CONTROL ORIENTED DYNAMIC PEM FUEL CELL SYSTEM MODEL

Fontalvo Morales Víctor[a]
vfontalvo@uninorte.edu.co

Sanjuan Mejía Marco[b]
msanjuan@uninorte.edu.co

Fecha de recepción: agosto de 2014. Fecha de aceptación: octubre de 2014

Abstract: hybrid energy generation systems allow a transition from conventional systems, and the opportunity to test and learn about fuel cell performance in a given setting. This paper presents an open cathode fuel cell dynamic model. This model can be used to design control strategies and design test benches to test fuel cells stacks. Results demonstrate that the predictions in voltage and current in the fuel cell stack are close to experimental data obtained from manufacturer.

Keywords: Fuel Cell, Dynamic model, Hydrogen, Electrical power generation, Dynamic simulation.

Resumen: Sistemas de generación de energía híbridos permiten una transición de los sistemas convencionales, y la oportunidad de probar y aprender sobre el rendimiento de células de combustible en un entorno dado. En este trabajo se presenta un modelo dinámico de celdas de combustible de cátodo abierto. Este modelo se puede utilizar para diseñar estrategias de control y diseño de bancos de pruebas para poner a prueba pilas de combustible. Los resultados demuestran que las predicciones en el voltaje y la corriente en la pila de células de combustible están cerca de los datos experimentales obtenidos del fabricante.

Palabras Claves: Fuel Cell, modelo dinámico, hidrógeno, generación de energía eléctrica, la simulación dinámica

1. INTRODUCTION

Energy is usually defined as the ability to do work; particularly electrical energy has become indispensable for the development of society. Our quality of life is completely dependent on availability of electricity both in industrial, commercial and residential sectors. Most of the electrical energy is currently obtained from fossil fuels (oil, coal and natural gas mostly), unfortunately the continued use of these non-renewable sources have severely impacted the environment due to continuous gas emissions from the combustion of these fuels. Fuel cells are electrochemical devices capable of producing electrical power as long as the fuel and oxidant supply is not interrupted. Although the operating principle of fuel cells has been known since the mid nineteenth century it was not until the mid-twentieth century when thanks to the space race fuel cells became a practical, providing power and drinking water aboard ships.

---

[a] Mechanical Engineer, MSc, Ph.D Student and researcher in Mechanical Engineering Department, Universidad del Norte, Barranquilla, Colombia

[b] Mechanical Engineer, Ph.D. Professor and researcher in Mechanical Engineering Department, Universidad del Norte, Barranquilla, Colombia

In recent decades it has resumed the interest in fuel cells as an alternative technology for generating electricity from renewable energy sources such as hydrogen, with greenhouse gas emissions almost null. It's not the first time that fuel cells are a topic of interest to the scientific community, but unlike previous waves, this time there is a strong interest from the industrial sector and the government sector which has helped early in his marketing development. While the basic principle of operation of fuel cells dates back more than a century, today there are many challenges to be addressed both in terms of the materials used in the cell and in the control strategies implemented to ensure its proper functioning. In terms of materials relates the biggest challenges for marketing are linked to high costs, especially of the catalysts and the membrane, the former being typically platinum based polymeric membrane normally, but with the necessary treatments to grant property very specific as its mechanical strength which allows to manufacture very thin thickness and permeability to gases but not to liquids and permeability mainly in the gas phase of protons only (the core) of the hydrogen atoms while forcing electrons to circulate through an external circuit, thereby generating current. The control system remains a challenge due to the strong non-linearities present in the systems formed by fuel cells, and hybrid systems that integrate the fuel cell with conventional systems, for example gas turbines in power generation plants, or systems based on renewable energy sources such as wind farms or solar. Nonlinearities make conventional control strategies loops using only PID controllers have poor performance because these controllers are tuned using identifications from an operating point of the system, and while this is in operation in these neighborhoods the answer is acceptable, but in the moment load conditions, fuel feed or oxidant (oxygen or air) and the operating point change, the response of the control system is spoiled.

2. FUEL CELL SYSTEM ANALYTICAL MODEL

The model used in the simulation takes account of three different phenomena:

a) Mass transfer
b) Thermodynamics
c) Electrochemical

Mass Transfer

The fuel cell uses hydrogen and air to generate electricity. The hydrogen is supplied to the fuel cell anode and the air is supplied to the fuel cell cathode.

This model allows the calculation of the pressure and mass flow circulating in the cell.

