

A Study in Development and Application of a Virtual Fuel Cell Test Platform

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Date of Submission: 08-05-2020

Date of Acceptance: 22-05-2020

| Symbols Symbols A I I V_{cell} | Units cm ² A/cm ² A V | Details Active cell area Current density Current Cell voltage |
|---|---|--|
| T P η_{act} | K atm | Cell temperature Cell pressure Activation losses |
| ${m \eta}_{_{ohm}}$ ${m \eta}_{_{diff}}$ | | Ohmic losses Diffusion losses |
| E E_{Nernst} | V V | Thermodynamic potential Equilibrium thermodynamic potential |
| E^{0} | V | Reference potential |
| $P_{H_2}^*, P_{O_2}^*$ | atm | Hydrogen and oxygen partial gas pressure at the surface of the catalyst At the anode and cathode |
| R F | | Gas constant Faraday's constant |
| eta_i | | Semi-empirical coefficients for calculation of activation losses |
| $C^*_{_{H_2}}$ | mol/cm ³ | Hydrogen concentration at the anode water-gas interface |
| $C^{*}_{H_{2}} \ C^{*}_{O_{2}}$ | mol/cm ³ | Oxygen concentration at the cathode water-gas interface |
| $R^{	ext{int}ernal}$ | Ωcm^2 | Total internal resistance |
| r_m | Ωcm | Membrane specific resistivity for the flow of hydrated proton |
| l | cm | Thickness of the polymer membrane |
| m,n | 2 | Mass transfer coefficients |
| р | W/cm ² | Power density |

| Abbreviations | |
|-----------------|--------------------------------|
| DC | Direct current |
| DMFC | Direct Methanol Fuel Cell |
| MEA | Membrane electrode assembly |
| MCFC | Molten Carbonate Fuel Cell |
| PEMFC Polymer | Electrolyte Membrane Fuel Cell |
| PAFC | Phosphoric Acid Fuel Cell |
| SOFC | Solid Oxide Fuel Cell |
| VFCTP Virtual I | Fuel Cell Test Platform |

I. INTRODUCTION

In 1800, British scientists William Nicholson and Anthony Carlisle had described the process of using electricity to decompose water into hydrogen and oxygen. But combining the gases to produce electricity and water was, according to Grove, "a step further that any hitherto recorded." Grove realized that by combining several sets of these electrodes in a series circuit he might "effect the decomposition of water by means of its composition." He soon accomplished this feat with the device he named a "gas battery" the first fuel cell [1].

William Robert Grove (1811-1896), a Welsh lawyer turned scientist, won renowned for his development of an improved wet-cell battery in 1838. The "Grove cell," as it came to be called, used a platinum electrode immersed in nitric acid and a zinc electrode in zinc sulfate to generate about 12 amps of current at about 1.8 volts [2].

Problems of global energy and factors effect on the earth's environment are pressing need with countries in the world. The human has started attention to new energies as wind energy, solar cell, nuclear energy, fuel cell et al. The fuel cells are received considerable attention. With motivations supply a tool for researches and studying fuel cell that we don't spend much money for experiment and component experiment. The computer language applications for developed computer program which help to test factors effect into fuel cells. Reducing the cost of research, studying, design, manufacturing fuel cell is by improving the performance of fuel cell itself.

In this paper, it is used a programming language, visual basic of Microsoft, to build a virtual fuel cell test platform (VFCTP). With friendly interface for users and simply used, this is related teaching materials to bring teaching and studying of the fuel cell into general school. Further, a VFCTP is useful tool for researches about fuel cell. Investigator can use it to accurately predict the fuel cell performance system for engineering applications and know important factors in determining the real performance of fuel cell. Using VFCTP, we will investigate the effect of different parameter such as pressure, temperature and channel geometry at different operating voltages. From that, a good design of fuel cell system was developed.

