

Modeling and Simulation of PEM Fuel Cell with Bond Graph and 20sim

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Abstract— Due to the increasing and highly promising use of fuel cells as an important electrical energy source, its modeling has been a major research issue for some years, trying to find mathematical models precise enough to accurately predict how a cell will behave in a real world system, without becoming too complex. Many attempts have been made using different techniques. In this paper, the authors describe a static model for the PEM (Proton Exchange Membrane) fuel cell, developed by means of Bond Graphs and simulated in 20sim. The model proves to be simple and accurate, reproducing the characteristic curve of a commercial PEM fuel cell.

I. INTRODUCTION

DESPITE its relatively slow evolution as a source for electrical energy, fuel cells (FC) have recently experienced a surge in research and use, driven by environmental concerns, high costs of fuel, and even political reasons. Fuel cell applications include small and medium sized electricity generating stations, automobiles, spacecrafts, portable electronic devices, etc. [1], [2].

Of all types of FC, companies and researchers are mostly focused on *Proton Exchange Membrane Fuel Cells* (PEMFC), envisioned as a major electricity source for electric automobiles. As a consequence, its modeling has become an important research issue [3]-[8].

On the other hand, *Bond Graphs* (BG) role as a tool for modeling and simulation of complex multi-domain systems has been steadily increasing since its original creation by Dr. H. M. Paynter in 1959. Since then, *Bond Graphs* have been successfully used in the analysis and synthesis of many kinds of systems: electrical, electronic, hydraulic, mechatronic, etc. Fuel cells, being a system comprising chemical and electrical domains, make a perfect ground for BG application. Having a BG model for a fuel cell allows its immediate integration with the BG model of the subsystem the FC is connected to (for example, the mechanical subsystem of an automobile), allowing an easier understanding of the whole system.

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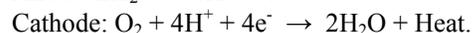
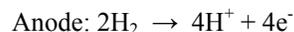
II. PROTON EXCHANGE MEMBRANE FUEL CELL (PEMFC)

A. Principle of Operation

Generally speaking, fuel cells are electrochemical devices capable of generating electricity from a chemical reaction. During operation, they must be constantly fed with a fuel (hydrogen or any hydrocarbon with a high hydrogen content) and an oxidant (oxygen or air).

Fig. 1 shows the principle of operation of a PEMFC, as well as its main components. Electrodes are made of carbon, and the membrane is a fine polymer film, which allows protons flow, while checking electrons passage. On the anode side, a constant hydrogen flow is injected into the cell. Hydrogen dissociates itself into hydrogen protons (H^+) and free electrons (e^-). Protons arrive at the cathode, passing through the membrane, but electrons are forced to flow through the external connections to the cell, thus providing energy to the load attached to it. On the cathode side, air is injected. Its oxygen combines with hydrogen protons and electrons, and water is produced. This water must be continuously extracted from the cell, in order to avoid excessive humidity, which can degrade its performance.

Chemical reactions in both electrodes are:



As a whole, the chemical reaction inside the FC is:

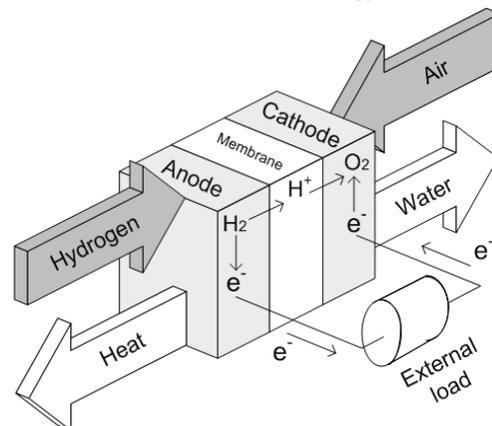


Fig. 1. Principle of operation of a PEMFC. Chemical reactions in both electrodes are also shown.

