# Analysis of the Parametric Effect on the Performance of a Polymer Electrolyte Membrane Electrolyzer

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*Abstract*—This paper presents the study on the impact of the operating parameters of a Polymer Electrolyte Membrane (PEM) electrolyzer on its performance using the numerical simulation method. The results showed that the increment of some parameters, including the operating temperature, the exchange current density, and the charge transfer coefficient could lead to the improvement of the PEM electrolyzer performance. But the increase of operating pressure reduces the electrolyzer performance.

*Index Terms*—water electrolysis, performance, numerical simulation, polymer electrolyte, electrolyzer

# I. INTRODUCTION

The demand for hydrogen gas is increasing due to its efficiency and capability in energy storage that can be used in energy conversion system such as fuel cells [1]. However, since hydrogen does not exist in its natural form, it has to be produced by either steam reforming form hydrocarbons, or thermolysis of water, or water electrolysis. The latter has the least pollutant emission because electrolysis of water generates only oxygen and hydrogen.

Nowadays, One the most attractive and efficient technology to produce hydrogen by water electrolysis is the Polymer Electrolyte Membrane (PEM) electrolyzer.

A PEM electrolyzer cell mainly consists of a solid polymer membrane (electrolyte), two electro-catalysts (anode and cathode), two gas diffusion layer, and two bipolar plates.

Basically, the electrolysis of water by the PEM electrolyzer is the electrochemical process that split water into hydrogen gas and oxygen gas by using the electric energy. The reactions in this process are defined as follow:

Anode (reduction):  $H_2 O \rightarrow 2H^+ + \frac{1}{2}O_2 + 2e^-$  (1)

Cathode (oxidation):  $2H + +2e \rightarrow H_2$  (2)

Total reaction:  $H_2 O \rightarrow H_2 + \frac{1}{2} O_2$  (3)



Figure 1. PEM water electrolysis principle

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The water supplied to the anode is reduced (Eq. 1) by the effect of electric energy to produce oxygen, hydrogen protons and electrons (Fig. 1). The oxygen is discharged at the anode side while protons traverse the membrane to the cathode and the electrons pass through the electrical conductor to the cathode side in order to merge with the protons to generate hydrogen which is discharged at the cathode side (Eq. 2).

The PEM electrolyzer has the ability to produce high purity hydrogen, the fast response in term of charging and discharging, the high dynamic operation and the compact system design [2]-[5]. But challenging majors with PEM electrolyzer development are durability, cost and performance [6].

This paper focuses on the study of PEM electrolyzer performance where we discuss the effect of different operating parameters on the performance. The study is conducted by using the numerical simulation.

# II. MODELING AND NUMERICAL SIMULATION

A 2D geometry modelling and numerical simulation were performed in COMSOL Multiphysics 5.1. In COMSOL Multiphysics, the electrochemical process of PEM electrolyzer cell is modeled with the Secondary Current Distribution interface that is found under the electrochemistry branch. This interface defines the transport of charged ions in an electrolyte and currentconduction electrodes using Ohm's law in combination with charge balance. The activation overpotentials are accounted and the relation between charge transfer and overpotential is described by Butler-Volmer equation.

The domains of charge transport are defined as electrodes for the Gas diffusion layers, the electrodeelectrolyte coupling (Porous electrodes) interface for the electrocatalysts, and the electrolyte for the membrane. The electric transport charges on the bipolar plates, which contain the channels, are not considered.



Figure 2. Domains and boundary conditions

For boundary conditions, the cell voltage was applied to the interface of anode channel and anode gas diffusion layer while the interface of cathode flow channel and cathode gas diffusion layer was grounded (see Fig. 2). The stationary study was chosen and the parametric analysis was solved by the Direct PARDISO method. The below Table I contains the design parameter used to simulation the model.

