



**NUMERICAL INVESTIGATIONS OF THE  
EFFECT OF OPERATION TEMPRETURE AND  
RELATIVE HUMIDITY ON THE PEM FUEL CELL  
PERFORMANCE**

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**NUMERICAL INVESTIGATION OF THE EFFECT OF OPERATING  
TEMPERATURE AND RELATIVE HUMIDITY ON THE PEM FUEL CELL  
PERFORMANCE**

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Omar Qasim Saleh AL-HADEETHI

## **ABSTRACT**

**M. Sc. Thesis**

### **NUMERICAL INVESTIGATION OF THE EFFECT OF OPERATING TEMPERATURE AND RELATIVE HUMIDITY ON THE PEM FUEL CELL PERFORMANCE**

**Omar Qasim Saleh AL-HADEETHI**

**Karabük University  
Institute of Graduate Programs  
Department of Mechanical Engineering**

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In this thesis, a three-dimensional single flow channel PEM fuel-cell for 4.8 cm<sup>2</sup> active area has been numerically investigated by using computational fluid dynamics (CFD) commercial program ANSYS-FLUENT. Required variables and boundary conditions have been defined. The essential objectives of this study are to study the impact of the Hydrogen and Oxygen relative humidity and cell operation temperature cell performance. The obtained results from the simulation have been verified with previous literature, verification results showed a good conformed to previous literature experiments.

Simulation results indicated a higher cell performance was obtained at 55°C operating temperature where the higher current density was obtained (0.3 A/cm<sup>2</sup>), cell voltage (0.6 V) and best power output equals to (0.1 W/cm<sup>2</sup>). Also, higher cell performance was obtained at 90% relative humidity values at the anode side and maximum current density (0.9 A/cm<sup>2</sup>), cell voltage (0.2 V) and maximum power output (0.3 W), similarly, when utilizing oxygen gas with 90% relative humidity, current density (0.9 A/cm<sup>2</sup>), cell voltage (0.2 V), and maximum power output (0.3 W).

The rational reasons for this results are an increase in the cell operating temperature between (45°C-55°C), the water evaporation rates becomes greater than water production rates, leads to membrane dehydration cases in decreases in cell protonic conductivity and increase ohmic loss leads to cell performance degradation moreover, an increase in the relative humidity of the Hydrogen and Oxygen gases leads to increases in membrane water content cases in increases in cell protonic conductivity and decrease ohmic loss leads to enhance the cell performance.

**Key Words** : PEM fuel-cell, operating temperature, relative humidity,  
Three-dimensional model, (CFD)

**Science Code** : 914048

## **ÖZET**

**Yüksek Lisans Tezi**

### **ÇALIŞMA SICAKLIĞI VE BAĞIL NEMLENDİRMENİN PEM YAKIT HÜCRE PERFORMANSINA ETKİSİNİN SAYISAL İNCELENMESİ**

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Bu tezde, 4.8 cm<sup>2</sup> aktif alan için üç boyutlu tek akışlı kanal PEM yakıt hücresi, sayısal akışkan dinamiği (CFD) ticari programı ANSYS-FLUENT kullanılarak sayısal olarak araştırılmıştır. Gerekli değişkenler ve sınır koşulları tanımlanmıştır. Bu çalışmanın temel amaçları Hidrojen ve Oksijen bağıl nemi ve hücre çalışma sıcaklığı hücre performansının etkisini incelemektir. Simülasyondan elde edilen sonuçlar önceki literatür ile doğrulanmıştır, doğrulama sonuçları önceki literatür deneylerine uygun olduğunu göstermiştir.

Simülasyon sonuçları, yüksek akım yoğunluğunun ( $0.3 \text{ A/cm}^2$ ), hücre voltajının ( $0.6 \text{ V}$ ) ve en iyi güç çıkışının ( $0.1 \text{ W/cm}^2$ ) olduğu  $55^\circ\text{C}$  temperature çalışma sıcaklığında yüksek PEM yakıt hücresi performansının elde edildiğini gösterdi. Ayrıca, anot tarafındaki % 90 bağıl nem değerlerinde ve maksimum oksijen yoğunluğu ( $0.9 \text{ A/cm}^2$ ), hücre voltajı ( $0.2 \text{ V}$ ) ve maksimum güç çıkışı ( $0.3 \text{ W}$ ) ile benzer şekilde oksijen gazı kullanılırken daha yüksek hücre performansı elde edildi. % 90 bağıl nem, akım yoğunluğu ( $0.9 \text{ A/cm}^2$ ), hücre voltajı ( $0.2 \text{ V}$ ) ve maksimum güç çıkışı ( $0.3 \text{ W}$ ).

Bu sonuçların rasyonel nedenleri, hücre çalışma sıcaklığında ( $45^\circ\text{C}$ - $55^\circ\text{C}$ - $55^\circ\text{C}$ ) arasında bir artış, su buharlaşma oranları su üretim oranlarından daha büyük olur, hücre protonik iletkenliğinde azalmalar ve ohm kaybının artmasıyla membran dehidratasyon vakalarına yol açar. Ayrıca, hücre performansında bozulmaya yol açar. Hidrojen ve Oksijen gazlarının bağıl nemi, hücre protonik iletkenlik artışlarında membran su içeriği vakalarında artışa yol açar ve omik kaybını azaltır PEM yakıt hücresi performansını artırır.

**Anahtar Kelimeler** : PEM yakıt hücresi, çalışma sıcaklığı, bağıl nem, üç boyutlu model, (CFD)

**Bilim Kodu** : 914048



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## SYMBOLS AND ABBREVIATIONS INDEX

### SYMBOLS

$\eta$	:	efficiency of the PEM fuel-cell
T	:	working temperature of the PEM fuel-cell (°C)
V	:	voltage of the PEM fuel-cell (V)
n	:	number of electrons transferred through the anode to cathode
P	:	working pressure of the PEM fuel-cell (kPa)
$\Psi$	:	relative humidity
$P_v$	:	water vapor pressure (kPa)
$P_{vs}$	:	saturation vapor pressure (kPa)
R	:	universal gas constant (J/mol.K)
E	:	potential (Volt)
F	:	faraday's constant (C/mol)
I	:	electric current (Amper)
M	:	mass flow rate (g/min)
L	:	liquid phase
$\Delta H$	:	change in the enthalpy (J/mol)
$Q_{H_2}$	:	fuel input to PEM fuel cell

- $P_{H_2O}$  : partial pressure of water vapor (kPa)
- $V_{Theory}$  : theoretical cell voltage (V)
- $V_{losses}$  : cell potential losses (V)
- $V_{Activ}$  : activation losses (V)
- $V_{Conc}$  : concentration losses (V)
- $V_{Ohmic}$  : ohmic losses (V)
- $i_{LM}$  : limitation current (A/cm<sup>2</sup>)
- $R_{elec}$  : electronic resistance ( $\Omega$ )
- $R_{ionic}$  : ionic resistance ( $\Omega$ )
- $P_{Output}$  : power output from the PEM fuel-cell (kW)



## ABBREVIATIONS

ICE	: Internal combustion engine
NASA	: National Aeronautics and Space Administration
USA	: United states of America
CO <sub>2</sub>	: Carbon dioxide
CO	: Carbon monoxide
NO <sub>x</sub>	: Nitrogen oxides
PM	: Particle matter
HC	: Hydrocarbons
PEMFC	: Polymer electrolyte membrane fuel cells
SOFC	: Solid oxide fuel cells
MCFC	: Molten carbonate fuel cells
AFC	: Alkaline fuel cell
HOR	: Hydrogen oxidation reaction
ORR	: Oxygen reduction reaction
MEA	: Membrane electrode assembly
PEM	: Proton exchange membrane
CLs	: Catalyst layers
GDL	: Gas diffusion layer
FCHs	: Flow channels
FFPs	: Flow filed plates
RHC	: Cathode Relative humidity
RHA	: Anode Relative humidity
HFCV	: Hydrogen fuel cell vehicle
CFD	: Computational fluid dynamic

BD	:	Back diffusion
EOD	:	Electro osmotic drag
OCV	:	Open circuit voltage
PTFE	:	Polytetrafluoroethylene
I-V	:	Current -voltage curve
PFSA	:	Perfluoro-sulfonic acid
EHM	:	External humidification methods
IHM	:	Humidification methods

## PART 1

### INTRODUCTION

Fossil fuels consider the main energy sources worldwide, all energy sectors like power plants, automotive, and industries are used fossil fuel for energy production. The energy demand increases around 15 billion metric tons per year, therefore, increase the concern for governments about fossil fuel depletion around the world. Electric production, industrialization, and transportation sectors considered the main energy consumption in the world. Figure 1.1. Shows energy consumption worldwide. The combustion of fossil fuels has an adverse impact on the environment as global warming and climate-changing, it emits risky gases the same soot, carbon monoxide CO, hydrocarbons HC, nitrogen oxides NO<sub>x</sub> [2].

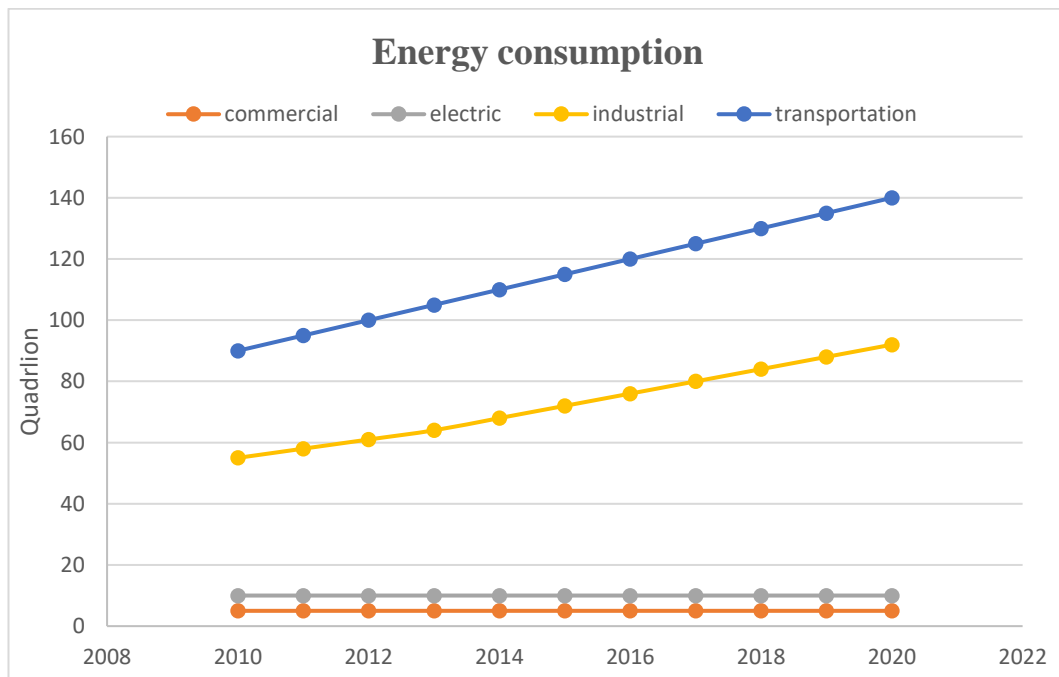


Figure 1.1. Energy consumption worldwide [3].

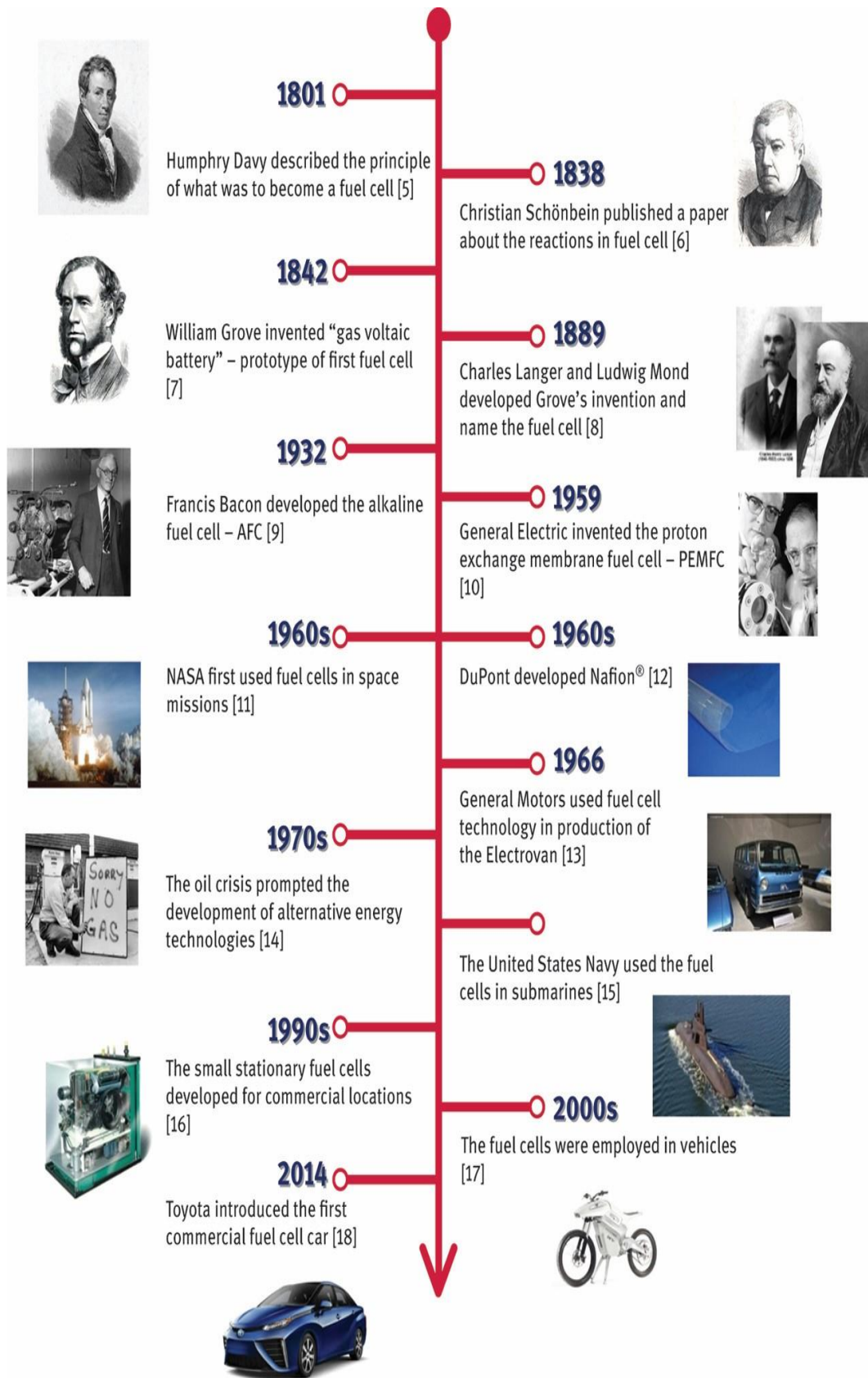


Figure 1.2. History of the fuel cell [4].

Fuel cell history started in 1842. Sir William Grove invented the gas voltaic battery which considered a prototype of the fuel cell. In 1960, National Aeronautics and Space Administration (NASA) used the fuel cell in the space missions. In 1966, General Motors Company developed first electric van powered by fuel cells, in 2014, Toyota Company produced hydrogen fuel cell vehicle called (MIRAI) as shown in Figure 1.2.

Unique functions of the fuel cells made them a strong candidate to replace the conventional energy sources particularly in automotive sector [5]. Fuel-cells are energy converter that converts the heat energy in the fuel (Hydrogen) to useful electricity. Various fuel cells technology can be classified depending on the membrane types and cell working temperature [6]. Different fuel cell types listed in Table 1.1.

Table 1.1. Different fuel cell types [7].

<b>Fuel cell types</b>	<b>Used electrolyte</b>	<b>Working temperature</b>	<b>Cell efficacy</b>	<b>Used Fuel</b>
Alkaline fuel cell AFCs	Potassium hydroxide solution	25-85 °C	70%	H <sub>2</sub> -O <sub>2</sub>
PEM fuel cell PEMFCs	Proton exchange membrane	50-95 °C	50-60%	H <sub>2</sub> -O <sub>2</sub>
Solid oxide fuel cell SOFCs	Oxide ion conducting ceramic	800-1000 °C	65%	CH <sub>4</sub> , H <sub>2</sub> -O <sub>2</sub>
Molten carbonate fuel cell MCFCs	Molten mixture of alkane metal carbonate	650 °C	65%	CH <sub>4</sub> , H <sub>2</sub> -O <sub>2</sub>

Good properties of PEM fuel-cells as low-temperature operation, high energy density, and zero-emission device made the PEM fuel-cells type are more desirable than other types of fuel cells, and made it strongest candidate to replace internal combustion engine ICE in automotive. It has many uses in portable, stationary power applications, and transportation sectors, particularly, in the automotive [8].

Generally, PEM fuel-cells like an automotive battery, it is consist of the positive side, negative side (Anode), and solid electrolyte. Anode side covered with platinum layers that catalyze the hydrogen molecules to one electron and one proton, concentrations of the platinum particles in the anode side ( $0.05 \text{ Mg/cm}^2$ ) as well as Cathode side covered with platinum layers that reduced the oxygen molecules and hydrogen proton to produce water, the platinum particles concentrations in the cathode side ( $0.2\text{-}0.4 \text{ Mg/cm}^2$ ). PEM fuel-cells operate at special conditions, as the following below:

- Operating temperature:  $50^\circ\text{C}\text{-}90^\circ\text{C}$ .
- Operating pressure:  $100\text{-}300 \text{ kPa}$ .
- Inlet gas relative humidity:  $50 \% - 100\%$ .
- Fuel tank pressurized to  $700 \text{ kPa}$  [9].

PEM fuel-cells are consumed hydrogen gases as an oxidize gases and oxygen gases as a reductant. In reality, hydrogen gases are not available in the earth but it combined with oxygen as water or combined with carbon as natural gas or in living thing as in biomass, hydrogen have high energy value than other fuels [10]. Hydrogen gases can be produced from the renewable energy sources like geothermal energy, hydroelectric wind, solar photovoltaics and direct photo electrochemical, it has a high heating energy. Table 1.2. Summarize the deferent fuel heating values used in automotive [11].

Table 1.2. High heating values of different fuels used in automotive [12].

<b>Fuel</b>	<b>Chemical symbol</b>	<b>Heating energy</b>	<b>Density</b>
		MJ/kg	$\text{kg/m}^3$
Hydrogen	$\text{H}_2$	141.8	0.0899
Gasoline	$\text{C}_6\text{H}_6$	47.3	719.79
Diesel	$\text{C}_{14}\text{H}_{30}$	44.4	832
Natural gas	-	50	0.8000

## 1.1. PEM FUEL-CELLS APPLICATIONS

Unique functions of the PEM fuel-cells as low-temperature operation, great energy density, and zero-emission device made this cells type are more desirable than other types of fuel cells. In reality, PEM fuel-cells have three main application as can be shown in Figure 1.3. As following:

- Transportation applications
- Portable applications
- Stationary applications

PEM fuel-cells have gained a huge interest from the automotive company because it has many benefits as no emission, no moving parts, high-efficiency device and environment friendly. Hydrogen fuel cell vehicle (HFCV) working is following:

- Air (oxygen) enters to automotive from the windows in front of automotive from the atmospheric air and enters to cell at a cathode side.
- Hydrogen gases are fed to cell from the high-pressure hydrogen tank. The hydrogen gases enter to fuel cell at an anode side where it oxidized into one negative electron and one positive proton.
- On the anode side: An electrochemical reaction occurs on the anode surface between the hydrogen and platinum particles on the catalyst layer interface result in splitting the hydrogen into one electron and one proton, protons are moved from the anode to the cathode across the proton exchange membrane PEM, electrons will moving through external load circuit from the anode to the cathode [13].
- On cathode side: An electrochemical reaction occurs on the cathode surface between the negative electrons and positive protons and oxygen atoms leads to generate water and release some heat [14].
- The generated electricity from the PEM fuel-cell are supplied to an electric motor to moves the wheels of automotive [16].



a) Transportation applications



b) Portable applications



c) Stationary applications

Figure 1.3. Three main applications of fuel cells.



## 1.2. BASIC COMPONENTS OF PEM FUEL-CELL

Figure 1.4. Explained the essential cell parts, PEM fuel-cell are consist of a membrane electrode assembly (MEA) laying between two flow field plates. (MEA) involve of the proton exchange membrane (PEM), catalyst layers (CLs), and gas diffusion layers (GDLs), each layer has a various function in the cell operation [17].

