

INVESTIGATE THE EFFECT OF OPERATING PRESSURE VARIATION ON THE PEM FUEL CELL PERFORMANCE

2022 MASTER THESIS MECHANICAL ENGINEERING

Sarah Suhail Gatea ALHUSAINI

Thesis Advisor Assoc. Prof. Dr. Selami SAĞIROĞLU

INVESTIGATE THE EFFECT OF OPERATING PRESSURE VARIATION ON THE PEM FUEL CELL PERFORMANCE

Sarah Suhail Gatea ALHUSAINI

T.C. Karabuk University Institute of Graduate Programs Department of Mechanical Engineering Prepared as Master Thesis

Thesis Advisor Assoc. Prof. Dr. Selami SAĞIROĞLU

> KARABUK July 2022

I certify that in my opinion the thesis submitted by Sarah Suhail Gatea ALHUSAINI titled "INVESTIGATE THE EFFECT OF OPERATING PRESSURE VARIATION ON THE PEM FUEL CELL PERFORMANCE" is fully adequate in scope and in quality as a thesis for the degree of Master of Science.

Assoc. Prof. Dr. Selami SAĞIROĞLU Thesis Advisor, Department of Mechanical Engineering

This thesis is accepted by the examining committee with a unanimous vote in the Department of Mechanical Engineering as a Master of Science thesis. July 29, 2022

Examining Committee Members (Institutions)		Signature
Chairman	: Prof. Dr. Mustafa Bahattin ÇELİK (KBU)	
Member	: Assoc. Prof. Dr. Selami SAĞIROĞLU (KBU)	
Member	: Assoc. Prof. Dr. Habib GÜRBÜZ (SDÜ)	

The degree of Master of Science by the thesis submitted is approved by the Administrative Board of the Institute of Graduate Programs, Karabuk University.

Prof. Dr. Hasan SOLMAZ Director of the Institute of Graduate Programs

"I declare that all the information within this thesis has been gathered and presented in accordance with academic regulations and ethical principles and I have according to the requirements of these regulations and principles cited all those which do not originate in this work as well."

Sarah Suhail Gatea ALHUSAINI

ABSTRACT

M. Sc. Thesis

INVESTIGATE THE EFFECT OF OPERATING PRESSURE VARIATION ON THE PEM FUEL CELL PERFORMANCE

Sarah Suhail Gatea ALHUSAINI

Karabük University Institute of Graduate Programs The Department of Mechanical Engineering

Thesis Advisor: Assoc. Prof. Dr. Selami SAĞIROĞLU July 2022, 71 pages

Due to fossil fuel depilation concerns, and effort to reduce environmental pollution to make our universe an eco-friendly place for all think life. The invention of new renewable energy sources is considered a vital issue. All countries around the world aim to produce clean and sustainable energy. The most common energy uses in daily life are hydrogen energy and solar energy. PEM Fuel cell model with (2.5e-05) active area and a single parallel flow channel have been presented in this study. PEM Fuel cell model implemented in the interface of ANSYS-WORKBENCH-FLUENT 19-2. As a computational fluid domain, CFD commercial software investigates, the behavior of the PEM fuel cell, by varying the operating pressure values (1-3-5 bar) and selecting the proper operation pressure values, and investigating the effect of operating pressure values on the current density and PEM Fuel cell performance.

It is observed that when the working pressure of the cell is increased, the flow rate of the reactant gases increases too, and therefore results in an increase in the performance of the fuel cell, it has been observed that increasing the operating pressure of the fuel cell leads to an increase in the rate of the electrochemical reaction. The highest mass fraction of hydrogen gases has been noted on the working pressure of 3 Bar. The highest cell working temperature has been noted on the 3 Bar.

Key Words : Fossil fuel, Eco-friendly, Renewable energy, PEM Fuel cell, ANSYS-WORKBENCH-FLUENT 19-2.

Science Code: 91408

ÖZET

Yüksek Lisans Tezi

ÇALIŞMA BASINCI DEĞİŞİMİNİN PEM YAKIT HÜCRE PERFORMANSI ÜZERİNDEKİ ETKİSİNİN ARAŞTIRILMASI

Sarah Suhail Gatea ALHUSAINI

Karabük Üniversitesi Lisansüstü Eğitim Enstitüsü Makine Mühendisliği Anabilim Dalı

Tez Danışmanı: Doç. Dr. Selami SAĞIROĞLU Temmuz 2022, 71 sayfa

Fosil yakıtların tükenme endişeleri ve çevre kirliliğini azaltma çabası nedeniyle evrenimizi tüm düşünen yaşam için çevre dostu bir yer haline getirmektedir. Yeni yenilenebilir enerji kaynaklarının icadı hayati bir konu olarak kabul edilmektedir. Dünyadaki tüm ülkeler temiz ve sürdürülebilir enerji üretmeyi hedeflemektedir. Günlük hayatta en yaygın enerji kullanımları hidrojen enerjisi ve güneş enerjisidir. Bu çalışmada (2.5e-05) aktif alana ve tek paralel akış kanalına sahip PEM yakıt hücresi modeli sunulmuştur. ANSYS-WORKBENCH-FLUENT19-2 arayüzünde uygulanan PEM yakıt hücresi modeli. Hesaplamalı bir akışkan alanı olarak CFD ticari yazılımı, çalışma basıncı değerlerini (1-3-5 bar) değiştirerek ve uygun çalışma basıncı değerlerini seçerek ve çalışma basıncı değerlerinin akım üzerindeki etkisini araştırarak PEMFC'lerin davranışını araştırmıştır.

PEM yakıt hücresi simülasyon sonuçları, artan PEMFC çalışma basıncının, hücrenin termodinamik özelliklerini iyileştirdiğini göstermiştir. Pilin çalışma basıncının Artmasıyla reaktan gazların akış hızının da arttığı ve dolayısıyla yakıt pilinin performansında bir artışa neden olduğu gözlenmiştir, yakıtın çalışma basıncının artması da gözlenmiştir. Hücre elektrokimyasal reaksiyon hızında bir artışa yol açar. Hidrojen gazlarının en yüksek kütle oranı 3 bar çalışma basıncında kaydedilmiştir. En yüksek hücre çalışma sıcaklığı 3 barda kaydedilmiştir.

Anahtar Kelimeler: Fosil yakıt, çevre dostu, yenilenebilir enerji, PEM yakıt hücresi, ANSYS-WORKBENCH-FLUENT19-2.

Bilim Kodu : 91408

ACKNOWLEDGMENT

First of all, I would like to express my thankful to my Lord (Allah Subhanahu Wa Ta'ala) for support me in along my journey. I would like to express my thankful to my supervisor Assoc. Prof. Dr. Selami SAĞIROĞLU. I would like to express my thankful to my family and all who supported me.

CONTENTS

	Page
APPROVAL	ii
ABSTRACT	iv
ÖZET	vi
ACKNOWLEDGMENT	viii
CONTENTS	ix
LIST OF FIGURES	xi
LIST OF TABLES	xiii
SYMBOLS AND ABBREVITIONS INDEX	xiv
PART 1	1
INTRODUCTION	1
1.1. RENEWABLE ENERGY	2
1.2. PEM FUEL CELLS HISTORY	
1.3. PEM FUEL-CELL APPLICATIONS	6
1.3.1. Automotive Applications	7
1.3.2. Stationary Backup Power (Industry)	
1.3.3. Portable Power Generation- Consumer Electronic Devices	
1.4. PEM FUEL-CELL PARTS	9
1.4.1. Proton Exchange Membrane (PEM)	
1.4.2. Catalyst Layer (CLs)	
1.4.3. Bipolar Plats BPs	
1.4.4. Micro-Porous Layers MPLs	13
1.4.5. Flow Channels FCHs	
1.5. THESIS MOTIVATIONS	15
1.6. THESIS OUTLINE	16

PART 2	. 18
LITERATURE REVIEW	. 18
2.1. WATER MANAGEMENT	. 19

Page

2.2. HEAT MANAGEMENT ISSUE IN PRM FUEL-CELLS	21
2.3. WORKING CONDITION PARAMETERS IN PEM FUEL-CELLS	23
2.3.1. Working Pressure	23
2.3.2. Working Temperature	24
2.3.3. Relative Humidity	27
2.4. RESEARCH PROBLEMS	81
PART 3	3
METHODOLOGY	3
3.1. MODEL ASSUMPTIONS	\$4
3.2. GEOMETRY DEFINITION	5
3.3. MESH GENERATION	6
3.4. BOUNDARY CONDITIONS	;7
PART 4	0
RESULTS	0
PART 5	9
CONCLUTIONS	9
5.1. RECOMMENDATION	9
REFERENCE	51
RESUME	55

LIST OF FIGURES

	Page
Figure 1.1.	Energy consumption in the world annually1
Figure 1.2.	Various type of renewable energy
Figure 1.3.	Hydrogen gases production and uses
Figure 1.4.	PEM fuel-cells history
Figure 1.5.	PEM fuel cell application in wide uses
Figure 1.6.	PEM Fuel-cells applications in automotive industrialization HFCV a) various types of pem fuel cell vehicle, b) vehicle structure powered with Hydrogen
Figure 1.7.	Large stationary power plants
Figure 1.8.	Proton exchange membrane PEM10
Figure 1.9.	Catalyst layer structures with Platinum particles
Figure 1.10.	Bipolar plates with serpentine flow channel design
Figure 1.11.	Gas diffusion layer with 100 um thickness
Figure 1.12.	Serpentine and parallel flow channels
Figure 2.1.	Water formation in cathode side
Figure 2.2.	Water molecules transportation mechanism in PEM Fuel-cells
Figure 2.3.	Heat management in PEM Fuel-cells
Figure 2.4.	Schematic diagram of the PEM fuel-cells operating temperature25
Figure 2.5.	Cell operate with various cell operating temperature
Figure 2.6.	PEM fuel-cells operate with various cell relative gas humidity
Figure 2.7.	Polarization curve of cell with different R.H values
Figure 2.8.	Polarization curve and power curve of cell with defferent anode and cathode R.H
Figure 2.9.	Impact of inlet gases humidity on the PEM Fuel-cells power output 30
Figure 2.10.	Schematic drawing of Yiming Xu experiment (2021)
Figure 3.1.	PEM fuel-cells model zones including solid zones, flued zones
Figure 3.2.	Steps of the (PEM) fuel cell simulation
Figure 3.3.	PEM fuel cell divided into finite elements
Figure 3.4.	PEM Fuel-cells Boundary conditions assignment
Figure 4.1.	PEM Fuel-cells behavior with various operating pressure a) 1 bar b) 3 bar) 5 bar

Page

Figure 4.2.	Change of Hydrogen gas mass fraction with deferent working pressure a) 1 bar b) 3 bar) 5 bar	
Figure 4.3.	Change of Oxygen gas mass fraction with deferent working pressure a 1 bar b) 3 bar) 5 bar	·
Figure 4.4.	Change of water molecules gas mass fraction with deferent working pressure a) 1 bar b) 3 bar) 5 bar	45
Figure 4.5.	Variation of PEM Fuel-cells operating temperature under various operating pressure a) 1 bar b) 3 bar) 5 bar	46

