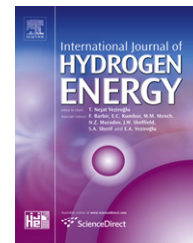




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# Modeling charge transfer in a PEM fuel cell using solar hydrogen

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## ABSTRACT

Hydrogen is an energy carrier that can be used in industry, residences, transportation, and mobile applications. One of the main attractions for hydrogen is the environmental advantage over fossil fuels. However, Polymer Electrolyte Membrane Fuel Cells, (PEMFC), is an integral part of the future hydrogen economy, they are highly efficient and a low-polluting technology. Numerous applications exist; one of the promising applications is the automotive industry. For this report a comprehensive literature survey is conducted. The findings of the literature survey include hydrogen production and fuel cell models that fit into two broad categories, that is, analytical and empirical. This work is a presentation of our original research and development regarding the production and utilization of a solar hydrogen and its use in a PEM single cell. In order to facilitate the understanding of the charge transfer phenomena in the PEM single cell, a modeling tool with visual basic was developed. All the experiences and results were illustrated in this work.

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## 1. Introduction

Hydrogen is an energy carrier that can be used to store, move, and deliver energy produced from other sources. It's the simplest element on Earth and the most abundant element in the universe; but despite its simplicity and abundance, hydrogen doesn't occur naturally as a gas on Earth. It is always combined with other elements. Water, for example, is a combination of hydrogen and oxygen. Hydrogen is also found in many organic compounds, notably the "hydrocarbons" that make up fuels such as gasoline, natural gas, methanol, and propane.

To generate electricity using hydrogen, pure hydrogen must first be extracted from a hydrogen containing compound. Then it can be used in a fuel cell. Hydrogen can be

produced using diverse, domestic resources including fossil fuels, such as coal (preferentially with carbon sequestration), natural gas, and biomass or using nuclear energy and renewable energy sources, such as wind, solar, geothermal, and hydroelectric power to split water. This great potential for diversity of supply is an important reason why hydrogen is such a promising energy carrier.

Hydrogen can be produced at large central plants, semi centrally, or in small distributed units located at or very near the point of use, such as at refueling stations or stationary power sites. The electrolysis uses an electric current to split water into hydrogen and oxygen. The electricity required can be generated using any of a number of resources. However, to minimize greenhouse gas emissions, electricity generation using renewable energy technologies, such as

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Nomenclature		Greek letters	
A	area, cm <sup>2</sup>	$\alpha$	charge transfer coefficient
A <sub>ac</sub>	empirical constant, V	$\Delta H$	enthalpy variation, J mol <sup>-1</sup>
b	empirical coefficient, mA/cm <sup>2</sup>	$\Delta H$	Gibbs free energy, J mol <sup>-1</sup>
E	reversible voltage, V	$\Delta H$	voltage losses, V
F	Faraday constant, C mol <sup>-1</sup>	$\zeta_{\text{air}}$	cathode air stoichiometric ratio
I	current, A	$\theta_{\text{H}_2}$	surface coverage of H <sub>2</sub>
i	current density, A/cm <sup>2</sup>	$\lambda$	wetness
i <sub>0</sub>	exchange current density, A/cm <sup>2</sup>	$\sigma$	resistivity of the membrane efficiency
L	width, $\mu\text{m}$	<i>Superscripts and subscripts</i>	
m	concentration loss coefficient, V	a	anode
n	concentration loss coefficient, cm <sup>2</sup> /mA	ac	anode cathode
n <sub>e</sub>	number of electrons transferred	act	activation
P	pressure, atm	c	cathode
X <sub>w</sub>	water fraction	conc	concentration
R	gas constant, J K <sup>-1</sup> mol <sup>-1</sup>	eh	electro-oxidation of hydrogen
R <sub>diff</sub>	diffusion resistance	m	membrane
r	specific surface resistance, $\Omega\text{ cm}^2$	max	maximum (current)
T	temperature, K	ohm	Ohmic
V	cell voltage, V	th	theoretical
We	electrical work, J	tot	total
k	electro – oxidation rate of H <sub>2</sub>	w	water

wind, solar, geothermal, and hydroelectric power, nuclear energy, or coal and natural gas with carbon sequestration are preferred.

However while fuel cells have advanced other technologies have as well and fuel cells have remained a few years behind. Fortunately fuel cells are now coming into the market.

For these systems designed to consume hydrogen directly, the only products are electricity, water and heat. Fuel cells are an important technology for a potentially wide variety of applications including on site electric power for households and commercial buildings; supplemental or auxiliary power to support car, truck and aircraft systems; power for personal, mass and commercial transportation; and the modular addition by utilities of new power generation closely tailored to meet growth in power consumption. One of these promising areas for fuel cells is the automotive industries which already have buses and cars running on fuel cells. PEM fuel cells are non emission energy conversion devices, and their main byproduct is water. Hydrogen and oxygen (air) are used as the fuel and oxidant respectively.

The desire is to use existing sustainable energy techniques such as wind power to produce the hydrogen using electrolysis. The advantages of fuel cells are many. They have the potential for zero emissions, high efficiency, quiet operation, high energy density, plus high reliability and long life due to few moving parts. Polymer Electrolyte Membrane (PEM) fuel cells are now an efficient and commonly used power source. The goal now is to fully penetrate well established markets [1,2].

In this Work; The first section concerns the fundamental operations regarding the Hydrogen production and the PEM fuel cell area, the second will be dedicated to the test of this modeling tool with results discussions and the final is dedicated to the conclusion.

## 1.1. The hydrogen production technologies

Researchers are developing a wide range of technologies to produce hydrogen economically from a variety of resources in environmentally friendly ways [2–4].

### 1.1.1. Natural gas reforming

Hydrogen can be produced from natural gas using high temperature steam. This process, called steam methane reforming, accounts for about 95% of the hydrogen used today in the U.S. Another method, called partial oxidation, produces hydrogen by burning methane in air. Both steam reforming and partial oxidation produce a “synthesis gas”, which is then reacted with additional steam to produce a higher hydrogen content gas stream.

