial and full load connection and disconnection and short circuits. The power performance of the PEMFC is also investigated as well as the effect of some model parameters in the FC operation.

II. PEMFC MODEL

The PEMFC under study is assumed to have an active area of 50 cm^2 and a maximum current density of 1 A/cm^2. The working temperature is considered constant at 70 °C. Diffusion inside the electrodes has not been taken into account, which means that the partial pressures are considered constant inside the anode and cathode of the fuel cell. Figure 1 shows the PEMFC model built using Matlab/Simulink [11]. The detailed equations of each block are presented in the following paragraphs.

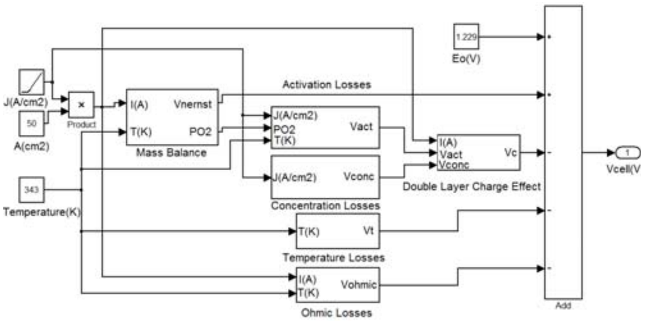

Figure 1. PEMFC Model built in Simulink

A. Ideal Cell Potential

The chemical reaction taking place inside a PEMFC when hydrogen is used is [9], [10]:

$$H_2 + \frac{1}{2} O_2 \rightarrow H_2O \tag{1}$$

The ideal open circuit potential of the above chemical reaction for standard temperature and pressure (25 °C, 1 atm) and liquid water product is 1.229 V. Using the Nernst equation [9], the open cell potential for other operating pressures can be adjusted. Different operating temperatures can also be taken into account by adding an extra term to the Nernst equation. Equation 2 gives the open cell potential for operating conditions inside the cell:

$$E_{nernst} = E^0 + \frac{\Delta S}{2F}(T - T_o) + \frac{RT}{2F}\ln\left(\frac{P_{H_2}\sqrt{P_{O_2}}}{P_{H_2O}}\right) \tag{2}$$

where ΔS is the change in entropy, F is the Faraday constant, R is the universal gas constant, T_o is the standard temperature (278 °K), T is the working temperature in °K and P_{H_2}, P_{O_2} and P_{H_2O} are the partial pressures of the reactant and product species inside the fuel cell [9].

B. Mass balance equations

The changes in the partial pressures inside the fuel cell can be determined using the ideal gas law [1]. It is assumed that the only gas inside the anode inlet is pure hydrogen, whereas only oxygen exists inside the cathode inlet. Water is also formed inside the cathode [1], [8]:

$$\frac{dp_{H_2}}{dt} = \frac{RT}{V_a}(q_{H_2}^{in} - q_{H_2}^{out} - q_{H_2}^{r}) \tag{3}$$

where p_{H_2} is the partial pressure inside the fuel cell in atm, V_a is the anode volume in l, $q_{H_2}^{in}$ is the hydrogen inlet flow rate in mol/s, $q_{H_2}^{out}$ is the part of the hydrogen that does not react and remains in the cell at this point and $q_{H_2}^{r}$ is the hydrogen that reacts:

$$q_{H_2}^{r} = \frac{I}{2F} \tag{4}$$

From the above equation the amount of hydrogen needed can be computed. Usually there is an excess of hydrogen inside the fuel cell.

The partial pressure of the hydrogen is linearly depended on the hydrogen flow:

$$\frac{q_{H_2}}{p_{H_2}} = \frac{K_a}{\sqrt{M_{H_2}}} = K_{H_2} \tag{5}$$

where K_{H_2} is the hydrogen molar flow constant given in mol/(s·atm) [2], [9]. Using the Laplace transformation:

$$p_{H_2} = \frac{1/K_{H_2}}{1+\tau_{H_2}s}(q_{H_2}^{in} - q_{H_2}^{out}) \tag{6}$$

where:

$$\tau_{H_2} = \frac{V_a}{K_{H_2}RT} \tag{7}$$

The same equations can be used on the cathode side for the determination of the partial pressure of oxygen and water taking into account that the inlet flows are different. The oxygen inlet is half the hydrogen inlet and zero water input both in the anode and cathode side is assumed. In reality the inlet flows contain more gases such as CO, CO_2 and probably other hydrocarbons in the anode and nitrogen and other substances contained in the air in the cathode. Both inlet gas streams are often humidified before entering the fuel cell.