LIST OF TABLES

Page

Table 1.1. PEM fuel-cells applications	9
Table 3.1. Enthalpy value of chemical reaction in PEM Fuel cells	19
Table 3.1. Explained the (PEM) fuel cell model geometries	36
Table 4.1. Variation of PEMFCs current density and power density with cell	
voltage, a) 1 bar b) 3 bar) 5 bar	48

SYMBOLS AND ABBREVITIONS INDEX

SYMBOLS

V_{Theory}	: theoretical cell voltage	Volt
V _{Losses}	s : cell potential losses Volt	
V _{Activ}	: activation losses	Volt
V_{Conc}	: concentration losses	Volt
V_{Ohmic}	: ohmic losses	Volt
η	: cell efficiency temperature	
Т	: cell working °C	
V	: cell Voltage	Volt
Р	: cell working pressure	kPa
Ν	: number of electrons transferred	
Ψ	: relative humidity	
R	: universal gas constant	J/mol. K
E	: cell potential	Volt
Ι	: electric current	ampere (A)
ΔH	change in the enthalpy	J/mol
т	: mass flow rate	g/min
Poutput	: power output from the PEM fuel cell	Kw
Q _{H2}	fuel input to PEM fuel cell	
F	: faraday's constant	C/mol

ABBREVITIONS

ICE : Internal combustion engineNASA : National Aeronautics and Space AdministrationUSA : United states of America

- CO₂ : Carbon dioxide
- CO : Carbon monoxide
- NO_x : Nitrogen oxides
- PM : Particle matter
- HC : hydrocarbon
- PEMFC : Polymer electrolyte membrane Fuel cell
- SOFC : Solid oxide Fuel cell
- MCFC : Molten carbonate Fuel cell
- AFC : Alkaline Fuel cell
- HOR : Hydrogen oxidation reaction
- ORR : Oxygen reduction reaction
- MEA : Membrane electrode assembly
- PEM : Proton exchange membrane
- CL : Catalyst layers
- GDL : Gas diffusion layer
- FCH : Flow channels
- BP : Bipolar 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 : Internal humidification methods

PART 1

INTRODUCTION

Sustainability in energy is considered is a key requirement for countries around the world. Fossil fuels are considered the biggest source of energy production, and all countries around the world depend on Fossil Fuels to meet their energy needs, as can be seen in Figure 1.1. Increasing demand for energy in transport sectors, electric production, and industrial processing, etc. Fossil fuel has a negative impact on the environmental by emitting harmful gases like Carbon monoxide CO, Carbon dioxide CO₂, Hydrocarbons HC, and Nitrogen oxides NO_x. Also, Fossil Fuels have a negative impact on ocean organisms, by absorbing Carbon dioxide and results in ocean acidification. Fossil fuel has a negative impact on the environment through extreme weather events including Wildfires, hurricanes wind, and flooding all of these disasters have been costing the United State of America USA between 2016 and 2022 \$ 607 billion [1].

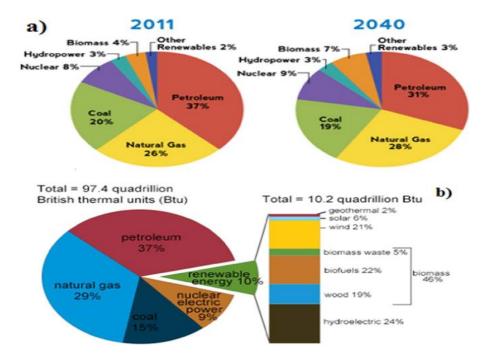


Figure 1.1. Energy consumption in the world annually [2].

1.1. RENEWABLE ENERGY

All countries around the world aim to produce clean and sustainable energy. Renewable energy is defined as the energy that can be replenished by nature and is categorized by its sustainable energy, eco-friendly sources. Energy sources that can be produced from natural sources, as can be seen in Figure 1.2. The most common sources of the renewable energy as:

- Solar energy [3].
- Wind energy.
- Biomass energy [4].
- Geothermal energy.
- Hydrogen energy.
- Hydropower energy [5].

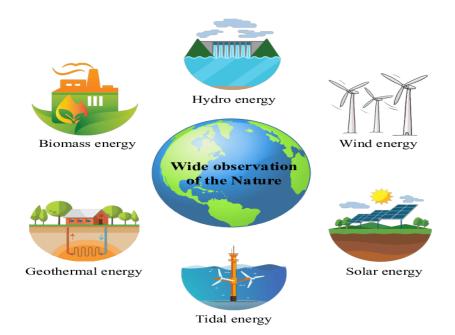


Figure 1.2. Various type of Renewable energy.

Hydrogen gas is colorless and odorless gas at standard conditions. Hydrogen gas is diatomic gas with two atomic making it the least dense among gases Hydrogen is the greatly abundant element in the universe.

Hydrogen gas is found on water molecules, fossil fuels, and living things, but it needed to be produced because it doesn't exist, it is a non-free element, but it shares strong bonds with other elements such as natural gas and Hydrocarbons. Hydrogen gas has a higher specific energy and higher heat energy than other elements as can be seen in the table. Today, many electric generations power plants depend on traditional sources as Fossil fuel but it has a negative impact on the environment because it emitting harmful gases. Hydrogen gas can be produced from fossil fuels such as natural gas, or from renewable sources such as wind energy.

In reality, there is a continuous increase in Hydrogen production, especially with most sectors heading to the production of clean energy, as nine million tons per year are produced in America. Hydrogen gas is characterized by high dispensability as can be seen in Figure 1.3. Due to Hydrogen gases have low density and high flammability. Therefore, it is a dangerous gas, and care must be taken when dealing with it. Today, there are 350 Hydrogen fueling stations around the world, most of them in America and Japan.

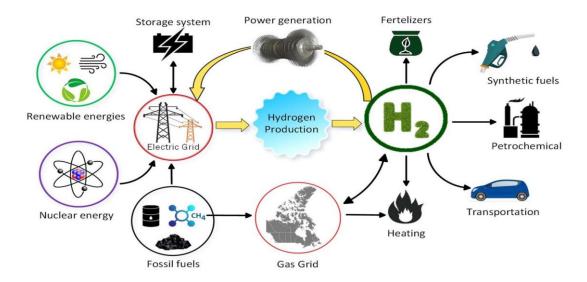


Figure 1.3. Hydrogen gases production and uses [6].

1.2. PEM FUEL CELLS HISTORY

Fundamentals of the fuels cell have been explained in the Nineteen centuries, and the development of PEM fuel cells through history has been explained and summarized

in Figure 1.4. Where the History of fuel cells had been beginning in Nineteen century, where, the British chemistry scientist Humphrey Davy described the principles and components of the fuel cell, in the 1842 year William grove invented the first gas voltaic battery which was considered an oldest prototype of the fuel cell in 1889 years.

Charles Langer and Ludwig Monad developed William Grove's invention and named it the fuel cell. In the 1932 year scientist Francis Bacon developed the Alkaline Fuel cell (AFC) which is considered one type of fuel cell, in the 1959 year, General Electric invented the proton exchange membrane fuel cell.

In 1960 years: National Aeronautics and Space Admiration (NASA) used fuel cells to power spacecraft in space flights, in 1966 General Motor Company used fuel cell technology to invent the first fuel cell vehicle called Electro van, wherein the 1970 United States navy (U.S Navy) used fuel cell in the submarines. In 1990 year, small stationary fuel cells were developed for commercial locations. In 2014, Toyota Company manufactured first fuel cell vehicle in Japan.

From the history of fuel cells, we can note that scientists have many continuous experiments to develop fuel cells because they have unique properties such as high energy density and zero-emission devices. In reality, fuel cells have various applications in the transportation sector especially, due to the desirable properties which characterized fuel cells and make them a strong candidate to replace traditional power sources (ICE) in automotive sectors. Manufactured and presented the first fuel-cell car.



1801 0

Humphry Davy described the principle of what was to become a fuel cell [5]

18420



William Grove invented "gas voltaic battery" - prototype of first fuel cell [7]

Francis Bacon developed the alkaline

fuel cell - AFC [9]

1932 🕩



1960so NASA first used fuel cells in space missions [11]

1970s O

1990sO

The oil crisis prompted the development of alternative energy

technologies [14]

0 1838



Christian Schönbein published a paper about the reactions in fuel cell [6]

0 1889

Charles Langer and Ludwig Mond developed Grove's invention and name the fuel cell [8]

• 1959 General Electric invented the proton exchange membrane fuel cell - PEMFC [10]

0 1960s DuPont developed Nafion[®] [12]

0 1966

General Motors used fuel cell technology in production of the Electrovan [13]

The United States Navy used the fuel cells in submarines [15]

O 2000s



The fuel cells were employed in vehicles [17]





The small stationary fuel cells developed for commercial locations [16]

2014 0

Toyota introduced the first commercial fuel cell car [18]



Figure 1.4. PEM fuel-cells history [7].

5















1.3. PEM FUEL-CELL APPLICATIONS

PEM fuel-cells are electrochemical converted devices that convert chemical energy in the fuel into electrical energy without emitting any harmful gases. Two electrochemical reactions Hydrogen oxidation reaction HOR. Oxygen reduction reaction ORR). Reactions results electrical current and pure water and some heat. This section summarizes the PEM Fuel cells applications. PEM Fuel cells application can be distinguished into four main groups as can be seen in Figure (1.5), and Table (1.1):

- High power applications (Call centers, high technology, communication).
- Emissions-reducing applications (Automotive, industrialization facilities, urban areas).
- Stationary backup power (industry).
- Portable power (consumer).

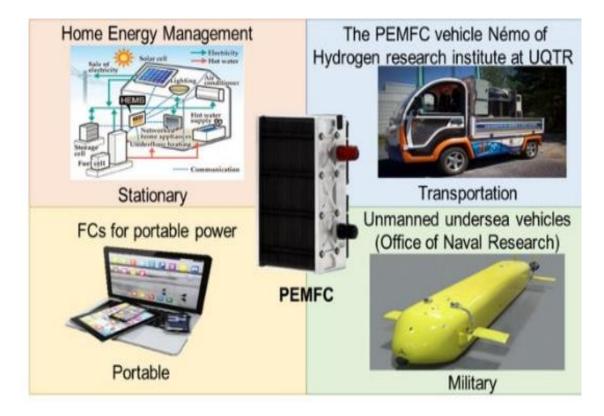


Figure 1.5. PEM fuel cell application in wide uses.

1.3.1. Automotive Applications

PEM Fuel cells have various applications in automotive industrialization companies as can be shown in Figure 1.6. PEM Fuel cells used a 100 kW stack. Honda FCX clarity has been manufactured in the Los Angeles region and it operates with a 100 Kw PEM Fuel cells stack also it operates with a lithium-ion battery pack (288 V) so it is considered a hybrid vehicle. Total range of the PEM Fuel cells automotive based on the size of Hydrogen tank in the vehicle, that is means the tank capacity to Hydrogen must be large to give us the required power.