### 1.1.2. Gasification

Gasification is a process in which coal or biomass is converted into gaseous components by applying heat under pressure and in the presence of air/oxygen and steam. A subsequent series of chemical reactions produces a synthesis gas, which is then reacted with steam to produce a gas stream with an increased hydrogen concentration that then can be separated and purified. With carbon capture and storage, hydrogen can be produced directly from coal with near zero greenhouse gas emissions. Since growing biomass consumes CO<sub>2</sub> from the atmosphere, producing hydrogen through biomass gasification releases near zero net greenhouse gases.

### 1.1.3. Renewable liquid reforming

Biomass can also be processed to make renewable liquid fuels, such as ethanol or bio oil, which are relatively convenient to transport and can be reacted with high temperature steam to produce hydrogen at or near the point of use. Researchers are

also exploring a variation of this technology known as aqueous phase reforming.

#### 1.1.4. Nuclear high temperature electrolysis

Heat from a nuclear reactor can be used to improve the efficiency of water electrolysis to produce hydrogen. By increasing the temperature of the water, less electricity is required to split it into hydrogen and oxygen, which reduces the total energy required.

#### 1.1.5. High temperature thermo chemical water splitting

Another water splitting method uses high temperatures generated by solar concentrators (mirrors that focus and intensify sunlight) or nuclear reactors to drive a series of chemical reactions to split water into hydrogen and oxygen through a series of chemical reactions. All of the intermediate process chemicals are recycled within the process.

#### 1.1.6. Biological

Microbes, such as green algae and cyanobacteria, produce hydrogen by splitting water in the presence of sunlight as a byproduct of their natural metabolic processes. Other microbes can extract hydrogen directly from biomass.

#### 1.1.7. Photo electrochemical

Hydrogen can be produced directly from water using sunlight and a special class of semiconductor materials. These highly specialized semiconductors absorb sunlight and use the light energy to completely separate water molecules into hydrogen and oxygen.

#### 1.1.8. Renewable electrolysis

Electrolysis uses an electric current to split water into hydrogen and oxygen. The electricity required can be generated using any of a number of resources. However, to minimize greenhouse gas emissions, electricity generation using renewable energy technologies, such as wind, solar, geothermal, and hydroelectric power, nuclear energy, or coal and natural gas with carbon sequestration are preferred.

### 1.2. Aim of the work

This research work is divided into two parts; the first part is the hydrogen production from solar energy, a solar photovoltaic (PV) panel with voltage regulator was used as a source of renewable electricity which feed an electrolytic device; then we have used the produced hydrogen into a PEM single cell to visualize the no load and load charge phenomena as well as voltage losses regions.

The second part of this work is to develop and test a charge transfer modeling tool with visual basic Excel that can be used to predict the PEMFCs performances while introducing the operating and technical data of the PEM fuel cell.

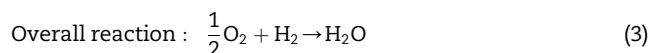
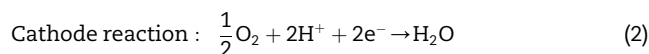
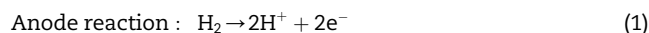
## 2. The Polymer Electrolyte Membrane Fuel Cells

A Polymer Electrolyte Membrane Fuel Cell (PEMFC) is a power generator from electrochemical reaction using hydrogen and

oxygen as fuel and oxidant respectively, the most important component is the membrane which is a thin ion conducting solid electrolyte and has its advantages over liquid electrolytes in that it has a high power density and reduced corrosion. The low temperature of these cells ensures a quick start up time and its wide application range includes the transport industry. One of the drawbacks to PEMFCs in the past was the fact that they required expensive platinum metal catalysts. Developments in recent years mean that only minute amounts of platinum are now used and the cost of platinum is now a small part of the total price of a PEM fuel cell [5]. The large number of applications for PEMFCs is mainly due to the enormous power range and versatility of the fuel cell. The power range is from a few watts to several hundred kilowatts, with temperature only varying from 25 °C to 100 °C. PEMFCs are particularly suited to the transport industry because they can start quickly due to a low operating temperature. Also there are no corrosive fluid hazards and the cell can work in any orientation. These factors set the PEMFCs apart from other fuel cells. This and the potential for PEMFCs to produce zero emissions create a great prospect for clean energy in the transport industry.

### 2.1. Fundamental operations

Hydrogen and oxygen are used to produce electricity, heat and water. The physics of the PEM fuel cell can be considered as the opposite of electrolysis. In electrolysis an electric current is passed through water to produce hydrogen and oxygen. In the fuel cell, hydrogen and oxygen gases are passed either side of a polymer electrolyte membrane which produces an electric current, heat and water. The electrochemical reactions for the PEM fuel cell are shown in Eqs. (1)–(3), [6].



A PEMFC primarily consists of three components: a negatively charged electrode (cathode), a positively charged electrode (anode), and a polymer electrolyte membrane. The simple chemistry of the fuel cell involves hydrogen being oxidized on the anode and oxygen reduced on the cathode. Protons ( $\text{H}^+$ ) are transported from the anode to the cathode through the polymer electrolyte membrane and electrons are carried to the cathode through an external circuit. On the cathode, oxygen reacts with protons and electrons forming water and producing heat. Both the anode and the cathode contain a catalyst, usually platinum, to speed up the electrochemical processes. The basic PEM fuel cell operation is given in Fig. 1 modified from Ref. [7].