Cathode

The cathode is supplied with moist air. It is assumed that moist air contains only water, oxygen and nitrogen.

Mass Balance

The water content contained in the air depends on the temperature and the relative humidity.

The water content contained in the air depends on the temperature and the relative humidity.

$$w_e = \frac{m_v}{m_a} = 0.622 \frac{\phi_e p_{sat}(T_e)}{p_e - \phi_e p_{sat}(T_e)} \qquad \text{1)}$$

The water saturation pressure can be estimated using the regression proposed by (Musio et al., 2011)

$$\begin{aligned} p_{sat}(T) = -2.1794 &+ 0.02953 \cdot T \\ &- 9.1873 \times 10^{-5} \cdot T^2 \\ &+ 1.4454 \times 10^{-7} \cdot T^3 \end{aligned} \qquad \text{2)}$$

The different components of moist air are related with the moist air mass flow. It is assumed dry air is formed by 79% nitrogen and 21 % oxygen.

The content of oxygenin the air supply is defined by:

$$\dot{m}_{O_2,,e} = 0.21 \frac{M_{O_2}}{M_a} \frac{1}{1 + w_e} \dot{m}_e \qquad \text{3)}$$

And for the nitrogen:

$$\dot{m}_{N_2,,e} = 0.79 \frac{M_{N_2}}{M_a} \frac{1}{1 + w_e} \dot{m}_e \qquad \text{4)}$$

Now the mass balance in the cathode can be written for each component.

For the water

$$\frac{dm_v^{ca}}{dt} = \dot{m}_{v,e}^{ca} - \dot{m}_{v,s}^{ca} + \dot{m}_v^{ca,GDL} + \dot{m}_{eva}^{ca} \qquad \text{5)}$$

Where,

$\dot{m}_{v,e}^{ca}$: Water input mass flow on the cathode side.

$$\dot{m}_{v,e}^{ca} = \frac{w}{1 + w_{r,e}} \dot{m}_{ah,e}^{ca} \qquad \text{6)}$$

And

$$\dot{m}_{ah,s}^{ca} = K^{ca}(p^{ca} - p_{suc}) \qquad \text{7)}$$

$\dot{m}_{v,s}^{ca}$: Water output mass flow on the cathode side

$$\dot{m}_{v,s}^{ca} = K^{ca} \frac{m_v^{ca}}{(m_a^{ca} + m_v^{ca})} (p^{ca} - p_{suc}) \qquad \text{8)}$$

$\dot{m}_v^{ca,GDL}$: Water mass flow through the GDL on the cathode side

$$\dot{m}_v^{ca,GDL} = A_{fc} \cdot n_c \langle D_v^{ca} \rangle \cdot \left(\frac{c_v^{ca,GDL} - c_v^{ca,can}}{\delta^{GDL}} \right) \qquad \text{9)}$$

c_v^j: Molar concentration

$$c_v^j = \frac{p_v^j}{RT_{fc}} \qquad \text{para} \qquad \text{10)}$$

$$j = ca, can; ca, GDL$$

Nam and Kaviany (Nam & Kaviany, 2003) propose the following relation for mass transport on porous media.

$$\langle D_v^{ca}\rangle = D_v\, \varepsilon \left(\frac{\varepsilon - 0.11}{1 - 0.11}\right)^{0.785} (1 - s^{ca})^2 \qquad 11)$$

And

ε: Media porosity (0.5 for carbon fibers paper)

s^{ca}: Media saturation. This is the relation between the volume occupied by the water and the total volume occupied by the porous $\frac{V_{H_2O}}{V_p}$

$\dot{m}_{eva}^{ca}$: Condensed/evaporated in the cathode.

Zemansky proposed in (Zemansky & Dittman, 1979) an equation to estimate the evaporation/condensation mass flow.

$$\dot{m}_{eva}^{ca} = \min\left(A_{fc}\big(p_{sat}(T_{fc}) - p_v^{ca}\big)\sqrt{\frac{M_v}{2\pi R T_{fc}}}, \dot{m}_l^{ca,GDL} \right) \qquad 12)$$

Notice, $\dot{m}_{evap}$ will be positive when $p_v^{ca} < p_{sat}(T_{fc})$ The logical restriction guarantee the model does not calculate mass flow greater than the available water in the cell (dynamic). The liquid water used as restriction for equation 12 is defined by the liquid water mass balance (see equation 13)

$$\rho_l^{H_2O} \cdot \frac{dV_l^{ca,GDL}}{dt} = \dot{m}_{cond}^{ca,GDL} - \dot{m}_l^{GDL\to ca} \qquad 13)$$