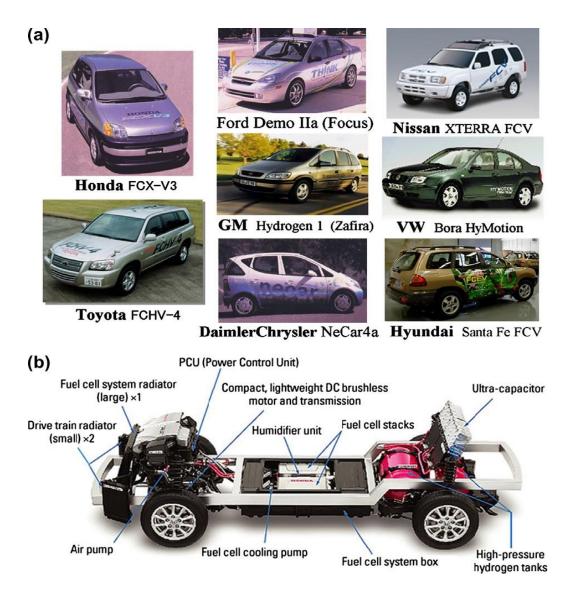


Figure 1.6. PEM Fuel cells applications in automotive industrialization HFCV a) various types of PEM Fuel cells vehicle, b) vehicle structure [9].

1.3.2. Stationary Backup Power (Industry)

Several types of fuel cells are used in stationary power applications, like Solid Oxide Fuel cells (SOFCs), Alkaline Fuel cells (AFCs), and Proton Exchange Membrane Fuel cells (PRMFCs). Appropriate properties of PEM Fuel cells types made them the most common type of fuel cells used in stationary power applications like a (high efficiency-high power Density and low operation Temperature-zero emotion). PEM Fuel cells stationary power plants can be distinguished into two groups:

- Large stationary power plants can be produced 20 MW as can be seen in Figure 1.7.
- Small stationary power plants can be produced 300 Kw.

1.3.3. Portable Power Generation- Consumer Electronic Devices

PEM Fuel cells have appropriate properties like a high power density, high efficiency, low cost, durability, and simple design making them a suitable device for the portable power production. Portable power production like a (cell phone, laptop and mini disc player) in this market there is a strong competition between all portable power because this electronic pieces must be smaller and cheaper, also PEM Fuel cells have a various applications in materials handling (Forklift), and, military [8].



Figure 1.7. Large stationary power plants.

Power output	Application
100 kw-1Mw	Large transportation buses
10-100 Kw	Small vehicle-small power station
1-10 Kw	Motorcycle- deferent portable power devices
100 w-1 Kw	Small raiding devices (bicycle-scooter-wheelchairs)
10-100 w	Portable power such as military equipment
<10 w	Cell phone

Table 1.1. PEM fuel-cells applications.

1.4. PEM FUEL-CELL PARTS

The unique properties of the PEM Fuel cells made them strongest candidate among various types of fuel cells as power sources. PEM Fuel cells are composed of electrolytes sandwiched between two electrodes, one positive called the Cathode side and the other negative called the Anode side, in fact, electrolytes consist of a proton exchange membrane, catalyst layer, and, gas diffusion layer. Briefly, PEM Fuel cells work like traditional automotive batteries, in the PEM Fuel cells, two main electrochemical reactions take place on anode side: Hydrogen Oxidation Reaction (HOR), on cathode side: Oxygen reduction reaction (ORR). Hydrogen gas enters to PEM Fuel cells from the Negative side (Anode), then, diffuses through the Gas diffusion layer and reaches to Catalyst layer, and oxidizes into one positive ion and one negative electron. The Proton exchange membrane allows for an ion to move through it while does not allow to electron to move through it, so the negative electron was forced to migrate due to an external load circuit generating an electrical current. On other hand, Oxygen gas enters to PEM Fuel cells from the positive side (Cathode), then, diffuses through the gas diffusion layer and reaches to catalyst layer, a composition occurs between a positive ion, one negative electron, and oxygen to produce water. Water production at the cathode side is considered a major problem facing the PEM Fuel cells, good water management must be applied to gain better cell performance, because excessive water leads to cell flooding and results in blockage of the pours area on the microporous layers and prevent reactant gas from reach the active site on the catalyst layer, thereby, reduce cell performance [10].

1.4.1. Proton Exchange Membrane (PEM)

Proton exchange membrane PEM is considered a key component of proton exchange membrane PEM Fuel cells. In reality, a Proton exchange membrane PEM is like Electrolyte in conventional automotive batteries. Proton exchange membrane PEM is made from Sulfonated polymer materials which have good properties like thermal and chemical stabilities, protonic conductivity, and good insulators for electrons. Main role of the Proton exchange membrane is protonic conductivity. Two main electrochemical reactions take place in the Proton exchange membrane (Hydrogen Oxidation Reaction (HOR)-Cathode side: Oxygen reduction reaction (ORR). As can be illustrated in Figure 1.8.

Proton exchange membrane required full hydration to achieve better performance of PEM Fuel cells, Proton exchange membrane must be hydrated with some of the water content carefully, because, excessive water results in electrodes flooding, resulting in clogging the porous media on the gas diffusion layers. Thereby, the obstruction of gas access to the reaction areas at catalyst layers results in Proton exchange membrane fuel cell's performance degradation.

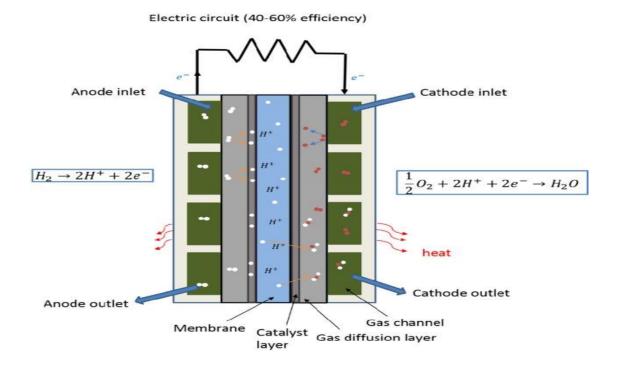


Figure 1.8. Proton exchange membrane (PEM) [11].

1.4.2. Catalyst Layer (CLs)

Catalyst layer (CLs) considered a thinner layer located between the proton exchange membrane (PEM) and gas diffusion layers, is often known as a membrane electrode assembly (MEA). Hydrogen Oxidation Reaction (HOR), and Oxygen reduction Reaction (ORR) take place on both sides of the PEM Fuel cells anode and cathode at the catalyst layer. The structure of the catalyst layers consist of carbon powder particles and have a thickness of 50 nm. Platinum particles are added to the carbon particles as can be illustrated in Figure 1.9. The diameter of the Platinum particles is 5 nm, as shown in the figure below. The main objective of adding platinum atoms is to stimulate the Hydrogen atoms to oxidize via Hydrogen Oxidation Reaction (HOR). Via Oxygen reduction reaction (ORR) Oxygen gas enters to PEM Fuel cell from the positive side (Cathode), then, diffuses through the microporous layer and reaches to catalyst layer, a composition occurs between a positive ion, one negative electron, and oxygen to produce water and some heat. In the last decade, the high cost of the catalyst layers represented a significant barrier to proton exchange membrane PEM Fuel cell commercialization. The material for the catalyst layers must-have characteristics such as: (High ionic conductivity-High electric conductivity-Preamble gases-High activity).

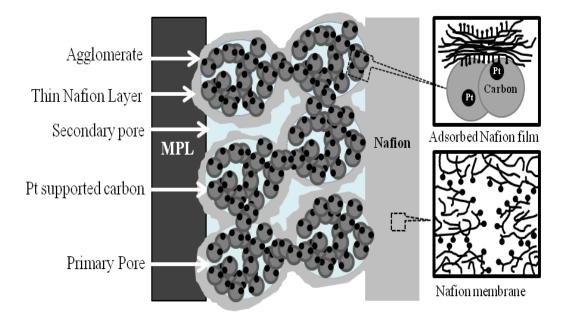


Figure 1.9. Catalyst layer structures with Platinum particles [12].

1.4.3. Bipolar Plats BPs

Bipolar plates are the biggest part of PEM Fuel cells, they account for 70% of cells' weight and 30% of cells cost. The gas flow channel is usually shaped with bipolar plates as can be illustrated in Figure 1.10. And various kinds like parallel type, zigzag design, serpentine design, and integrated design. Parallel design and serpentine design, are considered the most common type used in PEM Fuel cells, because of their advantages such as distributing the reactant gases equally to the reaction sites. Carbon (graphite) are the most common material used to manufacture bipolar plates because it has unique properties like:

- High electronic conductivity.
- High chemical stable.
- Good thermal conductivity.
- Good corrosion resistance.
- Easy to manufacture.
- Low cost.

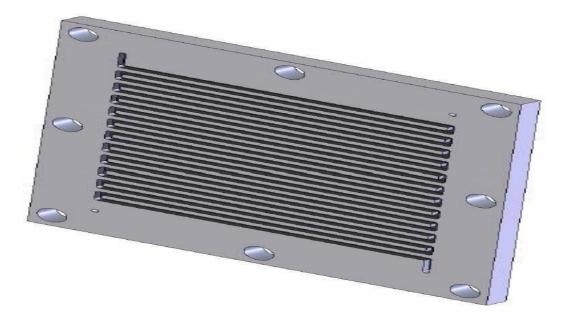
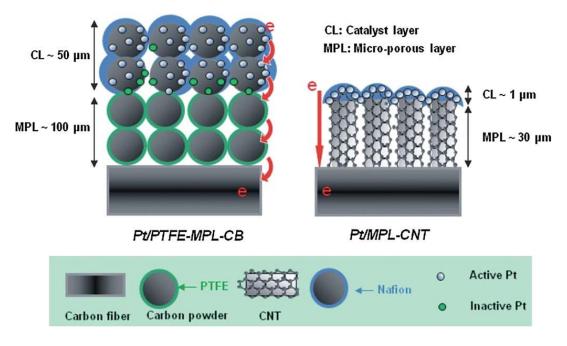


Figure 1.10. Bipolar plates with serpentine flow channel design [13].

1.4.4. Micro-Porous Layers MPLs

Micro-porous layers play a vitally important role inside the PEM Fuel cells, and they have a set of important functions like, they ensure diffuse, actively, and evenly diffuse the reactant reaches active sites on the catalyst layer and contribute in water management issues. The most common materials used to manufacture micro-porous layers MPLs are carbon cloth with 300 µm thickness as can be illustrated in Figure 1.11. Good gas diffusion layers must be characterized by some features as follows:

- Micro-porous layers provide chemical and mechanical stability for membrane and catalyst layers.
- Micro-porous layers have a high electron conductivity high thermal conductivity.