II. MATHEMATICAL MODEL AND DEVELOPMENT OF A VFCTP

2.1. Mathematical model of a fuel cell

In order to build a Virtual Fuel Cell Test Platform, a mathematical modeling of fuel cells needs to be developed. We need to study the internal working of the fuel cell and know the effects of various parameters. The electrochemical and thermodynamic principles of fuel cells are described and the effects of various parameters such as temperature, pressure and reactant composition on the fuel cell power output are studied.

A fuel cell produces the electrical energy (useful work) only when a current is drawn, but actually because of irreversible losses, cell voltage (V_{cell}) is decreased from its equilibrium thermodynamic potential (E_{Nernst}). When current flows, a deviation from the thermodynamic potential occurs corresponding to the electrical work performed by the cell. The deviation from the equilibrium value is called the overvoltage and has been given the symbol (η). The overvoltages originate mainly from activation loss (η_{act}), ohmic loss (η_{ohm}) and concentration loss (η_{diff}). The voltage for PEM fuel cell can be given by Eq. (1), [3, 4]:

$$V_{cell} = E_{Nernst} + \eta_{act} + \eta_{ohm} + \eta_{diff}$$
(1)

The pressure and concentration of the reactants affect the Gibb free energy, and thus the voltage. The Nernst equation gives to calculate the reversible thermodynamic potential of the $H_2 + O_2$ reaction previously described as follows:

$$E_{Nernst} = E^{0} + \frac{RT}{2F} \ln \left[P_{H_2}^{*} (P_{O_2}^{*})^{0.5} \right]$$
(2)

It is well-known that E^0 is a function of the cell operating temperature T, expressed as:

$$E^{0} = 1.229 - 0.85 \,\mathrm{x} \, 10^{-3} (T - 298.15) \tag{3}$$

To replace equation (2.3) with equation (2.2) we have derived the Nernst equation for the reaction described above as given by Eq. 4(4), [5, 6].

$$E^{0} = 1.229 - 0.85 \times 10^{-3} (T - 298.15) + 4.3085 \times 10^{-5} T[\ln(P_{H_{2}}^{*}) + 0.5 \ln(P_{O_{2}}^{*})]$$
(4)

The activation losses are a proportion of the voltage generated that is lost in driving the chemical reaction that transfers the electrons to or from the electrodes [7]. In order to mode the activation losses for a PEM fuel cell the following the semi-empirical equation is given by Eq. (5), [3, 8].

$$\eta_{act} = \beta_1 + \beta_2 T + \beta_3 \ln(C_{O_2}^*) + \beta_4 T \ln(iA)$$
(5)

with the works of Maxoulis et al. [6], the semi-empirical coefficients for calculation of activation losses were determined as following.

$$\beta_1 = 0.9514; \beta_2 = 0.00312; \beta_3 = 0.000074; \beta_4 = 0.000187$$

The Ohmic losses should result from electrical resistance losses in the cell. These resistances can be found in practically all fuel cell components: ionic resistance in the membrane, ionic and electronic resistance in the gas diffusion backings, bipolar plates and terminal connections [8]. Thus, the Ohmic losses depend on the material used in the electrodes and on the operating conditions of the cell, including the temperature, the current density and the membrane humidity [9]. This could be expressed using Ohm's Law equations such as:

$$\eta_{ohm} = \eta_{ohm}^{electronic} - \eta_{ohm}^{proton} - i(R^{electronic} - E^{proton}) - iR^{int\,ernal} \tag{6}$$

Diffusion Losses is caused by mass transfer limitations on the availability of the reactants near the electrodes. The electrode reactions require a constant supply of reactants in order to sustain the current flow. When the diffusion limitations reduce the availability of a reactant, part of the available reaction energy is used to drive the mass transfer, thus creating a corresponding loss in output voltage. Similar problems can develop if a reactants reaction product accumulates near the electrode surface and obstructs the diffusion paths or dilutes the reactants [8].

As proposed by Berning et al. [10], Chahine et al. [11], and Hamelin et al. [12], the total diffusion losses can be represented by Eq. (7), [8].

$$\eta_{diff} = -m \exp(ni) \tag{7}$$

The power for a fuel cell is calculated by the product of current and voltage is expressed by Eq. (8).

$$p = V_{cell} \mathbf{X} \mathbf{i} \tag{8}$$

Where V_{cell} is calculated at the above, i [A/cm²] is current density; p [W/cm²] is power density.