- Anode-flow filed plates (FFPs).
- Anode-flow channels (FCHs).
- Anode-gas diffusion layers (GDLs).
- Anode-catalyst layers (CLs).
- Proton exchange membrane (PEM).
- Cathode-catalyst layers (CLs).
- Cathode-gas diffusion layers (GDLs).
- Cathode-flow channels (FCHs).
- Cathode-flow filed plates (FFPs).

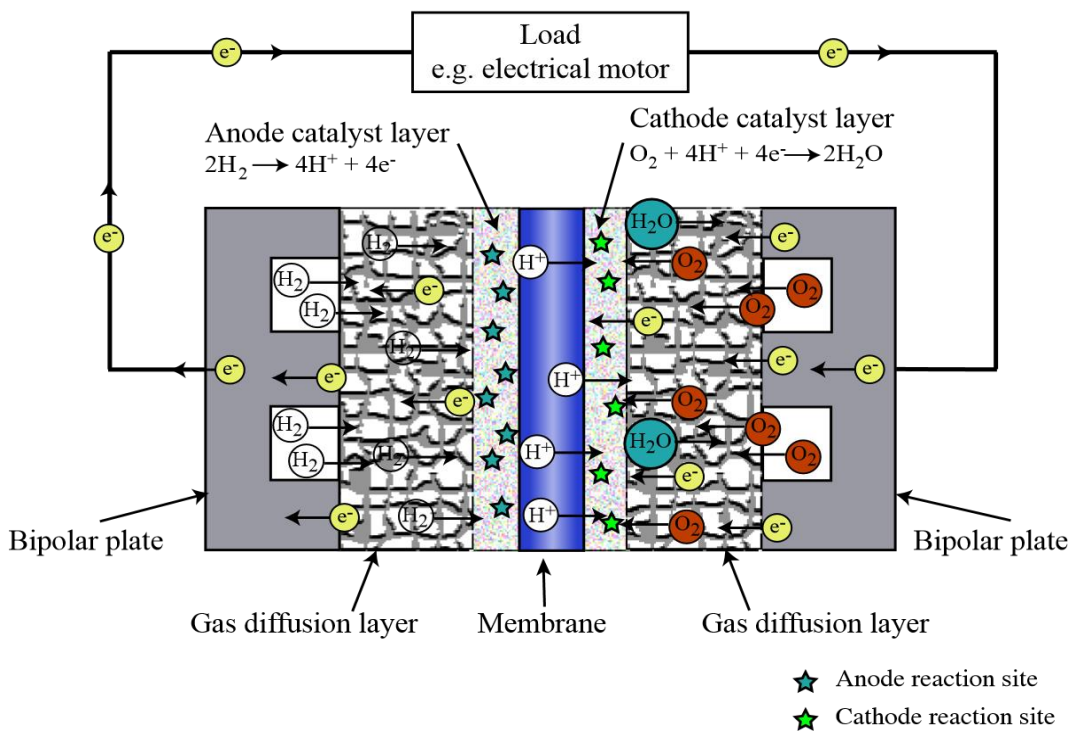


Figure 1.4. PEM fuel-cell components [7].

### 1.1.1. Flow Filed Plates (FFPs)

Flow filed plates (FFPs) are the biggest component in the cell, almost accounts 70% from the cell mass and 30% from the overall cell price. Flow channels shapes in the flow filed plates as shown in Figure 1.5. The most common material to fabricate flow filed plates (FFPs) is a graphite-carbon. Several functions for flow filed plates (FFPs) like it conduct cell to adjacent cell electrically, electrons transportation from the anode to cathode, uniformly distributed the reactant gases and contribute in water management, and heat contribute in management by removing the overheat from the reaction sites by coolant [20]. Good Flow Filed Plates (FFPs) must be characterized by:

- An impermeable for reactant gases, high electronic conductivity, chemically stability.
- Good thermal conductivity.
- Easy to manufactured and low cost.

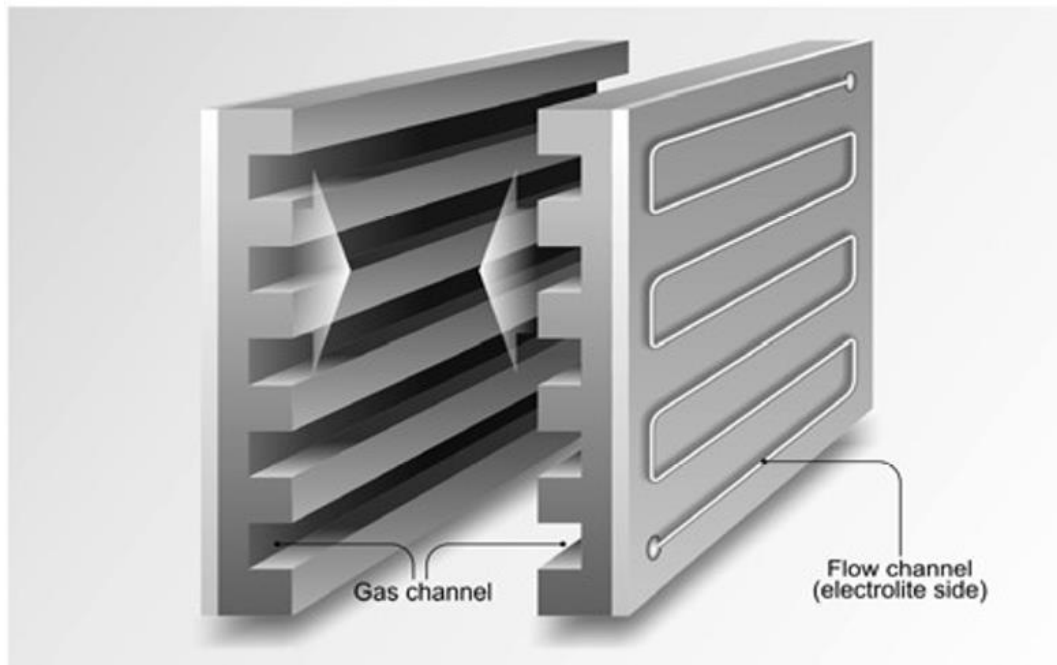


Figure 1.5. Flow Filed Plates (FFPs) [11].

### 1.1.2. Flow Channels (FCHs)

Flow channels have a vital importance in the PEM fuel-cell operation system, it has significant influence on the cell performance. The main function of the flow channels are distributed reactant gases to the reaction sites evenly and plays important roles in the water management where it removed the water molecules out of the cell. Flow channels have several designed as parallel, serpentine, zigzag straight channel, and integrated design, each design have a different influence on the cell performance [21]. Flow channels must have characterized by three aspects:

- Distribute the reactant gases on the reaction sites evenly.
- Small pressure difference between the inlet cell and outlet cell.
- Do not allow of the electrode flooding.

Parallel design, are most common used type, it has many advantages as the low-pressure difference of the reactant gases, simple design, can be treated any blockage in flow channel. Another common type is the serpentine channel, this type characterized by being a one-flow channel extending from cell inlet to outlet.

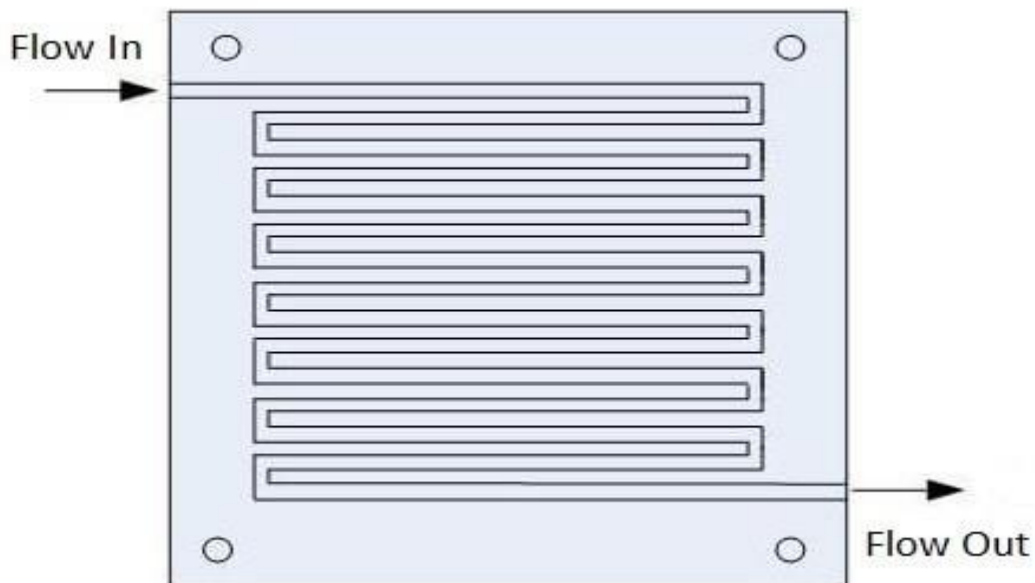


Figure 1.6. Serpentine types of flow channels (FCHs)

### 1.1.3. Gas Diffusion Layers (GDLs)

Gas Diffusion Layers (GDLs) consider a functional component in PEM fuel-cell; it consists of mixture with three layers (carbon, water, and polytetrafluoroethylene). Essential function of a polytetrafluoroethylene is facilitating the transport of water and gases during flooding phenomena conditions. Carbon clothes are most common materials for the (GDLs) [22]. It has a 300  $\mu\text{m}$  thick, it must have designed as a hydrophobic that is means (GDLs) are able to repel water molecules out of reaction sites to prevent the electrode flooding as can be seen in Figure 1.7 [18]. Main functions of the (GDLs) are:

- Diffuse and distribute the reactant gases to the reaction sites on the (CLs).
- Heat transportation from the reaction sites on the (CLs) to the (FFPs).
- Electrons transportation from the reaction sites on the (CLs) to the (FFPs).
- Contribute in the water and heat management.
- Electronic resistivity [23].

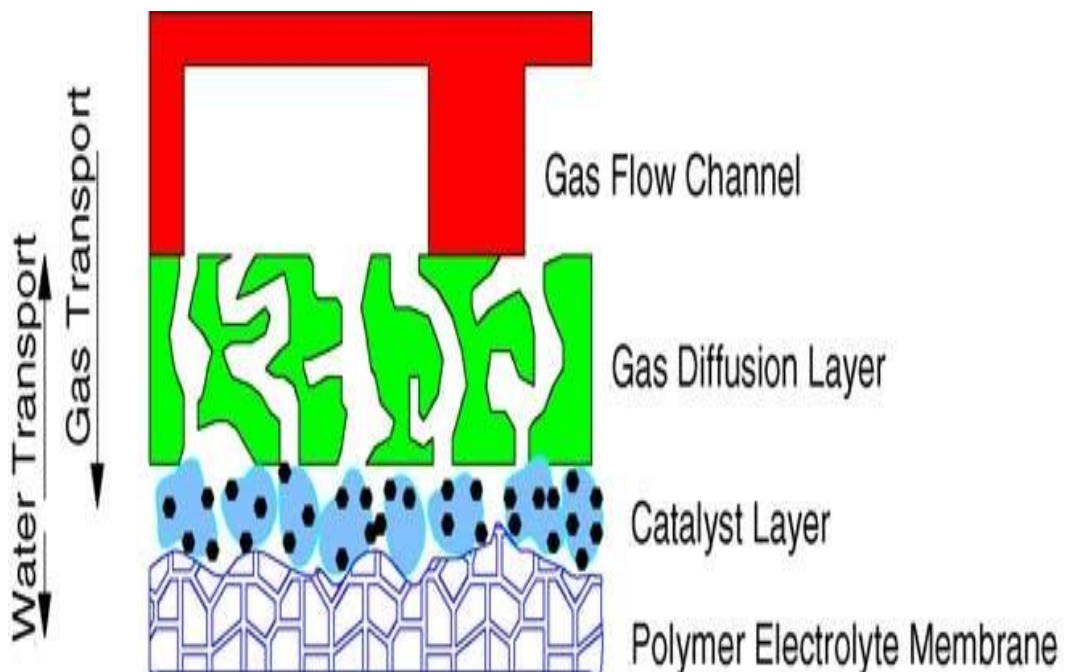


Figure 1.7. Gas diffusion layers (GDLs) [18].

#### 1.1.4. Catalyst Layers (CLs)

Catalyst layers (CLs) plays a major roles inside the PEM fuel-cell. Two electrochemical reaction takes place on the catalyst layers (CLs) interface for anode and cathode side as in the following equations below. Hydrogen oxidization reaction (HOR): where Hydrogen oxidize on the anode catalyst surface into on proton and one electron as shown in equation (1.1).

On the cathode side, Oxygen will reduce the proton and electron to form water and release some heat by Oxygen reduction reaction (ORR) as shown in equation (1.2) [24].



Catalyst layers consist of small carbon powder particles it has a 50 nm thickness and small platinum particles around 5 nm as shown in Figure 1.8. [25]. Platinum particles had used as a catalyst because it has high activity. Good catalyst layers must be having a special specification as following [39]:

- High ionic and electronic conductivity.
- Preamble gases.
- High activity.
- Low cost.

The main challenges in the catalyst layers operation are the hydrogen fuels are, containing impurities of CO that that has a containing impurities, several researchers were suggested addition the ruthenium with the platinum to solve problem of carbon impurities and enhance the PEM fuel-cell performance.

### 1.1.5. Proton Exchange Membrane (PEM)

Proton exchange membrane (PEM) represents the functional component in the PEM fuel-cells, it has the same functions of the electrolyte inside the conventional automotive battery, and it must have a special specification as following:

- Thermally and chemically stable.
- Highly protonic conductivity.
- Good insulator for electrons.
- Thin as possible [26].

Better material used in the membrane are sulfonated polymer, this material has unique feature which high proton conductivity as can be shown in Figure 1.9. Protonic conductivity is the major function of the proton exchange membrane (PEM). It must be maintain fully hydrated to achieve better performance from the cell, therefore, water molecules needed. On one hand, an excessive in the waters molecules lead to electrode flooding result in blockages the porous media in (GDLs) and retarded the reactants gas from reaching the active sites on the (CLs). Thereby reducing the protonic conductivity which can result in decreases the cell performance [13].

Proton exchange membrane (PEM) works with a normal level of water with the desirable cathode and anode relative humidity and desirable operating temperature it would lead to increase in cell performance.

The essential aims of this thesis are examine the cell performance at different working temperature and deferent relative humidity values, then select better operation values.

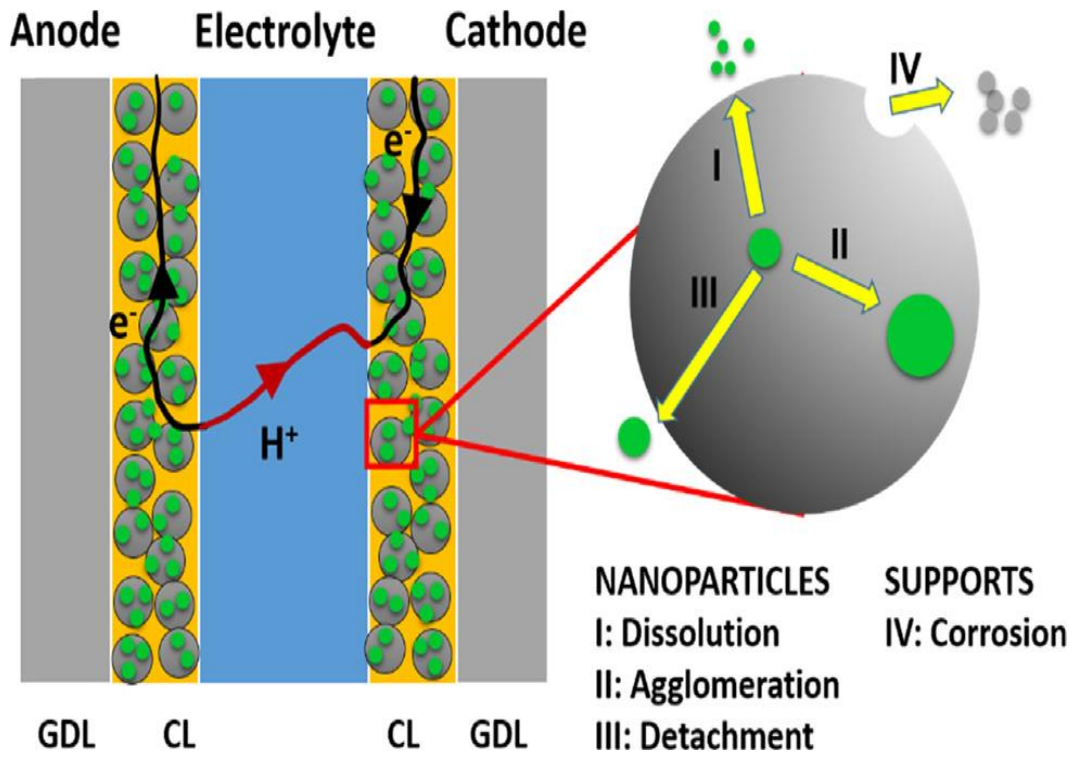


Figure 1.8. Catalyst layers in (CLs) [25].

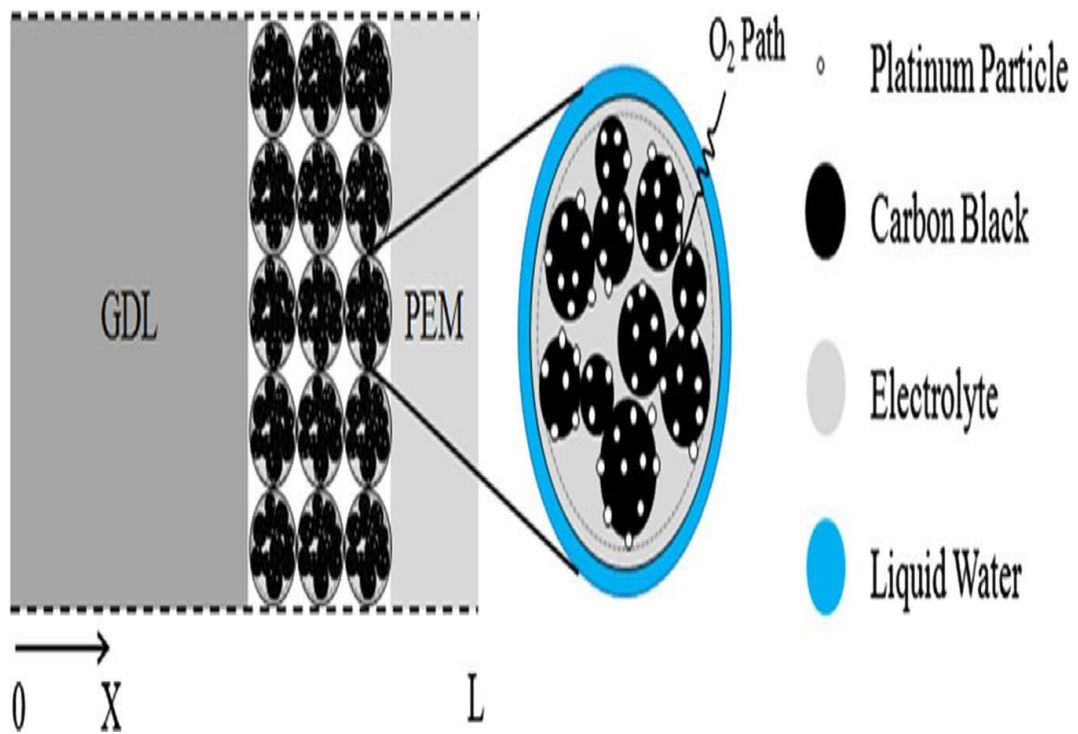


Figure 1.9. Proton exchange membrane (PEM) [27].