As mentioned before, there is an excess of hydrogen in the anode and an excess of oxygen in the cathode. The fuel utilization is a measure that gives the percentage of the fuel consumed inside the fuel cell. The rest of the fuel can be recirculated under certain circumstances. A small amount is lost due to back diffusion through the electrolyte. The utilization is kept around 0.8 to prevent fuel overusage leading to fuel starvation or fuel underusage leading to an increase in voltage output [7].

C. Operating Voltage

When current is drawn from the fuel cell the voltage drops due to the various losses. Even when there is no current drawn, the real open circuit voltage is less than the ideal because of certain losses occurring at zero current. The different types of losses are given below:

1) *Activation Losses:* The slow rate of the reaction taking place inside the fuel cell is the cause of the activation voltage drop. There is an activation energy that has to be surpassed for the reaction to take place inside the fuel cell. The Tafel equation is usually used in order to compute the activation voltage drop [9]. Semi-empirical equations are also commonly used for the computation. In the present work the following semi-empirical equation has been used [3]:

$$\begin{aligned}\eta_{act} &= -0.9514 + 0.00312T - 0.000187T\ln(i) \\ &+7.4\cdot 10^{-5}T\ln(c_{O_2})\end{aligned} \tag{8}$$

where T is the temperature in °K, i is the current density in A/cm^2 and c_{O_2} is the oxygen concentration. The oxygen concentration is calculated by the semi-empirical Eq. (9) after taking into consideration the pressure in the flow channels, diffusion in the electrodes and diffusion through a water film that is created by the presence of water in the electrodes [3]:

$$c_{O_2} = \frac{p_{O_2}}{5.08\cdot 10^6 \exp(\frac{-498}{T})} \tag{9}$$

2) *Ohmic Losses:* This voltage drop comes mainly from the ionic resistance of the electrolyte and from the electronic resistance of the electrodes, interconnections and other parts of the fuel cell. The voltage drop is proportional to the current drawn by the fuel cell [9]:

$$V_{ohmic} = R\cdot I \tag{10}$$

The membrane specific resistance in Ω·cm is computed using the following empirical equation [4]:

$$r_m = \frac{181.6[1+0.03\frac{i}{A}+0.062(\frac{T}{303})^2(\frac{i}{A})^{2.5}]}{(\lambda-0.634-3\frac{i}{A})\exp(4.18\frac{T-303}{T})} \tag{11}$$

where i is the current density in A/cm^2, A is the active cell area in cm^2, T is the temperature in °K and λ is an empirical parameter that shows the humidity percentage in the membrane. Parameter λ ranges from 14, when the membrane is considered 100% humidified, to 23, when the membrane is considered "flooded". To compute the resistance of the membrane in Ω the following expression is used:

$$R_m = \frac{r_m\cdot l}{A} \tag{12}$$

where l is the width of the membrane in cm. Nafion 117 is used as a membrane material with a width of 178 μm [6].

3) *Concentration Losses:* As the reactions in the anode and cathode take place and the reactants are consumed, the finite transport of mass causes a depletion of the reactants in the reaction sites. This depletion causes a drop on the output voltage, especially when high current is drawn. The voltage drop due to the concentration loss is computed using the following semi-empirical equation [6]:

$$\eta_{conc} = -B\ln(1-\frac{i}{i_{\max}}) \tag{13}$$

where i is the current density in A/cm^2 and i_{max} is the maximum current density of the fuel cell. The maximum current density that the fuel cell can withstand is assumed to be 1 A/cm^2.

4) *Charge Double Layer Effect:* In the surface where the electrode and the electrolyte are in contact, charge is built up due to diffusion effects and due to reactions between the electrons in the electrodes and the protons in the electrolyte. This acts like a capacitor which smoothes the voltage drop due to the activation and the concentration losses [6], [8]. This capacitance is given by:

$$C = \varepsilon \frac{A}{d} \tag{14}$$

where ε is the electrical permittivity, A is the effective cell area and d is the separation of the electrode-electrolyte. The capacitance is usually in the order of a few Farads [6]. In the present model it is considered to be 2 Farads.