2.2. Development of a Virtual Fuel Cell Test Platform

Visual Basic (VB) is the third-generation event-driven programming language and integrated development environment (IDE) from Microsoft for its COM programming model. A programming language and environment developed by Microsoft. Based on the BASIC language, Visual Basic was one of the first products to provide a graphical programming environment and a paint metaphor for developing user interfaces. Although not a true object-oriented programming language in the strictest sense, Visual Basic nevertheless has an object-oriented philosophy. It is sometimes called an event- driven language because each object can react to different events such as a mouse click.



Figure 1. Interface of function part



Figure 2. Interface of graphic part

With objective of program is built for beginner study fuel cell. The program needs to have visual interface, easy usage, and friendly for user. Therefore, its interface is built with two main part such as function part (Figure 1) and graphic part (Figure 2).

In a computer program, an algorithm is a finite sequence of instructions, an explicit, step-by-step procedure for solving a problem, often used for calculation and data processing as described as in Figure 3. Algorithms are essential to the way computers process information. Many computer programs contain algorithms that specify the specific instructions a computer should perform (in a specific order) to carry out a specified task, such as calculating employees' paychecks or printing students' report cards. In this study, I only bring out a basic algorithm of the program. It will describe step-by-step procedure for building the program.



Figure 3. Diagram of Virtual Fuel Cell Test Platform's algorithm

III. EXPERIMENTAL METHOD

The equipment systemisthe Prodigit 3311D Series DC Electronic Load and Instek GPS- 3030DD DC Power Supply 30V/3A.DC Electronic Load: Prodigit 3311D Series DC Electronic Load is shown in figure 4 below.



Figure 4. DC Electronic Load model Prodigit 3311D

DC Power Supply: Instek GPS-3030DD DC Power Supply 30V/3A is shown in figure 5 below. The specifications of DC Power Supply are shown in table 1.



Figure 5.Instek GPS-3030DD DC Power Supply 30V/3A

| Table 1. The | specifications | of DC Power Supply | |
|---------------|----------------|--------------------|--|
| I dole It Inc | specifications | | |

| Line Regulation | 3 mA |
|-------------------------------|-------------|
| Load Regulation V/C | 3 mV - 3 mA |
| Other Features | 3 mV |
| Output 1, Volts/ Max. Current | 30V - 3A |
| Total Power | 90W |
| Туре | DC |

The PEM fuel cell system considered in this study is the stack Model 10SR4-A. The stack is made with 9 bipolar plates, 2 collector plates, 8 membrane/electrode assemblies, 2 structural plates, and air fan is shown in figure 6 below.



Figure 6. PEM fuel cell with the experimental

The general features of fuel cell used with experimental are shown in table 2 below.

| Technology | |
|-----------------------------|--------------------------------|
| Туре | Proton Exchange membrane, PEM |
| Menbrane | Nafion [®] 111 |
| Fuel | High purity hydrogen |
| Oxidant | Oxygen (from air) |
| H2 pressure | 250 mbar relative |
| Fuel cell stack | 8 membranes (MEAs) |
| Reaction Area | 3.8 cm^2 by MEA |
| Working temperature | 30 to 40°C |
| Electrical Specifications | |
| Nominal power (theoretical) | 10W |
| Output Voltage | 3 to 8 V |
| Power density | $460 \mathrm{mW/cm^2}$ |
| Ohmic resistance per MEA | 345mohm/cm ² |
| Voltage decay at 0.5 A | 3mv/hr |
| Useful functioning lifetime | 1500hr |
| Other Specifications | |
| Dimensions | 45x55x20 mm |
| Weight | 132 g |
| Room temperature | Temperature between 5 and 40°C |