### 1.3. THEORETICAL LOSSES IN PEM FUEL-CELL

The relationship between the cell voltage and exchange current density defined as polarization curve or (I-V) curve. (I-V) curve used in the comparison between the quantities of the power output produced from two deferent cells, where the following relation as can calculate the voltage of the cell shown in Figure 1.10. Equations 1.3. Explained the cell voltage include the cell voltage losses.

$$V_{cell} = V_{Theory} - V_{Losses} \quad (1.3)$$

Where:

$V_{Cell}$  : Cell voltage in V

$V_{Theory}$  : Theoretical cell voltage in V

$V_{Losses}$  : Losses in the cell voltage in V

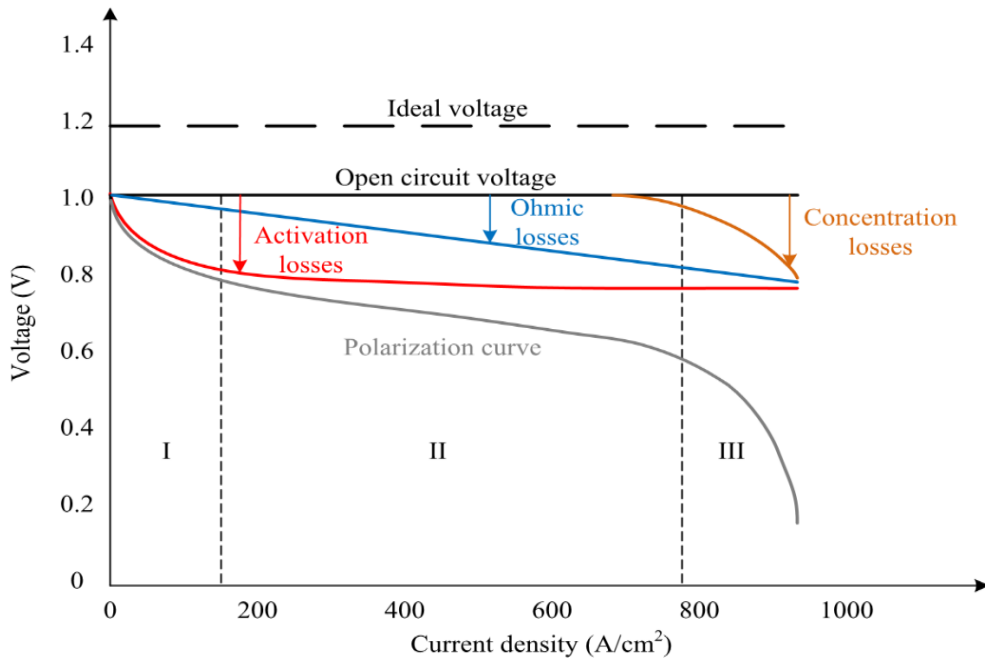


Figure 1.10. Various voltage losses and (I-V) curve [28].



Theoretical cell voltage  $V_{Theory}$  can determine from the Nernst equation as following as in equation (1.4), and cell voltage losses can calculated by using 1.5. Equation:

$$V_{Theory} = V_{Theory}^{\circ} + \frac{RT}{nF} \ln \frac{(P_{H_2} P_{O_2})^{1/2}}{P_{H_2O}} \quad (1.4)$$

$$V_{Losses} = V_{Activation} + V_{Consternation} + V_{Ohmic} \quad (1.5)$$

Where:

$V_{Theory}^{\circ}$ : Standard theoretical cell voltage.

T : Working temperature.

R : Universal gases constant 8.314 kJ/mol.K.

N : Number of electrons.

F : Faraday is constant 96.485 c/mol.

P : Hydrogen, oxygen, and water partial pressure in atm.

$V_{Activ}$  : Activation losses.

$V_{Cons}$  : Consternation losses.

$V_{Ohc}$  : Ohmic losses.

The electric power produced from the PEM fuel-cells governed by Faradays law takes in account the theoretical losses from the cell as mentioned in the second law of thermodynamics which state that impossible to transform all heat energy to useful work, some heat must be lost as a sink heat.

### 1.3.1. Activation Losses

Activation Losses define as voltage lost in driving the chemical reaction, which transfers electrons, from the anode side to the cathode side, this loss depend on the electrode type, ionic activity, ionic activity solvent, and electrode-electrolyte interface. These losses takes place on both side of electrode anode and cathode,

Oxygen reduction reaction (ORR) faster than the hydrogen oxidation reaction (HOR), so the activation losses on the anode side neglected. Activation losses dominated at the low exchange current density, increasing the exchange current density can be reduces these losses by increase many factories as following [29]:

- Working temperature.
- Flow rates of the reactant.
- Working pressure.
- Activity of the catalyst layers (CLs).
- Roughness of the electrode.

Activation losses can be calculated by using the following equation (1.6):

$$V_{Act} = \frac{RT}{\alpha nF} \ln \left( \frac{i + i_{LM}}{i} \right) \quad (1.6)$$

Where:

$V_{Act}$  : PEM fuel cell actual voltage losses.

$i_{LM}$  : Exchange current density limitation.

$T$  : PEM fuel cell operating temperature.

$F$  : Faraday is constant 96.485 c/mol.

$N$  : Number of electrons.

$\alpha$  : Transfer current coefficient .

$i$  : Exchange current density.

### 1.3.2. Concentration Losses

The concentration voltage losses occur because of reactant consumption on the electrode surface which leads in concentration gradient between bulk and electrode surface [30]. The concentration voltage losses dominated at high current density. Concentration loss can minimize by:

- Increase the hydrogen and oxygen concentrations.

- Increase the hydrogen and oxygen flow rates.
- Increase the hydrogen and oxygen pressure.
- Optimize the porosity of gas diffusion layers (GDLs).

This relation following below can calculate the cell concentration losses in equation (1.7):

$$V_{Cons} = \frac{RT}{nF} \left( \frac{i_{LM}}{i_{LM} - I} \right) \quad (1.7)$$

Where:

$V_{Cons}$  : Concentration Losses.

T : Working temperature.

R : Global gases constant 8.314 kJ/Mol.k.

N : Number of electrons.

F : Faraday is constant 96.485 c/mol.

$i_{LM}$  : Exchange current density limitation, the approximate value of the exchange current density limitation for PEM fuel-cell 1.2 A/cm<sup>2</sup>.

### 1.3.3. Ohmic Losses

The ohmic losses result in retired the electrons moving from the anode to the cathode. Major reasons for ohmic losses are resistance of the ionic current in the electrolyte and electronic current in the electrode, it dominant at the intermediate current density [31]. Using electrolyte with high ionic conductivity and an electrode with high protonic conductivity, contributed to lower these losses, ohmic losses have a significant impact on the cell performance, these losses shown in Figure 1.11. This relation following below can calculate the cell ohmic losses in Equation (1.8).

$$V_{Ohmic} = I * (R_{Elec} + R_{Ione}) \quad (1.8)$$

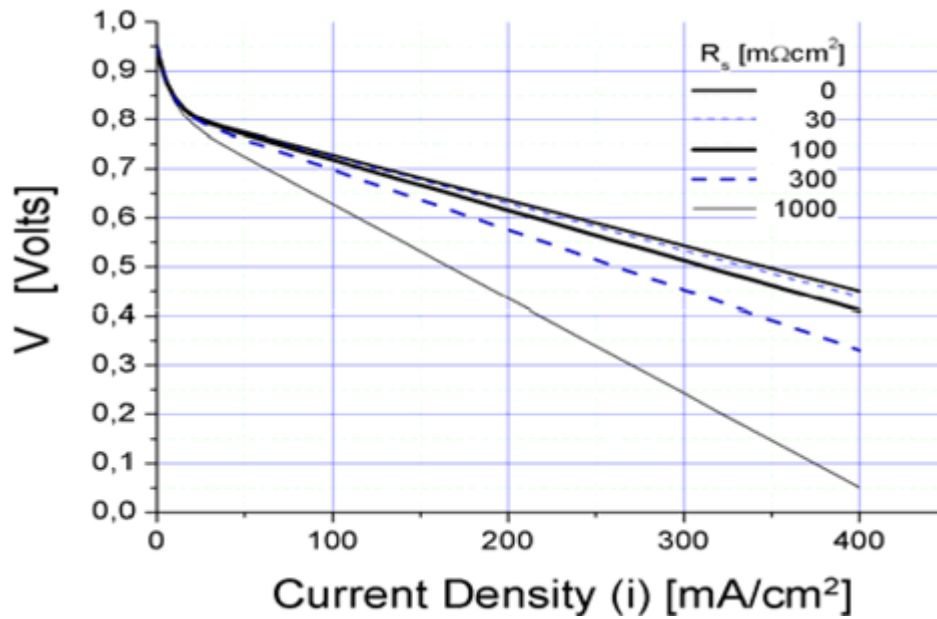


Figure 1.11. Impact of ohmic losses on the cell performance [32].

#### 1.4. PEM FUEL-CELL EFFICIENCY

The efficiency of any conversion device can evaluate by dividing the output to input energy. The output energy in the PEM fuel-cells can be represent by electrical work, on the other hand the input energy can be represent by the hydrogen heating value. Efficiency of cell equals to electric power output to fuel input. The expression ( $\frac{m \Delta H}{n F}$ ) represent a reversible potential includes thermal and electric energies from the electrochemical reaction has a value 1.482 V. In simple way, the cell efficiency is a ratio between actual operating voltage and reversible potential 1.482 V [33]. Electric power output from the cell are represent a product of the (current (I) multiply the cell voltage (V)). Fuel input to the cell are a product of hydrogen higher heating value (142000 J/g), and hydrogen consumption rate (g/s), the rates of the hydrogen consumption is governed by faraday's law as below. The set of equations below (1.9, 1.10, 1.11, 01.12) Explained the algebraically relation between the cell concepts.

$$P_{Output} = V * (I) \quad (1.9)$$

$$Q_{H2} = \frac{mI}{nF} \quad (1.10)$$

$$Q_{H2} * \Delta H = \frac{mI}{nF} * \Delta H \quad (1.11)$$

$$\eta = \frac{P_{Output}}{Q_{H2}} \quad (1.12)$$

## 1.5. RESEARCH OBJECTIVES

There are many advantages for PEM fuel-cell technology made them interesting for many researchers like:

- High-efficiency devices compared to (ICE) for vehicles.
- The main produce from the electrochemical reaction is pure water and heat so it is clean energy conservation devices.
- Alternative energy sources to fossil fuel.
- Fuel flexibility that is mean can operate on the hydrogen fuel and operate on other fuel like methanol.

In this thesis, three-dimensional model created for PEM fuel-cell with 4.8 cm<sup>2</sup> active area. From the previous studies, the author saw the investigations related to water management and operating conditions are very few. Obviously, cell operating with a proper level of water with the desirable cathode and anode relative humidity and desirable operating temperature it would lead to increase in cell performance. In present thesis, three-dimensional, PEM fuel-cell with single flow channel and membrane area 4.8 cm<sup>2</sup> have been developed to investigate the influence of the operating temperature and reactant relative humidity. Numerical investigating have been done by using CFD solver ANSYS–FLUENT, where the operating temperature have varied between (55°C-75°C-85°C) values, and Hydrogen and Oxygen gases relative humidity have varied between (50%, 70%, 90%) values.

## 1.6. OUTLINE OF THE STUDY

In this study, a three-dimensional mathematical PEM fuel-cell model have been created to study the effect of operating temperature and the effect of anode and cathode relative humidity on the cell performance. The biggest challenges towards cell operation are water formation due to electrochemical reaction.

Part 1, this part presented a brief introduction about the energy production in the worldwide, then explained the dependence on fossil fuel in the energy production, and clear up the common renewable energy sources as hydrogen energy, then deeply explained (fuel cell) device, that converts the energy Stord in fuel to electricity. Compressive information of cell parts then shed light on PEM fuel-cell working, cell applications, and cell efficacy, this part ends by presents the research objectives and outline for the study.

Part 2, this part presented previous studies about working conditions influencing the water management issue in the PEM fuel-cell include an influencing of (operating temperature, operating pressure, the relative humidity of the inlet gases on the cell performance). Part 2 ends by defining the research problems.

In the Part 3, this part presented three-dimensional single flow channel PEM fuel-cell model build by using ANSYS –FLUENT 2020 R1, the model includes all the transport phenomena processes. The model geometry was designed in ANSYS–SPACE CLAIM included nine layers then insert into ANSYS–DESIGN MODELER-MESH to discretization processes by finite volume method (FVM) then insert into ANSYS–FLUENT to set boundary conditions, finally , the discretize cell were insert to ANSYS-FLUENT to set up the proper operation conditions and solve initialization

Part 4, this part presented the numerical simulation results of the three-dimensional computational fluid dynamic (CFD) of PEM fuel-cell model as a graphical contour and current density and cell voltage and power density values, the polarization (I-V) curve was drawn to validate with literature experiment.

The chapter ends with illustration the effect of (working temperature, anode relative humidity (ARH), and cathode relative humidity (CRH) on the cell power output.

Part 5, this part presented conclusions of recent work and recommendations for next work. Three-dimensional single flow channel PEM fuel-cell model created for 4.8 cm<sup>2</sup> active area. From the previous studies. PEM fuel-cell operating with a proper level of water with the desirable cathode and anode relative humidity and desirable operating temperature it would lead to increase in cell performance.

The essential target of this thesis is to examine the cell performance at different working temperature and deferent relative humidity values, then select better operation values.

## PART 2

### LITERATURE REVIEW

PEM fuel-cell considered an energy conversion devices which transform the heat energy in the (Hydrogen) to electric energy and emit pure water and some heat. Figure 2.1. Explained the cell parts. Generally, PEM fuel-cell like an automotive battery which consist of two sides, positive side (cathode) negative side (anode). Two main electrochemical reaction takes place on its surface (Hydrogen oxidization reaction (HOR) - Oxygen reduction reaction (ORR)) [24].

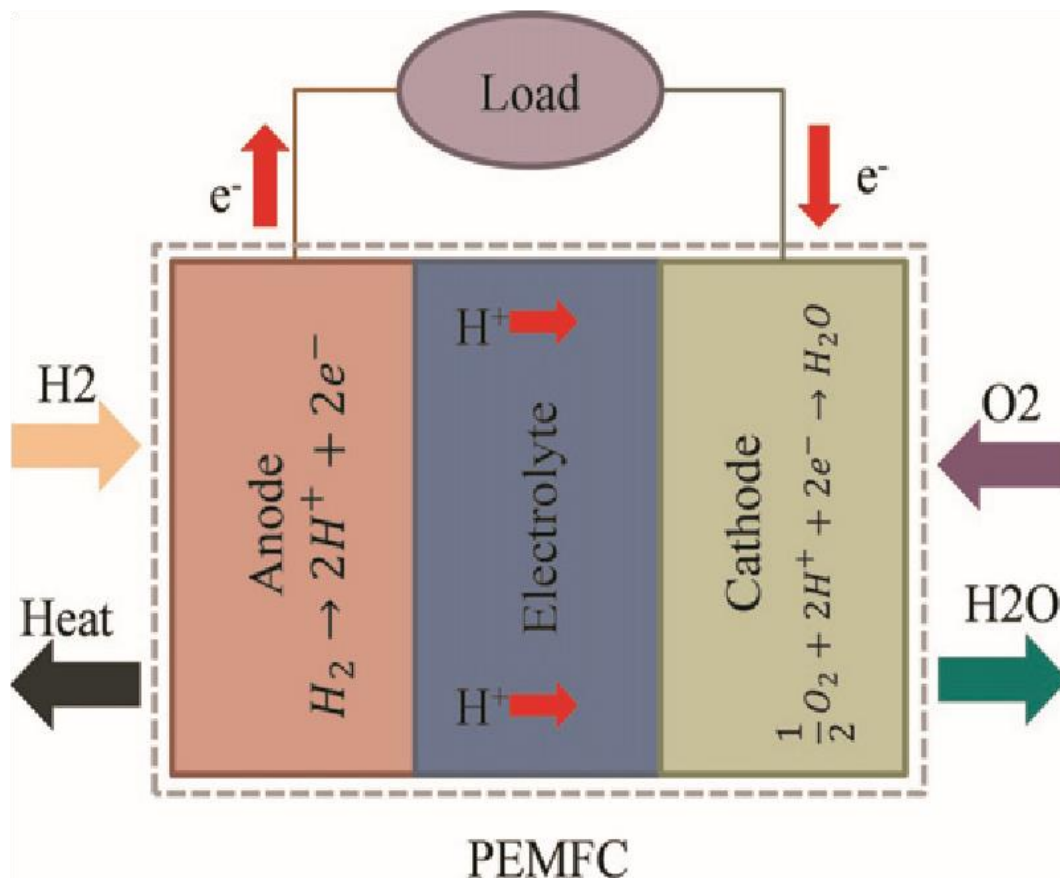


Figure 2.1. PEM fuel-cell parts and operation [8].



Hydrogen gases are delivering into anode side, while the oxygen gas are deliver into cathode side, hydrogen gas enters to the flow channels and diffuse through pours media In the (GDLs) then reach activities sits in catalyst layers (CLs). In (CLs) there are two electrochemical reaction occur as following:

- On the anode side an electrochemical reaction takes place on the anode side (CLs) surface between the hydrogen and platinum particles result in oxidizing the hydrogen to one electron and one proton. Protons are transfers from the anode to the cathode across the membrane, electrons moving via an outer load circuit from the anode to the cathode. (2.1) Equation express the electrochemical reaction on the anode side [13].
- On the cathode side an electrochemical reaction takes place (CLs) surface between the electrons and protons and oxygen on the cathode, result in water formation and release some heat equation (2.2) describes this reaction [14]. Equation Express the electrochemical reaction on the cathode side.



PEM fuel-cells consist of nine components as following as can be seen in Figure 2.2.

- Anode-flow filed plates (FFPs).
- Anode-flow channels (FCHs).
- Anode-gas diffusion layers (GDLs).
- Anode-catalyst layers (CLs).
- Proton exchange membrane (PEM).
- Cathode-catalyst layers (CLs).
- Cathode-gas diffusion layers (GDLs).
- Cathode-flow channels (FCHs).
- Cathode-flow filed plates (FFPs).

## 2.1. WATER MANAGEMENT

The water formation issue considered a major challenge in the PEM fuel-cell operational. To achieve high performance from the cells membrane must maintain fully humidified. Excessive water causes in blockages gas porous media lead to denying the reactant gases from reaching the active sites on the (CLs), cause in the decrease the cell performance. On other hands, insufficient water molecules maybe lead to membrane dehydration, increase in the ohmic resistance losses, which result in decrease in the cells performance.

(J. P. Owejan, et al, 2009), published a comprehensive review about the water management issues studied the impact of the water formation on the cell performance and durability [34]. He focused on the equilibrium between the membrane hydration and liquid water formation. The results showed, water formation depends on the reactants gases relative humidity, flow field layout and the structure of the (GDLs). Proper equilibrium in the membrane water contain, can be achieve a better cell performance [13]. The equilibrium in the water level means allows to reactant gases humidification without electrode flooding occurrence [11]. The main sources of water molecules in the cells are:

- Oxygen reduction reaction (ORR) on cathode catalyst interface.
- Water supplement via reactant gases during the humidification process.

Water molecules transported in the cell by three mechanism (Electro-mostic drag (EOD), back diffusion (BD) and hydraulic permeation) [37].

### 2.1.1. Electro-Mostic drag (EOD)

Darning cell operation, the electric current runs through the cell, and protons with water molecules will transfer from the anode Side to the cathode through the membrane, water molecules transportations depending on the humidification state of the membrane.

### 2.1.2. Back diffusion (BD)

Water molecules will accumulate on the cathode leads to high concentration water on the cathode after the oxygen reduction reaction (ORR), high concentration water molecules will migrate from the cathode side to anode side. The gradient in concentration water influence by many factors as reactant gases humidification, membrane water content, membrane thickness, cell temperature, and current density. Figure 2.2. Shows the water transport process inside the cell [35].

### 2.1.3. Hydraulic permeation

Water will transport in both side (anode and cathode) depended on the pressure differential, almost Hydraulic permeation effect is small compared with (EOD) and (BD) effect so in many cases it is negligible.