The modelling parameters that were used to construct the PEMFC model are shown in Table 1.

Table 1. Modelling Parameters

Modelling Parameter	**Value**
Effective Cell Area A	50cm^2
Membrane Width	178 μm
Temperature T	343 °K
Ideal Voltage E_o	1.229V
Hydrogen molar constant K_{H_2}	$4.7955 \cdot 10^{-7}$ kmol/(atm·s)
Oxygen molar constant K_{O_2}	$2.39773 \cdot 10^{-7}$ kmol/(atm·s)
Water molar constant K_{H_2O}	$8.768 \cdot 10^{-8}$ kmol/(atm·s)
Maximum current density J_{max}	1 A/cm^2
Constant λ	$14<\lambda<23$
Constant B	0.016 V
Anode Volume	0.0454 l
Cathode Volume	0.0454 l

D. V-I and P-I curves

Using the model described above the V-I curve shown in Figure 2 is derived. For low currents the main losses are the activation losses. There is also a linear drop in voltage, mainly due to the ohmic losses, and at high operating currents a sharp voltage drop due to the concentration losses. In Figure 3 the derived P-I curve is shown. The maximum power output of the fuel cell does not appear at maximum current, because of the sharp voltage drop that appears in high operating currents. It appears at around 40 A, which is approximately 80% of maximum load and is nearly 24 W. Since the fuel flow is considered steady at the maximum value, the x axis can be also considered to show the fuel utilization. The maximum power appears at around 0.8, which is the desired operating point as mentioned above.

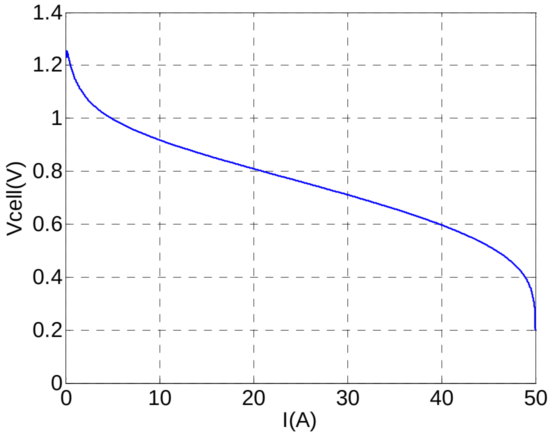

Figure 2. V-I curve

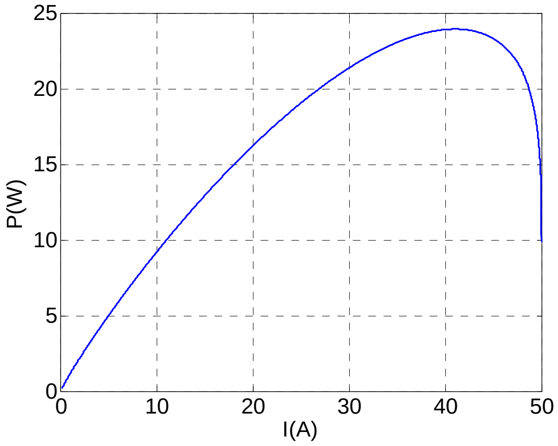

Figure 3. P-I curve

III. SIMULATION

Next the PEMFC model is used in three different simulation scenarios commonly encountered in DG networks.

A. Load Step Changes

The simulation lasts 200 s and a step change from minimum to maximum current is imposed at time 40 s. The fuel cell operates on maximum load for 80 s and then the load drops to half. In Figure 4 the step changes of the current in the right axis and the voltage response of the fuel cell on the left axis are presented.

The voltage output of the fuel cell reaches the steady-state in approximately 50 s in the large step. In the small step the voltage still changes for about 50 s but the change is very small, so it is assumed to reach steady state in approximately 20 s. The power output of the fuel cell has the same response as the voltage curve. When the load increases the fuel cell provides more power than needed for about 50 s until the voltage reaches the steady state. On the contrary, when the load decreases the power output is less than the load demand for about 50 s when the fuel cell reaches the steady state. This power excess, that actually comes from the overvoltage when the load increases and the undervoltage when the load decreases, can cause damage to the loads in case they are connected directly to the fuel cell.