Table 2. The general features of fuel cell

IV. EXPERIMENTAL RESULTS AND DISCUSSIONS

4.1.Relationship of fuel cell current density and voltage

The experimental results were based on the PEM fuel cell system, which are 8 cells with the active area by MEA is 3.8 cm² and specifications of fuel cell were considered in table 3. With the base-case operating conditions of the system temperature, pressure, and air stoichiometric are 25°C, 0.21 atm, and 1 respectively. Following this experimental, experimental data was stored as in Table 3, and shown in Figure 7. This figure showed that when the current density increased the voltage of fuel cell decreased.

|--|

| Current density(mAcm ⁻²) 0.035 0.084 0.166 0.279 0.423 0.564 0.695 Voltage(V) 0.685 0.626 0.562 0.499 0.438 0.374 0.313 | 14010 0 | · Emperime | inter result | e at temper | | , o. _ 1 aam | | |
|---|--------------------------------------|------------|--------------|-------------|-------|---------------------|-------|-------|
| Voltage(V) 0.685 0.626 0.562 0.499 0.438 0.374 0.313 | Current density(mAcm ⁻²) | 0.035 | 0.084 | 0.166 | 0.279 | 0.423 | 0.564 | 0.695 |
| | Voltage(V) | 0.685 | 0.626 | 0.562 | 0.499 | 0.438 | | 0.313 |



Figure 7. Experimental results at 25°C, 0.21 atm

4.2. Comparison of experimental and predicted results

The results show that the predicted polarization curve (or characteristic curve) of the program is good agreement with the experimental data curve as shown in Figure 8. The slight difference between two curves proved the program ability and its advantages. This difference is caused by variations in gases inlet, relative humidity and temperature, pressure, etc. between experimental and theoretical.From the verification results, it can be concluded that the VFCTP leaned on base-theoretical right. The VFCTP gives the predicted polarization curve exactly. Users can confirm that VFCTP supply for their studies and specially for studying of the fuel cell into general school.



Figure 8. Validation of analytical cell performance curve with experimental results

V. APPLICATION OF THE VFCTP

5.1. Prediction of the effect of temperature and pressure on the polarization curves

Polarization curves are the way to present fuel cell performance at the studies about fuel cell. It presents relation and the effect of change in current density i with the output voltage. With VFCTP, users easily have the predicted polarization curve at different operating temperatures and pressures of the fuel cell as shown in Figure 9 and Figure 10. The analyzed results showed that the fuel cell voltage increased with increasing of the temperature and pressure of the fuel cell.



Figure 9. Effect of change in the temperature to cell performance



Figure 10. Effect of change in the pressure to cell performance

5.2. Prediction of the power density

The power density is the measure of power generated per unit area. The power density is the product of voltage and the current density. Through VFCTP program, it obtains the power density curves for fuel cell at difference temperature and pressure.



Figure 11. Polarization curve and Power density curve at 40°C, 1 atm

Moreover, with VFCTP program, it can be used to obtain polarization curve and power density curve on a diagram. As in figure 11, shows the polarization curve and the power density curve at 40°C, 1 atm, respectively.

VI. CONCLUSIONS

In this paper, a mathematical model based on semi-empirical equation for a proton exchange membrane fuel cell, the Virtual Fuel Cell Test Platform (VFCTP) was developed to predict the current density and other process variations such as the gas pressure, temperature, diffusion to cover operating processes, and so on which are important factors in determining the real performance of PEMFC.

The VFCTP was built by using Visual Basic language. With visual interface, easy usage, and friendly for user, it guaranteed its objective is built for teaches, studies fuel cell, and especially for beginner study fuel cell. The VFCTP became a useful tool that users can predict polarization curve and power density curve at difference temperatures and pressure. It can be used to investigate the influence of process variables for optimization design of fuel cell and complete fuel cell power system.

The program results were compared well with experimental results. The comparison shows good agreements between the program results and the experimental data. The VFCTP programcan be applied as a useful tool for teaching and studying the fuel cell.

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Nguyen Hoai Son, et. al. "A Study in Development and Application of a Virtual Fuel Cell Test Platform." The International Journal of Engineering and Science (IJES), 9(5), (2020): pp. 29-37. _____