Where

$\dot{m}_l^{GDL\to ca}$: Liquid water flowing from GDL toward cathode channels due to capillary effect (the GDL is a porous media). This model is explained in detail in (Nam & Kaviany, 2003) and simplified by (del Real, Arce, & Bordons, 2007), where simplified concentration gradients are used.

$$\dot{m}_l^{GDL\to ca} = \frac{\rho_l \cdot A_{fc} \cdot n_{fc} \cdot K \cdot S^3}{\mu_l}\left|\frac{d\rho_c}{dS}\right| \frac{S^{ca}}{\delta^{GDL}} \qquad 14)$$

The term $\left|\frac{d\rho_c}{dS}\right|$ can be approximated to the constant value $30{,}312\ kPa$ (Nam & Kaviany, 2003) although it formally depends of the Leverette.

S^{ca}: The liquid saturation can be calculated with the model proposed by (Nam & Kaviany, 2003) and adapted by (del Real et al., 2007)

$$S^{ca} = \begin{cases} \dfrac{s^{ca} - s_{im}}{1 - s_{im}} & para\ s_{im} < s^{ca} \le 1 \\ 0 & para\ 0 \le s^{ca} \le s_{im} \end{cases} \qquad 15)$$

The remaining terms from equation1 are

ρ_l: Liquid water density $\left(978\frac{kg}{m^3}\right)$

A_{fc}: Fuel cell area
n_{fc}: Number of cells in the stack
S^3: Relative permeability
K: Absolute permeability$(2.55 \times 10^{-13} m^2)$
u_l: Water viscosity $(0.000405\ kg/ms)$
s_{im}: Immobile saturation(0.1)
From equation $m_{cond}^{ca,GDL}$ is the water condensation (or evaporation) rate in the porous media, and defined by (Nam & Kaviany, 2003)

$$\dot{m}_{evap}^{ca,GDL} = -\dot{m}_{cond}^{ca,GDL} = -M_{H_2O}\gamma\left[\frac{p_{ca}^{GDL} - p_{sat}(T_{fc})}{R_u T_{fc}}\right]\varepsilon V^{GDL} \qquad 16)$$

With the logical constraint

$$If\ V_l^{ca,GDL} = 0\ \&\ \dot{m}_{evap}^{ca,GDL} > 0 \rightarrow \dot{m}_{evap}^{ca,GDL} = 0$$

The volume of liquid water in the GDL is critical, it can flood the cell and thereby restricting gas flow through the GDL and delaying the reaction both the anode side and the cathode.

The remaining gases mass flow balances are as follows

For oxygen

$$\frac{dm_{O_2}^{ca}}{dt} = \dot{m}_{O_2,e} - \dot{m}_{O_2,s} - \dot{m}_{O_2,reac} \qquad 17)$$

Where

$$\dot{m}_{O_2,reac} = n_{fc} M_{O_2} \frac{I}{4F} \qquad 18)$$

This is the oxygen required in the electrochemical reaction in the cell.

$$\frac{dm_{N_2}^{ca}}{dt} = \dot{m}_{N_2,e} - \dot{m}_{N_2,s} \qquad 19)$$

Input flows were defined at the beginning of the section, and output flows can be estimated from

$$\dot{m}_{j,s}^{ca} = K^{ca} \frac{m_j^{ca}}{(m_a^{ca} + m_v^{ca})}(p^{ca} - p_{suc}) \qquad 20)$$

for $j = O_2, N_2$

For nitrogen

$$\frac{dm_{N_2}^{ca}}{dt} = \dot{m}_{N_2,e} - \dot{m}_{N_2,s} \qquad 21)$$

Pressures

The cathode must contain in a finite volume a variable amount of mass, this variation will depend mainly on the magnitude of the mass flows into the cell and from the load demand. Increases and decreases on the mass inside the cathode produce pressure changes depending on the operating temperatures and the gases included in the model can be estimated by using the ideal gas equation. Pressures have to be dynamically determined in the different volumes of the cathode since as shown in equation the concentrations of the gases and hence the magnitude and direction of mass transfer of these gases are functions of pressure.