### 2.2. Fuel cell voltage

The most important aspect in the cell modeling is the cell voltage, this is because the cell potential changes with different loads and operating conditions so it is essential that the cell voltage is known, the individual cell voltage and then

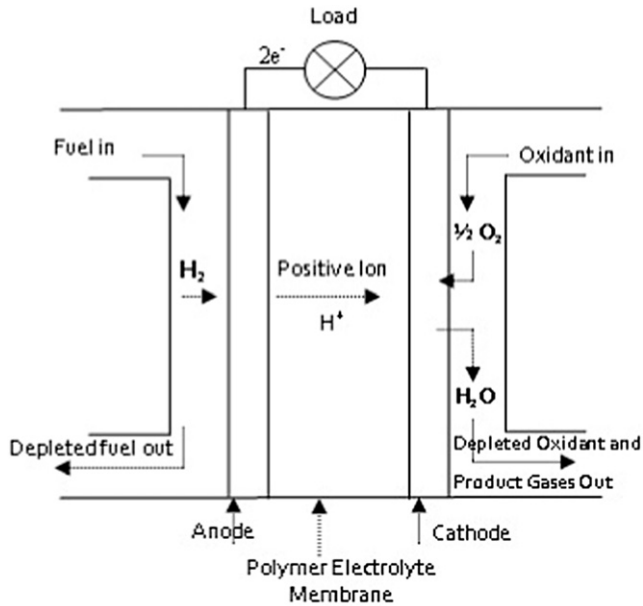


Fig. 1 – Basic PEM fuel cell operations.

the stack voltage and the major voltage losses. The losses include the activation, Ohmic, concentration and internal current losses. The internal current losses are modeled by an internal current integrated into the other loss mechanisms [8].

### 2.2.1. Reversible cell voltage

Each element of the PEM fuel cell realizes the direct conversion of the Hydrogen into electricity current, (electrical energy), in the theoretical case of a reversible reaction, the electrical work done is the product of the load by the voltage as presented in Eq. (4), which is equal to the enthalpy variation called also Gibbs free energy. The reversible voltage will be expressed as in Eq. (5), [6].

$$We = n_e \cdot F \cdot E = -\Delta G \quad (4)$$

$$E = \frac{-\Delta G}{2F} \quad (5)$$

The pressures of the products and reactants play a part in effecting the reversible voltage of the fuel cell. Basically increasing the pressure of the reactants increases the amount of reactants on the surface of the electroplates and so increases the frequency of chemical activity. The change in Gibbs free energy varies with different pressures and temperatures of the fuel cell. This in turn changes the reversible voltage of each cell. I will describe how  $(-\Delta G)$  varies from its standard value which is stated at Standard Temperature and Pressure. The effect of pressure on  $(-\Delta G)$  is displayed in literature with slight variations. Sometimes they approximate one bar to equal one atm, or vice versa. The difference is that 1 atm is equal to 1.01325 bar. Although this is not much, it is worthwhile minimizing errors when possible. In some papers such as Naso et al. [9] researchers do not make any assumptions but state their standard value of  $(-\Delta G^0)$  is stated at 1 bar, not 1atm. The deviation of pressure from  $(-\Delta G^0)$  assumes that "E" is at the standard temperature.

In this condition (E) is equal to  $E_{Nernst}$ . The effect of pressure on  $E_{Nernst}$  as shown in literature is presented in Eq. (6), [10]

$$E = E_T^\circ + \frac{RT}{2F} \ln \left( \frac{P_{H_2} \cdot \sqrt{P_{O_2}}}{P_{H_2O}} \right) \cdot \sqrt{\frac{1}{P_0}} \quad (6)$$

while:

$$E_T^\circ = 1.229 - 0.85 \cdot 10^{-3} \cdot (T - 298.15) \quad (7)$$

As a simplification, the partial pressures of  $H_2$ ,  $O_2$  and  $H_2O$  can be stated in atmospheres which reduces the term  $(1/P_0)^{1/2}$  to 1, [8].

### 2.2.2. The activation losses

A certain proportion of energy is needed to start the chemical reaction. This phenomenon produces a nonlinear voltage drop called activation polarization. These losses occur on both anode and cathode catalysts. However, the oxygen reduction reaction kinetics is much slower than hydrogen oxidation reaction, thus the reduction reaction produces a much larger magnitude of activation polarization loss. The oxidation reaction on the anode is much faster and practically constant throughout the current range. If only a single reaction is considered then the voltage loss due to activation polarization can be described in Eq. (8) by the Tafel relation mentioned by Husar et al. in Ref. [11]:

$$\Delta V_{act} = \frac{RT}{\alpha n F} \ln \left( \frac{i}{i_0} \right) - 2.3 \frac{RT}{\alpha n F} \log \left( \frac{i}{i_0} \right) \quad (8)$$

The parameter ( $\alpha$ ) expresses how the change in the electrical potential across the reaction interface changes the reaction rate. It depends on the type of reaction and the electrode material. Its value is theoretically between 0 and 1 depending on the catalyst material [5]. It physically represents the fraction of additional energy that goes toward the cathodic reduction reaction at an electrode. The charge transfer coefficient can also be thought of as a symmetry coefficient of the electrode reaction and it is typically considered to be around 0.5 with hydrogen and oxygen reacting on a platinum catalyst [12].

Another model of activation losses considers only the reaction of hydrogen with oxygen, while all other species are considered inactive. The diffusion resistance ( $R_{diff}$ ) is based on linear regressions evaluated experimentally by Korsgaard et al. in Ref. [13] and mentioned in Ref. [14]. The anode and cathode over potentials are given by the following Eqs. (9) and (10), respectively:

$$\Delta V_a = \frac{RT}{\alpha_a F} \sinh^{-1} \left( \frac{i}{2k_{eh} \theta_{H_2}} \right) \quad (9)$$

and

$$\Delta V_c = \frac{RT}{4\alpha_c F} \ln \left( \frac{i_0 + i}{i_0} \right) + R_{diff} \left( \frac{i}{\zeta_{air} - 1} \right) \quad (10)$$

### 2.2.3. The Ohmic losses

The Ohmic loss is due to the resistance of ions through the polymer electrolyte membrane and the resistance of imperfect electrodes. For a complete electrical circuit the membrane

is required to conduct protons. An ideal membrane would freely conduct  $H^+$  ions. Eq. (11) shows the expression of the Ohmic losses expressed by Ohm's law [11]:

$$\Delta V_{ohm} = r_m \cdot i \quad (11)$$

While the internal cell resistance ( $r_m$ ) is given by Eq. (12) from Ref. [15]

$$r_m = \frac{L_m}{A_m \cdot \sigma_m} \quad (12)$$

The electric and contact resistance can be considered constant with respect to current and temperature. Thus any change in the resistance is only dependent on membrane water concentration and membrane temperature [16], so it is the indicator for membrane ionic resistance. The resistivity ( $\sigma_m$ ), given by Eq. (13), depends on the temperature and the water content of the membrane in Ref. [17].

$$\sigma_m = (0.005139\lambda_m - 0.00326)\exp\left(1267\left(\frac{1}{303} - \frac{1}{T}\right)\right) \quad (13)$$

The water content of the membrane ( $\lambda_m$ ), is dependent on the dimensionless water activity in the membrane ( $a$ ) given by Eq. (14) according to experimental data [17].