• Micro-porous layers protect the catalyst layer from corrosion.

Figure 1.11. Gas diffusion layer with 100 μ m thickness [14].

1.4.5. Flow Channels FCHs

Flow channels play a significant role to account PEM Fuel cells performance, flow channels are considered a key component in PEM Fuel cells, usually, shaped inside bipolar plates, flow channels have an important function by contributing to water management (flow channels remove water molecules produced at the cathode side out of the cell by the reactant gases.), also, flow channels contribute to heat management by taking out the excessive heat and rejecting it out of the cell by the reactant gases, therefore, flow channels have a vitally important to determine cell performance, the major function of flow channels inside PEM Fuel cells are distributing the reactant gases evenly and reach it to the active site on the catalyst layers.

There are many types of flow channels like parallel design, serpentine design as can be shown in Figure 1.12. Zigzag design, and, integrated design. The most common flow channel designs in the market are parallel design and serpentine design. Flow channels with parallel design characterized by: serpentine flow channel have a low pressure drop, so it has poor liquid water removal and short channels with low velocity. Flow channels with serpentine design are characterized by a high-pressure drop, so they have good liquid water removal, and they have long channels with high velocity.

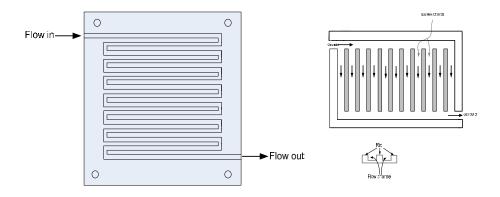


Figure 1.12. Serpentine and parallel flow channels [15].

1.5. THESIS MOTIVATIONS

Due to fossil fuel depilation concerns, and effort to reduce environmental pollution to make our universe an eco-friendly place for all think life. The invention of new renewable energy sources is considered a vital issue. All countries around the world aim to produce clean and sustainable energy. Renewable energy is defined as the energy that can be replenished by nature and it is categorized by its sustainable energy, eco-friendly sources, and energy sources that can be produced from natural sources, the most common sources of the renewable energy as:

- Solar energy is used in solar power plants.
- Wind energy is used in wind power plants.
- Biomass energy is used in Biofuels and Bio-power.
- Geothermal energy is used in heat pumps and power plants.
- Hydrogen energy is used in a fuel cell.
- Hydropower energy used in Hydropower plants.

The most common energy uses in daily life are hydrogen energy and solar energy, Hydrogen gas is colorless and odorless gas under standard conditions. Hydrogen gas is diatomic gas with two atomic making it the least dense among gases Hydrogen is the greatly abundant element in the universe. Hydrogen gas is found in water molecules, fossil fuels, and living things, but it needed to be produced because it doesn't exist, it is a non-free element, but it shares strong bonds with other elements such as natural gas and Hydrocarbons. In fact, Hydrogen gas has a higher specific energy and higher heat energy than other elements. PEM fuel-cells are electrochemical converted devices that convert chemical energy in the fuel into electrical energy by two electrochemical reactions Hydrogen oxidation reaction (HOR), and Oxygen reduction reaction (ORR)), the reactions result in an electrical current and pure water, and some heat. PEM fuel-cells have many uses as in the Automotive company, stationary power plant, portable power generation as smartphones.

1.6. THESIS OUTLINE

In this study, three-dimensional PEM fuel-cells model-single flow channel have been created using commercial CFD SOFTWARE-ANSYS-FLUENT to investigate the behavior of the PRMFCs by varying the operating pressure values (1-3-5 bar) and selecting the proper operation pressure values, and investigating the impact of operating pressure values variation on the current density and PEM fuel-cells performance. Using CFD SOFTWARE ANSYS-FLUENT has many benefits like it is available and easy to use, it provides accurate results, and the specification of the model was mentioned in part three. Single flow channel parallel type with proton exchange membrane active area (2.5e-05 m) have been used in the simulation process.

Part 1 has been introduced a brief background about the energy production and energy consumption in the world, and it shed light on the dependence on the fossil fuel in energy production. then it presents several solutions to decrease this dependence by inviting renewable sources doesn't have a negative impact on the environment, PEM Fuel-cells have appropriate properties like a high power density, high efficiency, low cost, durability, and simple design making them suitable devices for portable power production.

Part 2 introduced PEM fuel-cells basic thermodynamics then express a previous studies on the factors and modes of operation of the fuel cell (operating pressure/operating temperature/relative humidity), and then two important issues are highlighted, namely, water management and heat management within the fuel cell, and then the chapter ends with a statement of the main research problem.

Part 3 has introduced a methodology for the PEM fuel-cells model generated. PEM fuel-cells model building implementation has been done using commercial CFD SOFTWARE ANSYS-FLUENT 19.2 to solve all mass transport equations. Briefly, model development consists of FOUR steps:

- Model geometry definition in Solidworks include nine parts.
- Model meshing creation using FVM using ANSYS-DESIGN-MODELER-MESHER.
- Solver setup and entering boundary condition value using ANSYS-FLUENT.
- Results visualizing using ANSYS-CFD-POST PROCESSING.

Part 4 has presented a visualization of a three-dimensional PEMFCs model simulation results, as graphical, counters, figures, tables, and polarization curves (current density- cell voltage), also, this part discusses the effect of PRMFCs operation pressure variation on the ell performance and suggests the proper cell operation pressure.

Part 5 has presented the summarization of the conclusion obtained from the threedimensional PEM fuel-cells model in current study, and suggest a future work.

PART 2

LITERATURE REVIEW

Fuel cells are devices that convert the heat energy in the fuel to electric work directly without any combustion process, so they can be provided consumers clean energy, moreover, inside the fuel cell two electrochemical reactions as follows [16]. Hydrogen Oxidation Reaction (HOR) happens on the anode side as can be seen in equation (2.1). Oxygen Redaction Reaction (ORR) happens on the cathode side as can be seen in equation (2.2). Overall electrochemical reaction as can be seen in equation (2.3). Theoretical voltage of PEM fuel cell V_{Theoretical} can be calculated after take into account the cell voltage losses like V_{Ohmic} losses, concertation losses V_{Concertation}, activation losses V_{Activation}, and cell potential losses V_{Potential}.

$$H_2 \rightarrow H^+ + 2e^- \tag{2.1}$$

$$2H^{+}+2e^{-}+_{1/2}O_{2} \rightarrow H_{2}O$$
 (2.2)

$$H_{2+1/2}O_2 \rightarrow H_2O + Energy$$
 (2.3)

$$\Delta H_{f}(H_{2}O) - \Delta H_{f}(H_{2}) - \Delta H_{f}(H_{2}O_{2})$$

$$(2.4)$$

In the overall electrochemical reaction, overall electrochemical reaction represents a Hydrogen combustion process and this process can be named exothermic process, which means the Hydrogen combustion reaction produces energy (heat), to determine enthalpy of Hydrogen combustion reaction or amount of heat energy released from the Hydrogen combustion reaction by subtracting enthalpy of products from the Enthalpy of reactants as can be seen in equation (2.4).

Enthalpy values of both reactants and products are listed in thermodynamics as can be seen at the table. Refer to amount of water enthalpy (-286.02 KJ) negative sign of the enthalpy of water represents to being the Hydrogen combustion reaction (HCR) released heat. Amount of water enthalpy (-286.02 KJ) represent the maximum Hydrogen Heat Value (HHV), but according to second law of Thermodynamic which stats (only portion of energy can be converted to useful work, another portion goes as a losses by Entropy) [17].

According to him, this topology is useful for theoretical description of financial markets and search of economic common factors affecting specific groups of stocks. The topology and hierarchical structure associated to them could be obtained by using information in the time series of stock prices only. This result showed that time series of stock prices are carrying valuable (and detectable) economic information.

Table 2.1. Enthalpy value of chemical reaction in PEM Fuel cells [17].

Species of reactants	Enthalpy of reaction (KJ/Mol ⁻¹)	Entropy (KJ/Mol ⁻¹ K ⁻¹)
Hydrogen gases	0	0.133066
Oxygen gases	0	0.20517
Water	-286.02	0.06996

2.1. WATER MANAGEMENT

The main water sources inside PEM Fuel-cells are an electrochemical reaction in which their Oxygen gas reacts with Hydrogen gas on the cathode side to produce water as can be shown in the equation (2.5), and, Figure 2.1. In Oxygen reduction reaction (ORR), other important are the reactants them self which contain some molecules of water before entering to PEM Fuel-cells by humidification process, water management has vital importance and impact on cell lifetime.

$$H^+ + {}_{1/2}O_2 \to H_2O$$
 (2.5)

There are two phenomena that must be avoided during PEM Fuel cells designing (electrodes flooding and membrane dehydration) because they have a significant

impact on ionic conductivity which has the strongest effect on PEM Fuel cells performance. Produced water inside cells can be transport due to main three ways:

- Electroosmotic drag (EOD)
- Back diffusion (BD)
- Hydraulic permeation (HP)

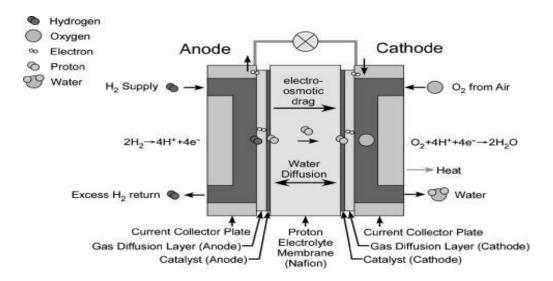


Figure 2.1. Water formation in cathode side [18].

Produced water Inside PEM Fuel cells can be transport due to main three ways as can be shown in Figure (2.2): Electroosmotic drag (EOD). Back diffusion (BD). Hydraulic permeation HP. Electroosmotic drag (EOD): This transition process occurs due to the electric current traveling from the, where the electric current is drawn from the anode side to the cathode side through the proton exchange membrane resulting in the transformation of water molecules. Electroosmotic drag (EOD) affected by membrane's humidification state. Back diffusion (BD) after the water molecules reach to the cathode side due to Electroosmotic drag, water Molecules accumulation occurs on the cathode side results in high water molecules concentration on the cathode side thereby water molecules migrate to the anode side through the electrolyte, water molecules transportation based on the proton exchange membrane thickness, proton exchange membrane humidification, and reactants gases humidification. Hydraulic permeation HP: Hydraulic permeation doesn't have a significant effect on cells performance, so, almost we can neglated this mechanism.

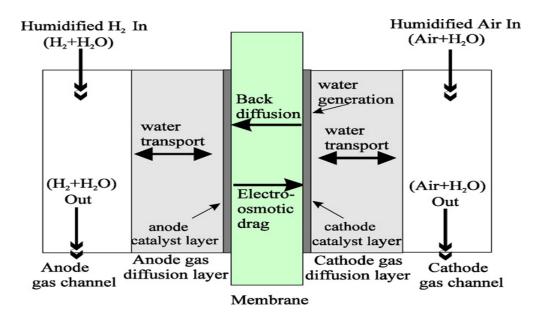


Figure 2.2. Water molecules transportation mechanism in PEM Fuel-cells [19].

