SIMULATION OF A PROTON EXCHANGE MEMBRANE FUEL CELL STACK USING AN ELECTRONIC EQUIVALENT CIRCUIT MODEL

J.P. Du Toit* and H.C. vZ. Pienaar**

** Dept. of Applied Electronics and Electronic Communications, Vaal University of Technology, Private Bag X021, Vanderbijlpark, 1900, South Africa.*
***Telkom Centre of Excellence, Vaal University of Technology, Private Bag X021, Vanderbijlpark, 1900, South Africa.*

Abstract: This article describes the method to calculate the parameters of an electronic equivalent circuit model of a proton exchange membrane fuel cell stack. The model is based on that of Yu and Yuvarajan [1], but very little detail is given by them on how to calculate the component values of the circuit model based on the experimental data of a fuel cell or fuel cell stack. Here, a method will be established in which the performance data of small fuel cell stacks can be used to simulate the behaviour of much larger stacks under the same operating conditions. It is crucial to be able to simulate a fuel cell stack using an electronic circuit equivalent model when designing power converters for fuel cells, since the fuel cell stack can then be simulated together with a power converter or any other electronic circuitry. First, a mathematical model of a small, two-cell, proton exchange membrane fuel cell was calculated based on experimental data. This model was then adapted to describe the characteristics of a much larger, 100 W, fuel cell stack. Finally, the mathematical model was used to calculate the parameters for an electronic circuit model by establishing a clear relationship between the two models.

Key words: Proton exchange membrane fuel cell (PEMFC), electronic circuit model

1. INTRODUCTION

Over recent years, much emphasis has been placed on the development of fuel cells (FCs) for the replacement of internal combustion engines (ICEs) in automobiles for both economic and environmental reasons. Although there are different types of FCs currently in development, the proton exchange membrane fuel cell (PEMFC) is the most likely candidate to replace ICEs because of its lightweight and low operating temperatures. A PEMFC is an electrochemical device that converts a fuel (hydrogen) and an oxidant (oxygen or air) into electricity. Unlike a battery, a FC can supply electrical energy for as long as it is being supplied with fuel. This, together with the fact that a FC contains no moving parts, results in much longer lifetimes of FCs compared to batteries and ICEs, resulting in long-term cost savings.

A number of technical and economic issues still prevent the widespread implementation of FCs in automobiles since the threat of global warming demands that hydrogen for cars be produced from sources that do not generate greenhouse gases. However, the use of FCs in stationary applications is much more plausible [2]. This is especially true for the use of FCs in backup power systems, even more so when the hydrogen needed to fuel these devices can be produced on-site from renewable sources.

The theoretical open-circuit output voltage of a PEMFC is 1.23 V. Due to losses in the various components of a FC, the open-circuit voltage is somewhat less, typically around 0.9 V. Furthermore, as the output current of a FC increases, its voltage drops in a non-linear fashion. The various losses in a FC, together with their influence on the cell's output characteristics, will be discussed in the next section. If a FC stack is to be implemented in a system that would provide backup power for telecommunications equipment, for example, some form of power converter would be needed to increase the output voltage of a FC stack to a required level and that would be able to maintain a constant output voltage even under changes in load conditions.

In order to facilitate the design of a DC-DC boost converter to condition the output voltage of a FC stack, it is necessary to be able to simulate a FC stack as it operates in combination with such a converter. For this reason an electronic equivalent circuit model of a PEMFC stack has been developed [1]. Very little detail is available on the calculation of the parameters of the above-mentioned model. Furthermore, Yu and Yuvarajan [1] only calculated the parameters of the model based on already existing performance data of a PEMFC stack and did not use the model to predict the characteristics of larger stacks.