Since the volume of the cathode is a constant value the partial pressure of each gas can be calculated as follows:

$$p_j^{ca} = \frac{m_j R T_{fc}}{M_j V^{ca}} \text{ for } j = O_2, N_2, v \qquad 22)$$

Pressure inside the cathode will be the addition of the gases partial pressures.

$$p^{ca} = \sum_{j=1}^{3} p_j^{ca} \quad \text{for} \quad j = O_2, N_2, v \qquad 23)$$

Finally pressures in the cathode side are defined with the variations of them in the GDL

$$\frac{dp_v^{ca,GDL}}{dt} = RT_{fc}\left(\frac{N_v^{mem} - N_v^{ca,ca}}{\delta^{GDL}} + \frac{N_v^{gen}}{V^{GDL}} + \frac{\dot{m}_{evap}^{ca,GDL}}{M_{H_2O}V^{GDL}}\right) \qquad 24)$$

This last equation assumes a gas ideal behavior, and therefore is only valid for the gas phase.

The term N_v^{gen} depends on the load, the electrochemical reaction and can be calculated as

$$N_v^{gen} = \frac{I}{2F} \qquad 25)$$

Membrane

There are many mechanisms that allow water to flow through the various components of the fuel cell. In the case of the membrane vapor flow coming from this can be estimated by the equation proposed by which considers two phenomena; an electro-osmotic drag due to the presence of an electrical potential in a porous medium (Nafion membrane), also is present the phenomenon of vapor diffusion to the anode due to the concentration gradient.

$$N_v^{mem} = n_d \frac{I}{A_{fc}F} - \alpha_w D_w \frac{c_v^{ca} - c_v^{an}}{\delta^{mem}} \qquad 26)$$

The term $\left(n_d \frac{I}{A_{fc}F}\right)$ makes reference to the electrosmotic drag due to hydrogen, and the electro-osmotic drag factor nd is defined by (Dutta & Shimpalee, 2001) as:

$$n_d = 0.0029\lambda_{an,ca}^2 + 0.05\,\lambda_{an,ca} - 3.4 \times 10^{-19} \qquad 27)$$

and

$$\lambda_j = 0.043 + 17.81\,a_j - 39.85\,a_j^2 + 36a_j^3 \text{ for } j = an, ca \qquad 28)$$

$$a_j = \frac{y_{H_2O}p_j}{p_{sat}(T_{fc})} \qquad 29)$$

Notice that, a_j from equation 29 is in this study the relative humidity in each membrane side.

The second term on equation 26 is the back diffusion of vapor from the cathode towards the anode due to concentration gradient. The diffusion mass transfer coefficient is calculated using the equations proposed by (Dutta & Shimpalee, 2001)

$$D_w = D_{\lambda_{an}} \exp(2416\left(\frac{1}{303} - \frac{1}{T_{fc}}\right) \qquad 30)$$

$$D_{\lambda_{an}} = \begin{cases} 10^{-10} & \lambda_{an} < 2 \\ 10^{-10}\left(1 + 2(\lambda_{an} - 2)\right) & 2 \le \lambda_{an} \le 3 \\ 10^{-10}\left(3 - 1.67(\lambda_{an} - 3)\right) & 3 < \lambda_{an} < 4.5 \\ 1.25 \times 10^{-10} & \lambda_{an} \ge 4.5 \end{cases} \qquad 31)$$

Note that mass transfer is increased when the cell temperature increases and the relative humidity in the anode decreases.

α_w Correction factor is used to adjust the transport vapor through the membrane as these correlations may be outdated since were developed for approximately ten years

$$c_v^j = \frac{\rho^{mem,seca}}{M^{mem,seca}}\lambda_j \text{ for } j = an, ca \qquad 32)$$

Ballard membrane has the following parameters

$$\delta^{mem} = 35\ \mu m$$
$$\rho^{mem,seca} = 2 \times 10^{-3}\ kg/m^3$$
$$M^{mem,seca} = 1.1\ kg/kmol$$

Anode

The analysis of the mass transfer phenomena for the anode is similar to the one showed for the cathode governing equations. Mass transfer and pressure in the anode are summarized

Mass Balances

For Hydrogen

$$\frac{dm_{H_2}^{an}}{dt} = \dot{m}_{H_2,,e} - \dot{m}_{H_2,,s} - \dot{m}_{H_2,,reac} \qquad 33)$$