 TABLE I.
 PARAMETERS OF NUMERICAL SIMULATION [7]

Parameters	Values
Membrane thickness	0.18 mm
Cathode catalyst thickness	0.01 mm
Anode catalyst thickness	0.005 mm
Anode GDL thickness	0.35 mm
Cathode GDL thickness	0.19 mm
Cathode catalyst electric conductivity (Pt/C)	2x10 <sup>8</sup> S/m
Anode catalyst electric conductivity (Ir)	$2 \mathrm{x} 10^7  \mathrm{S/m}$
Anode GDL electric conductivity(Titanium)	2x10 <sup>6</sup> S/m
Cathode GDL electric conductivity (Carbon	6x10 <sup>4</sup> S/m
Paper)	
Operating temperature	313 K
Operating pressure	1 atm
Cathodic exchange current density	$0.027 \text{ A/cm}^2$
Anode exchange current density	5x10-6 A/cm <sup>2</sup>
Membrane conductivity	10 S/m
Anode GDL Porosity	0.76
Cathode GDL Porosity	0.78
Catalysts Porosity	0.3
Catalysts Permeability	$1.18 \times 10^{-11} \text{ m}^2$

# III. RESULTS AND DISCUSSIONS

#### A. The Effect of Operating Temperature

The variation of the operating temperature can affect the performance of a PEM electrolyzer cell. As shown in Fig. 3, the parametric study, with the operating temperature varying from 313 K to 403 K, indicates that when the operating temperature increases, the voltage decreases which leads to a better performance of the cell. Basically, when the temperature rises, the electrochemical reactions become faster which causes higher exchange current density and less voltage loss.



Figure 3. Effect of operating temperature the performance

The above observation can also be seen in the Fig. 4, Fig. 5 and Fig. 6 that show the distribution of electric potential and electrolyte potential. For the applied voltage of 2.5V, it can be seen that when the cell temperatures are 323K, 363K and 403K, the maximum electrolyte voltages are 1.1V, 1.07V and 1.05 V respectively.



## B. The Effect of Operating Pressure

The influence of the operating pressure on the polarization curve was studied by defining the operating pressure at the anode as parameters (1MPa, 10MPa, 20MPa), and at the cathode, the pressure was kept at 1atm. The results are shown in Figure 7.The Fig.8 shows the results obtained when the values of cathodic operating pressures (1MPa, 15MPa, 25MPa, 40MPa) were used as parameters while the anodic operating pressure was 1atm.

As shown in Fig. 7 and Fig. 8, the increase of operating pressure at the anode  $(p_a)$  and cathode  $(p_c)$  results in an increase of voltage, therefore, reduces the performance of a PEM electrolyzer.



Figure 7. Effect of operating pressure (at anode) on the performance



Figure 8. Effect of operating pressure (at cathode) on the performance

#### C. The Effect of Exchange Current Density

There is not an exact value for exchange current density for the catalysts that have been developed until now. However, the exchange current density is one of the parameters that has to be given attention while analysing the performance of an electrochemical cell. Fig. 9 shows the effect of anodic exchange current density  $(i_{0,a})$  on polarization curve while Fig. 10 presents the influence of the cathodic exchange current  $(i_{0,c})$ . The results shown in Fig. 9 and Fig. 10 indicate that the higher the exchange current density is, the better the performance of the cell is.



Figure 9. Effect of anodic exchange current density



Figure 10. Effect of cathodic exchange current density



Figure 11. Effect of charge transfer coefficient (anode)

## D. The Effect of Charge Transfer Coefficient

Usually, without any indications, the charge transfer coefficient is considered to be 0.5 when solving the Bulter-Volmer equation for the PEM electrolyzer. However, the choice of the value of this coefficient has a significant impact on the performance of the cell. The

results of a parametric study of the anodic charge transfer coefficient and the anodic charge transfer coefficient are shown in Fig. 11 and Fig. 12 respectively. The results show that when the value of the charge transfer coefficient increases, the voltage of cell decreases which results in a good performance of the cell. But, the Fig. 11 shows that the increase of the anodic charge transfer coefficient from 0.5 to 2, the potential difference is large, whereas in Fig. 12, when the cathodic charge transfer coefficient increment from 0.5 to 2, the potential difference is large, and the anodic charge transfer coefficient increment from 0.5 to 2, the potential difference is very small. Thus, the appropriate choice for anodic charge transfer coefficient would be 2.



Figure 12. Effect of charge transfer coefficient (cathode)

## IV. CONCLUSIONS

The performance of a PEM electrolyzer was studied numerical simulation in using the COMSOL Multiphysics 5.1 and the effect of different parameters on the performance was presented for a 2D model of the electrolyzer. The results indicated that the increase of parameters, such as the operating temperature, the exchange current density, and charge transfer coefficient can cause the decrease of the cell voltage. At low current density, the effect of these parameters on the cell voltage was very small, but as the current density increased the potential difference is increased which lead to the improvement of the performance. However, when the operating pressure increases the cell voltage also increase and as results, the performance of a PEM electrolyzer drops.

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