This paper will discuss the method used to calculate the parameters of an electronic circuit equivalent model of a

PEMFC stack. This was done by obtaining a mathematical model of a small, two-cell stack, based on experimental data. The mathematical model was then adapted to model the behaviour of a larger stack and verified by comparing the model with experimental data of such a stack. Finally, the model was adapted for an even larger, 100 W FC stack, and then used to calculate the needed parameters for an electronic circuit model by establishing a relationship between the mathematical and electronic equivalent circuit model.

2. V-I CHARACTERISTICS OF A FC STACK

As the current drawn from a FC stack increases, the output voltage of the stack decreases due to various losses present in the components of the stack. The voltage-current curve of a typical FC is shown in Figure 1 and is also referred to as a polarisation curve or a V-I curve.

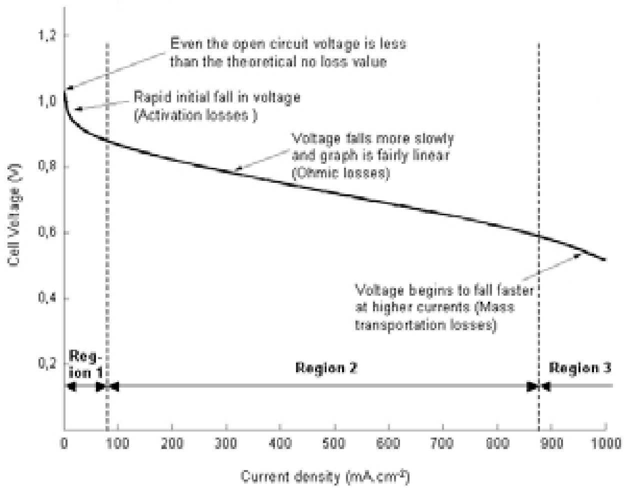

Figure 1: Polarisation curve of a FC stack [3].

Note that a polarisation curve shows the output voltage of a FC with regards to current density which makes it easier to compare cells with different membrane surface areas since the amount of current that can be supplied by a FC increases as its membrane surface area increases. Figure 1 shows that there are three regions of a FC polarisation curve in which the output voltage exhibits different characteristics. The following sections will discuss each of these regions as well as the mathematical equations that describe them [3].

2.1 Activation losses, fuel crossover and internal currents

Activation losses comprise the portion of the cell voltage that is lost in providing activation energy for the chemical reaction that transfers electrons between the electrodes. This voltage drop has a very non-linear form and contributes, in part, to the first region of the graph in Figure 1. Activation losses, $V_{act,}$ can be described by the equation shown in (1) where, i is the current density in mA.cm^{-2} and i_0 is the current density at which the voltage drop begins to move away from zero. For example, if i_0 is 100 mA.cm^{-2} there will be no voltage drop until the current density i is greater than 100 mA.cm^{-2}. In (1), A is a constant which value depends on the electrode material as well as the type of reaction taking place.

$$\Delta V_{act} = A \ln\left(\frac{i + i_n}{i_0}\right) \approx A\ln(i) - A\ln(i_0) \qquad (1)$$

Another cause of voltage drop in a FC is from fuel crossover and internal currents. Although the electrolyte membrane in a FC is designed to be impermeable to gas flow and to be only proton conductive, it is still possible for a small amount of the reactants (H_2 and air) to permeate through the membrane from one side of the cell to the other. This, together with a small amount of electron flow through the membrane, causes a voltage drop in the open circuit voltage of low-temperature FCs. If a total internal current density i_n is caused to flow through the cell by fuel crossover and internal currents, this voltage drop can be combined with the activation losses given in the first part of (1). Since the crossover current is usually very small and only useful in explaining the initial drop in FC voltage, it can be omitted [3].

2.2 Ohmic losses

The second region of a FC polarisation curve is fairly linear and is caused by the electrical resistance of the electrodes as well as the resistance to proton flow through the membrane. This voltage drop is proportional to the current density i and can be modeled by:

$$\Delta V_{ohm=ir} \qquad (2)$$

where r is an area specific resistance in terms of kΩ.cm^2.