B. Internal Regions or Zones of a PEMFC

The internal zones of a PEMFC are visible in Fig. 2. First, both hydrogen and air are injected into the cell. Next, gases diffuse through the porous electrodes, where liquid water is found (mostly on the cathode side, where the chemical reaction (mostly involves water generation), which causes an important opposition to gases flows, due to the effective reduction of the electrodes pores sizes. After leaving the diffusion zone, gases arrive in the so-called “active zone”, where the chemical reactions previously stated take place. It is in this zone where chemical energy is transformed into electrical. In this zone there is liquid water, too, which means an additional opposition to the diffusion of gases. Forced by the anode-cathode electrical field, protons flow from the anode to the cathode, passing through the water wet membrane, which plays the electrolyte role. Due to the resistivity of the membrane (which is dependent on moisture and temperature) this flow of protons causes important energy losses. Finally, water and heat expulsion mechanisms must be provided in order to keep the cell working properly.

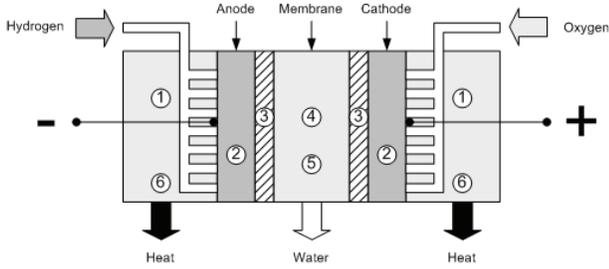


Fig. 2. Cutaway view of a PEMFC. (1) Injection of hydrogen and air, (2) Diffusion zone, (3) Active zone, (4) Membrane, (5) Water and (6) Heat expulsion.

C. Mathematical Model of a PEMFC with no Load

In fuel cells, the chemical reaction is responsible for the transformation of chemical energy into electrical; nevertheless, this ideal conversion is accompanied by irreversible phenomena like those of activation, diffusion, electric and ionic conduction, etc. All these must be taken into consideration in order to develop a reliable model of the cell.

If the reaction is an ideal one, the theoretical electromotive forces of the anode and cathode (E_{theo_anode} and $E_{theo_cathode}$) in equilibrium (no load current) are [3,4]:

$$E_{theo_anode} = \frac{\Delta G_{anode}}{nF} \quad (1)$$

$$E_{theo_cathode} = -\frac{\Delta G_{cathode}}{nF} \quad (2)$$

where ΔG_{anode} and $\Delta G_{cathode}$ are the variations of the enthalpies, or Gibbs free energy, n is the number of free

electrons (in our case of study, $n = 2$), and F is the Faraday constant (96,485.3383 C/mol). The theoretical potential (E_{theo}) of the whole cell is:

$$E_{theo} = E_{theo_cathode} - E_{theo_anode} \quad (3)$$

Nernst's law states that ΔG_{anode} and $\Delta G_{cathode}$ can be formulated in terms of standard free enthalpies (ΔG_{anode}^0 and

TABLE I
STANDARD ENTHALPIES AND ENTROPIES FOR HYDROGEN, OXYGEN,
AND LIQUID WATER

Substance	ΔH^0 (J . mol ⁻¹)	ΔS^0 (J . mol ⁻¹ . K ⁻¹)
Hydrogen	0	130.684
Oxygen	0	205.138
Water	-285.83 x 10 ³	69.91

$\Delta G_{cathode}^0$), temperature (T) and the pressures of gases at each electrode (P_{oxyg} and P_{hydro}):

$$\Delta G_{anode} = \Delta G_{anode}^0 - RT \ln(P_{hydro}) \quad (4)$$

$$\Delta G_{cathode} = \Delta G_{cathode}^0 - \frac{RT}{2} \ln(P_{oxyg}) \quad (5)$$

where $R = 8.314472$ J . K⁻¹ . mol⁻¹ is the universal or ideal gas constant.

ΔG_{anode}^0 and $\Delta G_{cathode}^0$ can be calculated by means of:

TABLE II
COEFFICIENTS OF EQUATIONS 8 AND 9

Substance	α (J.mol ⁻¹ .K ⁻¹)	β (J.mol ⁻¹ .K ⁻²)	γ (J . mol ⁻¹ . K ⁻³)
Hydrogen	29.038	-0.8356 x 10 ⁻³	2.0097 x 10 ⁻⁶
Oxygen	25.699	12.966 x 10 ⁻³	-3.8581 x 10 ⁻⁶
Water	30.33	9.6056 x 10 ⁻³	1.1829 x 10 ⁻⁶

$$\Delta G_{anode}^0 = \Delta H_{anode}^0 - T\Delta S_{anode}^0 \quad (6)$$

$$\Delta G_{cathode}^0 = \Delta H_{cathode}^0 - T\Delta S_{cathode}^0 \quad (7)$$

where ΔH_{anode}^0 and $\Delta H_{cathode}^0$ are the variations of the standard enthalpies, and ΔS_{anode}^0 and $\Delta S_{cathode}^0$ are the changes in the standard entropies.