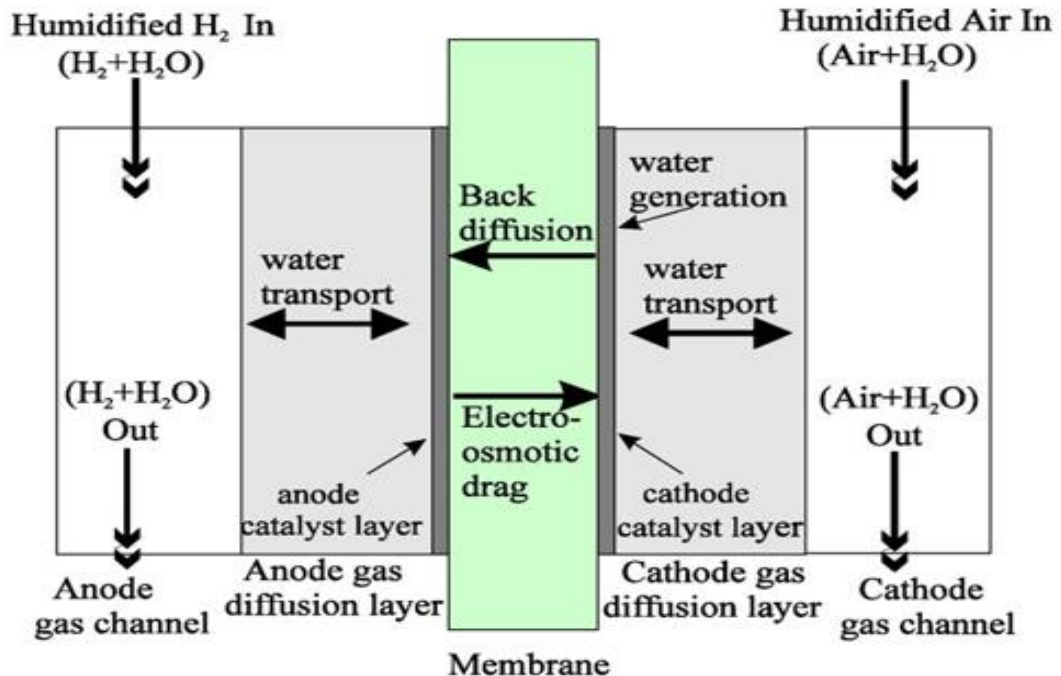


Figure 2.2. Water transportation mechanisms in the PEM fuel-cells [36-37].

## 2.2. INLET GASES RELATIVE HUMIDITY

Humidity is a parameter express about water content inside the gases or the water mixture, several ways to express for humidity as "absolute humidity, relative humidity, dew point temperature, and mixing ratio, relative humidity" almost, relative humidity is most common commercial idiom using in cell [45].

$$\Psi = \frac{P_v}{p_{vs}} \quad (2.1)$$

The temperature of the inlet gases is a " ratio between the partial pressure for the water vapor divided to saturated pressure for the water vapor [46]. The saturated pressure of the vapor is the same as the partial pressure of vapor for "mixture of air and water in equilibrium" that means; the rates of the water evaporation equals to rates of water condensation as shown in equation 2.3. [47].

PEM fuel-cells are used (Perfluoro-Sulfonic acid) ionomer membranes Nafion® PFSA as a proton exchange membrane (PEM), this type of membrane has a protonic conductivity characterized by the need to high water content level, consequently, in this type of membrane must be continues supplied sufficient water molecules and humidified a reactant gases to achieve better performance. In fact, there are two methods for reactant gases humidification internal humidification and external humidification. External humidification methods (EHM) are much better than internal humidification methods (IHM), for many reasons as: Reducing in total PEM fuel-cells cost and reducing in total weight and reducing in parasitic power consumption [38].

Water formation rate must be equal to water removal rate in order to maintain on the membrane fully hydrated and gained smoothly operated. In last century, (Staschewski & Technics, 1996) first work on the internal humidification (IHM), they developed a porous flow filed plats (FPPs), where linked with hot water loop and supplied hot water to humidify the membrane electrode assembly (MEA).

The study concluded that the internal humidification method was better than internal humidification method where leads to optimization the cell performance. Figure 2.3. Explained the external humidification in the PEM fuel-cells cells type [48].

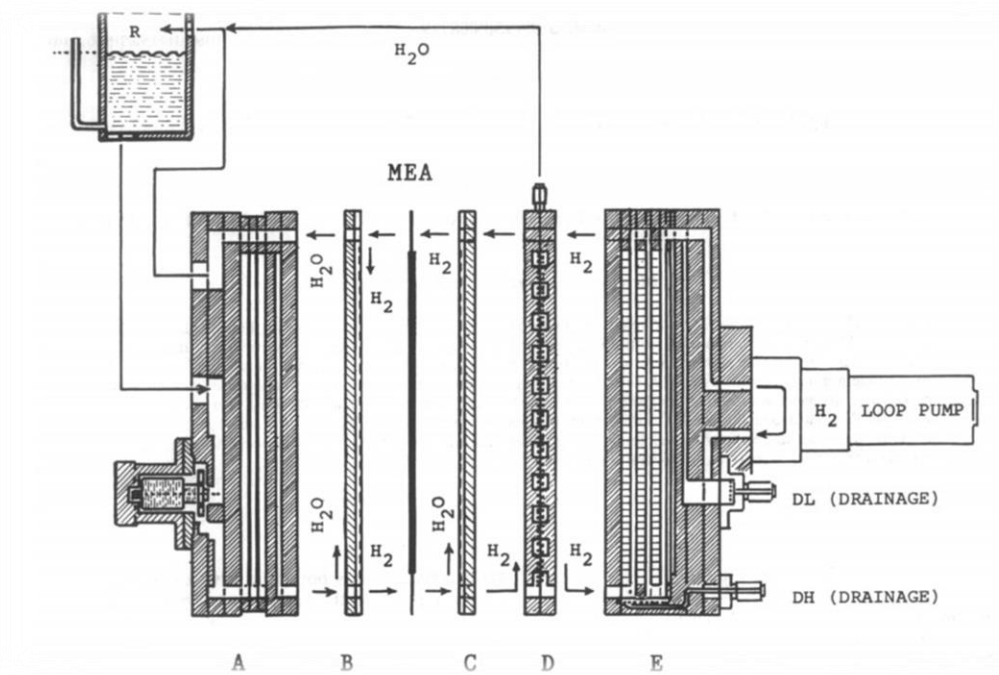


Figure 2.3. An external humidification method in PEM fuel-cells [48].

The conventional method and used widely is bubble humidification. Figure 2.4. Explain the schematic of the bubble humidification. Bubble humidification was considered the better method for controlling reactant gases humidity can be controlling both the water contained in the bubble's reservoir and water temperature inside the bubble's reservoir. Bubble humidification has several advantages like:

- Inexpensive method.
- Not requirement more power.
- Simplicity method.

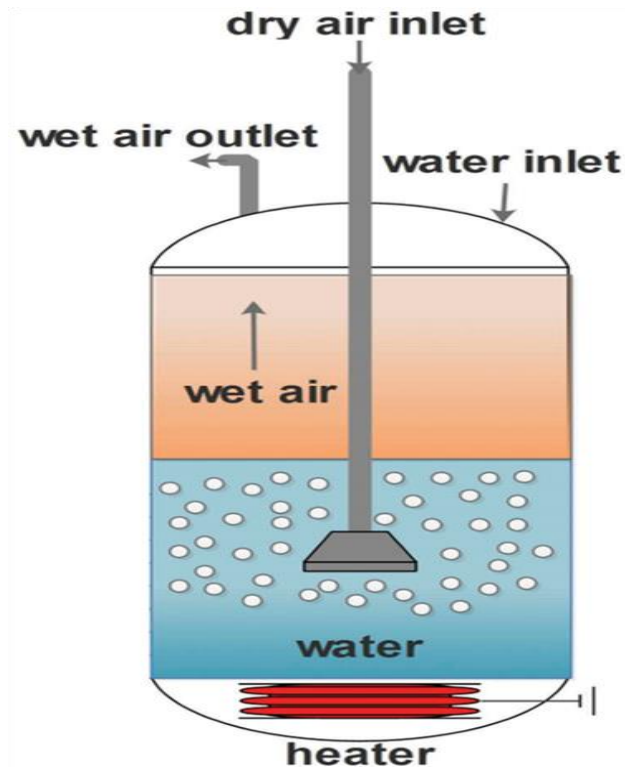


Figure 2.4. Bubble humidification [48].

(Ahmaditaba et al, 2018) designed and fabricated a bubble humidifier the and experimentally tested it, and examine the influence of water temperature and the water contain in the reservoir and the inlet airflow on the humidifier performance as shown in Figure 2.5.

The result showed that the relative humidity of the outlet air was decreased about (6% -11%) with an increasing inlet airflow rate from the  $1 \text{ m}^3 \text{ h}^{-1}$  to  $3 \text{ m}^3 \text{ h}^{-1}$ . Any increase in the water temperature in the reservoir and water contain in the reservoir resulting in improvements in the cell performance.

In addition, he concluded, humidifier operation at the  $20^\circ\text{C}$  and increasing the water contain in reservoir from 5 cm to 7.5 cm has a strong effect on the humidifier performance [48].

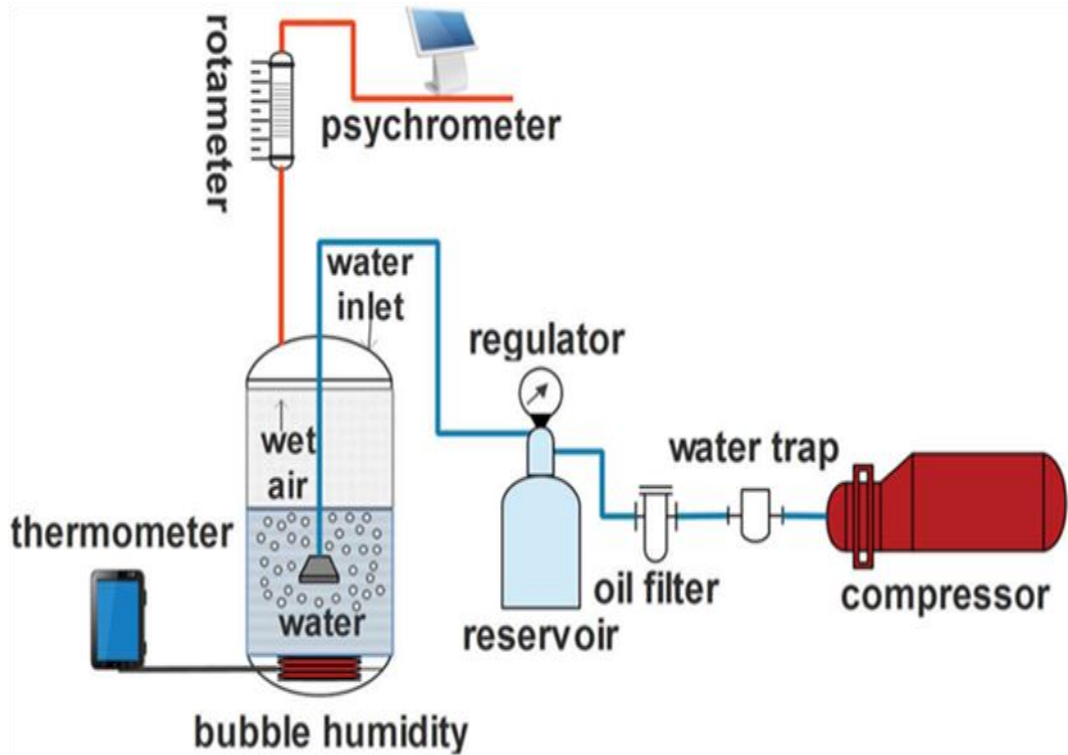


Figure 2.5. Schematic diagram of bubble humidification system [48].

Many researchers had investigated in the effect of reactant gases relative humidity on the cell performance. (Y. Liu, S. Bai et al 2020) studied experimentally and theoretically, the effect of symmetrical humidification and asymmetrical humidification as seen in Figure 2.6. The study performed at three operating temperature, where the three-dimensional model built using ANSYS-FLUENT. Temperature and heat transfer (T and HT) model. The result showed that the cathode and anode relative humidity have a different effect on the cell performance, the cathode relative humidity has an effect on the cell performance greater than anode relative humidity, any increase in the cell operating temperature leads to decrease in the cell performance under low humidity.

The rational reasons for these results are increase in the relative humidity leads to increase in the membrane water contains thereby enhance the protonic conductivity and decreases the ohmic losses lead to optimizing the cell performance [32].

(Elif Eker Kahveci and Imdat Taymaz 2015) investigated the effect of reactant gases humidification on the (PEM) fuel cell performance, so for this purpose, they developed a three-dimensional computational fluid dynamic single phase of the PEM fuel-cells model, the results were shown, the anode side inlet gas humidification has a strong effect on the cell performance.

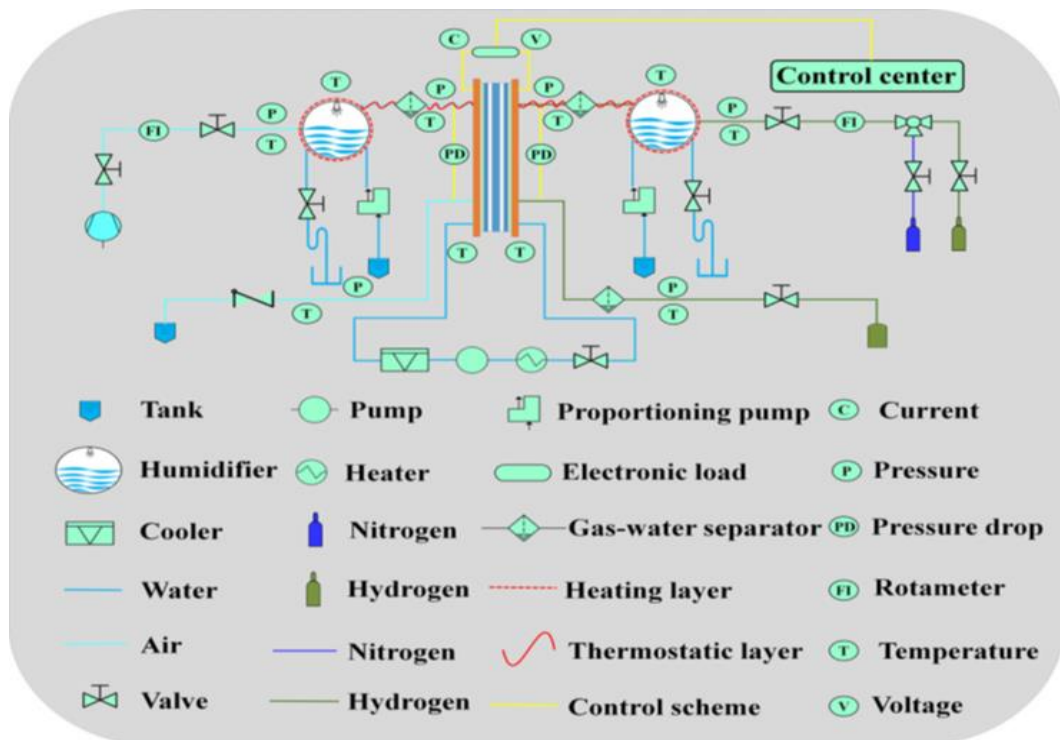


Figure 2.6. Symmetrical and asymmetrical humidification system [32].

(Burcu özsan, 2012) experimentally investigated the impact of the relative gas humidity and operating temperature on the cell performance by changing the operating temperature and relative gases humidity values as seen in Figure 2.7. The results were shown, the highest cell performance when the cell operated on 50% relative humidity for air and 100 % relative humidity for hydrogen at 60°C operating temperature, the experiment results gave an indication the humidification process has vital importance of the on the cell operation [47].



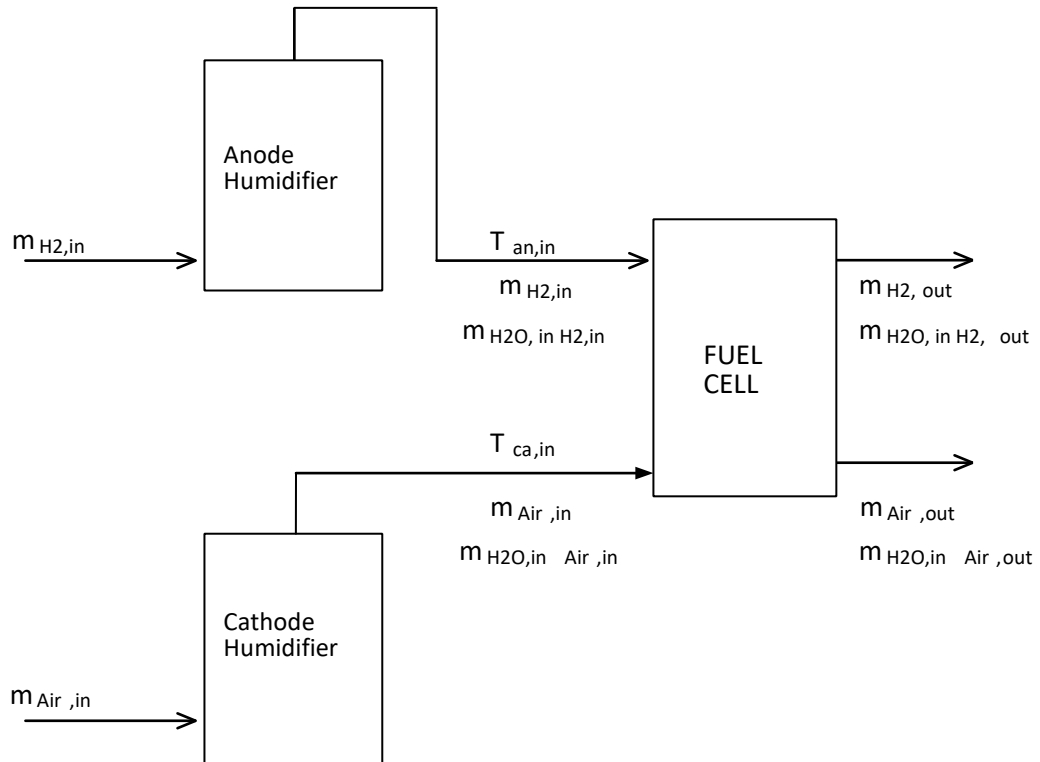


Figure 2.7. Schematic diagram for PEM fuel-cells humidification system [47].

(Iranzo et al, 2015) developed three-dimensional PEM fuel-cells model to study the impact of the reactant relative humidity on the cell performance. By using an external humidifier, the results indicated that a high hydrogen relative humidity leads to increase in the current density, in addition, high oxygen relative humidity leads to increase in the current density, the biggest value of the PEM fuel-cells performance at (0.6 V) with 90 % cathode relative humidity [49].

That is clear from the deep study in the literature working on the relative humidity close to 100% is difficult to obtained high performance from the PEM fuel-cells because the high cost of steam production. Moreover, increasing the probability to occur the electrodes flooding which can be blocks the porous of gas diffusion layers (GDLs) thereby it prevents the gases from reaching the active sites on the catalyst layers (CLs) causes in a decrease in the cell performance. Strong relationship between hydrogen and oxygen relative humidity and cell performance. Strong relationship between water management inside the cell and hydrogen and oxygen relative humidity.

### 2.3. OPERATING TEMPERATURE

Operation temperature considers the most important conditions, it has a significant impact on the cell lifetime and performance, increasing in the operation temperature result in better cell performance. But must be adjusted desired operating temperature (50°C-80°C) [40]. Some of heat quantities inside PEM fuel-cells which had been generated via electrochemical reaction this heat had a negative impact on the cell performance so an excess heat must be taken away from the cell through coolant liquid, reactant gases or the dissipation through an outer surface of the cell via heat transfer phenomena. Make a better heat management on of the vital importance issue inside the cell, this issue made by add the heat generated with electrochemical reaction and quantities of heat enters with reactant gases must be equals the heat dissipated from the cell.

(Subin & Jithesh, 2018) studied experimentally the impact of the operation temperature, self-humidification on the cell performance by using a mixed flow distributor without any modification of the cell design. The result shown that an improvement in the cell performance when he used a mixed flow distributor which he found a mixed flow distributor is a suitable for dry air operation. They were concluded; an optimum operation temperature at high cell performance under dry feeding conditions, a high-temperature result in performance losses due to water evaporation rate where contribute in the membrane dehydration [50].

(Ozen et al, 2016) investigated the influence of the inlet gases humidity experimentally, cell temperature and the oxidized type on the cell performance, the experiment performed on the (25 cm<sup>2</sup>) active area as shown in Figure 2.8 [40]. The result showed that the reactant humidification process has a positive impact on the cell performance where the ohmic resistance decreased and the membrane water content increases result in an enhancement in the protonic conductivity leads to increase in cell performance.