2.2. HEAT MANAGEMENT ISSUE IN PRM FUEL-CELLS

PEM Fuel-cells heat management has vital importance, PEM Fuel cells operate between (50-90 °C). PEM Fuel-cells operated with high operating temperature, it will lead to: increase in the rate of the electrochemical reaction, a decrease in efficiency, and an increase in the rate of mass transfer. Experimental results have been reported PEM Fuel cells that operated with high operating temperature (there are an increase in water molecule removal on both sides of the PEM Fuel cells (anode-cathode) which, result in membrane dehydration and high ohmic resistance leads to decreased protonic conductivity thereby, PEM Fuel cells performance decreases.

The electrochemical reaction in both side of the PEM Fuel cells (anode-cathode) result in heat generated, amount of heat included (55 % Entropy of reactants, and 35 % Irreversibility of electrochemical reaction, 10 % ohmic resistance). Generated heat must be removed from PEM Fuel cells because they result in protonic conductivity decreased leads to PEM Fuel cells performance degradation. So, cell cooling process has a significant effect on PEM Fuel cells performance improvement. On the other hand, experimens results have reported PEM Fuel cells that operated with low operating temperature leads to decreased protonic conductivity thereby, cells

performance decreases, in both cases, there are decreases in PEM Fuel cells performance, so proper thermal management have a big effect on cell performance [20].

In order to determine the cells operating temperature equals to the heat generated inside PEM Fuel-cells minus heat removal from cells as following in equation (2.6), (2.7) and figure (2.3).

$$Q_{\rm In} = Q_{\rm Out} \tag{2.6}$$

$$(Q_{\text{Generated}} + Q_{\text{Reactants}})_{\text{In}} = Q_{\text{Dissipated}} + (Q_{\text{Reactants}})_{\text{Out}} + Q_{\text{Cooling}}$$
(2.7)

PEM Fuel cells generates heat during an electrochemical reaction takes place, this heat is undesirable because it has a negative impact on the PEM Fuel-cells performance, for main PEM Fuel-cells operate at desirable operation temperature. Excessive heat must be removed from PEM Fuel-cell, some heat dissipated by outer surface, and other some must be removed by the coolant liquid.

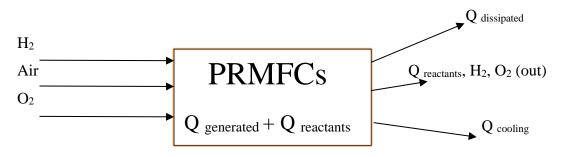


Figure 2.3. Heat management in PEM Fuel cells [21].

Heat sources in PEM Fuel cells:

- Protons movements from anode side to cathode side through proton exchange membrane leads to change in enthalpy.
- Hydrogen oxidation reactions (HOR), and Oxygen reduction reactions (ORR).
- Water evaporation and condensation, in Gas diffusion layers (GDLs).

2.3. WORKING CONDITION PARAMETERS IN PEM FUEL-CELLS

Some of the working conditions must be takin into account during PEM Fuel cells designing like good proton exchange membrane humidification, reactant gases pressurized, proper reactant gases working temperature and good design that allowing heat transfer phenomena occur from PEM Fuel cells, all of these working conditions must be adjustable in order to get the highest electric work with the highest efficiency of cells [22]. PEM Fuel cells performance affected by several parameters like:

- Working temperature.
- Working pressure.
- Relative humidity (water content level).
- Electrolyte thickness.
- Electrolyte active area.
- Species purity.
- Gases concentration.
- Water production.

2.3.1. Working Pressure

PEM Fuel cells working pressure plays an important role to determine cell performance. cells working pressure can be affected directly on many cell parameters like open-circuit voltage (OCV), reactant gases partial pressure, mass transfer, and, exchange current density, PEM Fuel cells working by a wide range of working pressure between (1-5 atm), many studied were conducted that any increasing in the reactant gases pressure result in an increase in PEM Fuel cells cost and that considered the strongest barrier to cell commercialization.

In addition, another's Havre been conducted that increase in the PEM Fuel cells working pressure can lead to lowering the cell efficacy and increasing the cell complexity, also, increase in the PEM Fuel cells working pressure can result in increased cell weight, size of components, parasitic energy losses, generally, an increase in cell working pressure results in cell thermodynamics parameters enhancement. (Al-Baghdadi et al) developed three dimensional model to study the effect of operating pressure on PEM Fuel cells performance.

Results showed the cell operating with high working pressure could be generating more distribution of exchange current density evenly by high Oxygen gases concentration on the catalyst layer. There are various types of the reactants flow field as parallel or serpentine as can be seen in the figure, therefore, differences in reactant gases distribution occur during reactant gases flows in the flow field, this difference pressure can be expressed in equation(2.8.-2.9), also, pressure on the anode side and cathode side too difference and can be expressed in equation (2.10), where the total anode side pressure represent sum of Hydrogen pressure H_2 and water pressure H_2O and can be expressed in equation [23].

$$P_{\text{Inlet}} = P_{\text{Outlet}} + P \tag{2.8}$$

$$P_{Anode} = \frac{1}{2} (2P_{Anode}_{Outlet} + P_{Anode})$$
(2.9)

 $P_{Cathode} = \frac{1}{2} (2P_{Cathode}_{Outlet} + P_{Anode})$ (2.10)

2.3.2. Working Temperature

PEM Fuel cells working temperature considered functional parameters it has a significant impact on the cells performance, in reality, PEM Fuel cells works under a limited range between (50-90 °C), where, any increase above this rang leads to, water evaporation rate becomes larger than water producing rate on cathode side results in membrane dehydration and leads to lower protonic conductivity, thereby, degradation cells performance. On the other hand, excessive heat generated due to electrochemical reaction must be removed from the cell to get high cell performance

therefore, the outer surface of PEMFCs is must made from high thermal conductivity materials which allow heat transfer phenomena to occur [7]. PEM fuel-cells are classified into cells operate with a high temperature above 100 °C, characterized by features like, durable in high CO concentration. Good heat-dissipating system, and, reactant gases humidification, not necessary. On the other hand, PEM fuel-cells operate with a low temperature between (60-80 °C), characterized by features like: High resistance to gas permeability, and, normal cost [24]. Qiangu Yan et al (2006) experimentally investigated the effect of working temperature on the PEM fuel-cells performance by using a single cell with 25 cm² electrolyte active area and serpentine flow pattern, and hydrogen stoichiometric ratio 1.2, air stoichiometric ratio 2, and PEM fuel-cells stack configuration.

The experiment results showed PEM fuel-cells operation temperature has a significant effect on the cell performance because it affects the electrolyte protonic conductivity, and, water transport in the microporous layer (MPLs) and catalyst layer (CLs). Polarization curve refers to an increase in cell working temperature from 65 °C to 75 °C as can be seen in Figure 2.5 [26].

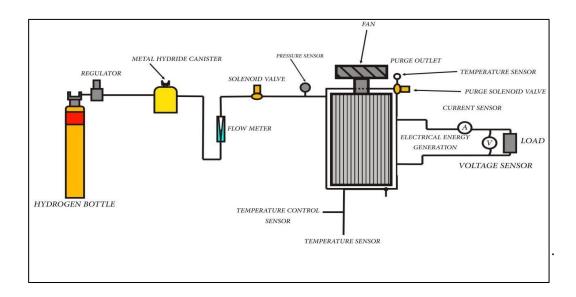


Figure 2.4. Schematic diagram of the PEM fuel-cells operating temperature

(H. A. Dhahad et al, 2016) experimentally studied the effect of operating temperature on the cell performance, the schematic of the studied experiment as can be seen in Figure 2.4, under different electrical loads and different Hydrogen flow rate, experiment results can be summarized as follows:

- PEM fuel-cells efficiency decreased when operation temperature increased.
- Operating temperature of the PEM fuel-cells has a strong effect on water management issues in PEM fuel cells, which assign cells performance as membrane dehydration and cathode flooding.
- Ionic resistance increased when membrane dehydration result in PEM fuelcells performance degradation.
- PEM fuel-cells performance developed due to increasing in cells operation temperature, but cells efficiency decreased.
- PEM fuel-cells operated ideally with operation temperature between (50-65°C), a cells performance decreasing had been showing when operation temperature increased than 65°C, the reasons beyond that the (operation temperature increasing leads to ionic conductivity decreasing because relative humidity reduced. When the operating temperature rises above 65 °C, the water begins to evaporate, so the amount of evaporated water becomes higher than the amount of water produced, and the drying of the membrane begins, which leads to a decrease in proton conductivity and, consequently, a decrease in the efficiency of the fuel cell) [25].

Salam. et al (2020) discussed elaborately the impact of working temperature on the efficiency and durability of PEM Fuel cells results showed an development in working temperature leads to an increase in cell performance, efficiency, power production, and leakage current, also reported, development in working temperature leads to decrease in cell durability, and mass crossover [24].

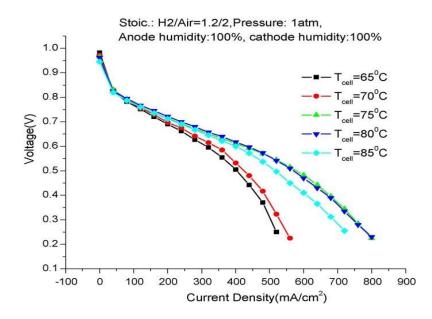


Figure 2.5. Cell operate with various cell operating temperature [26].

2.3.3. Relative Humidity

PEM fuel-cells utilize (Perfluorosulfonic acid) ionomer membrane Nation as a electrolyte PEM, so, this type of material require a high-level water content to provide the PEM fuel-cells with high protonic conductivity, for this reason, reactant gases must be humidified before entering to PEM fuel-cells. Relative humidity is a key parameter and it plays a significant role in the PEM Fuel cells, there are different ways to express about relative humidity like a (mixture ratio, absolute humidity, dew point), in fact there are two types of humidification method (internal humidification method, external humidification method) most common type is an external humidification method because many reasons as reduces the cell cost, reduces cell weight, and reduces cell parasitic power consumption [21].

Many studies had been performed to investigate of the impact of inlet gases relative humidity on the PEM fuel-cells performance. Y. liu (2020) experimentally studied the impact of inlet gases' relative humidity on the cell power output. results had shown, cathode side humidification and anode side humidification have different impact on the cell performance, and cathode side humidification have a large effect than anode side humidification on the PEM fuel-cells performance as can be seen in Figure 2.6 [27].