The activity is assumed uniform over the membrane and the physical meaning of relative humidity is this ratio, which is defined as the gas partial pressure of water ( $P_w$ ) at equilibrium with the membrane divided by the saturation pressure of water vapor ( $P_{sat}$ ) at the operating temperature [18].

$$a = \frac{P_w}{P_{sat}} = \frac{X_w P}{P_{sat}} \quad (14)$$

The saturation pressure of water can be computed from Eq. (15), ( $T$ ) is in [ $^{\circ}C$ ].

$$\log_{10} P_{sat} = -2.1794 + 0.02953T - 9.1837 \times 10^{-5} T^2 + 1.4454 \times 10^{-7} T^3 \quad (15)$$

In our case and for simplification reasons, the membrane resistance ( $r_m$ ) is given and it's considered to be constant, so we don't take in consideration the variation of the membrane wetness.

#### 2.2.4. The concentration losses

A concentration loss relates to the reduction of the reactant's concentration in the gas channels. The fuel and oxidant are used at the surface of the electrodes. The incoming gas must then take the place of the used reactant. The concentration of the fuel and oxidant is reduced at the various points in the fuel cell gas channels and is less than the concentration at the inlet value of the stack. This loss becomes significant at higher currents when the fuel and oxidant are used at higher rates and the concentration in the gas channel is at a minimum.

To approximate this phenomenon, an empirical equation better describes the concentration losses given in Eq. (16) shows the expression of the concentration loss [6]:

$$\Delta V_{conc} = m \cdot \exp^{(n \cdot i)} \quad (16)$$

where ( $m$ ) and ( $n$ ) are empirical coefficients with typical values close to  $3.10^{-5}$  V and  $8 \text{ cm}^2/\text{A}$ , respectively.

#### 2.2.5. The internal current loss

The internal current is due to the wasted fuel and oxidant that passes through the membrane and does not produce any useful work. It is also to a lesser extent, due to electron conduction in the membrane. This loss affects the fuel cell's performance most at open circuit and is insignificant at higher currents. It is mathematically represented in each of the other losses and often absent from PEM fuel cell models. An internal current loss means that excess chemical activity in the fuel cell is always occurring. Even at open circuit voltage, losses are evident when ideally there are none. Since the activation loss is the most pronounced loss at low currents, the internal current affects the activation loss the most significantly.

#### 2.2.6. The real cell voltage

The combined effects of all irreversibility's (losses) could be summarized in the Eq. (17) which presents the real cell voltage according to each current density, pressure and temperature  $V(P, T, i)$  [19]. In the widely published [20] basic fuel cell model used in this work, the fuel cell voltage  $V(P, T, i)$  is equal to the thermodynamic reversible potential ( $E$ ) of a PEM fuel cell minus the three major losses: activation ( $\Delta V_{act}$ ), mass transport ( $\Delta V_{conc}$ ) and ohmic ( $\Delta V_{ohm}$ ) [11]:

$$V(P, T, i) = E - \Delta V_{act} - \Delta V_{ohm} - \Delta V_{conc} \quad (17)$$

### 2.3. The polarization curve

A typical polarization curve from Wood et al. [21] is presented in Fig. 2, it is the characteristic graph of voltage versus current for a set of operating conditions. It summarizes the three parts of the voltage losses, activation, Ohmic and concentration

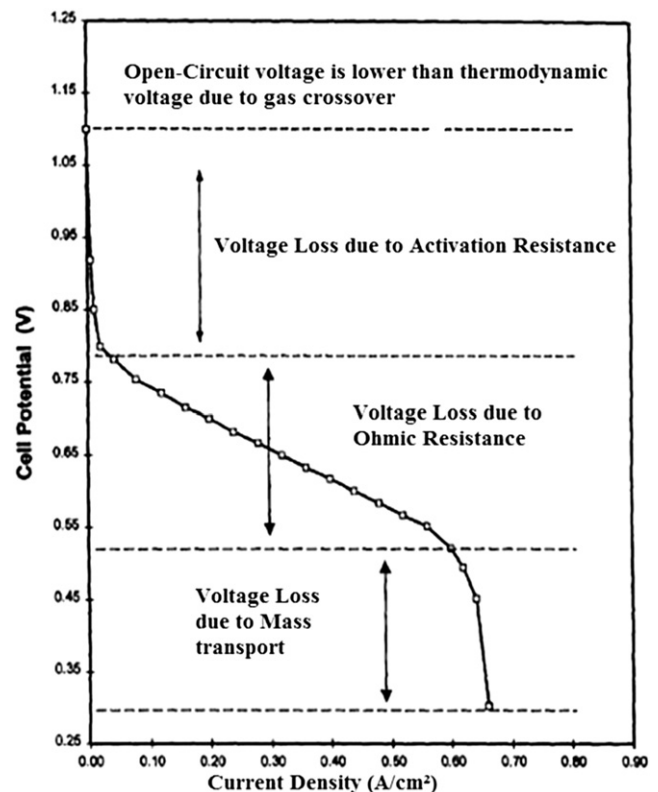


Fig. 2 – Typical polarization curve.