2.3 Mass transport or concentration losses

The final cause of voltage drop in a FC is shown in region 3 of Figure 1. This loss is caused by mass transportation loss or concentration losses. When the oxygen needed by the cell is supplied in the form of air, there will be a reduction of the concentration of oxygen in the air around the electrodes as the oxygen is used by the cell. On the anode side, where hydrogen is used, there will also be a reduction of hydrogen pressure as more hydrogen is consumed as a result of higher currents being drawn from the cell. The concentration loss, V_{trans} is given by:

$$\Delta V_{trans} = me^{ni} \qquad (3)$$

where m and n are constants in terms of V and $cm^2.mA^{-1}$ respectively.

2.4 Complete mathematical model for a FC stack

Equations (1)-(3) can be combined and subtracted from the theoretical open circuit voltage E (E = 1.23 V), to give the actual FC output voltage over its entire current range:

$$V = E + A\ln(i_0) - ir - A\ln(i) - me^{ni} \quad (4)$$

The first two terms in the above equation are constant, regardless of the cell current, and can be replaced by a practical open circuit voltage, E_{OC}:

$$V = E_{oc} - ir - A\ln(i) - me^{ni} \quad (5)$$

In the case of a FC stack, comprised of N_C identical cells, Equation (5) can be rewritten as [4]:

$$V_{STACK} = N_c E_{oc} - N_c ir - N_c A\ln(i) - N_c me^{ni} \quad (6)$$

The constants in the above equation (r, A, m and n) were determined from the analysis of experimental data from small FC stacks of only two cells. The value of N_C was then adjusted to predict the behaviour of a larger, 100 W, FC stack. The resulting equation was then used to design an equivalent electronic circuit model of a 100 W FC stack to enable the simulation of the stack together with other electronic circuitry.

In order to verify the model in Equation (6), a small two-cell stack was constructed and used to obtain an experimental polarisation curve [5]. A typical value of n was chosen as 0.008 $cm^2.mA^{-1}$.

From the data in Table I, it can be seen that the open circuit voltage of the two-cell stack, NE_{OC} is equal to 1.97 V. This means that the open circuit voltage of a single cell would be 0.985 V. By substituting values from Table I into Equation (6), the values of r, A and m were calculated. This was done by forming six equations from the data in Table I:

$$\begin{aligned}
8r &+ 2.7726A + 2.0650m = 0.15\\
24r &+ 4.9698A + 2.2015m = 0.22\\
160r &+ 8.7641A + 3.7930m = 0.40\\
320r &+ 10.1503A + 7.1933m = 0.55\\
560r &+ 11.2696A + 18.7867m = 0.88\\
640r &+ 11.5366A + 25.8716m = 0.96
\end{aligned}$$

The above equations can be written in matrix form:

$$\mathbf{A}x = \mathbf{b}, \quad (7)$$

where:

$$\mathbf{A} = \begin{bmatrix} 8 & 2.7726 & 2.0650 \\ 24 & 4.9698 & 2.2015 \\ 160 & 8.7641 & 3.7930 \\ 320 & 10.1503 & 7.1933 \\ 560 & 11.2696 & 18.7867 \\ 640 & 11.5366 & 25.8716 \end{bmatrix}, \quad x = \begin{bmatrix} r \\ A \\ m \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} 0.15 \\ 0.22 \\ 0.40 \\ 0.55 \\ 0.88 \\ 0.96 \end{bmatrix}$$

Table I: Two-cell stack performance data.