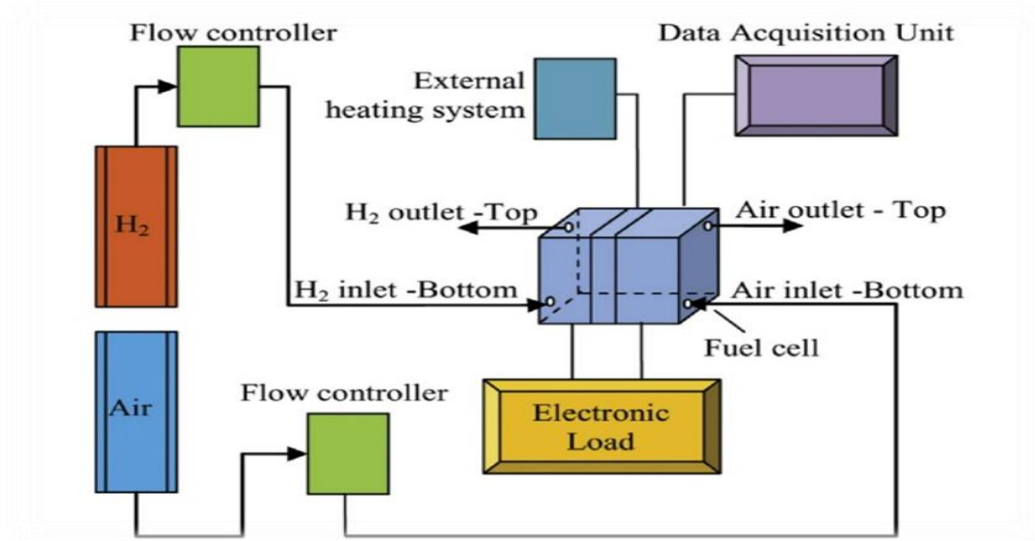


Figure 2.8. Schematic diagram of Self-humidification PEM fuel-cells system [40].

On the other hand, the impact of the cell temperature has a major importance; they also noted cell performance improvement when using pure oxygen. They concluded the strong relationship between the inlet gases humidification process and the cell performance [40]. Other study (Taymaz, 2020) developed a three-dimensional steady-state single flow channel and counter flow numerical PEM fuel-cells model to investigate the operating conditions on the cell performance. The result showed the cell operating temperature play an import role in the cell performance they founded the adverse impact on the cell temperature when operating on the 343k [52].

(H. A. Dhahad, W. H. Alawee, 2018) studied experimentally the impact of operating temperature on the cell performance, when the cell operates at a variable hydrogen flow rate and under variable electrical load as can be shown in Figure 2.9. The results were showed, when the cell operates at high operating temperature the proton exchange membrane can be dried because at high operating temperature the water evaporate rapidly due to electrochemical reaction leads to proton exchange membrane dehydration causes in decreases in the membrane protonic conductivity result in a decrease in the cell performance.

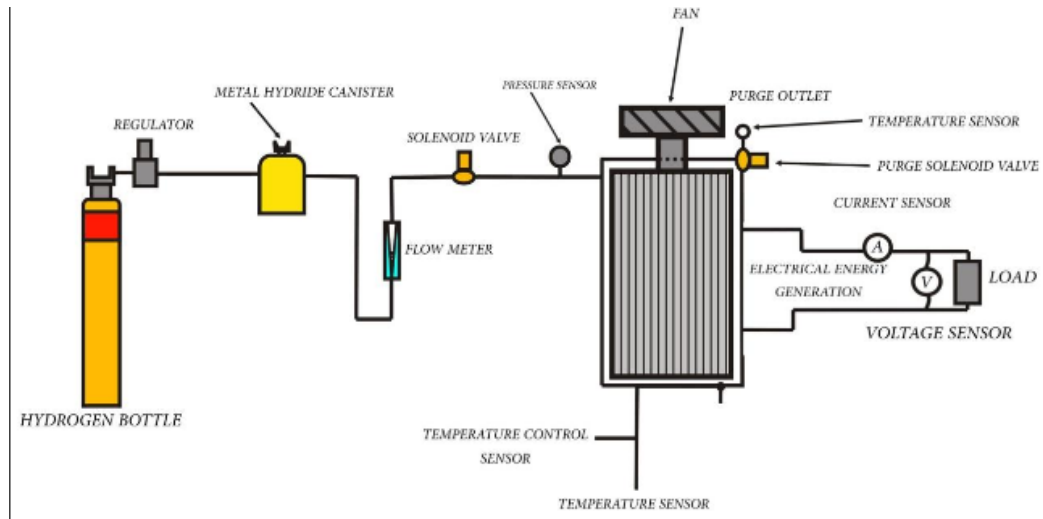


Figure 2.9. Schematic diagram of fuel cell used in experimental [41].

(E. G. Barakat, A. K. et al, 2010) experimentally studied the influence of the operating conditions such as cell operating temperature, cell-operating pressure, and relative humidity of the cell inlet gases on the cell performance as shown in Figure 2.10. The results showed: Better cell performance have been achieved at fully hydrated proton exchange membrane (PEM), an increasing in the relative humidity of the cell inlet gases leads to increase in the cell power output, an increasing in the cell operating pressure causes in increase in the cell power output, and an increasing in the cell operating temperature leads to decrease in the cell power output [53].

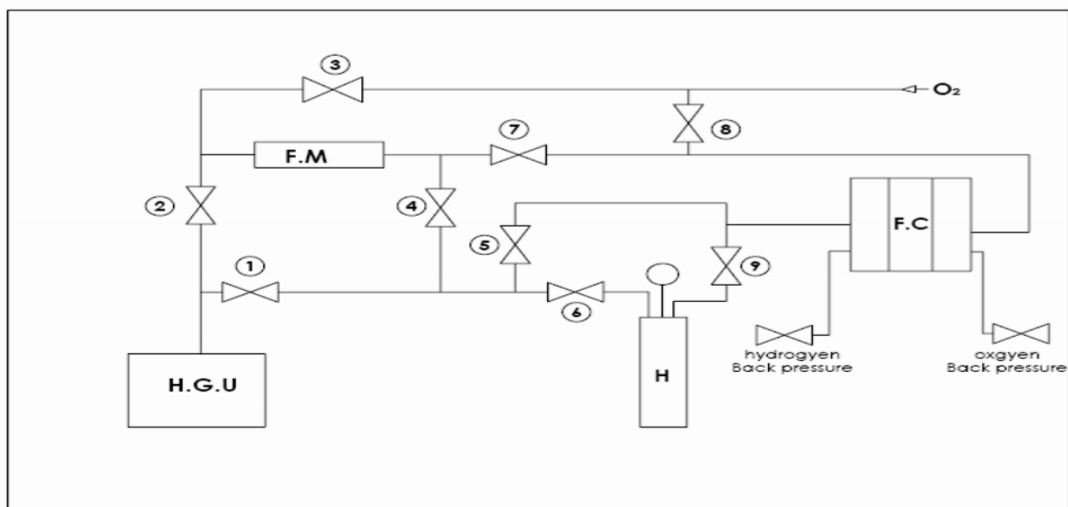


Figure 2.10. Schematic diagram of PEM fuel-cells system used in experiment [53].

## 2.4. RESEARCH PROBLEMS

Water molecules are main product from the electrochemical reactions in the PEM fuel-cell. The essential challenge toward the cell operation is membrane must maintain fully hydrated. Excessive water molecules lead blockage the flow channels, and prevent the reactant gases from reach the active sites thereby decrease the cells performance on the other hand, insufficient water maybe leads to membrane dehydration leads to increase in the ohmic resistance so decrease in the Proton exchange membrane PEM fuel-cell performance. From the deep investigate in the previous literature, it can be clear the strong relationship between the cell operation temperature and cell performance. Operation temperature considers the most important operation working.

Deep investigation in the previous literature, good cell working is achieved by good water management strategies, that is done by adjusting the proper operating temperature and inlet gases humidity so the research problems assigned in the water management issue as and the research aims to following:

- Working with proper proton exchange membrane water levels by select proper cell operating temperature and proper inlet gases relative humidity.
- Study the effect of various values of inlet gases relative humidity on the cell performance to select the proper value.
- Study the impact of various values of cell operating temperature on the cell performance to select the proper value.

### PART 3

### METHODOLOGY

This Part presents a numerical simulation of the PEM fuel-cell. The process had performed on the ANSYS-FLUENT included solving all governing equation as show in Figure 3.1. Part 3 aims to develop a three-dimensional PEM fuel-cell model to examined cell performance under three operating temperatures (55-65-75°C) and three values of hydrogen and oxygen relative humidity (50%-70%-90%) by select optimum operating temperature and select inlet humidification values.

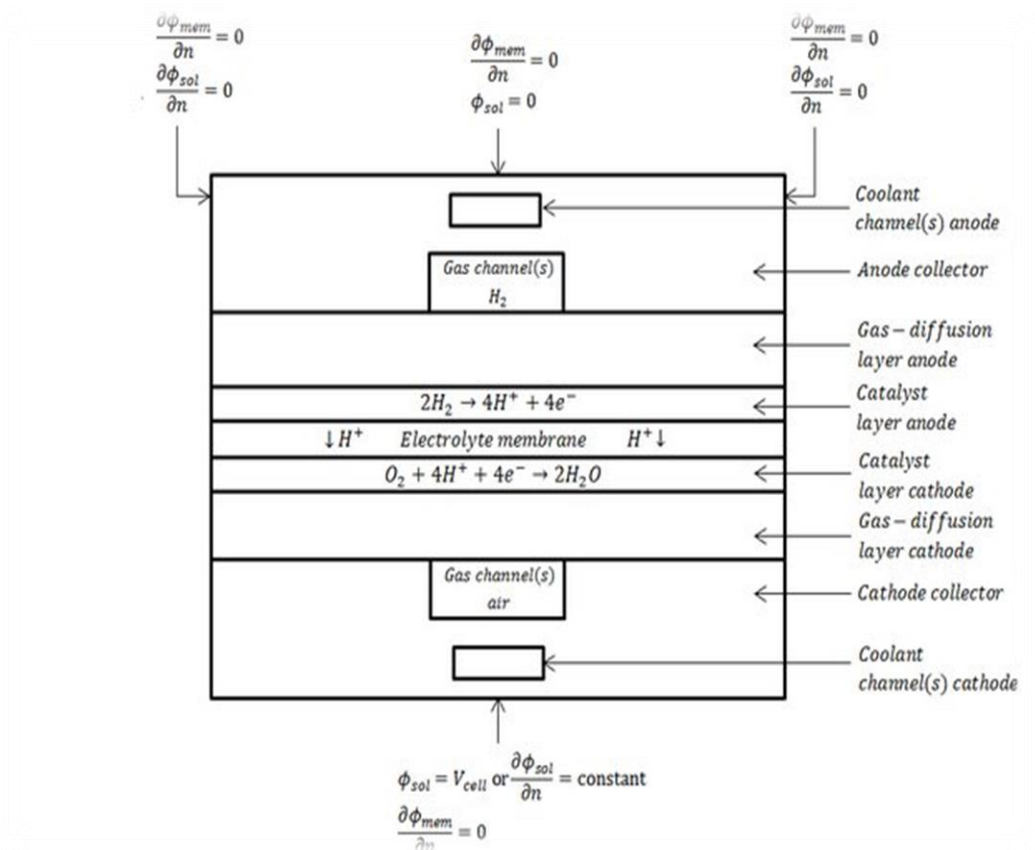


Figure 3.1. Equations which describes an electrochemical reactions in the cell [54].

### 3.1. NUMERICAL MODEL

Three-dimensional PEM fuel-cell model has been created using (CFD) commercial software ANSYS–FLUENT. The main objective of the cell modelling is to describe chemical and physical phenomenon that occurs inside the cells as can be seen in Figure 3.1. PEM fuel-cell simulation process includes three steps namely, preprocessing, processing, and post-processing as can be shown in Figure 3.2.

- Preprocessing: include the Three-dimensional model designing process in the SolidWorks 2020 software. [58].
- Processing: includes solving the conversation governing equation and electrochemical equation numerically to capture the flow properties of the PEM fuel-cell.
- Post-processing: provide a clear understanding for simulation results and includes the display of the obtained results from the three-dimensional model simulation as contours or curves or video animation [59].

### 3.2. MODEL ASSUMPTIONS

In order to simplify the complex phenomena that is takes place inside the cell including a mass, momentum, electrochemical reactions take place and heat transport, the fallowing assumption are used for modeling process:

- Fluid flow is study state and obey to Ideal gas law.
- Fluid flow inside the cell channel are laminar.
- The operating voltage was fixed 0.7 V.
- Thermodynamics properties of the gases and the cell sold materials were assumed a constant.
- Butler-volmer equations are used for electrochemical rate.

- Iso- isotropic and (GDLs), (CLs) and (PEM) were assumed to be homogenous electrodes.
- Non iso -thermal operating temperature was varying from 70°C- 80°C-90°C, to investigate the effect of operating temperature on the (PEM) fuel cells.
- Catalyst layers (CLs) and gas diffusion layers (GDLs) and proton exchange membrane were considered a porous zones.
- The effect of the gravity assumed as a negligible value.

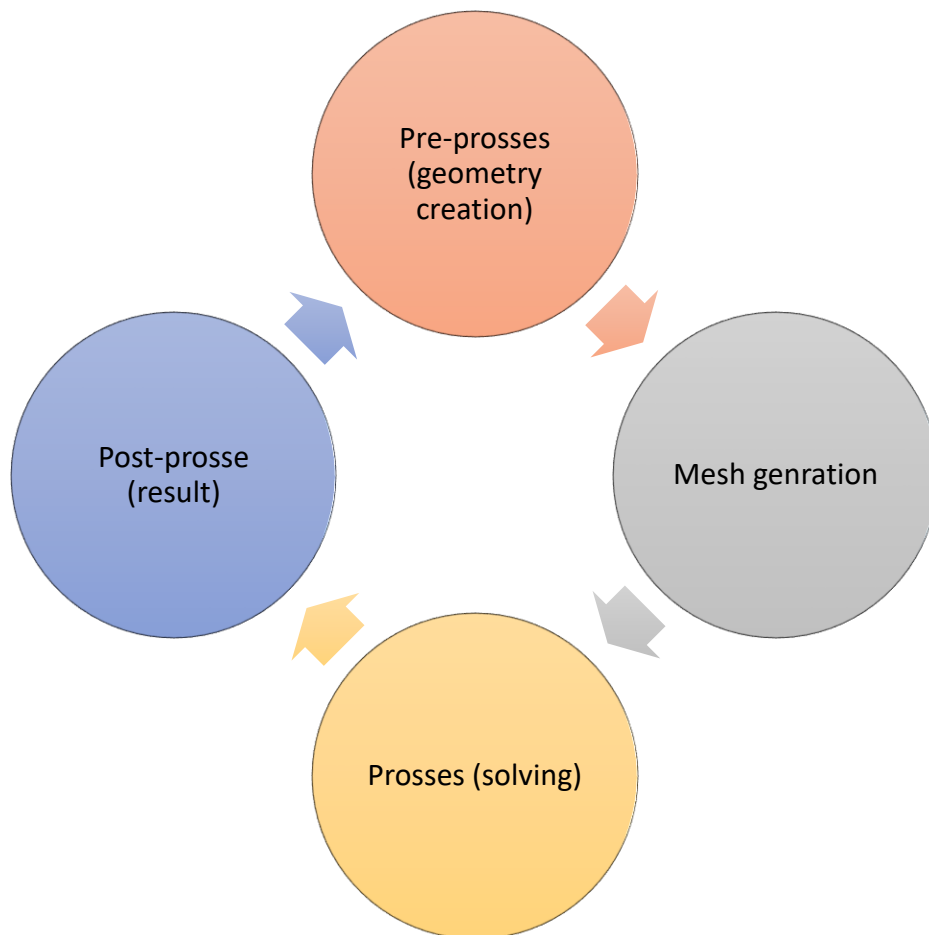


Figure 3.2. PEM fuel-cell simulation steps.



### 3.3. GEOMETRY CREATION

PEM fuel-cell geometry creation is the first step in the cell simulation proses. Many of the computer-aided design software is available to do this task like SOLDWORK, GAMBIT, AUTOCAD, NT, ANSYS-DESIGN MODELER, and ANSYS–Space Claim. In this study. PEM fuel-cell geometry has been created by using ANSYS–Space Claim. Major aim of the geometry creation is to capture the physical dimensions of the real cell [60]. By using ANSYS–Space Claim cell geometry had been designed, including a nine layers: anode flow filed plates (FFPs-A), anode flow channels (FCHs-A), anode gas diffusion layers (GDLs-A), anode catalyst layers (CLs-A), proton exchange membrane (PEM), cathode catalyst layers (CLs-C), cathode gas diffusion layers (GDLs-C), cathode flow channels (FCHs-C), cathode flow filed plates (FFPs-C) as shown in Figure 3.3.

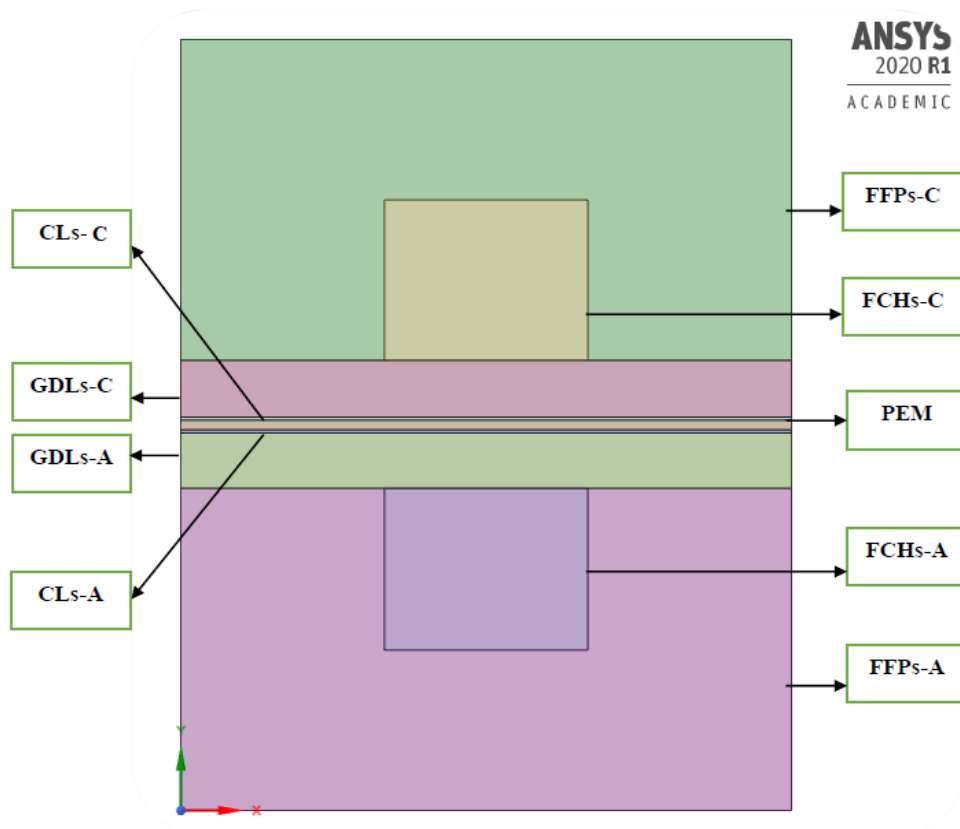


Figure 3.3. Nine parts of the PEM fuel-cell used in geometry creation.

### 3.4. MESH GENERATION

PEM fuel-cell mesh generation process has been implemented by using ANSYS-DESIGN MODDELER-MESHING. By using hexahedral meshing method. The mesh generation process has a strong effect on the model results accuracy, so the good mesh generation is one of the difficult steps during the cell simulation. In order to obtain a high result accuracy, must be a balance between the cell geometry and the number of mesh elements and available memory of the computer. Where the specifications of the used hardware in the simulation process in a quad-core HP Elite Book 8560 p workstation with 4.0 GB as a RAM, 2.50 GHz with windows 10 as an operating system, the solver used 3.5 GB RAM". (PEM) fuel cell divided into 270000 finite elements to prepare the model for enters to the solver "FLUENT ", the time of computation in this thesis 12 hour. Three-dimensional model has been discrete to 270000 elements with 15 components. Figure 3.4. Shows the cell with mesh generated. The total number and the number of the elements generated for each component of cells listed in Table 3.2.