[22]. This curve is the most common output of models and is seen as the most important performance criteria. Modeling this graph is the primary goal of the proposed modeling tool.

#### 2.4. The efficiency of the PEM fuel cell

Electrical and heat energy are produced by the overall reaction in Eq. (3). Theoretically, the Gibbs free energy of the reaction is available as electrical energy and the rest of the reaction enthalpy is released as heat. In practice, a part of the Gibbs energy is also converted into heat via the loss mechanisms [23]. The thermal efficiency of an energy conversion device is defined as the amount of useful energy produced relative to the change in stored chemical energy (commonly referred to as thermal energy) that is released when a fuel is reacted with an oxidant [7]. The amount of useful electrical energy in the system is the Gibbs free energy of the reaction. Some energy in the system is not available to do useful work and is always output as heat [8].

##### 2.4.1. Theoretical efficiency (maximum)

A PEM fuel cell working under constant pressure and temperature and with reversible conditions has a maximum efficiency which can be defined by the relationship between the electrical energy produced and the thermal energy released during the chemical reaction. Eq. (18) presents the expression of the Maximum efficiency:

$$\eta_{th} = \frac{W_e}{-\Delta H} = \frac{\Delta G}{\Delta H} \quad (18)$$

##### 2.4.2. Load efficiency (voltage)

The efficiency of a fuel cell delivering a load with a current density ( $i$ ) is defined as the ratio of the actual voltage of the fuel cell and the theoretical voltage, reversible, ( $E$ ).

Eq. (19) presents the expression of the load efficiency:

$$\eta_v = \frac{V(P, T, i)}{E} \quad (19)$$

##### 2.4.3. Faradic efficiency

The faradic efficiency is defined as the ratio of the delivered current “ $I$ ” and the maximum current which corresponds to the global reaction “ $I_{max}$ ”, we can have also another definition of the faradic efficiency which is the ratio of electrons really exchanged during the reaction those theoretical. Eq. (20) shows the expression of the faradic efficiency:

$$\eta_F = \frac{I}{I_{max}} = \frac{n_{e,ex}}{n_e} \quad (20)$$

##### 2.4.4. The total efficiency

If we consider only what happens inside the fuel cell, we can have the following configuration of the total efficiency of each fuel cell as well as presented in Eq. (21)

$$\eta_{tot} = \eta_{th} \cdot \eta_v \cdot \eta_F \quad (21)$$

### 3. Material description

As shown in Fig. 3, the hydrogen generating device is composed from the left to the right of the solar PV panel,

voltage regulator, electrolyzer and the device of hydrogen and oxygen measurement and it is similar to that presented in Ref. [24] but under different conditions. The PV panel deliver a 26 Volt (V) and 7.85 Ampere (A) in normal conditions, to vary the voltage, we have used a power transformer. An electrolyzer is designed for this experiments, it's a recipient of 1.5 l with four electrodes; two anodes connected in series, and two cathodes with the same type of connection, these electrodes are from graphite with 0.5 mm of diameter. Hydrogen and oxygen produced by the electrolysis are connected by pipes into a measurement device, it's a set of two bells overturned into two graduated cylinder in which we can read the hydrogen ( $H_2$ ) and oxygen ( $O_2$ ) volume by milliliter (ml).

#### 3.1. The hydrogen production experiment

Initially, we want to know the hydrogen production by this set device under different voltages to obtain a 10 ml of  $H_2$  as an element of comparison. We put the water in the electrolyzer and we turn on the switch. Under normal conditions the PV panel delivers up to 26 V in which a power transformer has been used to vary the voltage, Fig. 4 shows the time to produce 10 ml of hydrogen under different voltages, a generalization of these results give us an idea about the hydrogen flow in ml/hour presented in Fig. 5.

We observe that the time to produce the same hydrogen volume decreases each time we increase the voltage with an intensity of the current of 4.5 A, the experiment's results shows that we can have an average of 70 ml/h with 24 V.

#### 3.2. The PEM fuel cell experiment

To complete the second part of this research work, we use a PEM fuel cell kit and we make the connections as given in Fig. 6. Once the PEM fuel cell is connected with hydrogen and oxygen we can read the voltage and the current, so we can deduce the electrical power. With only 10 ml of Hydrogen the PEM fuel cell and without any resistor load shows a voltage of 1.41 V, and because there is no load the current will be zero, it's what we call the Activation region. This will define a part of the Polarization Curve. In the next experiments we will register the voltage, current and the time.

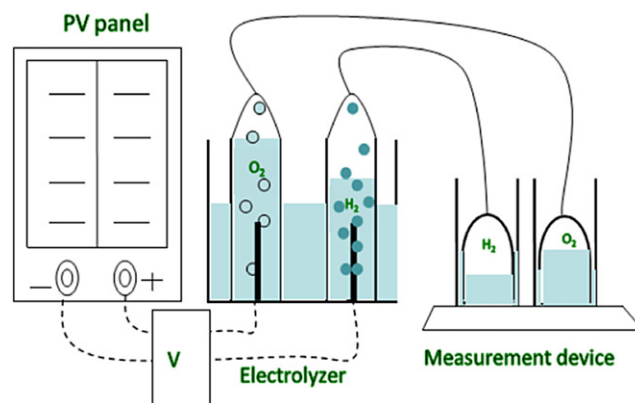


Fig. 3 – The experimental device for solar hydrogen production.