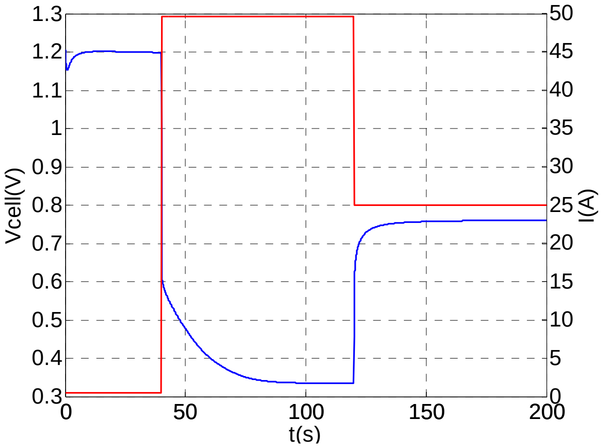

Figure 4. Step Changes

B. Load Rejection

The fuel cell is operating at full load and for 100 ms the load is rejected and then connected again. We assume maximum hydrogen flow. Figure 5a presents the voltage response of the fuel cell. In Figure 5b, which presents a partial zoomed area of Fig. 5.a, the above voltage response for the duration of the load rejection can be seen more clearly. In the right axis of Figure 5b the current change, which simulates a load rejection scenario, is also shown. A spike appears in the fuel cell output voltage reaching up to 0.65 V followed by a sudden drop. The voltage reaches the steady state in approximately 25 s. This sudden drop is caused mainly by the ohmic losses which are related directly to the current. The smooth curve is caused mainly by the double layer charge effect. The oxygen concentration and thus the oxygen partial pressure and the utilization also play an important role. The power excess discussed earlier will last for about 25 s and may cause damage to directly connected loads. In this case the utilization is near 1 at normal operation and it drops sharply near 0 at load rejection.

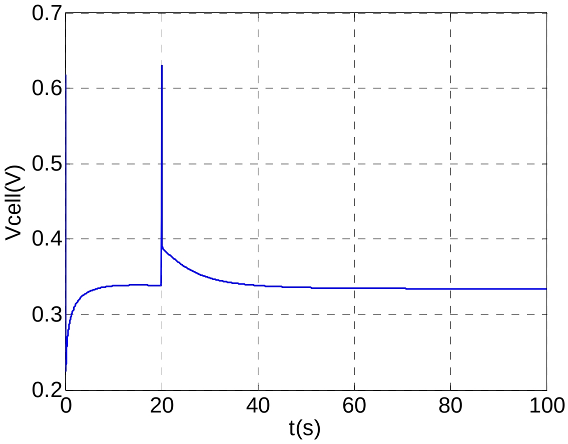

Figure 5.a. Voltage response for Load Rejection

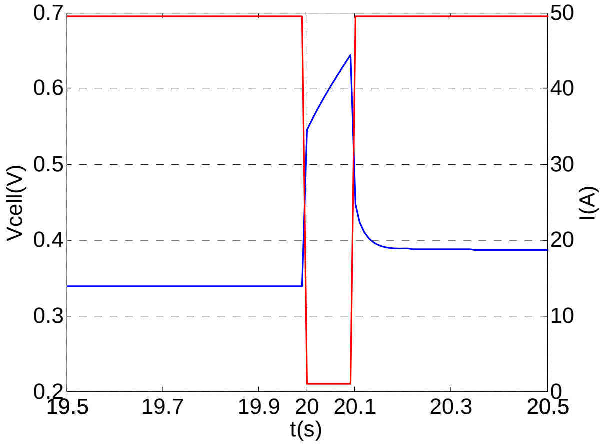

Figure 5.b. Zoom area for Load Rejection

C. Short circuit

A short circuit can be simulated by increasing the current from the operating point and further. In the simulated case the current is raised from the operating point, which is considered to be at 5 A, to its maximum acceptable value for a duration of 100 ms. Maximum hydrogen flow is assumed. The results are shown in Figures 6a and 6b. In Figure 6a the voltage response is shown for the whole duration of the simulation. In Figure 6b a more detailed graph of the voltage response can be seen for the duration of the short circuit. The current change is also presented on the right axis. The voltage drops sharply during the short circuit and returns to its original value rapidly in approximately 0.5 s. The fast response is mainly due to the large capacitance from the charge double layer effect and also due to the small change in the oxygen concentration, as the short circuit lasts only 100 ms. The oxygen partial pressure is also high, due to the low utilization, which decreases activation losses. In this scenario the utilization is 0.1, which is very small, and increases sharply near 1 during the short circuit. In practice the current could rise to a greater value and the fuel cell could suffer damages due to fuel starvation or increase of the temperature. It is obvious that there is need for a control system to recognise the faults and to isolate the fuel cell or to limit the fault current.