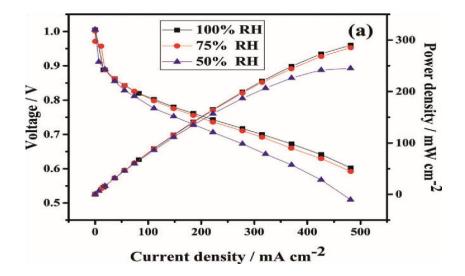


Figure 2.6. PEM fuel-cells operate with various cell relative gas humidity [27].

Burcu (2012) experimentally studied the impact of inlet gases' relative humidity on the PEM fuel-cells current density, results had shown the highest cell performance were obtained at 50% air relative humidity and 100% Hydrogen relative humidity, at 60 °C operation temperature as can be seen in polarization curve in Figure 2.7 [28].

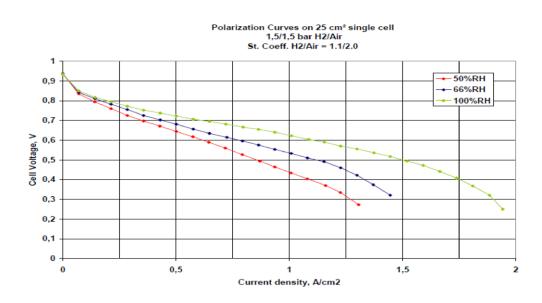


Figure 2.7. Polarization curve of cell with different R.H values [28].

O.Alhadethi and S. Saraoglu (2020) developed a three-dimensional single flow channel with a 4.8 cm² active area PEM fuel-cells to investigate the effect of inlet gases relative humidity on the cells performance theoretically. Results had shown the inlet gases humidification have vital importance on cell performance, at 90% relative

humidity for both anode side and cathode side cell performance high were showed as can be shown in Figure 2.8.

Reasons for the results for all previous studied can be summarized (any increase in inlet gases relative humidity for both anode or cathode side can be a help to maintain a membrane with high water content level that leads to enhance a protonic conductivity thereby cell performance enhancement) [7].

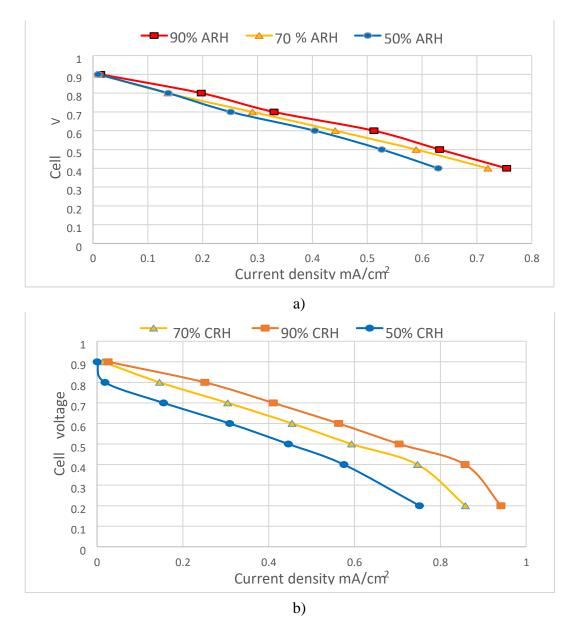


Figure 2.8. Polarization curve a) current density and cell voltage with different cell relative humidity, and b) power density of cell with defferent anode and cathode R.H [7].

Wilberforce et al, (2019) experimentally studied the impact of inlet gases relative humidity on the PEM fuel-cells performance, using one stack PEM fuel-cells fitted with Nafion electrolyte, using in experiment both dry and humidified hydrogen and air, the experiment set up as can be seen in Figure 2.9. Results shown:

- Inlet gas's R.H has significant importance to determine PRMFCs performance.
- All levels of inlet gases relative to humidification produce better cell power output than dry hydrogen or dry air.
- Using hydrogen and air with 100 % R.H gives a better cell performance.
- Using hydrogen and air with 50 % R.H causes a drop in cell performance [29].

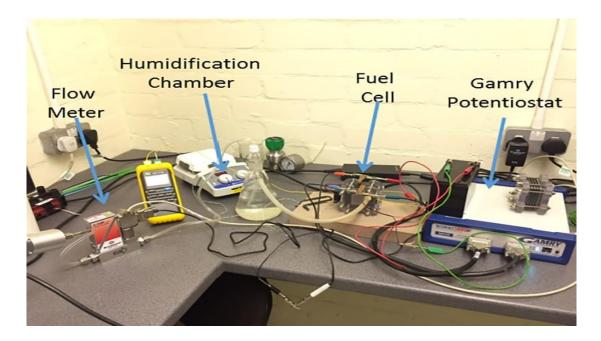
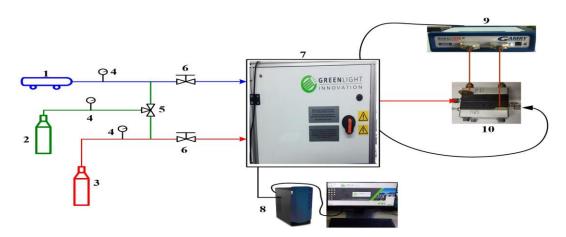


Figure 2.9. Impact of inlet gases humidity on the PEM Fuel cells power output [29].

Yiming Xu et al, (2021) investigated experimentally the effect of inlet gases relative humidity in the anode side (RHA), and cathode side (RHC) on the PEM fuel-cells performance, as can be seen in Figure 2.10. Results shown:

• Highest PEM fuel-cells performance on the (RHA=90%) - (RHC=90%).

- Highest ohmic resistance on the dry case in (RHA=50%) (RHC=50%).
- Better output cell current about 1 A/cm², because low mass transfer resistance.
- Maximum amount of cell power output can be achieved when anode side humidified with 90%, and cathode side humidified with 50%.
- Cell efficiency η can be reached to 24.4% when anode side humidified with 90%, and cathode side humidified with 50% [30].



1. Air compressor/ 2. N₂/ 3. H₂/ 4. Pressure gauge/ 5. Triple valve/ 6. Reducing valve/ 7. G20/ 8. Desktop/ 9. Electrochemical workstation/ 10. PEM fuel cell

Figure 2.10. Schematic drawing of Yiming Xu experiment (2021) [30].

2.4. RESEARCH PROBLEMS

PEM Fuel-cells thermal management has vital importance, PEM fuel-cells operates between (50-90°C), cell operated with high operating temperature, and it will lead to: increase in the rate of the electrochemical reaction, a decrease in efficiency, and an increase in the rate of mass transfer. Experimental results have been reported PEM Fuel-cells that operated with high operating temperature (there are an increase in water molecule removal on both sides of the PEM Fuel cells (anode-cathode) which, result in membrane dehydration and high ohmic resistance leads to decreased protonic conductivity thereby, cell performance decreases. The electrochemical reaction in both side of the PEM Fuel cells (anode-cathode) result in heat generated, these amounts of heat included (55 % Entropy of reactants, and 35 % Irreversibility of electrochemical reaction, 10 % ohmic resistance). Generated heat must be

removed from PEM Fuel cells because they result in protonic conductivity decreased leads to cell performance degradation. so, cell cooling process has a significant effect on cell performance improvement [31]. On the other hand, several experimental results have reported PEM Fuel cells that operated with low operating temperature leads to decreased protonic conductivity thereby, cells performance decreases, in both cases, there are decreases in PEM Fuel cells performance, so proper thermal management have a big effect on cells performance [32]. In order to determine the cells operating temperature equals to the heat generated inside PEM Fuel cells minus heat removal from PEM Fuel cells .

Several factors can be affected cells operation conditions including proton exchange membrane ionic conductivity, electrode kinetics, water management, heat management, and mass transport issues [33]. In this study, a three-dimensional PEM Fuel cells model have been created using commercial CFD SOFTWARE to investigate the behavior of the PEM Fuel cells by varying the operating pressure values (1-3-5 bar) and selecting the proper operation pressure values, and investigating the effect of operating pressure values on the current density and PEM Fuel cells performance.

PART 3

METHODOLOGY

PEM fuel-cells model with (2.5e-05) active area and single parallel flow channel have been presented in this part. PEM Fuel cells model implemented in the interface of ANSYS-WORKBENCH-FLUENT19-2. As a computational fluid domain CFD commercial software, it has many advantages as easy to use and available. PEM Fuel cells model has been developed including three main steps as follows:

- Pre-processing: this process includes PEM fuel cell modeling and geometry defining, and zone assignment, this process are performed in ANSYS-WORKBENCH-DESIGN MODELER, and SOLIDWORKS [34].
- Processing: this process includes PEM fuel-cells model divided into small shapes, and PEM fuel cell model boundary condition assignment, this process is performed in ANSYS-WORKBENCH-DESIGN MODELER-MESHER-FLUENT.
- Post-processing: this process include PEM fuel-cells model results visualization and analysis of final results, this process is performed in ANSYS-WORKBENCH-CFD-POSTPROCESSING[35].

Figure 3.1. Explain all PEM fuel-cells model zones including solid zones, flued zones, and anode oxidation reaction where Hydrogen gas enters to PEM fuel-cells from the Negative side (Anode), then, diffuses through the Gas diffusion layer and reaches to Catalyst layer, and oxidizes into one positive ion and one negative electron.

Proton exchange membrane allows for an ion to move through it while does not allow to electron to move through it, so the negative electron was forced to migrate due to an external load circuit generating an electrical current. On other hand, Oxygen gas enters to PEM fuel-cells from the positive side (Cathode), then, diffuses through the gas diffusion layer and reaches to catalyst layer, a composition occurs between a positive ion, one negative electron, and oxygen to produce water.

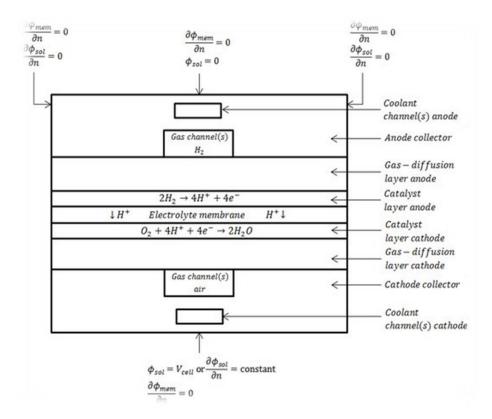


Figure 3.1. PEM fuel-cells model zones including solid zones, flued zones [36].

3.1. MODEL ASSUMPTIONS

In order to implement the three-dimensional PEM fuel-cells modeling process, some assumptions must be imposed for the cell to work on, as well, as, simplify the solution of equations that represent the phenomena that occur inside the PEM fuel-cells to which the momentum equation, mass equations, electrochemical reaction equation, and the heat transport equation, these assumptions can be written as follows:

- Thermodynamics properties of the gases and the solid materials constant.
- Gases flow under steady-state conditions.
- Isothermal operation condition.

- Isentropic and homogenous of electrode and proton exchange membrane (PEM).
- The gases flow in the flow channels are laminar flow.
- Gravity is negligible.
- The mixture of gases inside the PEM Fuel cells obeys to ideal gas law.