The input flow is function of anode pressure, hydrogen supply line pressure and control valve. The output flow is function of the purge valve; the system is designed to operate in a “dead-end” configuration, which means the hydrogen leave the anode side using periodically purges. The last term is function of the electrochemical reaction, basically depends on the current demanded to the system.

$$\dot{m}_{H_2,,reac} = n_{fc} M_{H_2} \frac{I}{2F} \qquad 34)$$

Output flows of hydrogen and vapor can be calculated with the following equation

$$\dot{m}_{j,s}^{an} = K^{an} \frac{m_j^{an}}{\left(m_{H_2}^{an} + m_v^{an}\right)} \left(p^{an} - p_{atm}\right) \text{ for } j = H_2, v \qquad 35)$$

To evaluate the water content in the anode is necessary to consider the two phases in

$$\frac{dm_v^{an}}{dt} = \dot{m}_v^{an,GDL} + \dot{m}_{evap}^{an} - \dot{m}_{v,s}^{an} \qquad 36)$$

The definition of the flow mass balance is similarly to what was proposed for the cathode.

$$\dot{m}_v^{an,GDL} = A_{fc} \cdot n_c \left[D_v \, \varepsilon \left(\frac{\varepsilon - 0.11}{1 - 0.11} \right)^{0.785} (1 - s^{an})^2 \right] \cdot \left(\frac{c_v^{an,GDL} - c_v^{an,can}}{\delta^{GDL}} \right) \qquad 37)$$

$$\dot{m}_{eva}^{an} = \min \left(A_{fc} \left(p_{sat}(T_{fc}) - p_v^{ca} \right) \sqrt{\frac{M_v}{2\pi R T_{fc}}}, \dot{m}_l^{an,GDL} \right) \qquad 38)$$

For the liquid phase

$$\frac{dm_v^{an}}{dt} = \dot{m}_v^{an,GDL} + \dot{m}_{evap}^{an} - \dot{m}_{v,s}^{an} \qquad 39)$$

The terms of the mass balance for the liquid phase are detailed below.

$$\dot{m}_l^{GDL\to an} = \frac{\rho_l \cdot A_{fc} \cdot n_{fc} \cdot K \cdot S^3}{\mu_l}\left|\frac{d\rho_c}{dS}\right|\frac{S^{an}}{\delta^{GDL}} \qquad 40)$$

Evaporating flow calculation is determined previously during the balance of the gaseous phase and the flow of liquid water that is dragged of the anode during purge can be estimated on the assumption that all liquid water that may have condensed in the anode channel exits in each purge.

$$\dot{m}_{l,s}^{an} = \frac{m_l^{an}}{t_{purga}} \quad \text{If } \sum \dot{m}_{j,s}^{an} > 0 \qquad 41)$$

Pressures

Since the volume of the anode is a constant value the partial pressure of each gas can be calculated as follows:

$$p_j^{an} = \frac{m_j R T_{fc}}{M_j V^{ca}} \text{ for } j = H_2, v \qquad 42)$$

Pressure inside the anode will be the addition of the gases partial pressures.

$$p^{an} = \sum_{j=1}^{2} p_j^{an} \text{ for } j = H_2, v \qquad 43)$$

To complete the calculation of the pressures in the anode is necessary to consider changes in partial pressure of vapor in the GDL.

$$\frac{dm_v^{an,GDL}}{dt} = \dot{m}_v^{mem} + \dot{m}_{evap}^{ca,GDL} - m_v^{ca,ca} + \dot{m}_v^{gen} \qquad 44)$$

Using an ideal gas model

$$\frac{dp_v^{an,GDL}}{dt} = RT_{fc}\left(\frac{\dot{m}_{evap}^{an,GDL}}{M_{H_2O}V^{GDL}} - \frac{N_v^{mem} + N_v^{an,can}}{\delta^{GDL}}\right) \qquad 45)$$

The molar flow per unit area into the channels of the anode can be calculated using equation ; if the vapor concentration is higher in the GDL than in the channels, towards them will be the direction of flow; positives values indicate that the steam leaves the GDL.

$$N_v^{an} = \langle D_v^{an}\rangle\left(\frac{c_v^{an,GDL} - c_v^{an,can}}{\delta^{GDL}}\right) \qquad 46)$$

Similar to cathode and with the same restriction, the flow of steam that evaporates or condenses can be determined by

$$\dot{m}_{evap}^{an,GD\dot{L}} = -m_{cond}^{an,GDL} = -M_{H_2O}\gamma\left[\frac{p_{an}^{GDL} - p_{sat}(T_{fc})}{R_u T_{fc}}\right]\varepsilon V^{GDL} \qquad 47)$$