Stack Voltage (V)	Current (A)	Current ($mA.cm^{-2}$)
1.82	0.1	4
1.76	0.2	8
1.75	0.3	12
1.73	0.4	16
1.72	0.5	20
1.70	0.6	24
1.69	0.7	28
1.68	0.8	32
1.67	0.9	36
1.65	1.0	40
1.61	1.5	60
1.57	2.0	80
1.53	2.5	100
1.50	3.0	120
1.46	3.5	140
1.42	4.0	160
1.38	4.5	180
1.33	5.0	200
1.26	5.5	220
1.23	6.0	240
1.16	6.5	260
1.09	7.0	280
1.01	8.0	320

To solve for the solution matrix, x, Equation (7) can be rewritten in the form

$$x = \mathbf{A}^{-1}\mathbf{b} \quad (8)$$

The above equation was solved and the following values were found:

$r = 0.0006$ kΩ.cm^2
$A = 0.0351$ V
$m = 0.0147$ V

Based on the above values, the mathematical model of any N_C – cell stack under the same operating conditions would be:

$$V_{STACK} = N_C(0{,}986) - N_C(0{,}0003)i - N_C(0{,}0351)\ln(i) - N_C(0{,}0147)e^{0{,}008i} \quad (9)$$

Note that Equation (9) only holds true when i is given in terms of current density (mA.cm^{-2}). The equation was converted to express i in terms of Amperes (A) so that it can be used to determine the parameters of an electronic equivalent circuit model:

$$V_{STACK} = N_C(0{,}986) - N_C(0{,}012)I_O - N_C(0{,}0351)\ln(I_O) - N_C(0{,}0147)e^{0{,}32I_O} - N_C(0{,}13) \quad (10)$$

where I_0 is the stack current in terms of Amperes (A). Also note that a second constant term is introduced in Equation (10) because of the nature of the natural logarithm term in Equation (9). The next section discusses the development of the electronic circuit equivalent model of a FC stack as proposed by Yu and Yuvarajan [1] that allows a FC stack containing any number of cells to be simulated using an electronic simulation package.

3. ELECTRONIC EQUIVALENT CIRCUIT MODEL

In the previous section, the mathematical model of a FC stack consisting of N_C cells was discussed. As stated earlier, an electronic circuit equivalent model was proposed by Yu and Yuvarajan [1]. However, no details were given on a method of calculating the values of the components in the equivalent circuit model based on a mathematical equation obtained from experimental data.

The electronic circuit model of a PEMFC stack is shown in Figure 2. The model is based on the non-linearity of a diode and the current control feature of bipolar junction transistors (BJTs). The diode is used to model the ohmic losses and activation losses, while the two BJTs (Q1 and Q2) are used to model concentration losses. The capacitor C and inductor L are used to measure the dynamic behaviour of the stack. Typical values of 1F and 10 mH were chosen for these two components respectively.

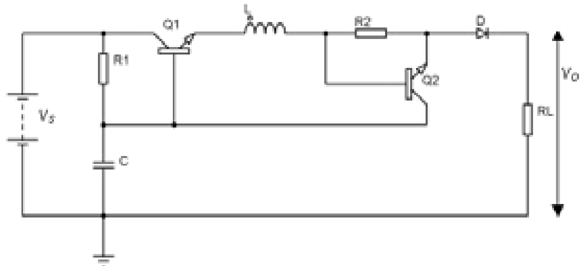

Figure 2: Electronic circuit model of a PEMFC [1].

The relationship between the voltage across a diode (V_D) and the current through it (I_D) is given by the equation:

$$V_D = nV_T \ln\left(\frac{I_D}{I_{SD}}\right), \text{ and } V_T = \frac{kT}{q} \quad (11)$$

where n is the emission coefficient, I_{SD} is the saturation current and V_T is the thermal voltage in terms of the Boltzmann's constant (k), absolute temperature (T) and electronic charge, q. This equation exactly resembles Equation (1) for the activation losses in a FC [1].

The transistors, Q1 and Q2, together with R1 and R2 form a current limiting circuit used to model the concentration losses of the FC stack. R2 acts a current sensing resistor so that when the current through it exceeds a certain limit, Q2 will start conducting, reducing the base voltage of Q1. This will cause the emitter voltage of Q1 to decrease at an exponential rate. The two transistors are assumed to be identical with current gain β and base-emitter voltage V_{BE}. The variation of the output voltage (V_0) as a function of load current (I_0) can be determined using the circuit in Figure 3.