ΔH_{anode}^0 , $\Delta H_{cathode}^0$, ΔS_{anode}^0 and $\Delta S_{cathode}^0$ at $T = 298$ K are obtained from Table I [6], where oxygen and hydrogen are considered as ideal gases, and water is in its liquid state.

Equations (8) and (9) [1] allow us to calculate standard enthalpies and entropies for a temperature other than 298 K:

$$\Delta H^0(T) = \Delta H^0_{298} + \alpha(T - 298) + \beta \frac{T^2 - 298^2}{2} + \gamma \frac{T^3 - 298^3}{3} \quad (8)$$

$$\Delta S^0(T) = \Delta S^0_{298} + \alpha \ln\left(\frac{T}{298}\right) + \beta(T - 298) + \gamma \frac{T^2 - 298^2}{2} \quad (9)$$

where the coefficients α , β , and γ can be obtained from Table II [1].

In a chemical reaction, the changes in standard enthalpies and entropies are calculated by means of:

$$\Delta H_{reaction} = \Delta H^0_{products} - \Delta H^0_{reactants} \quad (10)$$

$$\Delta S_{reaction} = \Delta S^0_{products} - \Delta S^0_{reactants} \quad (11)$$

At the anode this means:

$$\Delta H_{anode} = 0 - \Delta H^0_{Hydro} \quad (12)$$

$$\Delta S_{anode} = 0 - \Delta S^0_{Hydro} \quad (13)$$

and, at the cathode:

$$\Delta H_{cathode} = \Delta H^0_{water} - \frac{1}{2} \Delta H^0_{oxygen} \quad (14)$$

$$\Delta S_{cathode} = \Delta S^0_{water} - \frac{1}{2} \Delta S^0_{oxygen} \quad (15)$$

These equations and tables allow us to calculate the anode and cathode theoretical potentials, at any given temperature.

D. The PEMFC and Load Current

Anytime the PEMFC is delivering energy to an external load, the activation phenomena must be considered. This means that electrodes voltages (E_{anode} and $E_{cathode}$) will deviate from their theoretical values, calculated in the former section. These voltage variations are known as anode and cathode over voltages (η_{anode} and $\eta_{cathode}$).

Tafel's law states that, if:

$$\eta_{anode} = E_{anode} - E_{theo_anode} \quad (16)$$

$$\eta_{cathode} = E_{cathode} - E_{theo_cathode} \quad (17)$$

then:

$$\eta_{anode} = -\frac{RT}{\alpha_{anode} nF} \ln\left(\frac{I}{I_{0_anode}}\right) \quad (18)$$

$$\eta_{cathode} = -\frac{RT}{\alpha_{cathode} nF} \ln\left(\frac{I}{I_{0_cathode}}\right) \quad (19)$$

α_{anode} is the symmetry factor (or transfer factor) of the anode (oxidation), and $\alpha_{cathode}$ is the factor of the cathode (reduction). I_{0_anode} and $I_{0_cathode}$ are the exchange currents in the anode and cathode. I is the current that the cell delivers to its external load.

In [3] these equations are simplified by means of an

equivalent symmetry factor (α):

$$\alpha_{anode} n_{anode} = 3\alpha \quad (20)$$

$$\alpha_{cathode} n_{cathode} = \frac{3}{2}\alpha \quad (21)$$

where n_{anode} and $n_{cathode}$ are the numbers of electrons exchanged at the elementary reactions taking place at the anode and the cathode.

Another simplification in [3] is:

$$I_{0_anode} = 100I_0 \quad (22)$$

and:

$$I_{0_cathode} = \frac{I_0}{10} \quad (23)$$

where I_0 is the so called activation or exchange current.

Ohmic losses at the membrane must be considered. The resistivity (σ) of this element depends on the temperature and wetness of the membrane. Resistance of the membrane is:

$$R_{membrane} = \frac{L}{A\sigma} \quad (24)$$

where L is the width of the membrane and A is its area.