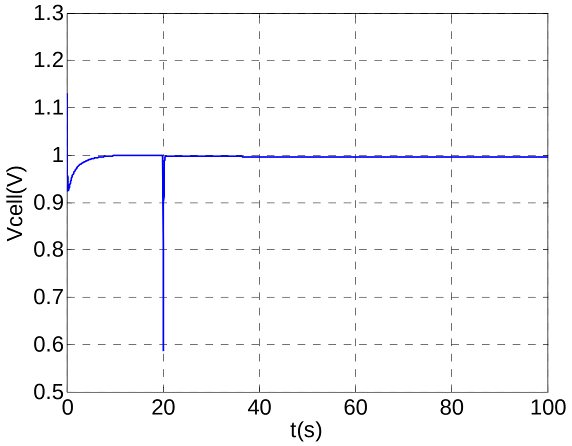

Figure 6.a. Voltage response for short circuit

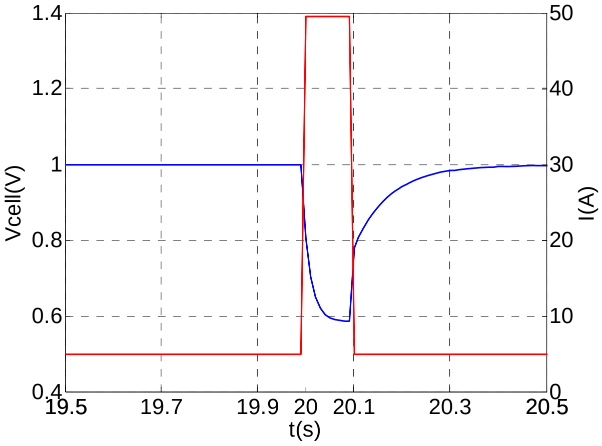

Figure 6.b. Zoom area for short circuit

IV. POWER CONDITIONING UNIT (PCU)

A. Block Diagram

In order to connect the fuel cell to the existing grid a Power Conditioning Unit (PCU) is needed to convert the dc output of the fuel cell into ac. Many different topologies have been proposed [9], [10]. A simple topology is given in Figure 7. A dc-dc converter is used to boost the usually low dc output voltage of the fuel cell. Then a dc-ac three-phase inverter is used to convert the voltage into three-phase ac set of voltages. After the dc-ac inverter a L-C filter is used to cut-off higher harmonics. Finally, a transformer is usually used both to boost the voltage and provide isolation. A backup power device, such as a battery or an ultra-capacitor, is usually connected in parallel to provide power for the start-up of the fuel cell and also to provide the extra power needed at sudden load changes or even faults. When the fuel cell is connected to the grid the need of a back-up power source is not as important as in islanding operation.

B. Simulink model

A model of a simple power conditioning unit connecting a fuel cell stack to the grid has been build using Simulink. A simple dc-dc boost converter was used to boost the output of a fuel cell stack containing 200 cells at 300 V.

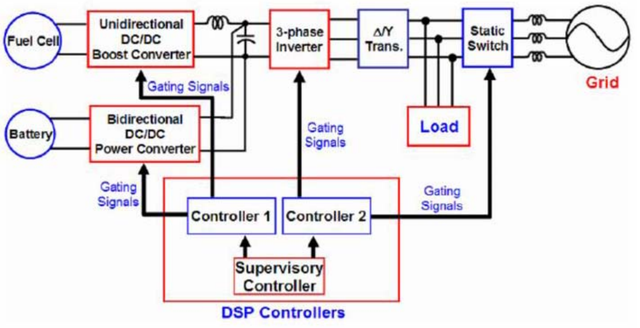

Figure 7. PCU block diagram

A 3-phase dc-ac inverter using Sinusoidal Pulse Width Modulation (SPWM) converts the dc voltage into 3-phase, 50 Hz, 130 V phase to phase. After the inverter a LC filter is used to reduce harmonics. Finally, a D-Y transformer is used to step up the voltage at 400 V phase to phase and connect the system to the power distribution network. The dc-dc boost converter and the dc-ac inverter are controlled using simple PI controllers.