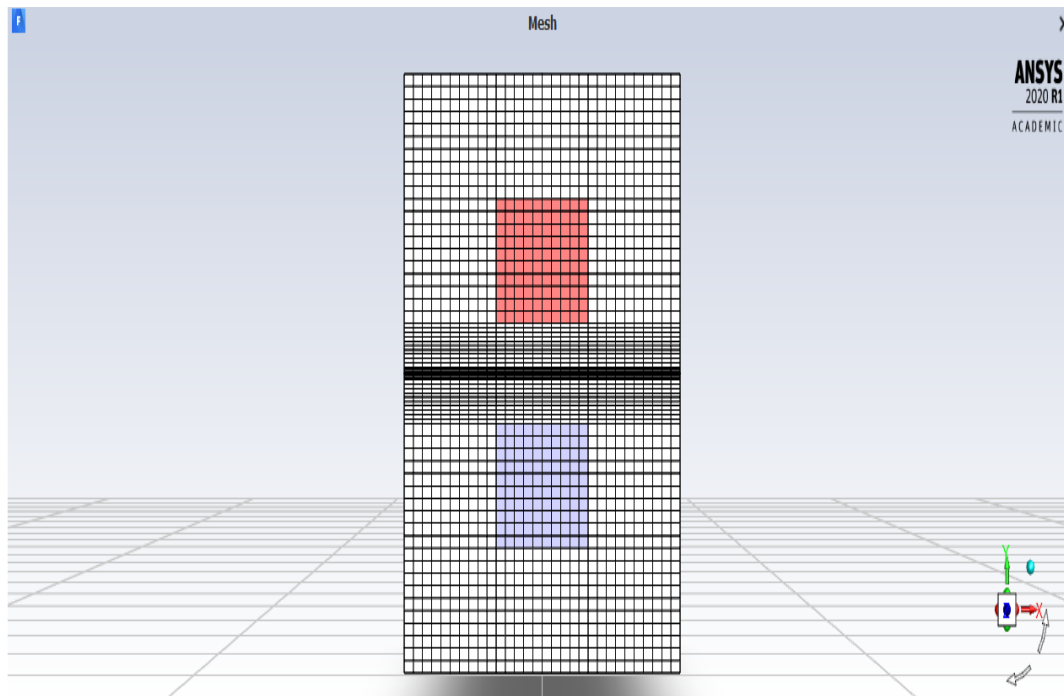


Figure 3.4. Mesh generation process.

Table 3.1.Explained the PEM fuel-cell model geometries.

<b>Layers</b>	<b>Units</b>	<b>Dimensions</b>
Flow filed plates thickness	Mm	1.2
Flow filed plates width	Mm	2.4
Flow channels length	Mm	20
Flow channels high	Mm	0.6
Flow channels width	Mm	0.8

Table 3.2. Number of cell generated elements

<b>Layers</b>	<b>Number of generated elements</b>
Flow filed plates	62500
Flow channels (FCHs)	12500
Gas diffusion layers (GDLs)	37500
Catalyst layers (CLs)	15000
Proton exchange membrane (PEM)	30000
Overall cell ELEMENTS	270000
Minimum Orthogonal Quality	2.3
Maximum Aspect Ratio	3.3

Name selection step performed in ANSYS-DESIGN MESHER where the PEM fuel-cells have been divided into eight as (Cathode flow field plats (CFFPs), Anode flow field plats (AFFPs), Hydrogen flow fields, Oxygen flow fields, Cathode-terminal, Anode-terminal, Membrane electrode assembly, PEM fuel-cell -side wall) components as shown in Figure 3.5. And named each component to prepare their to insert to the ANSYS-FLUNET solver.

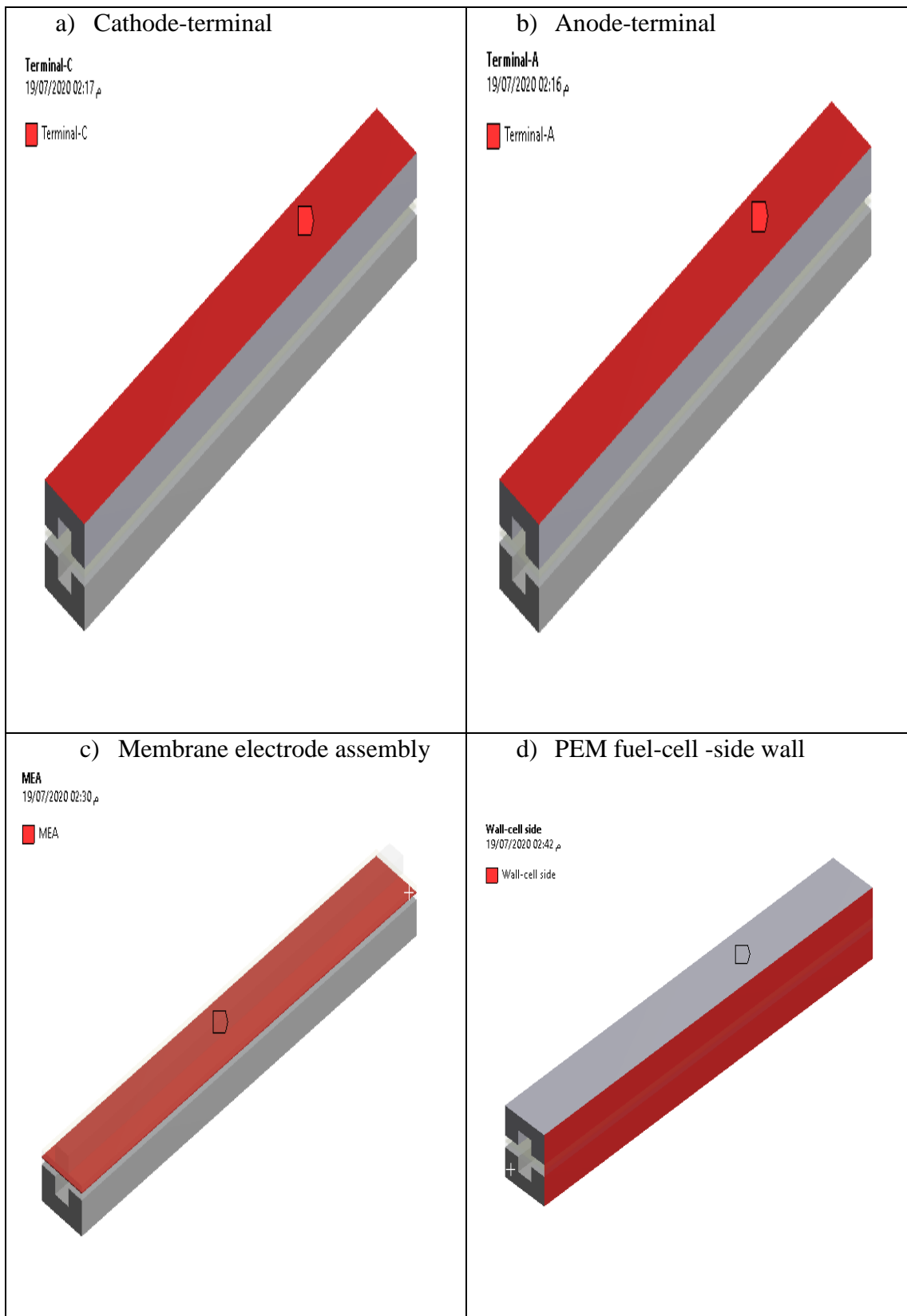


Figure 3.5. Name selection of PEM fuel-cell used in simulation.

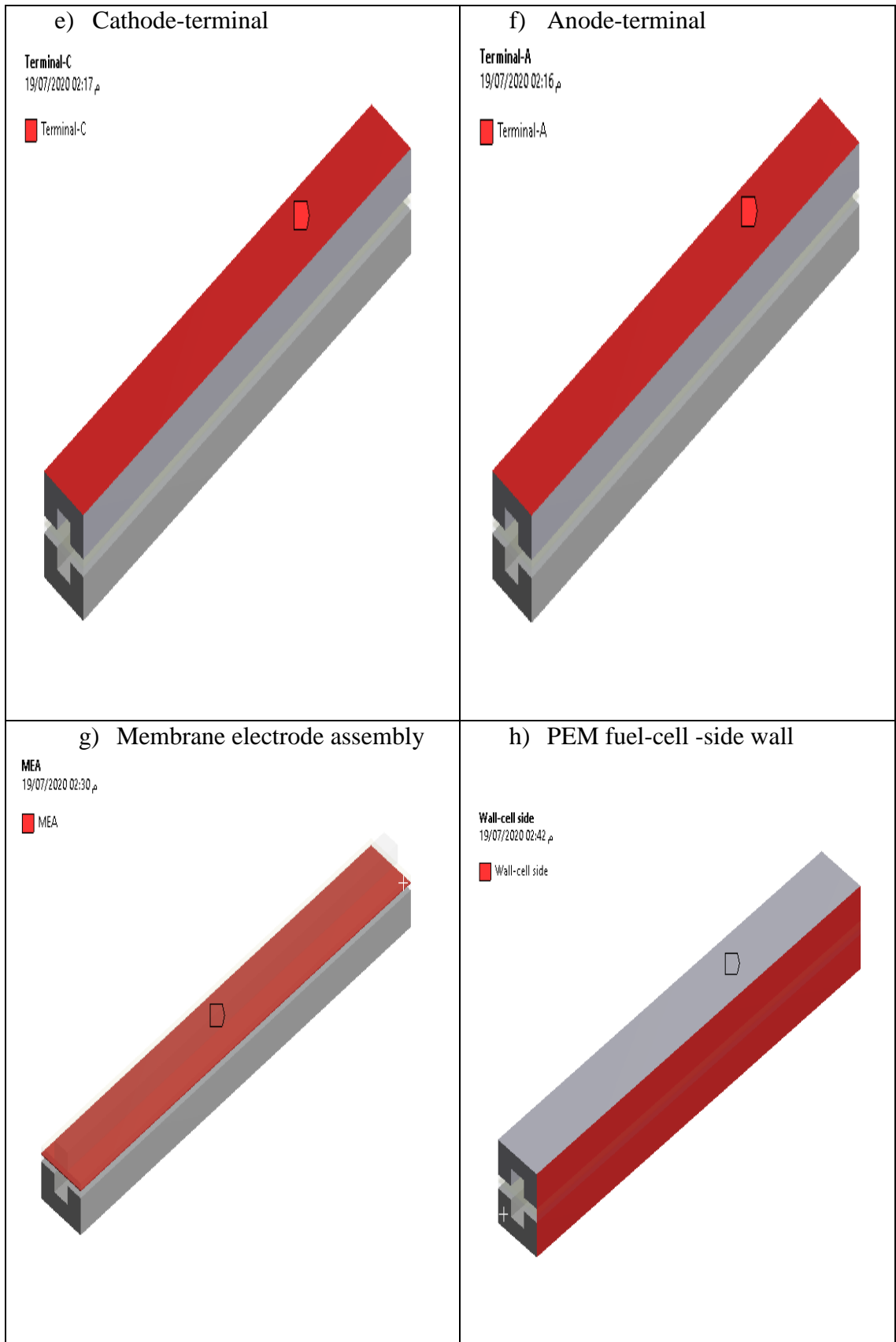


Figure 3.5. (Continued)

### 3.5. BOUNDARY CONDITIONS

Hydrogen gases are enters to fuel cell through the flow channels (FCHs) in anode side then diffused through the gas diffusion layers (GDLs) to reach the active sits on the catalyst layers (CLs), an electrochemical reaction occurs on the catalyst layer surface result in oxidizing hydrogen atoms into electron and proton. Proton migrate from anode side to the cathode side through the proton exchange membrane while the electrons travel from the anode side to cathode side via an external load.

On the anode side an electrochemical reaction takes place on the anode side (CLs) surface between the hydrogen and platinum particles result in oxidizing the hydrogen to one electron and one proton. Protons are transfers from the anode to the cathode across the membrane, electrons moving via an outer load circuit from the anode to the cathode. On the cathode side an electrochemical reaction takes place (CLs) surface between the electrons and protons and oxygen on the cathode, result in water formation and release some heat equation.

The boundary condition and solver setup process has been implemented by using ANSYS-FLUENT. Refer to Figure 3.4. The boundary location 3-5. Anode and cathode inlet zones are set to be mass flow rates, where the gases flow (*hydrogen on the anode side–oxygen on the cathode side*) will enters through the cell. The boundary location at other side from flow channels are set to be pressure outlet condition specified where the flow leave from the cell. At the boundary location 2-6. Anode and cathode flow filed plats were sets, there are no proton leaves the cell so we enforce the membrane sloid potential equal to zero. Boundary location 1-7. Were set to be anode and cathode terminals.

The cell potential will difference. At the cathode terminal the  $V_{CELL}$  = membrane solid potential, where membrane solid potential equals to zero at anode side. Anode flow channels, (GDLs), (CLs), (PEM), and cathode flow channels, (GDLs), (CLs) were set to be fluid zones where the anode and cathode flow filed plates were set to solid zones, table 3.3. Summarize the main parameter condition used in the simulation.

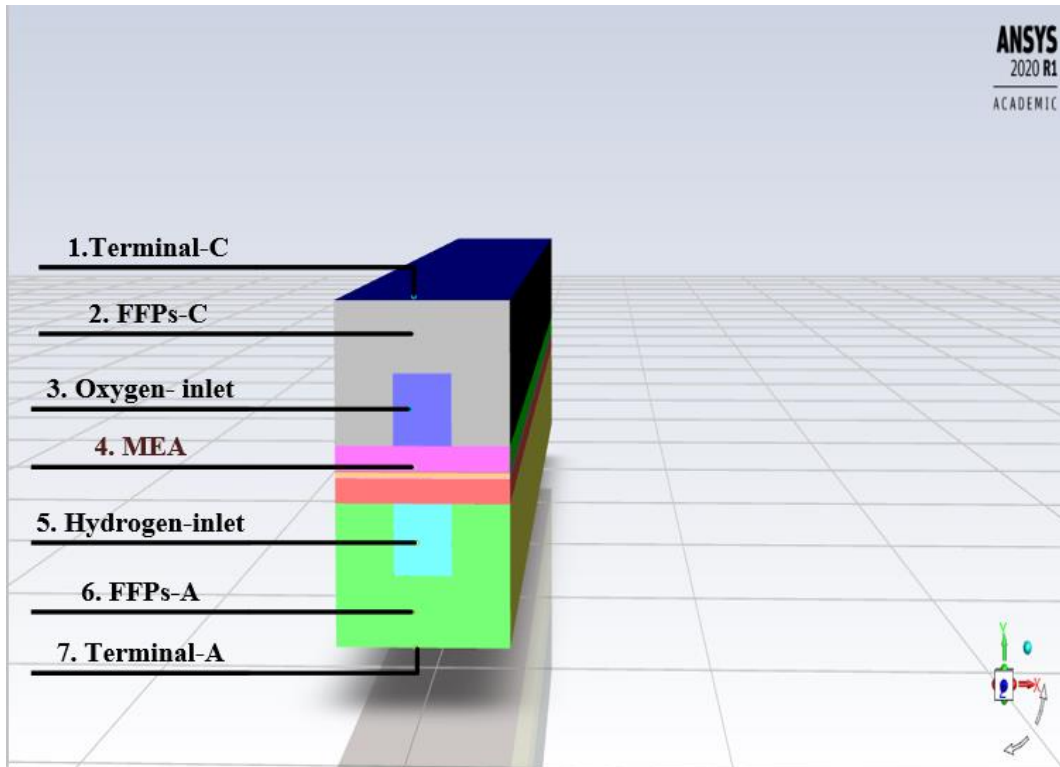


Figure 3.6. Boundaries assignment in the PEM fuel-cell modeling

Table 3.3. Necessary parameters and boundaries for requirement studies model.

Parameters	values	Units
Operating temperature	Uninform	K
Operating pressure	200000	Pa
H <sub>2</sub> mass flow rates	4.1996e-8	Kg/s
O <sub>2</sub> mass flow rates	5.2e-7	Kg/s
Anode outlet gas pressure	0	Pa (gage)
cathode outlet gas pressure	0	Pa (gage)
Anode inlet mass friction H <sub>2</sub>	0.85	-
O <sub>2</sub> cathode inlet mass friction	0.2	-
H <sub>2</sub> O inlet mass friction	0.1	-
H <sub>2</sub> O inlet mass friction	0.08	-

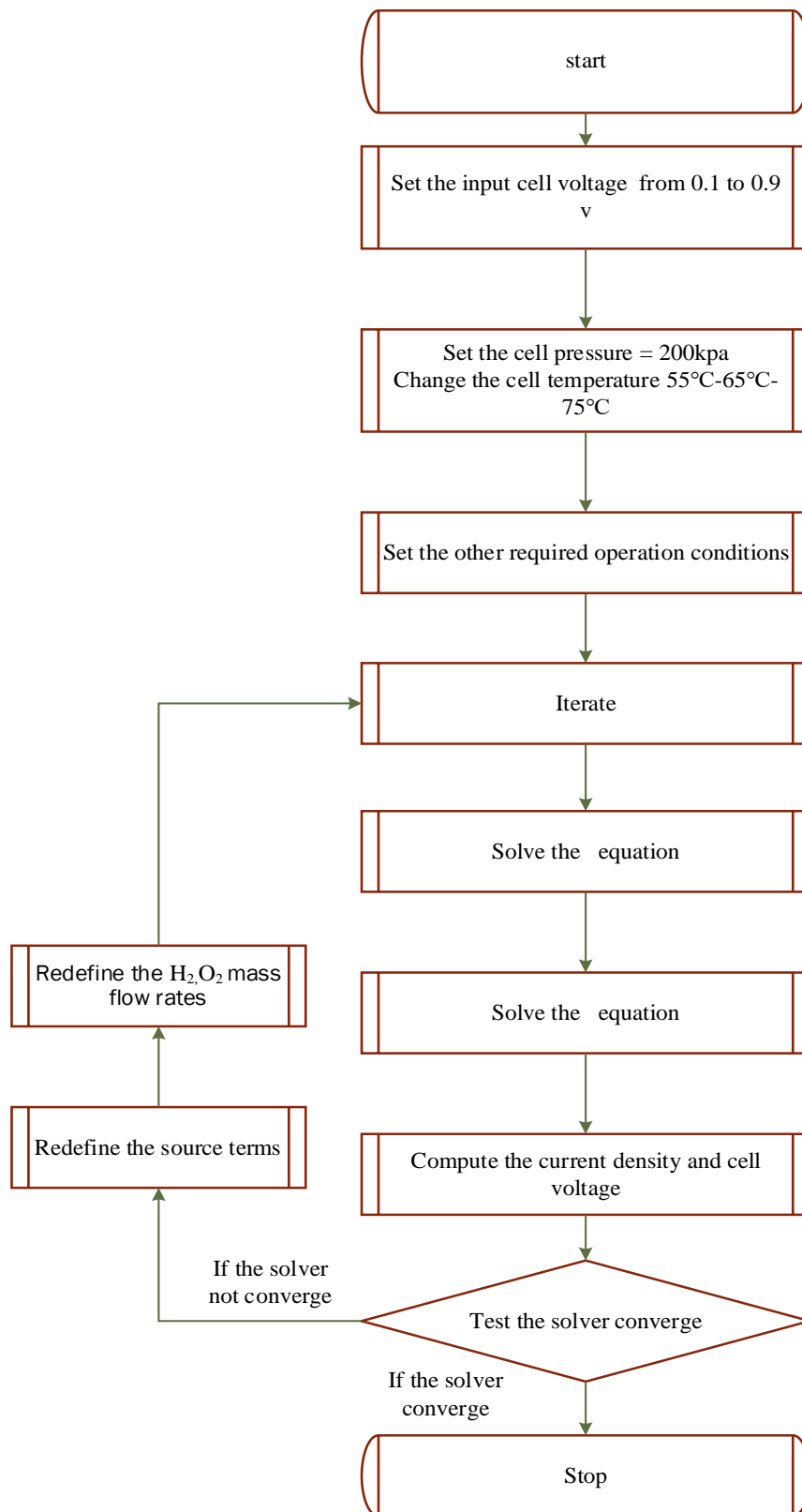


Figure 3.7. Flow chart of the PEM fuel-cell simulation process.



## PART 4

### SIMULATION RESULTS AND MODEL VALIDATION

#### 4.1. MODEL VALIDATION

Simulation results have been processed using ANSYS-CFD-POST, simulation results have validated with the experimental data which was taken from Wilberforce 2019 [1]. Good agreement was obtained between the currently computational model and Wilberforce 2019 experiment, expect the small difference in the current density value ( $0.0072A/cm^2$ ), the current density difference due to poor cell performance because of the negative effect of the electrode flooding which was neglected in mathematical model. Table 4.1. Listed the cell dimension used in the experiment experiment. Polarization curve and power output curve obtained from the mathematical model were compared with the polarization curve and power output curves obtained from mentioned experiment. Figure 4.1. Figure4.2. shows the variation of the cell performance and power output respectively.

Table 4.1.Cell dimensions used in the experiment [1].