Phenomena associated with diffusion generate energy losses, too. Butler – Vollmer law allows us to calculate them:

$$\eta_{diffusion} = \frac{RT}{\beta nF} \ln\left(1 - \frac{I}{I_{lim}}\right) \quad (25)$$

where $\eta_{diffusion}$ is the over voltage associated to diffusion, β is an empirical coefficient associated to diffusion phenomena, and I_{lim} is the so called limit equivalent diffusion current.

Voltage at the cell terminals (V_{cell}) is:

$$V_{cell} = E_{theo_cathode} - E_{theo_anode} - \eta_{cathode} - \eta_{anode} - |\eta_{diffusion}| - IR_{membrane} \quad (26)$$

III. MODEL DEVELOPED

Modeling of any real-world system demands some simplifications; otherwise, models become cumbersome and unmanageable. Our PEMFC model has the following restrictions:

- It is a one-dimensional model,
- The gases injected to the cell are pure hydrogen and oxygen,
- Gas pressure is constant, regardless of the volume flowing,
- Pressure losses are not considered,
- Only diffusion phenomena at the cathode are taken into account,
- Temperature is constant,
- Temperature is the same all over the cell,
- Wetness of the membrane is constant and satisfactory

for a normal operation of the cell, and

i) Our model is valid only for steady state analysis. Transients cannot be simulated with it.

IV. BOND GRAPH MODELING OF A PEMFC

One of the most remarkable features of BG modeling is that the model retains a general resemblance to the original physical system modeled [9].

Watching our BG model of a PEMFC in Fig. 3 it is clear that the layout of the elements is very close to the way these devices are built. The basic elements (anode, membrane, and cathode) have associated regions of the diagram, which are located at their correct positions.

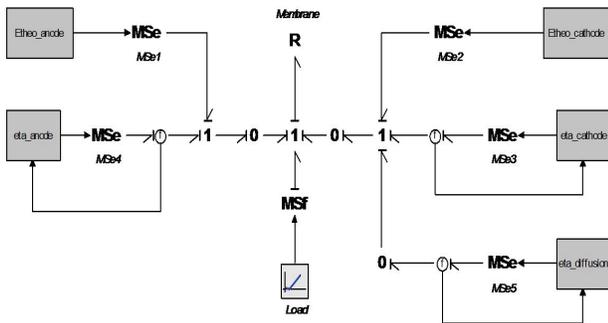


Fig. 3. Bond graph model of a PEMFC.

Figs. 4 and 5 show diagrams of the theoretical anode and cathode potentials. Inside their blocks equations of sections II-C and II-D have been programmed.

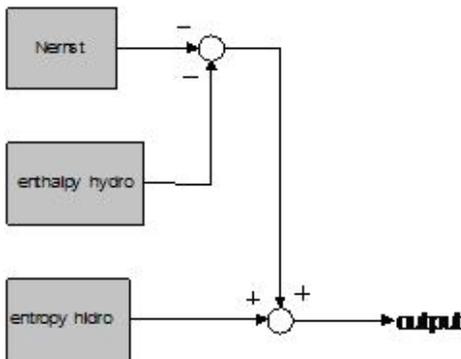


Fig. 4. Bond graph model of the anode of a PEMFC.

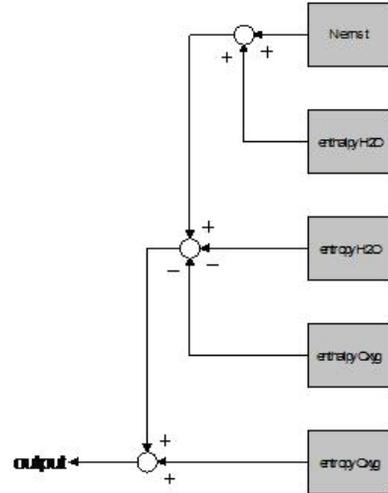


Fig. 5. Bond graph model of the cathode of a PEMFC.

V. SIMULATION OF A REAL FUEL CELL

A. Real Fuel Cell Data

From [3] we extracted the curve shown in Fig. 6. These data belong to a commercial fuel cell model, operating at 338 K, hydrogen and oxygen pressures, both at 200,000 Pa, a limit current of 100 A, and a membrane resistance of 8 mΩ.