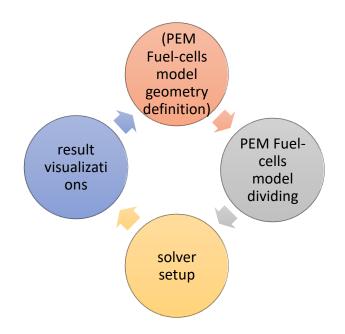


Figure 3.2. Steps of the (PEM) Fuel cells simulation.

3.2. GEOMETRY DEFINITION

PEM fuel-cells geometry can be designed in various software like GAMBIT, ANSYS-DESIGN MODELER, NT, SOLIDWORK, etc. In this study PEM fuel-cells modeling has been designed in SOLID WORK software, due to the facility in modeling cell zones provided by SOLID WORK software. The main objectives of cell geometry creation are to capture the physical dimensions for the real cell parts, and the fine cell geometry can provide a good basis to create a good computational domain. PEM fuel-cells consists of 10 zones that must be considered account during the designing proses. Ten regions have been sketched as two dimensions then extruded in three dimensions, Due to the effect of different physical zones in PEM fuel cell, the following regions must be present in the PEM fuel-cells modeling. High accuracy in geometry creation may be affected on the PEM fuel-cells simulation results particularly on the gases flow channels [37],[36].

3.3. MESH GENERATION

Computational domain creation is considered an important step to gain high accuracy model results, meshing generation means dividing one region into finite elements, then solving transport equations numerical approximation technique, then integrating to give us a final solution of modeling. Mesh generation proses strongly affected the simulation final results, so it must be generated carefully, it requires a balance between a Number of computational cells with available memory on the meshing hardware that is means create enough computational cells to capture the physical phenomena without create computational cells. In this study mesh generation proses have been done in ANSYS-DESIGN MODELLER-MESHER by hardware with the following specifications (HP elite book 8560P workstation-6 Gb, 2.5 GHz), the overall PEM Fuel cells was distracted into (81400) cells as can be seen in Figure (3.3), and, consumed (3 hours) as a time to perform this mesh generation Process. Table refer to a number of computational cells for each zone of PEM Fuel cells

Parts	Units of measure	Dimensions
Bipolar Plate Thickness	mm	0.4
Bipolar Plate Width	mm	1.5
Flow Channel Length	mm	54
Flow Channel High	mm	1
Flow Channel Width	mm	1
Microporouse Layer	mm	0.260
Thickness		
Catalyst Layer Thickness	mm	0.05
Proton Exchange Membrane	mm	0.20

Table 3.1. Explained the (PEM) Fuel cells model geometries.

Physics preference	CFD
Solver preference	Fluent
Element size (m)	1.2E-4
Number of meshed bodies	9
Number of generated Nodes	88578
Number of generated elements	81400
Average of mesh skewness	1.3E-10
Derivations	7.9E-12
Defeature size (m)	1E-010
Span angle center	Fine
Average Surface Area (m ²)	8.72E-006

Table 3.2. Physics parameters used in mesh generation.

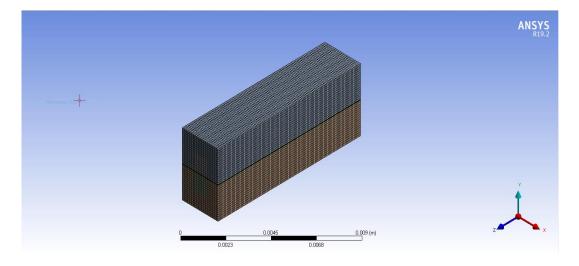
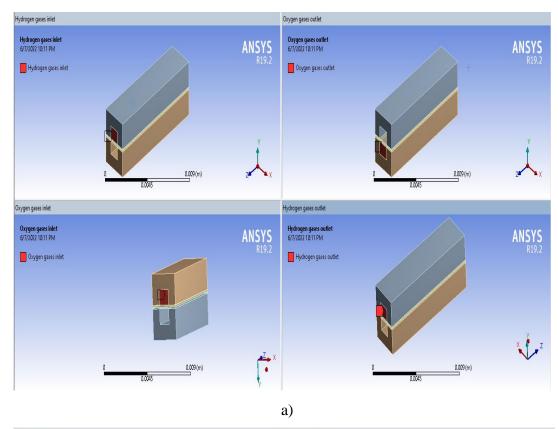


Figure 3.3. (PEM) fuel cell divided into finite elements.

3.4. BOUNDARY CONDITIONS

Generating electric current (I) in PEM fuel-cells can be summarized during two main chemical reactions; Anodic electrochemical reaction; one the Anode side Hydrogen gases fed to PEMFCs through flow channels and diffused through porous media in microporous layers to reach active sites on the catalyst layers, an electrochemical reaction take place on the catalyst layer results in conversion Hydrogen atoms into one proton, and one electron. Positive proton Immigrates from Anode side to Cathode side through proton exchange membrane. Electron travels from the Anode side to the Cathode side via electric load circuit generates electricity, on the other hand, chemical reaction take place on the Cathode side between the electrons and protons and Oxygen gases result in water generation and produce some heat. Humidified reactants (Hydrogen gas) enter to cell through the flow Channels, in this study the Anode side inlet, and, cathode side inlet is set to be the mass flow rate of the Hydrogen and oxygen gases. The values of the Hydrogen mass flow rate 3E-07 (kg/s), the values of the Oxygen gas mass flow rate 2E-06 (kg/s), with 353.15 K operation temperature, and the number of reactants determined based on the Faraday's Law of electric generation on the PEM Fuel cells . Figure 3.4. Demonstrate the various zones which specified as PEM fuel-cells boundary conditions. Anode flow channels inlet where the flow enters to the PEM Fuel cells . Hydrogen gas inlet zone are specified, when the flow of the Hydrogen gas leaves the flow channels at the other side of the Anode flow channel, this boundary assigned as pressure outlet conditions. Cathode flow channels inlet where Oxygen gases enter to the PEM Fuel cells. Oxygen gas inlet zone are specified, when the flow of the Oxygen gas leaves the flow channels at the other side of the Cathode flow channel, this boundary assigned as the pressure outlet conditions. At the boundary of Anode current collector where no proton ion Immigrates from the cell surface that's means no any different between cell voltage (Cell potential=0), this boundary sets as Anode side terminal, on the other hand, at the Cathode side the cell potential difference are applied, where the sold phase PEMFCs potential.



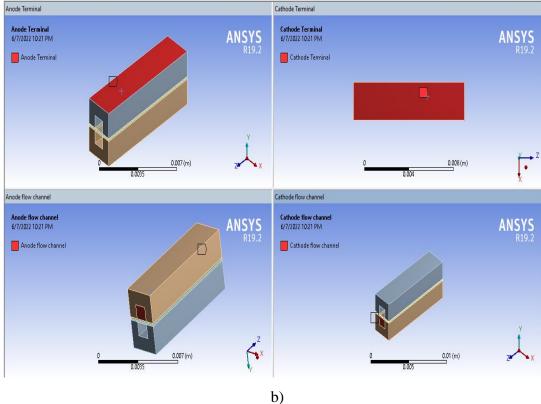


Figure 3.4. a) and b) PEM Fuel cells boundary conditions assignment.

PART4

RESULTS

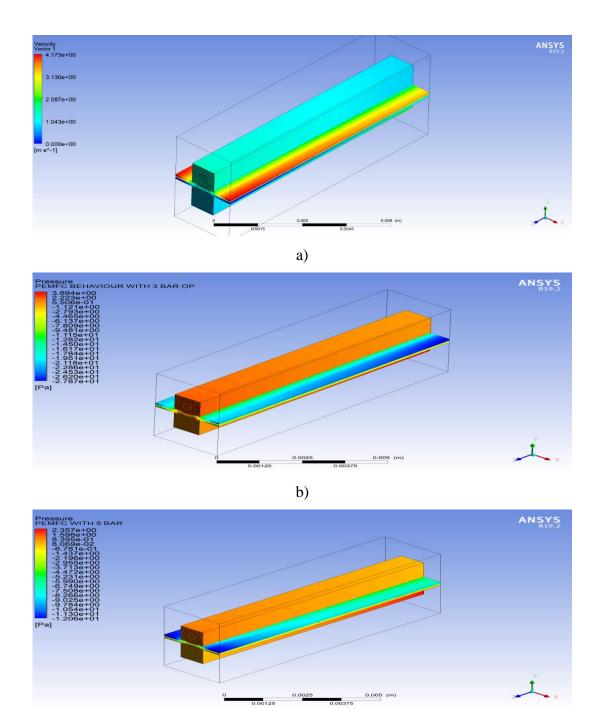
Flow rate of the reactant gases must be greater than the rate of the consumed reactant gases, the flow rate of the reactant gases equation is governed by faradays low. Generally, the high mass flow rate of the reactants can result in high voltage thereby high efficiency of the PEM fuel-cell. Operation temperature has a significant impact on the PEM fuel-cells performance, it is operates under 50-90 °C, any decrease in cell operation temperature of 50 °C can result in a water condensation rate, and contribute in electrode flooding, thereby, decrease in ionic conductivity and low power output, also, any increase in cell operation temperature than 90 °C can result in an increase the cell potential losses by generating more entropy, thereby, decrease in ionic conductivity and low power output, therefore PEM fuel-cells working temperature must be chosen carefully to get the desired cell performance.

Relative humidity of reactant gases play a vital role in cell performance, higher level of reactant relative humidity can provide high performance, because, the humidified reactants may be maintained on the desired water content of the proton exchange membrane thereby increase the ionic conductivity of proton exchange membrane results in high cell performance.

Operation pressure considers a key parameter in cells operation condition as it has a significant effect on the cell performance, to gain proper cell performance must be chosen operation pressure values carefully. In this study, a three-dimensional cells model has been created using commercial CFD SOFTWARE to investigate the behavior of the cells by varying the operating pressure values (1-3-5 bar) and selecting the proper operation pressure values, and investigating the effect of operating pressure values on the current density and cells performance.

Using CFD SOFTWARE ANSYS-FLUENT has many benefits like it is available and easy to use, it provides accurate results, and the specification of the model was mentioned in part three. Single flow channel parallel type with proton exchange membrane active area (2.5e-05 m) have been used in the simulation process. Increasing PEM fuel-cells working pressure results in cell performance enhancement by increasing the exchange current density, and improve the thermodynamic properties of the PEM Fuel cells, and accelerating the anodic and cathodic chemical reaction kinetics. On the hand, increasing the cell operating pressure over 5 bar can be lowering the cell performance due to membrane resistance, and mass transport issues. It is observed that when the working pressure of the cell is increased, the flow rate of the reactant gases increases too, and therefore results in an increase in the performance of the fuel cell, and, power output Q_{Output} increases too.

