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# Performances prediction study for proton exchange membrane fuel cells

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#### ABSTRACT

In this work, we propose to study the influence of the membrane physical properties on the performance of a single PEM cell through the polarization curve. A thermal approach describing the main heat transfer aspects was also discussed. For this study, we have developed and used a simulation tool called Performances Prediction Fuel Cell tool (2PFC tool) based on simplified charge, mass and even heat transfer equations. This tool aims to visualize the main evolutions in the heart of a single cell, and the results should help users to understand the variation of some operating conditions and component properties on the output cell voltage by offering a variety of sensitivity parameter studies. For this sensitivity analysis, three separated simulations are launched. The first simulation regards the effect of the resistive losses and charge transfer coefficient on the cell voltage. The second simulation concerns the influence of the water content of the membrane and the cell operating temperature on it proton conductivity. The last simulation takes in consideration the effect of water activity variation on the proton membrane conductivity, and the results proved the direct and strong relation of the charge transfer coefficient and of the water content of the membrane on the output cell voltage. In the thermal approach part, we have proposed to study the temperature distribution between two cathodes with the presence of an implemented cooling channel.

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#### Introduction

One of the main factors that have influenced the development of fuel cells has been the increasing concern about the environmental consequences of fossil fuel utilization in the production of electricity and for the propulsion of vehicles [1]. In a Polymer Electrolyte Membrane Fuel Cell, electrical energy is generated directly through the electrochemical reaction of oxidant (oxygen from air) and hydrogen at two electrodes separated by an electrolyte. When pure hydrogen is used, the only products of this process are heat, electricity and water [2].

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А	area. cm <sup>2</sup>	
а	water activity	
b	empirical coefficient, mA/cm <sup>2</sup>	
с	heat capacity. J kg <sup>-1</sup> K <sup>-1</sup>	
D	diffusion coefficient. $m^2 s^{-1}$	
EW	equivalent weight, g mol <sup>-1</sup>	
F	Faraday constant, C mol <sup>-1</sup>	
h	coefficient of convection, W $m^{-2} K^{-1}$	
Ι	current, A	
i	current density, A/cm <sup>2</sup>	
i <sub>o</sub>	exchange current density, A/cm <sup>2</sup>	
L	width (thickness), µm	
m	concentration loss coefficient, V	
n	concentration loss coefficient, cm²/mA	
Ν	molar flux, mol s <sup>-1</sup>	
n <sub>e</sub>	number of electrons transferred	
р	partial pressure, atm	
Q	heat extract or released, W	
R	gas constant, J K $^{-1}$ mol $^{-1}$	
R <sub>m</sub>	membrane resistance, $\Omega$ cm <sup>2</sup>	
S	heat source term	
Т	temperature, K	
V <sub>cell</sub>	cell voltage, V	
ρ	density, kg m <sup>-3</sup>	
Greek letters		
α	charge transfer coefficient	
λm	water content (membrane)	
λ	thermal conductivity, W m <sup><math>-1</math></sup> K <sup><math>-1</math></sup>	
$\sigma_{\rm H^+}$	membrane proton conductivity, S m $^{-1}$	
Superscripts and subscripts		
a	anode	
ac	anode cathode	
act	activation	
с	cathode	
conc	concentration	
dry	dry (membrane)	
L	limiting (current)	
m	membrane	
ohm	ohmic	
ext	extracted	

As well as presented in Fig. 1, hydrogen and oxygen are separately fed to anode and cathode channels, they diffuse through the porous electrodes and reach the catalytic layer respectively. At the catalytic layer of the anode, hydrogen splits into protons and electrons, and protons permeate through the membrane to the cathode side. The electrons are transported to the cathode by an external electric circuit. At the catalytic layer of the cathode, oxygen combines with protons and electrons to produce water.

The electrochemical reactions for a single cell of the PEM fuel cell are shown in the following equations [3].

Anode reaction :  $H_2 \rightarrow 2H^+ + 2e^-$ 

Cathode reaction : 
$$\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O$$
 (2)

Overall reaction : 
$$\frac{1}{2}O_2 + H_2 \rightarrow H_2O$$
 (3)

PEMFCs are low-temperature, high-efficiency (40–60%), high-power density, fast-start up Fuel Cells. The electrolyte is a solid polymer semi-permeable membrane, usually Nafion, carbon paper or cloth constitutes the basic mechanical structure of the electrodes and a platinum alloy catalyst is applied on it [4].

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  $^{\circ}$ C to 100  $^{\circ}$ 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.

A PEMFC system can be a part of a hybrid system for standalone applications, a good investigation, Rekioua et al. [5] conducted a recent work on this topic.

These factors set the PEMFCs apart from other fuel cells. This reason and the potential for PEMFCs to produce zero emissions create a great prospect for clean energy in the transport industry.

However, predicting the performances of these devices in theoretical cases becomes an important step to popularize and disseminate the basic knowledge to the students and young researchers working on this topic before starting their experimental works or even to compare their models and results with real performances.

#### The output cell voltage modeling

This part presents the mathematical model used to describe the (I-V) characteristics of the PEM fuel cell. A polarization curve is often used to describe the charge transfer phenomena in a single cell. It is a characteristic graph of voltage versus current for a set of operating conditions. This curve is the most common output of the models and it is seen as the most important criteria for the electrical performances prediction.

Modeling this graph is among the primary goals of the 2PFC tool. It can be done thanks to the following relation of the real cell voltage [6]:

$$V_{cell} = V_{cell,reversible} - \eta_{act} - \eta_{ohm} - \eta_{conc}$$
(4)

with

$$V_{\text{cell,reversible}} = 1.229 - 4.308 \times 10^{-5} \cdot T \cdot \ln\left(\frac{p_{\text{H}_2} \cdot \sqrt{p_{\text{O}_2}}}{p_{\text{H}_2\text{O}}}\right) - 8.453 \times 10^{-4} \cdot (T - 298.15)$$
(5)

There are three major types of fuel cell losses (voltage drop), which occurred in the PEM fuel cells as follow [7-11]:

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