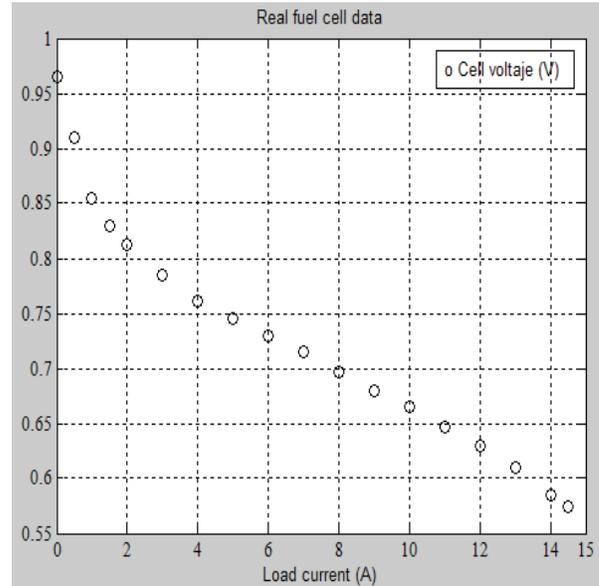


Fig. 6. Polarization curve of a commercial PEMFC.

B. Simulation of a Real Fuel Cell

To validate our model, we decided to replicate the data of Fig. 6. This implied an iterative work in order to find best values for α and β . At the end, we came to $\alpha = 0.53$, and $\beta = 0.0064$. It is interesting to remark that when α changes, it particularly influences the left side of the curve, while β changes basically modify the right side.

Fig. 7 shows the polarization curve obtained from our model. In order to make a better comparison between both

curves, in Table III we included values from Figs. 6 and 7. It is clear that, in the middle and right regions of the curves, errors are small. It is only on the left side of the curves (corresponding to very low load currents, less than 1 A) that noticeable errors are present.

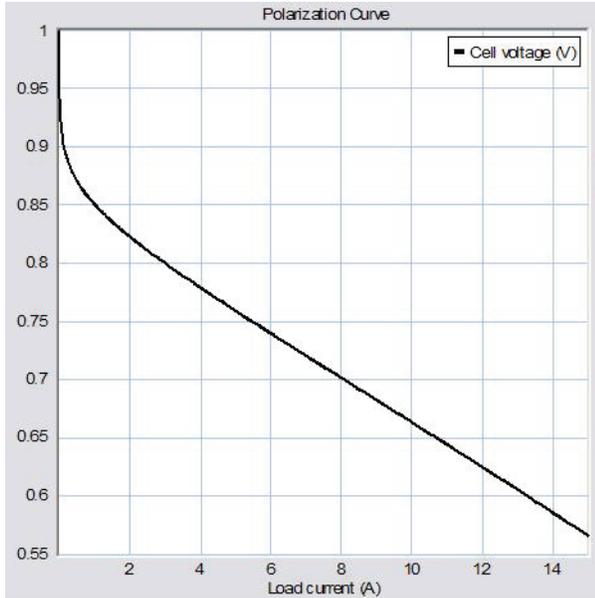


Fig. 7. Polarization curve obtained from the BG model.

In Table III we summarize the comparison between Figs. 6 and 7. Simulation of PEM fuel cell was realized using the software 20sim [10]-[12].

VI. CONCLUSION

Our Bond Graph model of a PEMFC has proved to be simple, yet accurate. Simulation results obtained through the software 20sim showed that the model proves to be very useful in the analysis and study of real world performance for this type of fuel cell. Further research can be accomplished with other types of fuel cells. The model can also be improved in order to deal with the dynamic behavior of PEMFC and analyze its performance.

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TABLE III
VALIDATION OF THE BG PEMFC MODEL

Load (A)	Real Cell Voltage (V)	Model Cell Voltage (V)	Error (%)
0	0.97	0.95	2.1
0.5	0.94	0.87	7.4
1.0	0.86	0.85	1.2
1.5	0.83	0.84	-1.2
2.0	0.81	0.82	-1.2
3.0	0.80	0.80	0.0
4.0	0.76	0.78	-2.6
5.0	0.75	0.76	-1.3
6.0	0.73	0.74	-1.4
7.0	0.71	0.72	-1.4
8.0	0.70	0.70	0.0
9.0	0.68	0.68	0.0
10.0	0.66	0.66	0.0
11.0	0.65	0.64	1.5
12.0	0.63	0.63	0.0
13.0	0.61	0.61	0.0
14.0	0.59	0.59	0.0
14.5	0.57	0.57	0.0