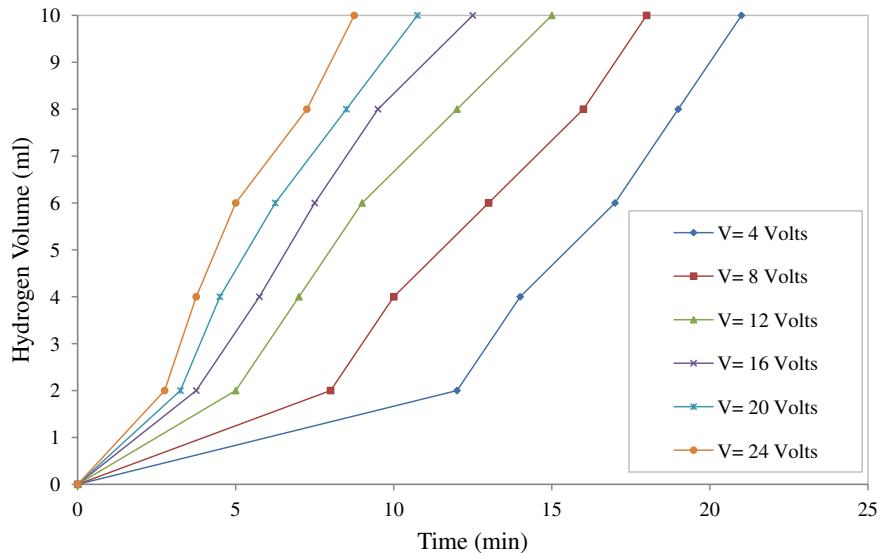


Fig. 4 – The hydrogen volume produced under different voltages.

Now we apply a single 100 Ohm resistor across the fuel cell's terminals. We observe that the voltage decreases. The fuel cell is transitioning from the Activation to the Ohmic region. In order to discover the specification of this Ohmic region we wait about one minute then we apply a second 100 Ohm resistor in parallel with the first one. The parallel resistance is 50 Ohms; we observe another decrease in voltage and an increase in current. After two minutes, we note that the voltage and current stay at the same level.

This is the advantage of the Ohmic region since the power to the load remains steady. We add a third 100 Ohm resistor in parallel with the other two in order to hasten the transition from the Ohmic to the Mass Transport region. This may take a few seconds to a few minutes to accomplish, it depends on the fuel cells hydrogen supply, and in our case we take a 10 ml of hydrogen. The data results are shown in Table 1.

Figs. 7 and 8 illustrate the voltage, current and the power of the fuel during the load.

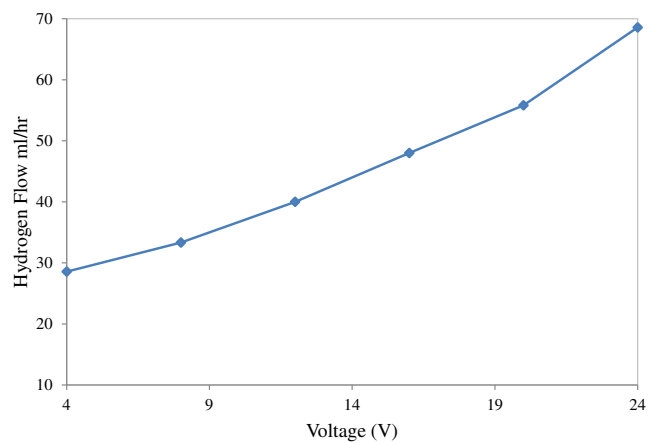


Fig. 5 – The hydrogen flow produced under different voltages.

This experiment demonstrates how the voltage and current start at a high value (Activation Region) and then quickly settle to a steady and consistent value (Ohmic Region). Only at the very end when the hydrogen began to run out, it finally fade to zero voltage, current and power (the Mass Transport Region).

#### 4. The charge transfer modeling tool

There are several types and levels of fuel cells modeling [8]:

- The static modeling which characterize the fuel cell performances in the steady state.
- The dynamic modeling which characterize the fuel cell performances in the transient regime.

In the tool that we have developed, only the static modeling is presented, because the dynamic one is still in the research and development level. All the previous equations were put in the database of this tool.

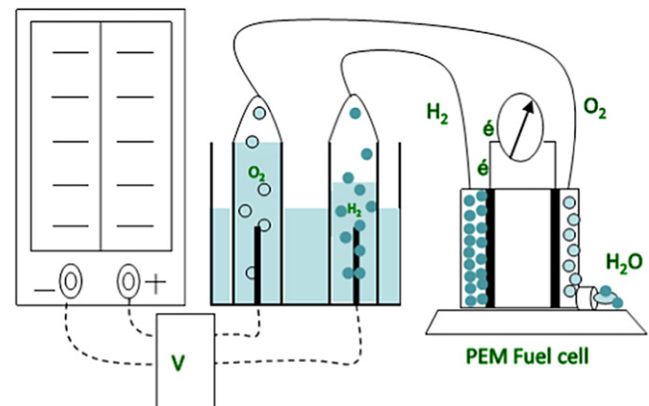


Fig. 6 – The hydrogen for fuel cell' device.

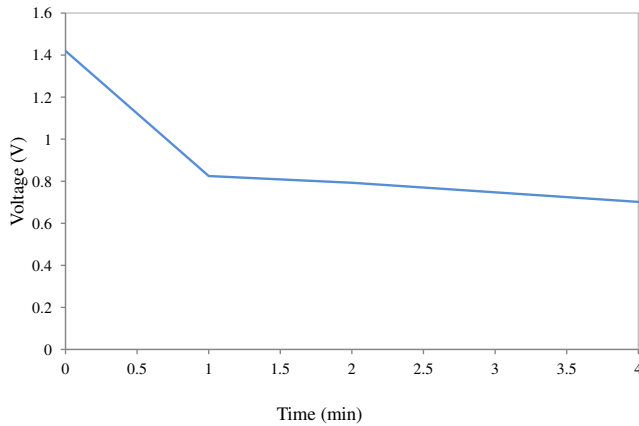


Fig. 7 – The voltage evolution in the single cell.

#### 4.1. Model review

Two main modeling approaches are presented in the literature. The first approach includes structural models that aim to simulate the heat transfer, mass transport and electrochemical phenomena produced in cells combustible. The second approach includes models based on empirical or semi empirical equations, applied to predict the effect of various operating parameters on the ( $I - V$ ) characteristics of the fuel cell. In our case we are interested by modeling the charge transfer in a PEM fuel cell expressed by the polarization curve, which is a graph of the voltage versus the load current for a given set of operating conditions [2].