To complete the fluid dynamic equations are required to evaluate the variations of liquid water content in the anode GDL

$$\rho_l^{H_2O}\cdot\frac{dV_l^{an,GDL}}{dt}=M_{H_2O}\gamma\left[\frac{p_{ca}^{GDL}-p_{sat}(T_{fc})}{R_uT_{fc}}\right]\varepsilon V^{GDL}-\frac{\rho_l^{H_2O}\cdot A_{fc}\cdot n_{fc}\cdot K\cdot S^3}{\mu_l}\left|\frac{d\rho_c}{dS}\right|\frac{S^{ca}}{\delta^{GDL}}\qquad 48)$$

Thermodynamic model

It has been shown up to this point the fuel cell stack model by analyzing variations in mass per volume of the cells that compose it, assuming that all behave in a similar manner within these. Essentially, pressures and mass transfer phenomena on mostly gaseous components are strongly affected by temperature variations as reflected in the equations so far presented.

The energy balance proposed includes the electrochemical reaction that is exothermic and the heat transfer to the air flowing through the cathode which has to supply the electrochemical reaction with the oxygen required and regulate the stack temperature. The analysis is based on the law of Dalton , so that it assumes that the enthalpy change in the system is equivalent to the sum of the enthalpies of each gas in the fuel cell. An uniform distribution it is assumed, so that a relaxation calculations once the simulation control system incorporates the following energy balance calculation is simplified and computational requirements are reduced.

$$\begin{aligned}m_{fc}C_{fc}\frac{dT_{fc}}{dt}&=\dot H^{reac}-\Delta\dot H_{H_2}^{pur}-\Delta\dot H_{H_2O}^{pur}\\&\quad-\Delta\dot H_{aire}^{enf}-\dot W^{elec}\end{aligned}\qquad 49)$$

$$\begin{aligned}\dot H^{reac}&=\dot m_{H_{2,},reac}\left(h_f^0+\Delta h\right)_{H_2}\\&\quad+\dot m_{O_{2,},reac}\left(h_f^0+\Delta h\right)_{O_2}\\&\quad-\dot m_{H_{2,}0,reac}\left(h_f^0\right.\\&\quad\left.+\Delta h\right)_{H_20(g)}\end{aligned}\qquad 50)$$

$\Delta\dot H_{H_2}^{pur}$ Energy lost with the hydrogen released in each purge. It did not reacted but changed its temperature

$$\Delta\dot H_{H_2}^{pur}=\dot m_{H_2,s}^{an}\Delta h_{H_2}\big|_{@T_{fc}-T_{amb}}\qquad 51)$$

$\Delta\dot H_{aire}^{enf}$ Energy transferred to excess air flowing through the fuel cell stack.

$$\begin{aligned}\Delta\dot H_{aire}^{enf}&=\dot m_{N_2,s}^{ca}\ \Delta h_{N_2}\big|_{@T_{fc}-T_{ref}}\\&\quad+\dot m_{O_2,s}^{ca}\ \Delta h_{O_2}\big|_{@T_{fc}-T_{ref}}\\&\quad+\dot m_{v,s}^{ca}\ \Delta h_v\big|_{@T_{fc}-T_{ref}}\\&\quad+\dot m_{l,s}^{ca}\ c_p\left(T_{fc}-T_{ref}\right)\end{aligned}\qquad 52)$$

During the purge of the anode water may exist in both the liquid phase and the gas phase (see equations and) present in the flow being dragged by purging hydrogen.

$$\Delta \dot{H}_{H_2O}^{pur} = \dot{m}_{v,s}^{an}\,\Delta h_{H_2O(g)}\Big|_{@T_{fc}-T_{ref}} + \dot{m}_{l,s}^{an}\,c_{p_{H_2O(l)}}\left(T_{fc} - T_{ref}\right) \qquad 53)$$

Finally, the energy balance is defined by calculating the electric power of the cell which is a function of the operating voltage and current. It will be shown in the next section of the paper, the cell voltage is a function of the partial pressures of the gases inside the cell and its operating temperature, variables which have been defined in the dynamic model presented so far.