The base current of Q1 (I_{B1}) and the collector current of Q2 (I_{C2}) can be written as

$$I_{B1} = \frac{I_O - I_{C2}}{1+\beta} \quad (12)$$

$$I_{C2} \approx I_S e^{\frac{I_O R2}{V_T}} \quad (13)$$

where I_S is the saturation current of Q1 and Q2 and V_T is the thermal voltage as given by Equation (11).

The output voltage can then be written as

$$V_O = V_S - \mathrm{R1}(I_{B1} + I_{C2}) - V_{BE1} - \mathrm{R2}(I_O - I_{C2} - I_{B2}) \quad (14)$$

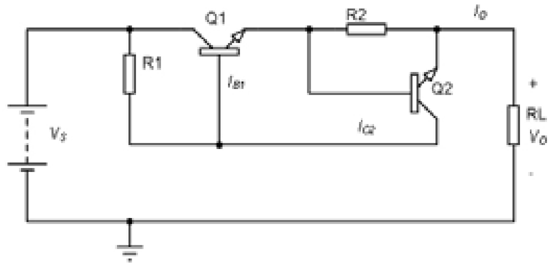

Figure 3: Modelling the concentration losses of a FC.

By substituting Equations (12) and (13) into Equation (14) and assuming that β is large, the output voltage can be simplified to

$$V_O = V_S - \mathrm{R2}\cdot I_O - \mathrm{R1}\cdot I_S e^{\frac{\mathrm{R2}\cdot I_O}{V_T}} - V_{BE} \tag{15}$$

Combining Equations (11) and (15), as well as taking the ohmic resistance of the diode ($\mathrm{R_D}$) into account, the total FC stack output voltage can be written as:

$$\begin{aligned} V_O &= V_S + nV_T \ln\left(I_{SD}\right) - V_{BE} - I_O(\mathrm{R2}+\mathrm{R_D}) \\ &\quad - nV_T \ln\left(I_O\right) - \mathrm{R1}\cdot I_S e^{\frac{I_O \mathrm{R2}}{V_T}} \end{aligned} \tag{16}$$

It can be seen that Equation (16) has the same form as the mathematical model of a FC stack given in Equation (10). By comparing these two equations, the following values must be calculated in order to finalise the circuit model of a FC (the thermal voltage V_T is 25 mV at room temperature):

- V_S (Voltage of the battery)
- R1 and R2
- The emission coefficient of the diode, n
- Saturation current of the diode, I_{SD}
- Saturation current of Q1 and Q2, I_S
- Ohmic resistance of the diode, $\mathrm{R_D}$

For a two-cell stack (N_C = 2), the above values can be determined by comparing Equation (16) with Equation (10) and establishing the following relationships:

- $V_S + nV_T \ln\left(I_{SD}\right) = 1{,}972$, where V_S is the theoretical output voltage of 2.46 V.
- $\left(\mathrm{R2}+\mathrm{R_D}\right) = 0{,}024$
- $nV_T = 0{,}07$
- $\mathrm{R1}.I_S = 0{,}0294$
- $\frac{\mathrm{R2}}{V_T} = 0{,}32$

A value for R1 was chosen as 10 Ω. The values for Equation (16) were then calculated to be:

- R2 = 0.008 Ω
- I_S = 0.00294 A
- $n = 2.8 \approx 3$
- $\mathrm{R_D}$ = 0.016 Ω
- I_{SD} = 0.000938 A

4. SIMULATION RESULTS

The graph in Figure 4 shows the polarisation curves of a two-cell FC stack obtained from experimental data (Table I), the mathematical model (Equation (10)) as well as the results of simulating the proposed electronic circuit equivalent using the Proteus VSM simulation package.