Thirumalai et al. [25] completed a good sensitivity analysis on an earlier model [26] to find the most important operating conditions of the PEM fuel cell stack. They found that the following factors were particularly important: Gas mass flows (pressure and stoichiometry of the inlet gases), Operating temperature of the fuel cell stack, and Relative humidity of the reactant gases, primarily of the anode gas.

PEM fuel cell models can also be divided into two broad categories, analytical and empirical. Analytical models are based on theory while empirical models are based on experimentation. Unfortunately, PEM fuel cell stacks are complex

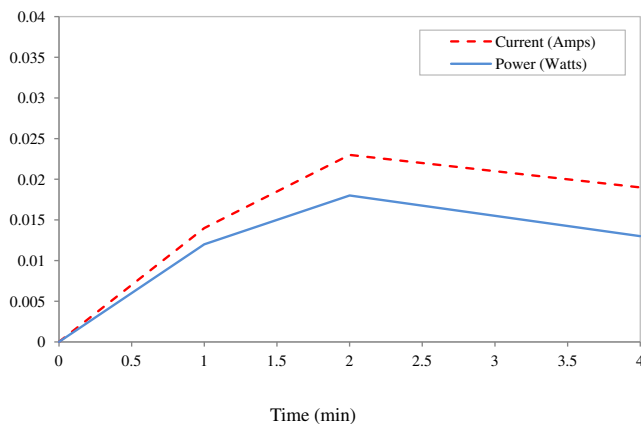


Fig. 8 – The current and power evolutions in the single cell.

Table 1 – The results for the fuel cell power delivery.

Load	Volts	Amps	Watts
No load	1.420	0	0
Single 100 Ohm	0.825	0.014	0.012
2 × 100 Ohm (in Parallel)	0.793	0.023	0.018
3 × 100 Ohm (in Parallel)	0.702	0.019	0.013

systems and are difficult to completely model analytically. For this reason, in general the analytical fuel cell models have a theoretical basis while still holding some empirical features. The analytical models can be classified as either simple or complex. Simple models examine the operating fuel cell stack voltage in respect to the maximum theoretical voltage and the major voltage losses.

Berger [27], provided the theoretical background and methodology for calculating the major voltage losses. Other groups aiming to describe the losses in a simple and accurate model developed these further. Amphlett et al. have produced the most comprehensive of these models based on the Ballard IV PEM fuel cell stack [28,29] and have attempted to develop this further into a general PEM fuel cell model [30]. Other models include that of Larminie and Dicks [5] which include the internal current and a simplified dynamic performance model of the fuel cell stack. Complex models use more detailed techniques and require detailed information on the materials and make up of the fuel cell stack.

Because of the complexity and interdependence of variables on the performance of the fuel cell stack an empirical equation can be used to predict the polarization curve. The advantage of this approach is that it is relatively simple to accurately predict a particular polarization curve. The disadvantage of this approach is that the polarization curve must be re-calculated for any change in operating conditions, such as humidity or temperature.

A landmark empirical equation was presented in 1995 by Kim et al. [31] that gave an accurate prediction of the polarization curve without complete consideration for the electrochemistry. The empirical equation, Eq. (17), has been used to model the polarization curve for various types of PEM fuel cells [32,33].

Another type of empirical model was used by Amphlett et al. [29]. When the analytical constants were not fully understood they went about finding an empirical equation for each parameter and for the entire irreversible losses. This technique issued as a supplement to analytical models and will be used in the proposed model.

In our modeling tool we have envisaged to use the semi empirical model of Amphlett because it's the most comprehensive one and which include more details on the voltage losses.

#### 4.2. The modeling tool test

We have considered studying the performances of a Ballard Mark V fuel cell with this tool [34]; the data input are shown in Table 2.

Many simplifications were taken in consideration as well as the water management and the temperature variations. However, "i" should take the values where  $i \in [0, 1000]$ .



**Table 2 – The data input of the PEM fuel cell.**

Parameters	Values
T	80 [°C]
$A_{ac}$	$2.89 \cdot 10^{-2}$ [V]
b	0.04 [mA/cm <sup>2</sup> ]
r	$2.114 \cdot 10^{-4}$ [kΩ/cm <sup>2</sup> ]
m	$1.4 \cdot 10^{-5}$ [V]
n	$8 \cdot 10^{-3}$ [cm <sup>2</sup> /mA]
$P_{H_2O}, P_{H_2}$	1 bar
$P_{O_2}$	0.21 bar

#### 4.3. The results and discussions

Two kinds of results can be provided by this tool; numerical results (calculations) and graphical representations.

##### 4.3.1. The calculations

A values of  $E = 179$  V and  $E_{80}^\circ = 1.182$  V were calculated by the tool, so we can observe that the value of  $E_{80}^\circ$  is smaller than  $E$  and this is due to the oxygen pressure (0, 21 bar) which has an impact on the logarithm part in the Nernst equation.

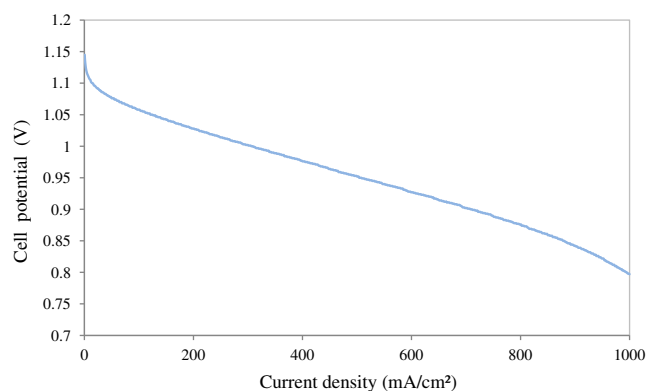
##### 4.3.2. The graphical results

The proposed modeling tool can also provide graphical results as well as the polarization curve shown in Fig. 9.