Parameters	Dimensions (mm)
Membrane thickness	0.05
Catalyst layers thickness	0.15
Gas diffusion layers thickness	0.5
Width of flow channel	1.99

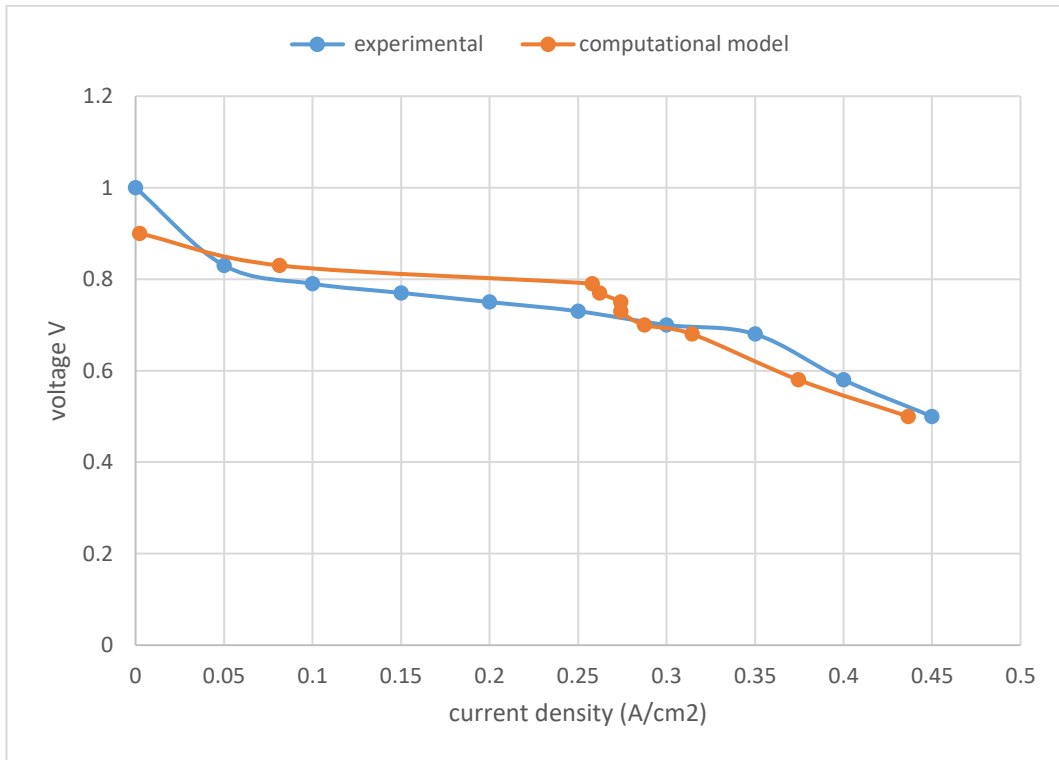


Figure 4.1. Numerical validation with Wilberforce 2019 experiment.

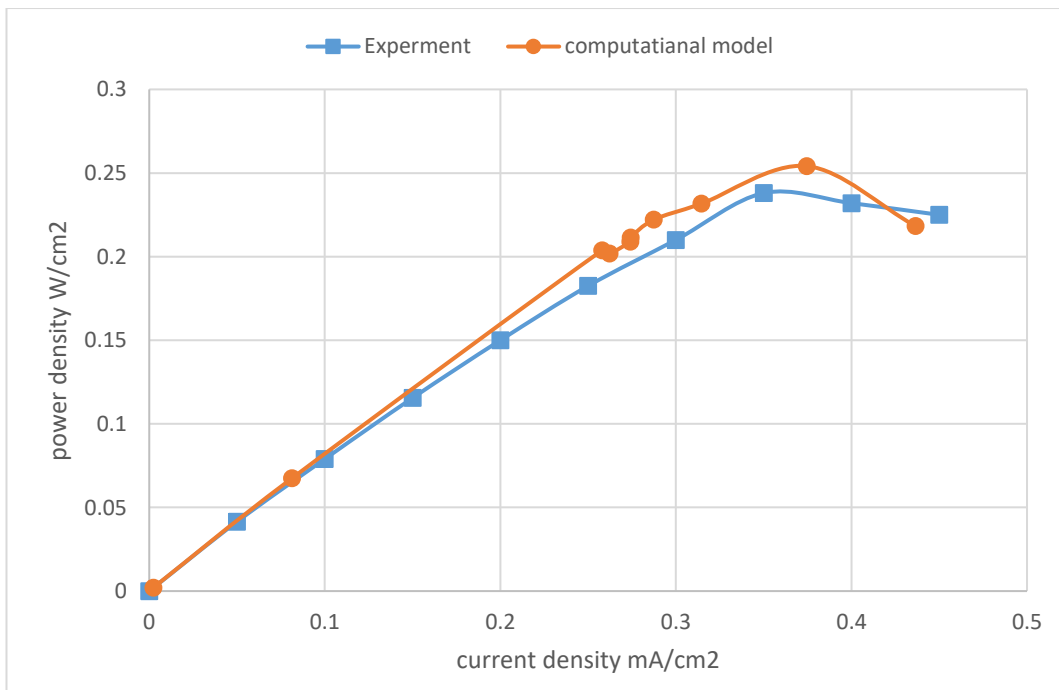


Figure 4.2. Numerical validation of the (I-P) with Wilberforce 2019 experiment.

## 4.2. OPERATING TEMPERATURE

The PEM fuel-cells performance influenced by many parameters as operating pressure stoichiometric ratio, reactant gas relative humidity and operating temperature. Operating temperature has a strong effect on the (PEM) fuel cells performance.

Generally, PEM fuel-cells operate at operating temperature between (50°C–90°C). Any decreasing in the cell working temperature less than (50°C), result in increasing in water condensation rates and increase the possibility of the electrode flooding, which result in decreases in the protonic conductivity of the proton exchange membrane (PEM). Any decreasing in the cell operating temperature less than (50°C) caused in decrease the cells performance, on the other hand, any increase in the cell operating temperature over than (90°C) result in an:

- Increase in the cell potential losses due to entropy generation from the electrochemical reaction.
- Decreasing the open-circuit voltage (OCV).
- Increase in the electrochemical rates.
- Decrease the over- potential activity.
- Increase the water removal rates may result in membrane dehydration thereby decrease in the protonic conductivity of the proton exchange membrane (PEM).

Therefore, any increase in the cell operating temperature than 90°C caused in decrease the cell performance, increase and decrease in the operating temperature influenced on the cell performance, so suitable operating temperature must be selected carefully, in this thesis three values of the operating temperature have been examined (55°C- 65°C- 75°C).

The effect of operating temperature on the PEM fuel-cells have been studied and analyzed, the simulation results indicated the cell performance strongly affected by the operating temperature as show in Figure 4.3. Similarly, cell power density strongly affected by the operating temperature too. Figure 4.4. Polarization curve (I-V) indicates that the cell performance was decreasing when the cell operated on high temperature.

In this study, operating temperature varied between (55°C-65°C-75°C) to investigate the effect of operating temperature on the cell performance. The result was showed the greatest cell performance was obtained at 55°C, and the cell performance slightly decreases when the cell operates on the 65°C. Figure 4.3. Explained the polarization curve indicates the cell performance was decreases with high operating temperature, so, ionic conductivity for membrane decreases with high operating temperature, therefore the cell performance were decreases with 75°C, operating temperature because at the high operating temperature causes leads to water evaporation rate due to condensation process greater than water formation rate due to electrochemical reaction.

And the decreasing in the reactant gases relative humidity, So the proton exchange membrane (PEM) suffer from the decrease in the water content result in decrease in the ionic conductivity of membrane causes in cell performance decreases. Table 4.2. Variations in the current density and power density. The operating temperature influence on the activation energy, ohmic resistance, open circuit voltage (OCV), gases diffusivity, and ionic conductivity of proton exchange membrane (PEM).

Where at 75°C operating temperature power density and current density decrease because of the high water evaporation rate, thereby decreases the water content in the proton exchange membrane (PEM) result in decreases in cell efficiency due to activation losses, on the other hand, the maximum cell power output was obtained on the 55°C operating temperature. Figure 4.5. Explained graphically the distribution of the Exchange current density on the Z.Y Plan.

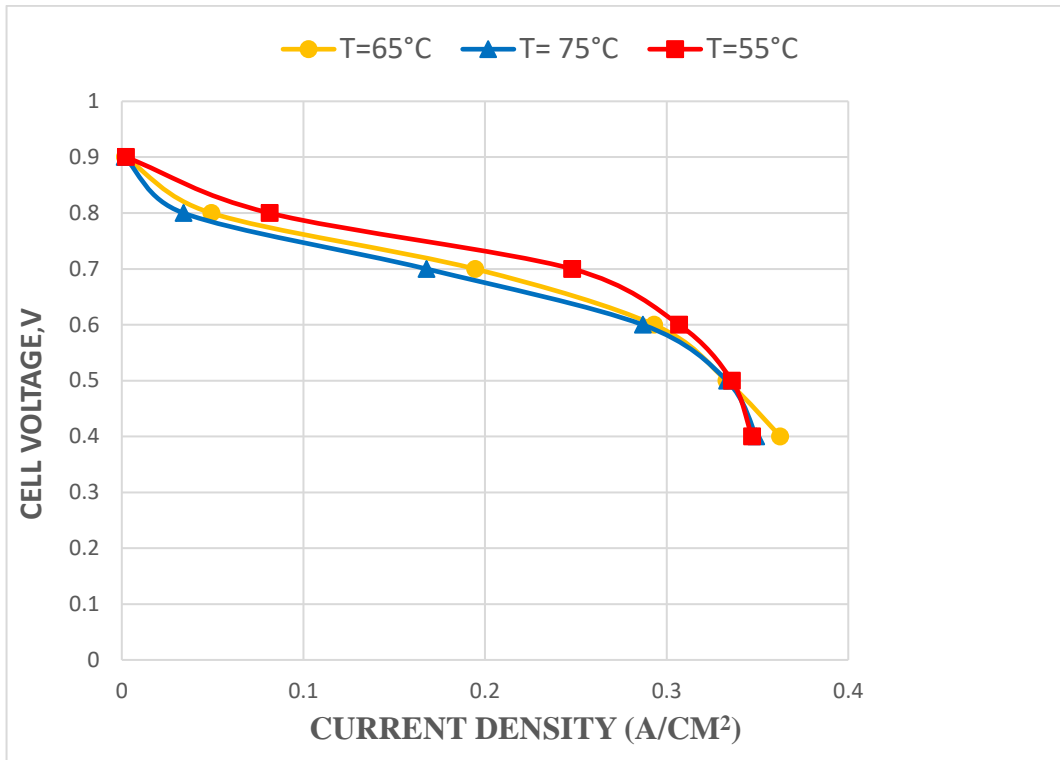


Figure 4.3. (I-V) Curve at various cell operating temperature.

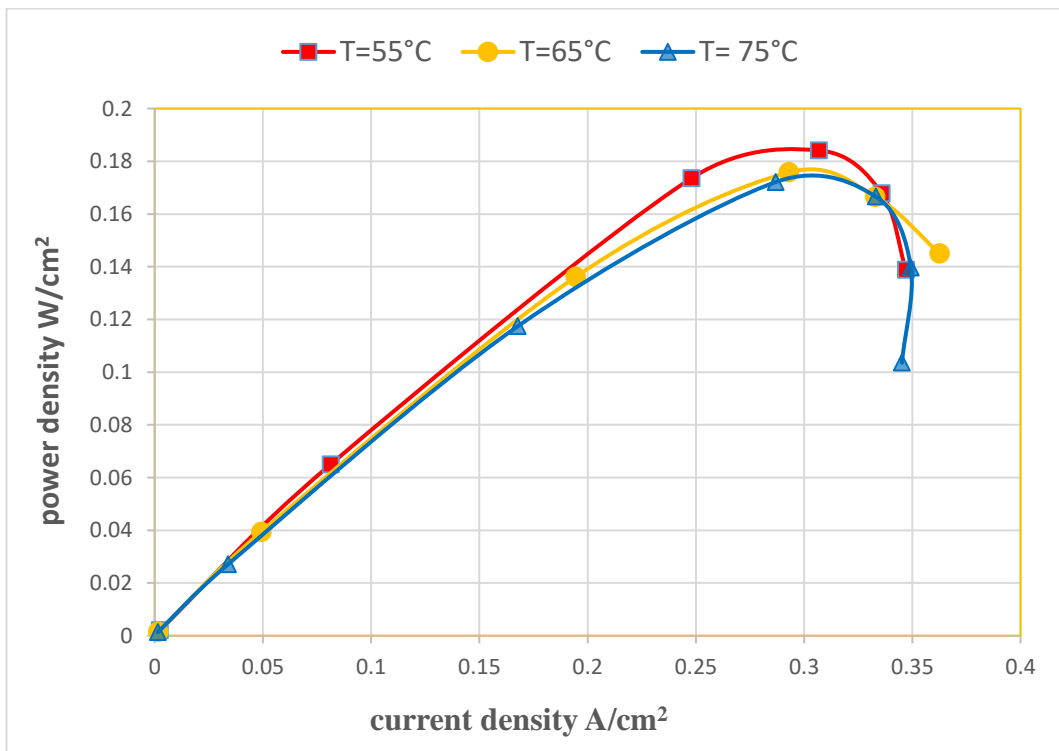


Figure 4.4. (I-P) Curve at various cell operating temperature.

Table 4.2. Cell current, voltage and power output at a) 55°C, b) 65°C, c) 75°C

a)

<b>Current density A/cm<sup>2</sup></b>	<b>Cell voltage V</b>	<b>Cell power density W/cm<sup>2</sup></b>
0.002279	0.9	0.002051
0.081305	0.8	0.065044
0.247974	0.7	0.173582
0.306831	0.6	0.184099
0.335807	0.5	0.167904
0.347028	0.4	0.138811

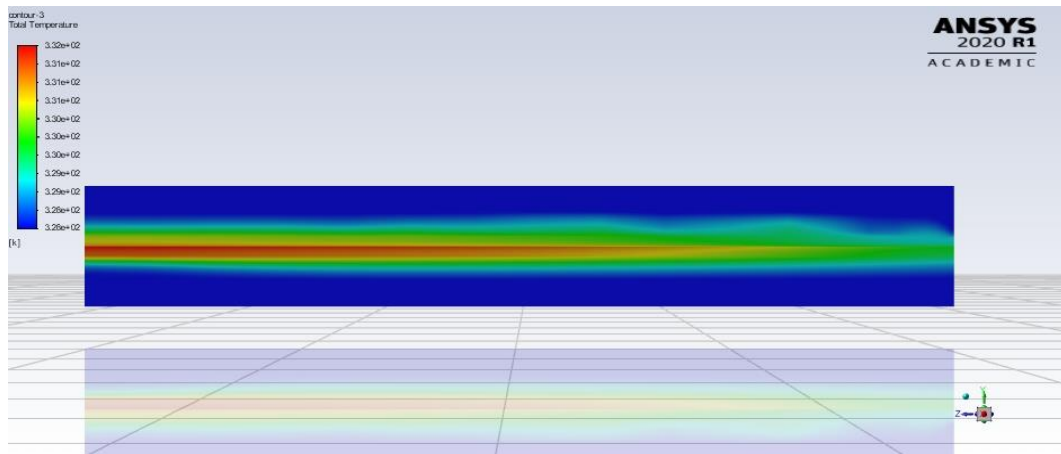
b)

<b>Current density A/cm<sup>2</sup></b>	<b>Cell voltage V</b>	<b>Cell power density W/cm<sup>2</sup></b>
0.001658	0.9	0.001492
0.049183	0.8	0.039346
0.194421	0.7	0.136095
0.292999	0.6	0.175799
0.332922	0.5	0.166461
0.362614	0.4	0.145046

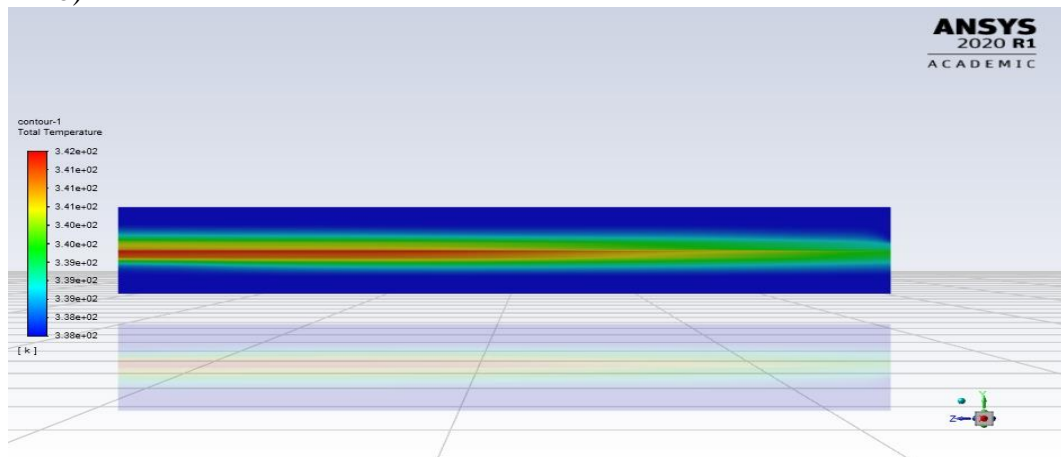
c)

<b>Current density A/cm<sup>2</sup></b>	<b>Cell voltage V</b>	<b>Cell power density W/cm<sup>2</sup></b>
0.001508	0.9	0.0013572
0.033905	0.8	0.027124
0.167742	0.7	0.1174194
0.286842	0.6	0.1721052
0.333146	0.5	0.166573
0.382614	0.4	0.147046

a)



b)



c)

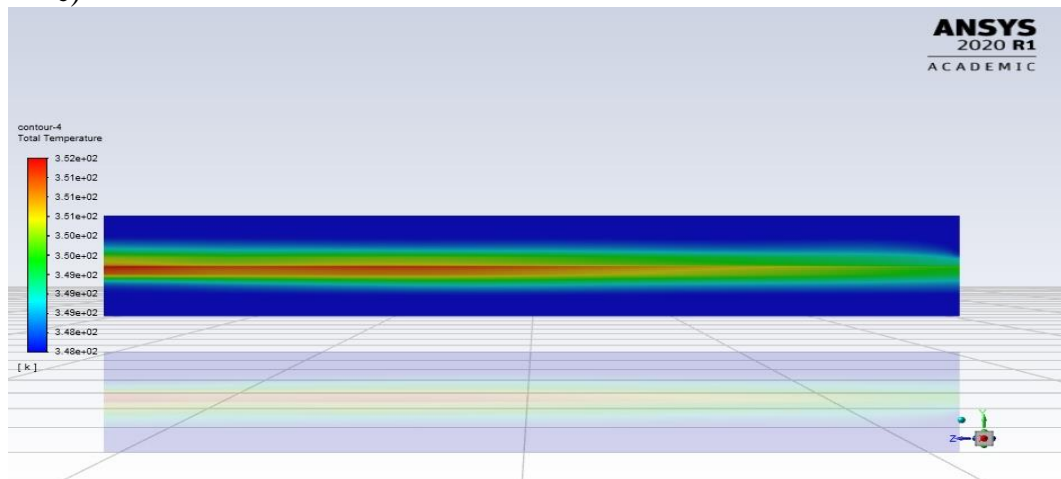


Figure 4.5. An Exchange current density distribution on the PEM fuel-cells at a) 55°C cell operation temperature, b) 65°C cell operation temperature, c) 75°C cell operation temperature.

### **4.3. RELATIVE HUMIDITY**

In this study, the effect of the hydrogen and oxygen relative humidity had investigated. Three ratios of hydrogen and oxygen relative humidity (50%-70%-90%) have been examined, obtained results from the (CFD) simulation were indicated the following: There are strong relationships between the hydrogen and oxygen gases relative humidity and the cell performance. The working on the relative humidity close to 100% considered major challenge to obtained high performance from the PEM fuel-cells because the high cost of steam production. In addition, increasing the probability to occur the electrodes flooding which blocks the porous of gas diffusion layers (GDLs) thereby it prevents the gases from reaching the active sites on the catalyst layers (CLs) causes in a decrease in the cell performance. Strong relationship between hydrogen and oxygen relative humidity and cell performance strong relationship between water management inside the cell and hydrogen and oxygen relative humidity.