Electrochemical model

The ideal electric potential of a fuel cell is defined by the Nernst equation.

$$E(T,p) = -\left(\frac{\Delta H}{nF} - \frac{T\Delta S}{nF}\right) + \frac{RT}{nF}\ln\left[\frac{p_{H_2}p_{O_2}^{0.5}}{p_{H_2O}}\right] \qquad 54)$$

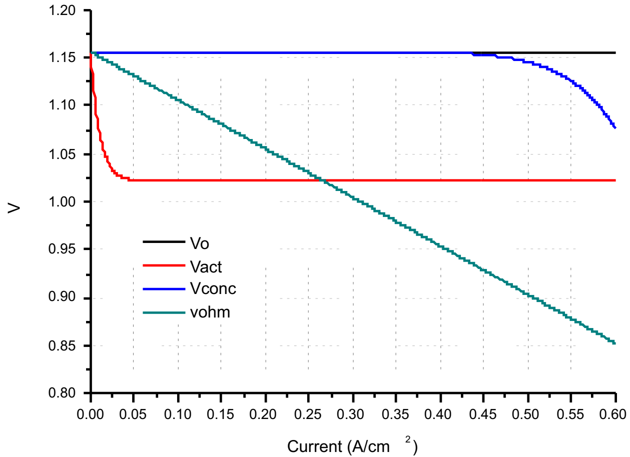
The Nernst equation alone is not enough to describe the electrical potential during the actual operation of the system. The main sources of voltage loss are presented. Observe the three voltage losses on .

1. Activation: The chemical reaction requires a voltage different to the equilibrium potential, otherwise the reaction stops. This phenomena is typically associated with the slower electrode (cathode) and is inversely related with the activation current.

2. Electrical resistance: All the fuel cell stack components has its own electrical resistance which induce a voltage drop that can be modeled with the Ohm law, that means greater currents has greater ohmic losses.

3. Concentration: An uniform concentration was assumed for cathode and anode in the model presented so far, but in the practice there is a different concentration on the surface in contact with the catalyst, therefore there is a concentration gradient, and greater currents induce greater gradients, due to the rate of the reaction (greater at higher currents) therefore higher the load, higher the voltage loss.

***Figure 1**. Voltage losses*



The actual voltage vs. current curve is known as polarization curve, and there are a couple of ways to plot it, proposed the following equation

$$V_{fc} = a_1 + a_2\left(T_{fc} - T_{fc}^{0}\right) + a_3\left(0.5\ln\left(p_{O_2}^{ca}\right) + \ln\left(p_{H_2}^{an}\right)\right) - a_4\left(1 - \exp\left(-\frac{I_{st}}{A_{fc}^{efec}\, a_5}\right)\right) - a_6\frac{I_{st}}{A_{fc}^{efec}} - a_7\left(\frac{I_{st}}{A_{fc}^{efec}}\right)^{1+a_8} \qquad 55)$$

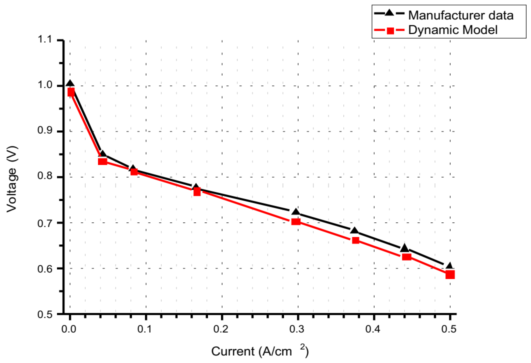
For the stack used as reference the constants are the following

***Table 1.** Electrochemical model parameters*

a_1	1.1564
a_2	2.9300×10^{-3}
a_3	3.0440×10^{-1}
a_4	1.3482×10^{-1}
a_5	1.0475×10^{-2}
a_6	5.0548×10^{-1}
a_7	2.1888×10^{1}
a_8	10

The model response was compared with experimental data supplied by the manufacturer

***Figure 2**. Polarization curve*



3. FUEL CELL STACK CONTROL VALVE

A control valve is required to control the hydrogen flow supplied to the fuel cell stack. The flow in the can be modeled by

$$\dot{V}_{H_2} = K_v N_9 P_1 Y \sqrt{\frac{x}{M T_1 Z}}$$

The valve dynamics can be represented with a first order differential equation.

$$\tau_v \frac{dK_v}{dt} + K_v = \frac{K_{v,max}}{100} m$$

Where represent the valve time constant and m is the control signal. Parameters of the valve are shown in table 2.