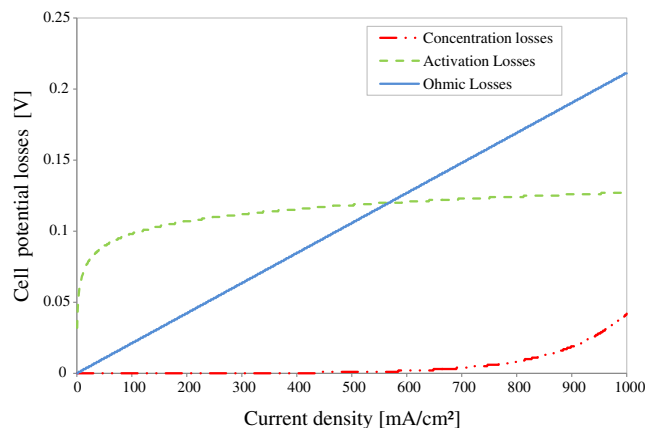
We can observe in Fig. 10 that the activation losses can be negligible against the others and the major losses are in the Ohmic region due to the joule effect in the membrane, then activation losses are in the second rank. Furthermore, the shape of the activation losses curve is logarithmic unlike the concentration one which is exponential, and main difference is that the activation losses can be summarized only in the beginning of the operation before the establishment while the concentration losses starts shortly before the end and continue increasing. The Ohmic losses increase during all the operation.

We try to vary the hydrogen and oxygen pressures, Fig. 11 presents the polarization curve under different pressures given by the graphical tool.

We can observe that there is a relationship between the increase of the pressure and the cell potential, so each time we increase pressure it will be better for the cell performances.



**Fig. 9 – The polarization curve given by the graphical tool.**



**Fig. 10 – The different voltage losses.**

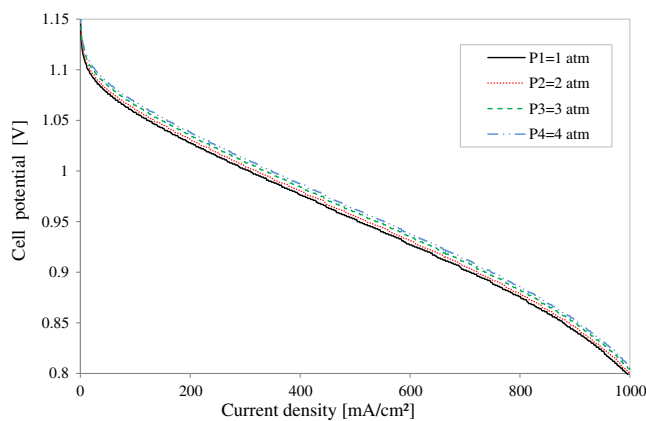
Latha et al. [10] found experimentally that the performance of the fuel cell improves with the increase of pressure of the inlet gases. Fig. 11 shows polarization curve shifts positively as the pressure increases from 1 to 4 atm.

We can also try to vary the operating temperature of the PEM single cell, Fig. 12 gives the polarization curve under different temperature given by the graphical tool.

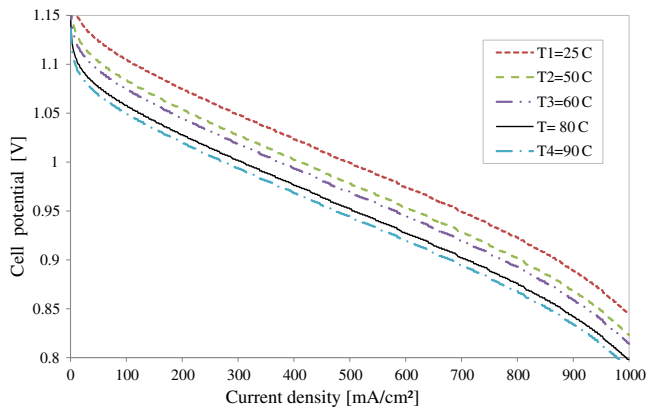
We can observe that there is a remarkable difference between these different curves.

Indeed, the cell voltage increase each time the temperature decrease, so with high operating temperature we need to maintain the cell in better conditions by using a chiller device.

Generally, In the case of Nafion membrane, water is easily condensed at lower temperature, water flooding may deteriorate gas diffusivity in the gas diffusion layer. The gas diffusivity of the fuel cell is improved with increased fuel cell temperature. Therefore, fuel cell performance is improved at higher temperature. However, membrane conductivity decreases at higher temperature because of the reduction in the relative humidity of reactant gases and water content in the membrane. As the temperature increases, there will be a greater rate of water evaporation. When the temperature reaches a critical temperature where the amount of evaporated water exceeds the amount of produced water, the



**Fig. 11 – The polarization curve under different pressure (T = 80 °C).**



**Fig. 12 – The polarization curve under different temperature ( $P_{H_2} = 1 \text{ atm}$ ,  $P_{O_2} = 0.21 \text{ atm}$ ).**

membrane will start to dry out. The resistance will increase as the membrane dried out and thereby, decreases both the current and water production [10].

## 5. Conclusion

The hydrogen can be produced by electrolysis, the current to supply the electrolyzer can be derived from solar energy source, and a variation on the voltage influences the hydrogen flow. A hydrogen PEM fuel cell is one of the applications of hydrogen; we can produce energy for vehicles by using these PEM fuel cells provided that hydrogen supply is not interrupted. The results in the second part of this research have shown that we can have three polarization regions in the PEM fuel cell functioning.

One of the goals of this research was to increase the knowledge of PEM fuel cells, because the field of fuel cell research and application is at an early stage of development. This research work provides an accurate and detailed summary of PEM fuel cell static modeling. It will be useful for future researchers in that they will not only be able to grasp the key issues and operation of the PEMFC but will also be able to continue to add to the body of knowledge. It is anticipated that development in fuel cell research and application will continue for years and this first step in modeling helps to lay the foundation for fuel cells in future works.

The proposed modeling tool was developed to be used for PEM Fuel Cells charge transfer modeling, it can provide several calculations according to data input such as the Nernst Potential Cell and the various voltage Losses and can also provide graphical representation of the results. The user can make many tests on this tool including the pressure and temperature variation and the fuel cell characteristics.

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