It can be seen from Figure 4 that the three results closely match each other, proving that the two models can be used to accurately describe the behaviour of a FC stack. In order to further test the models, Equation (10) was used to calculate the performance of a four-cell stack. The resulting equation was then used to determine the parameters of the equivalent circuit model for such a stack. The simulation results, together with those obtained from calculating (10), were compared to the actual performance data obtained from a four-cell stack constructed in the laboratory. These graphs (Figure 5) show that the model can be used to predict the behaviour of larger FC stacks based in the performance data of smaller ones.

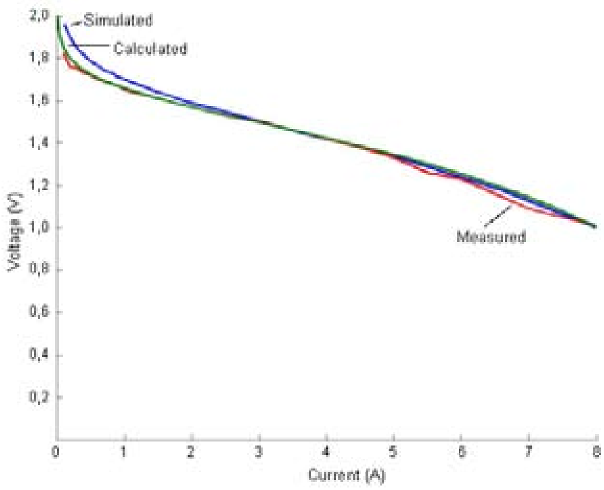

Figure 4: Simulated, calculated and measured polarisation curves of a two-cell PEMFC stack.

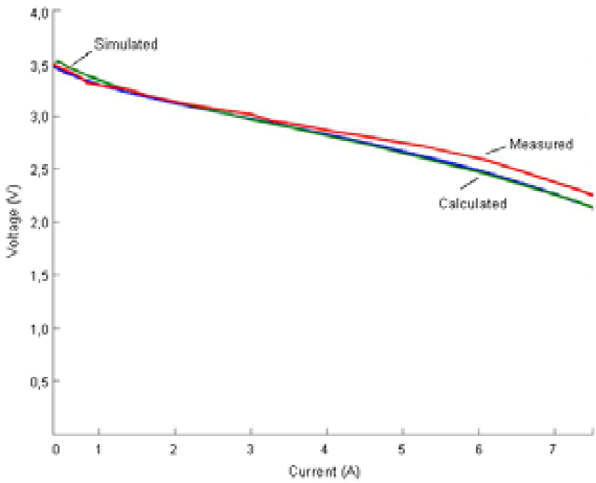

Figure 5: Simulated, calculated and measured polarisation curve of a four-cell stack.

5. CONCLUSION

The various losses present in a FC were discussed in terms of mathematical equations which were then used to mathematically model the behaviour of a FC stack. An already existing electronic circuit equivalent model of a FC stack was defined and the mathematical model of the FC used in order to make the circuit equivalent model more adaptable and easier to use for a wide variety of applications. It could be seen that the data collected from testing a small FC stack could be used to model and simulate the behaviour of larger stacks.

ACKNOWLEDGEMENTS

Telkom SA Ltd., M-TEC and TFMC have graciously provided funding for this project.

6. REFERENCES

[1] D. Yu, S. Yuvarajan: "Electronic circuit model for proton exchange membrane fuel cells", *J. Power Sources*, vol 142, pp. 238-242, 2005.

[2] J. Romm: *The hype about hydrogen, fact and fiction in the race to save the climate*, 1st edition, Washington, Island Press, 2004.

[3] J. Larmine, and A. Dicks: *Fuel cell system explained*, 2nd ed, West Sussex, Wiley, 2003.

[4] R. Jiang, D. Chu: "Comparative studies of polymer electrolyte membrane fuel cell stack and single cell", *J. Power Sources*, vol 80, pp.226-234, 1999.

[5] J. Du Toit: *Design and development of a 100 W proton exchange membrane fuel cell*, Vaal University of Technology, 2006.