The PCU changes the dynamic behaviour of the fuel cell. The response to the load changes is much faster because the voltage controllers monitor the output voltage and try to keep it constant. Especially when the system is connected to the grid, the voltage is supported and the dynamic response during transients is much better. The control strategy and the inverter modulation technique are also very important and play a major role in the response of the whole system.

C. Simulation

A very simple scenario where the fuel cell is providing power to loads connected to the power distribution network has been simulated to show some preliminary results of the way the PCU changes the overall response. The fuel cell is connected at t=1s. The load changes from 2kW to 5 kW at t=3s and the power needed is provided only by the fuel cell. The fuel cell dc voltage output does not reach the steady-state but the load voltage and the power provided reaches steady-state fast.

Figure 8 shows the load voltage. When the step change happens the voltage drop is very small. The grid supports the load voltage and keeps it constant around 230V phase to ground.

In Figure 9 the real power provided by the fuel cell is shown. When the load is increased it takes less than 0.5s for the fuel cell to provide the power needed. The problem with the overvoltage and the corresponding power excess is not present here. When the fuel cell is connected to the grid at 1s a spike appears. This is due to the original operating conditions that are considered for the fuel cell when it operates alone.

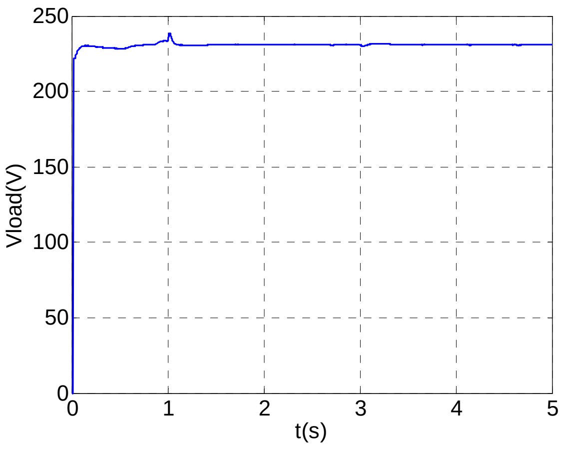

Figure 8. Load Voltage

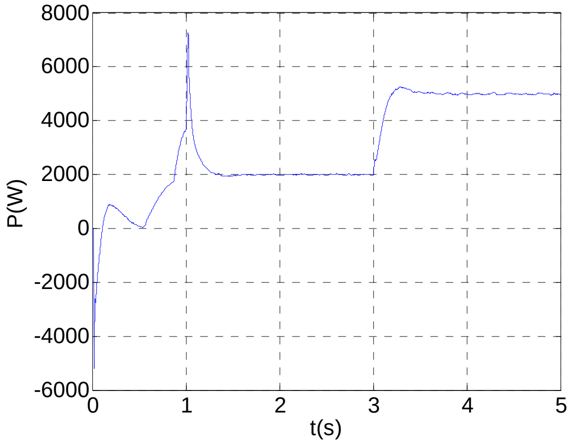

Figure 9. Power provided by the fuel cell

V. CONCLUSIONS

A model of a PEM fuel cell has been developed using mass balance and semi-empirical equations. Various simulations have been carried out using the model. The slow dynamic response of the fuel cell makes it hard to use fuel cells to provide power to isolated loads. In such a case a backup power device, such as a battery or an ultra-capacitor, is needed to provide the extra power.

In case of sudden load changes or short circuits there exists danger of damage to the fuel cell, especially to the electrolyte, due to fuel starvation or heat accumulation. To avoid or minimize this possibility, excess fuel is provided inside the fuel cell to prevent fuel starvation. In very high operating currents, which appear in short circuits, the fuel cell must be disconnected or the short circuit current must be limited. Thus a proper control system that senses sudden changes in current is needed.

When the fuel cell is connected to the grid using a PCU the dynamic response is even better. During load changes or faults the extra power needed can be provided by the grid. Another issue that has to be addressed when the fuel cell is connected at the distribution side is the islanding mode of operation. With a proper PCU and control system design the fuel cell can be used as a Distributed Generator to provide both active and reactive power.

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VII. BIOGRAPHIES

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