#### **4.3.1. Anode side relative humidity**

The polarization curve in Figure 4.6. Shows high performance obtained when the oxygen gases 90% humidified, while the cell performance slightly decreases when the oxygen 50 % humidified. The variation of the hydrogen gases relative humidity values from the 90% to 50% at a low current density has a little effect on the cell performance because of the water transport From the cathode side to anode side via back diffusion mechanism which contributed to maintain the anode side humidified. Figure 4.7. Shows the utilizing humidified hydrogen gases as a reactant gas has a positive impact on the cell power output because the proper membrane water content which enhance the membrane protonic conductivity and decreases the ohmic resistance hence improve the cell performance. PEM fuel-cells will generate more current when using 90% relative humidity of the hydrogen gases. Figure 4.7. Shows the maximum power density was obtained when the hydrogen gases were 90 % humidified and operated at (3.2 W/cm<sup>2</sup>) and current density (0.62 A/cm<sup>2</sup>). The important reason for this result are humidified hydrogen gas contributes to marinated high membrane water content level leads to optimize the protonic conductivity and decreases the ohmic resistance causes in increasing in the cell performance.



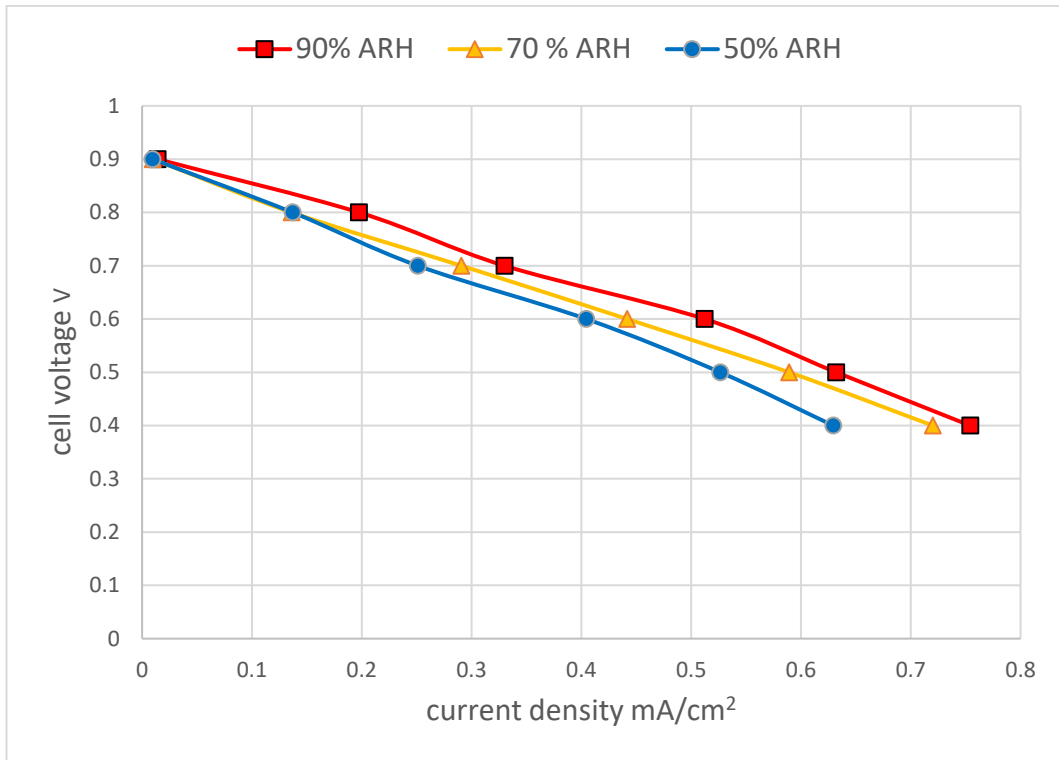


Figure 4.6. (I-V) Curve at various cell anode relative humidity.

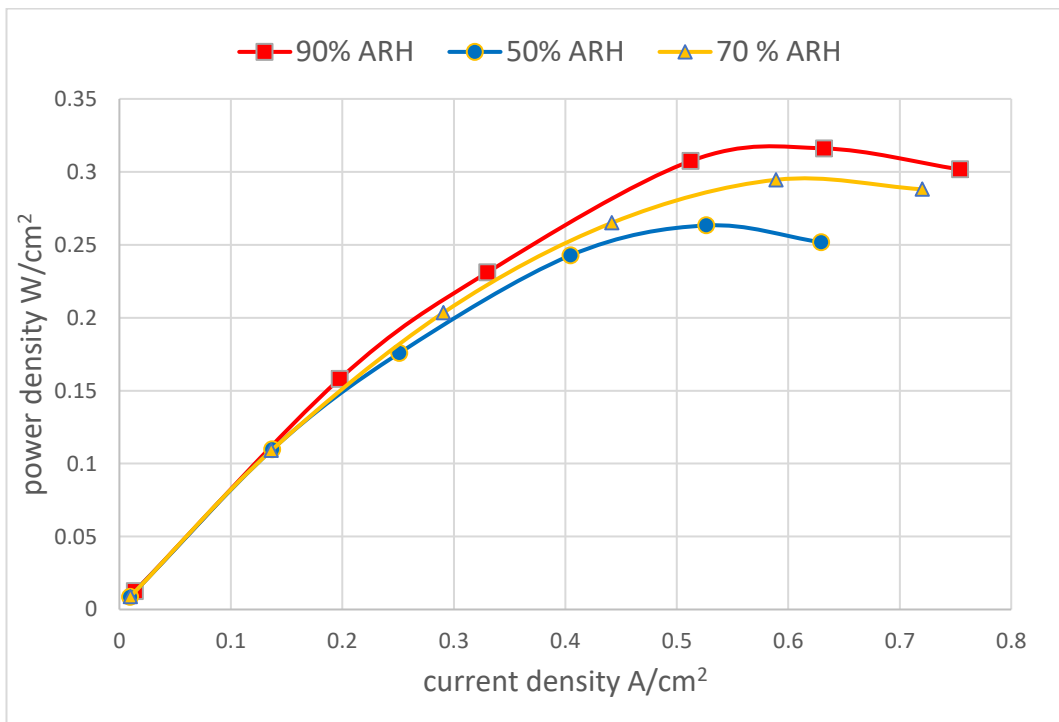


Figure 4.7. (I-P) Curve at various cell anode relative humidity.

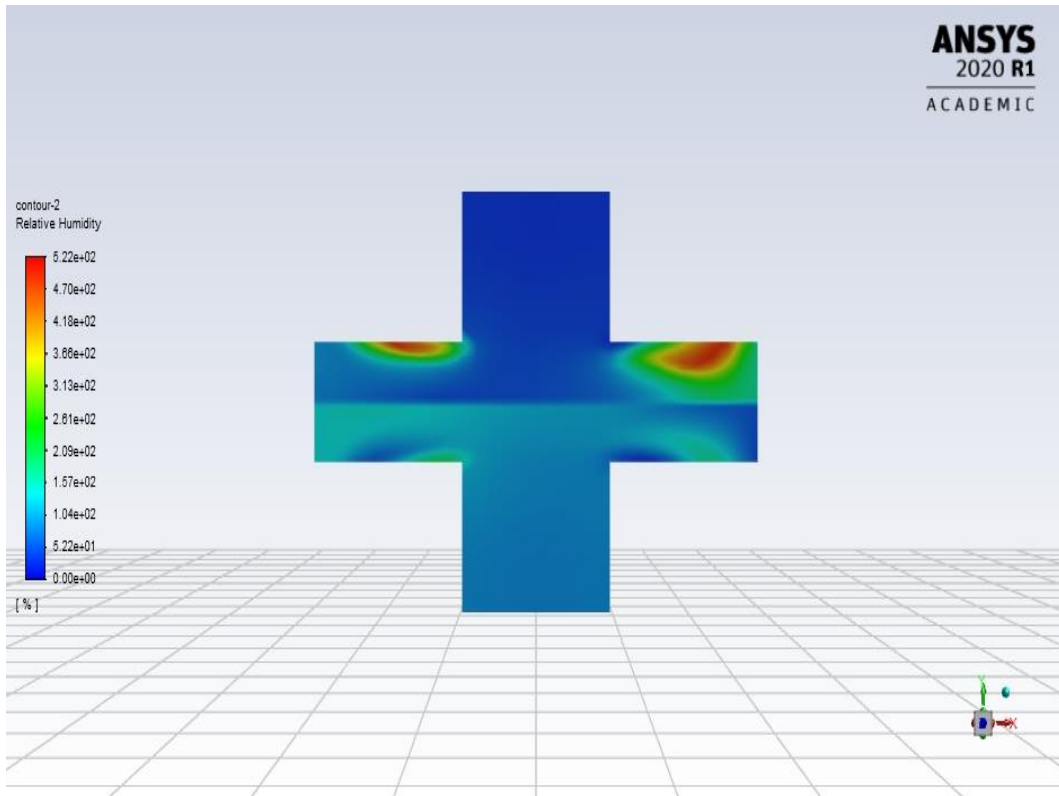


Figure 4.8. Graphical counters explain the anode relative humidity.

Table 4.3. Variations in the (I-P) at the anode side with 90% (ARH)

<b>Current density A/cm<sup>2</sup></b>	<b>Cell voltage V</b>	<b>Cell power density W/cm<sup>2</sup></b>
0.014231	0.9	0.012612
0.197545	0.8	0.1580324
0.330142	0.7	0.2315444
0.512365	0.6	0.3074195
0.632145	0.5	0.3160725
0.7541232	0.4	0.30164928

### 4.3.2. Cathode side relative humidity

The simulation results indicated the (CRH) has a positive impact on the cell performance, in this study three ratios of (CRH) (90%-70%-50%) have been examined. The results were showed the better cell performance and cell power output when the cell fed oxygen gases with 90% relative humidity as shown in Figure 4.9. Figure 4.10. Figure 4.11. The observed results indicated (Increase in membrane water content level with 90% (CRH), causes in enhances the cell protonic conductivity) causes in easy proton transportation from the anode side to cathode.

And decreases the ohmic loss, leads to improve the cell performance, On the other hand, when the cell fed oxygen gases with 50% relative humidity as shown in Figure 4.9. And Figure 4.10. Which observed degradation in the cell performance. The rational reasons for this phenomenon are the membrane water content level decreases with poor (CRH) result in a decrease in the cell protonic conductivity, leads to difficult proton transportation from the anode side to cathode side and increases the ohmic loss.

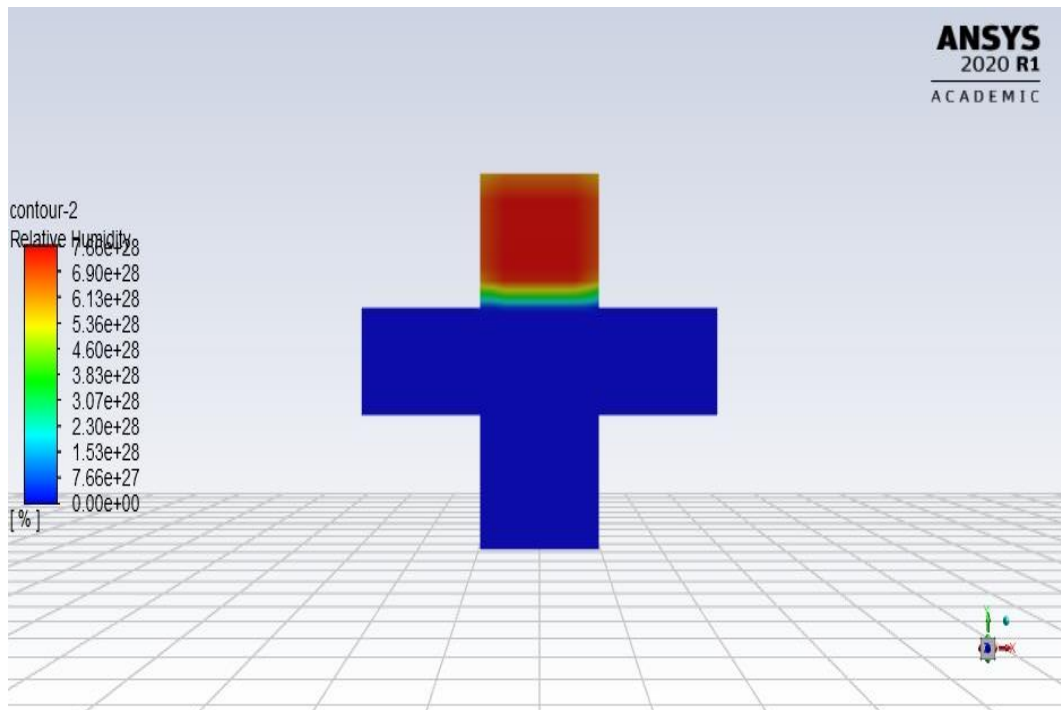


Figure 4.9. Graphical counters explain the cathode relative humidity.

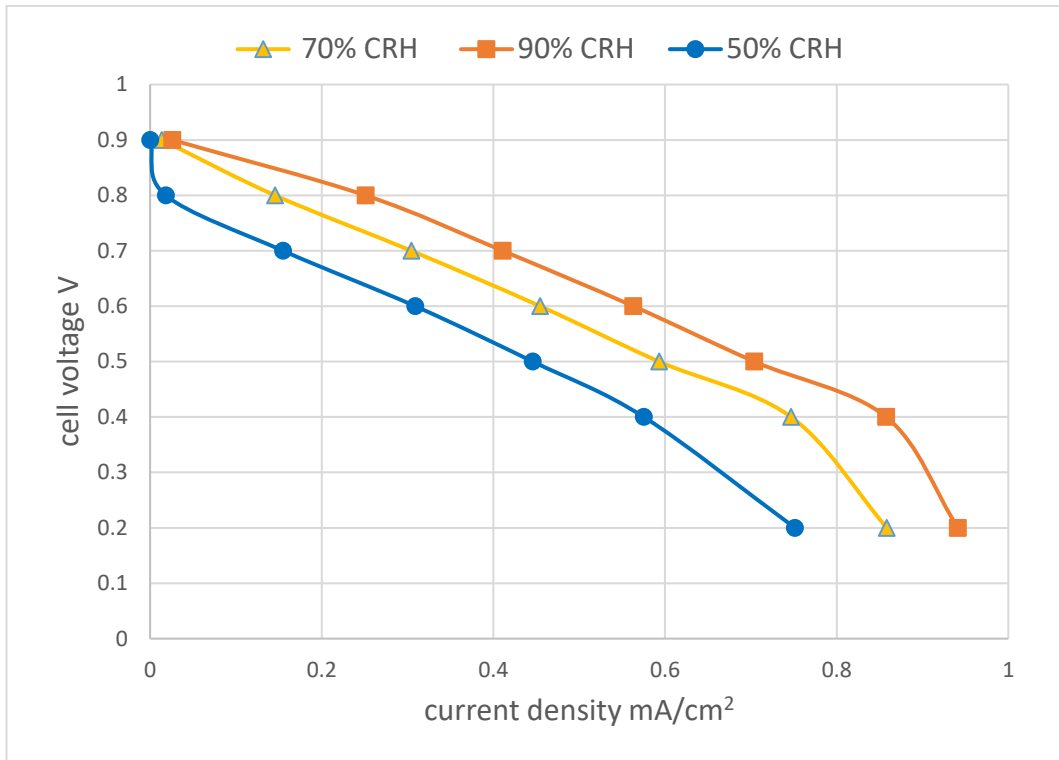


Figure 4.10. (I-V) Curve at various cell cathode relative humidity (CRH).

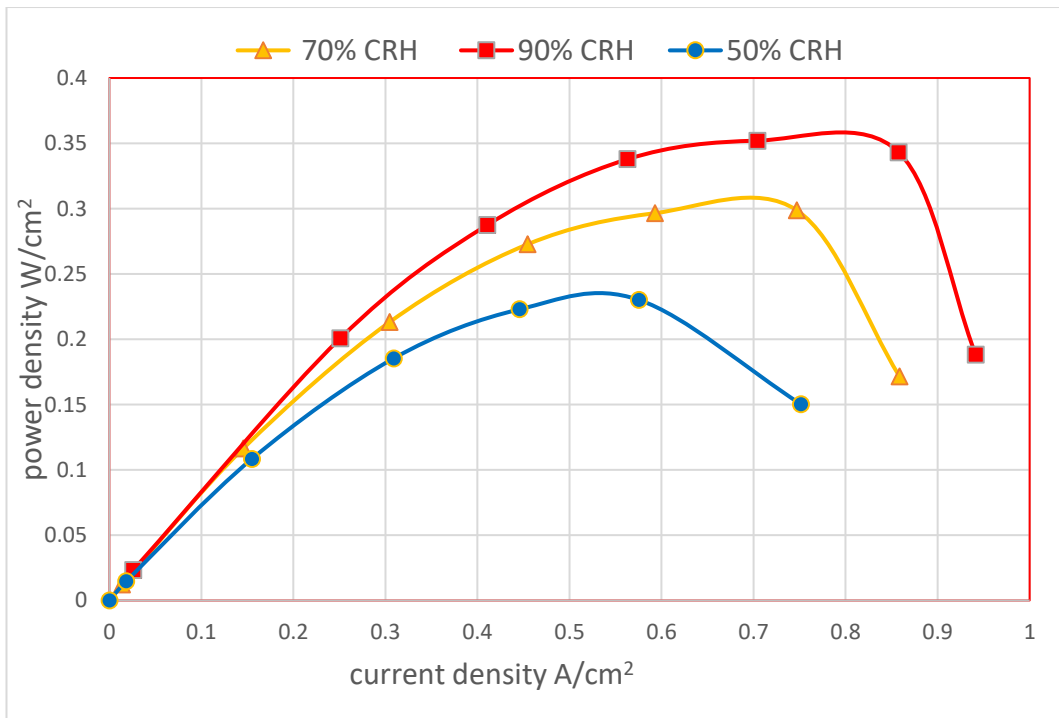


Figure 4.11 . (I-P) Curve at various cell cathode relative humidity (CHR).

## PART 5

### SUMMARY

In the present study, three-dimensional-single flow channel for single cell with an active area  $4.8 \text{ cm}^2$  PEM fuel-cells model developed were study the effect of the operating temperature and cathode relative humidity and anode relative humidity. The study done by (CFD) software ANSYS–FLUENT 2020. Three operating temperature values ( $55^\circ\text{C}$ ,  $75^\circ\text{C}$ ,  $85^\circ\text{C}$ ) examined to select a proper operation temperature. Observed results from the PEM fuel-cells simulation showed the strong relationships between the cell operating temperature and cell performance, the maximum cell performance and cell power output obtained when the cell operated at ( $55^\circ\text{C}$ ) as shown in Figure 1.1. Figure 1.4.

Refer to polarization curve and power output curve in Figure (4.3), (4.4). The maximum current density ( $0.3\text{A}/\text{cm}^2$ ) on the cell voltage ( $0.6\text{V}$ ), where the maximum power output equals to ( $0.1 \text{ W}/\text{cm}^2$ ).The rational reasons for this results are (an increase in the cell operating temperature greater than ( $55^\circ\text{C}$ ), the water evaporation rates becomes greater than water production rates, leads to membrane dehydration, particularly on the cathode side cases in decreases in cell protonic conductivity and increase ohmic loss leads to cell performance degradation).

Also, in this study an effect of the cathode and anode relative humidity on the cell performance had been investigated, three hydrogen and oxygen gases relative humidity values were varied 50%, 70%, 90%.

The result showed, the hydrogen and oxygen gases relative humidification have a positive impact on the cell performance. The maximum cell performance and cell power output was obtained when hydrogen and oxygen gases 90% humidified,

As can be seen in Figure 4.6. Figure 4.7. Figure 4.8. Figure 4.9. Refer to polarization curve and power output curve as shown in Figure 4.6. Figure 4.7. Utilize hydrogen gas on the anode side with 90% relative humidity the maximum current density were ( $0.6 \text{ A/cm}^2$ ) at cell voltage ( $0.5\text{V}$ ) . Where the maximum power output equals to ( $0.3\text{W}$ ), on the other hand , the maximum current density were ( $0.9\text{A/cm}^2$ ) on the cell voltage ( $0.2\text{V}$ ) where the maximum power output equals to ( $0.3\text{W}$ ) when utilize oxygen gas on the cathode side with 90% relative humidity.

The rational reasons for this result are (an increase in the relative humidity of the hydrogen and oxygen gases leads to increases in membrane water content, causes in increases in cell protonic conductivity and decrease ohmic loss leads to enhance the cell performance).

## **5.2. RECOMMENDATIONS FOR FUTURE WORK**

At future studies, can investigate the effect of operating pressure and reactant gases flow rates on the cell performance and can be examining the effect of different fuel stoichiometric ratios of the fuel on the cell performance and analysis of the water management in the (MEA) interface by commercial (CFD) software ANSYS-FLUENT.

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## **RESUME**

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