***Table 2** . Valve parameters*

Description	Symbol	Magnitude
Specific Heat Relation	γ	1.4
Supply temperature	T_1	$298\ K$
Kinematic viscosity	ν	$80.29 \times 10^{-6} \frac{m^2}{s}$
Molecular mass	M	$2.016 \frac{kg}{kmol}$
Compressibility factor	Z	1.001
Supply Pressure	P_1	$1.5\ bar$
Discharge Pressure	P_2	$1{\cdot}37\ bar$
Relation between pressure drop and the supply pressure $\left(\frac{\Delta P}{P_1}\right)$	x	0.09
Expansion factor	Y	0.9
Numerical constant $\left(\frac{m^3}{h}; bar\right)$	N_9	2.46×10^3
Valve coefficient	K_v	$K_v = 6{,}6 \times 10^{-2}$

4. CONCLUSIONS

The fuel cell power is defined by the polarization curve, although this may be moved depending on the partial pressures of hydrogen, oxygen and water vapor; polarization thus limited power conditions suitable for the operation of the equipment, how much greater difference exists between the couple voltage and current to the values obtained in the polarization voltage-current curve, greater the control challenge.

For the test bench simulation a dynamic model that considers phenomena of mass transfer through the main components of the cell (GDL and membrane) on both sides (cathode and anode) was implemented for this mass balances were used for component that enters and leaves the cell, as well as phase changes if there is a possibility that this occurs (water vapor). Temperature changes were contemplated in the cell using energy balances that include the energy associated with the chemical reactions that take place inside the cell. Finally thanks to the fluid dynamic model mentioned can be known pressures and temperatures within the cell and incorporated by the electrochemical model (a regression model from manufacturer's operating data) was used to calculate the voltage and current in the fuel cell for a given operating condition. Due to the complexity of the model was implemented into a numerical simulation software Matlab-Simulink in which for 150 second simulation time was required about 60 minutes of machine time and for operation in closed loop of about 200 second time simulation machine was in the range 100 to 120 minutes

REFERENCES

Barbir, F. (2005). *PEM fuel cells: theory and practice*. Elsevier. Retrieved from http://scholar.google.com/scholar?hl=en&btnG=Search&q=intitle:PEM+Fuel+Cells+Theory+and+Practice#0

Del Real, A. J., Arce, A., & Bordons, C. (2007). Development and experimental validation of a PEM fuel cell dynamic model.*Journal of Power Sources*, *173*(1), 310–324. doi:10.1016/j.jpowsour.2007.04.066

Dutta, S., & Shimpalee, S. (2001). Numerical prediction of mass-exchange between cathode and anode channels in a PEM fuel cell. *Journal of Heat and Mass Transfer*, *44*(11), 2029–2042. doi:10.1016/S0017-9310(00)00257-X

Grove, W. (1839). On Voltaic Series and the Combiantion of Gases by Platinum. *The London and Edinburgh Philosphical Magazine and Journal of Science*, *XIV*, 127–131.

Müller, E. A., & Stefanopoulou, A. G. (2006). Analysis, modeling, and validation for the thermal dynamics of a polymer electrolyte membrane fuel cell system. *Of Fuel Cell Science and Technology*. Retrieved from http://link.aip.org/link/?JFCSAU/3/99/1

Musio, F., Tacchi, F., Omati, L., Gallo Stampino, P., Dotelli, G., Limonta, S., … Grassini, P. (2011). PEMFC system simulation in MATLAB-Simulink® environment. *International Journal of Hydrogen Energy*, *36*(13), 8045–8052. doi:10.1016/j.ijhydene.2011.01.093

Nam, J. H., & Kaviany, M. (2003). Effective diffusivity and water-saturation distribution in single- and two-layer PEMFC diffusion medium. *International Journal of Heat and Mass Transfer*, *46*(24), 4595–4611. doi:10.1016/S0017-9310(03)00305-3

Zemansky, M. W., & Dittman, R. H. (1979). Calor y Termodinámica. Retrieved from http://orton.catie.ac.cr/cgi-bin/wxis.exe/?IsisScript=UNCPE.xis&method=post&formato=2&cantidad=1&expresion=mfn=001128

Ziogou, C., Voutetakis, S., Papadopoulou, S., & Georgiadis, M. C. (2011). Modeling, simulation and experimental validation of a PEM fuel cell system. *Computers & Chemical Engineering*, *35*(9), 1886–1900. doi:10.1016/j.compchemeng.2011.03.013