Rational reason for that, is the high reactant gases flow rate, results in a high concentration of hydrogen and oxygen gas is maintained, and when the flow rate of the reactant gases increases, the water molecules formed on the cathode side is as shown in the Figure 4.1.c. On the other hand, when the operating pressure of the fuel cell is increased, transfer rates of protons from the anode side to the cathode side increase, and they carry water molecules due to the EOD water transfer mechanism. It has been observed that increasing the operating pressure of the fuel cell leads to an increase in the rate of the electrochemical reaction as shown in Table 4.1. A high reaction rate means a high current rate and therefore a high performance resulting from the fuel cell. The highest mass fraction of hydrogen gases has been noted on the working pressure of 3 bar as can be seen in Figure 4.2.b. The highest mass fraction of hydrogen gases has been noted on the working pressure of 3 bar as can be seen in Figure 4.2. that means the highest cell performance can be achieved on the 3 bar working pressure, also, the highest oxygen mass fraction has been noted under 3 bar working pressure as can be seen in figure 4.3.b. Change of water molecules gas mass fraction with working pressure 3-5 bar have been noted the same value as can be seen in Figure 4.4.b.c, that is mean on the 3-5 bar working pressure must be made good water management strategies. The highest cell working temperature has been noted on the 3 bar as can be seen in Figure 4.5.b. that means the highest cell performance can be achieved on the 3 bar working temperature.



c)

Figure 3.5. PEM Fuel cells behavior with various operating pressure a) 1 Bar, b) 3 Bar, and c) 5 Bar.

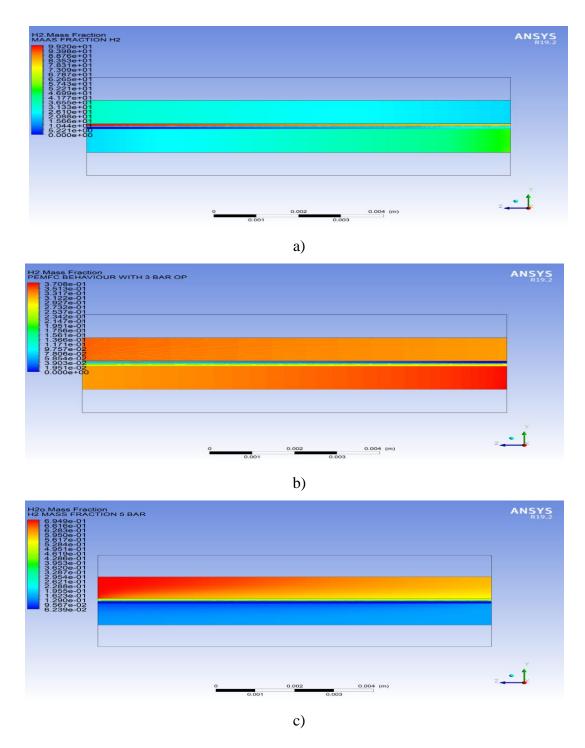


Figure 3.6. Change of Hydrogen gas mass fraction with deferent working pressure a) 1 Bar, b) 3 Bar, and c) 5 Bar.

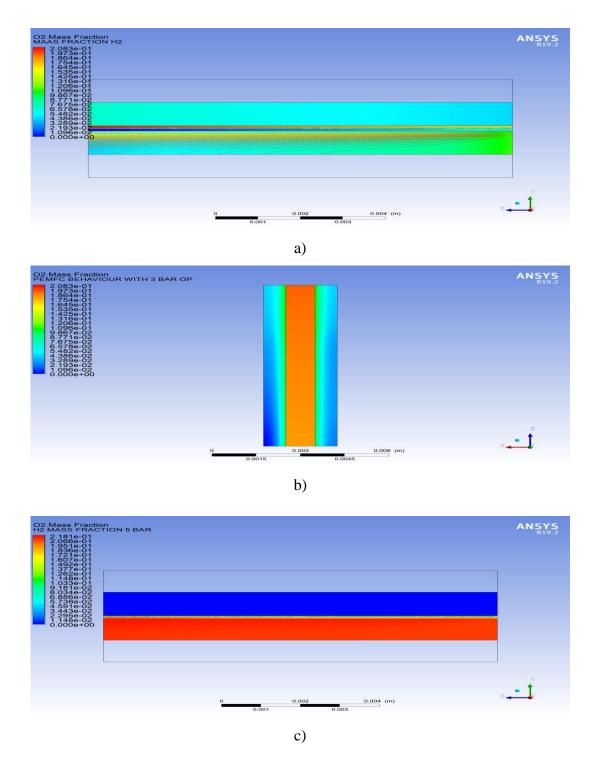
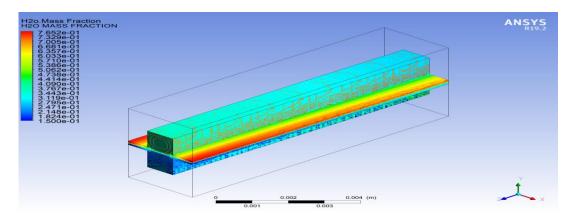
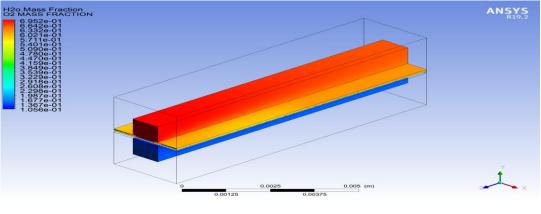


Figure 3.7. Change of Oxygen gas mass fraction with deferent working pressure a) 1 Bar, b) 3 Bar, and c) 5 Bar.



a)





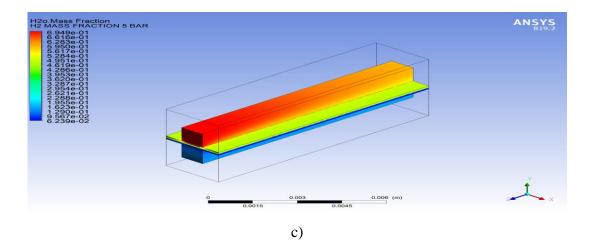
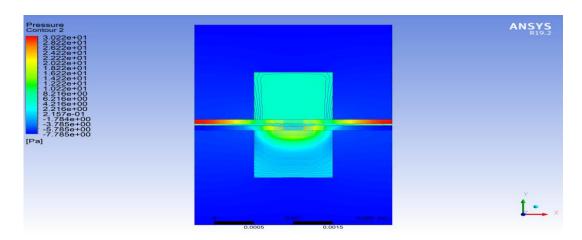
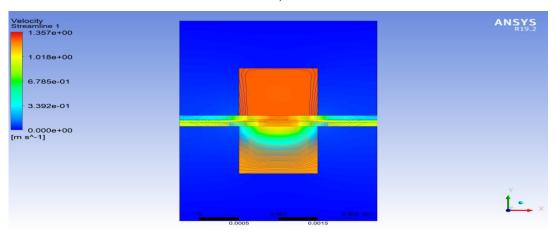


Figure 3.8. Change of water molecules gas mass fraction with deferent working pressure a) 1 Bar, b) 3 Bar, and c) 5 Bar.



a)





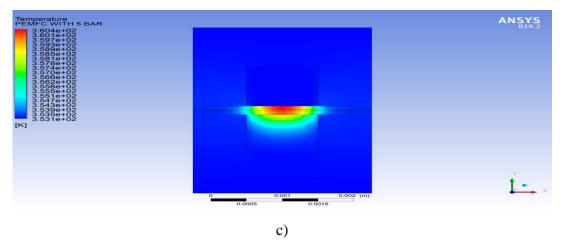
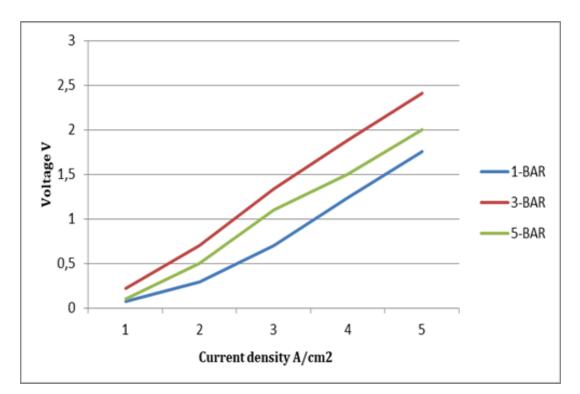
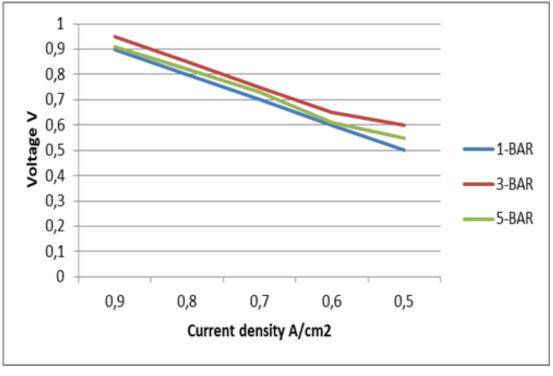


Figure 3.9. Variation of PEM Fuel cells operating temperature under various operating pressure a) 1 Bar, b) 3 Bar, and c) 5 Bar.



a)



b)

Figure 3.10. PEM Fuel cells performance variation a) Power density, and b) Current density.

Table 3.3. Variation of PEM Fuel cells current density and power density with cell voltage, a) 1 Bar, b) 3 Bar, and c) 5 Bar.

а	l)
	•/

Exchange current density A/cm ²	Voltage V	Power density W/cm ²
0.073	0.9	0.0657
0.289	0.8	0.2312
0.697	0.7	0.4879
1.240	0.6	0.744
1.760	0.5	0.88

b)

Exchange current density A/cm ²	Voltage V	Power density W/cm ²
0.1087	0.9	0.09783
0.61	0.8	0.488
1.2	0.7	0.84
1.80	0.6	1.08
2.40	0.5	1.2

c)

Exchange current density A/cm ²	Voltage V	Power density W/cm ²
0.219087	0.9	0.197178
0.699845	0.8	0.559876
1.336542	0.7	0.935579
1.880372	0.6	1.128223
2.406420	0.5	1.20321

PART5

CONCLUTIONS

In this study, a three-dimensional PEM Fuel cells model have been created using ANSYS-FLUENT to investigate the behavior of the PEM Fuel cells by varying the operating pressure values (1-3-5 bar) and selecting the proper operation pressure values, also, investigate the effect of operating pressure values variation on the current density and PEM Fuel cells performance.

PEM Fuel cells simulation results indicated that, Increasing PEM Fuel cells working pressure results in cell performance enhancement by increasing the exchange current density, and improve the thermodynamic properties of the PEM Fuel cells, and accelerating the anodic and cathodic chemical reaction kinetics. On the hand, increasing the cell operating pressure over 5 Bar can be lowering the cell performance due to membrane resistance, and mass transport issues, also, lowest PEM Fuel cells performance was gained when PEM Fuel cells operated with 1 bar as operating pressure.

Rational reason for these results the mass transport issues. The highest cell working temperature has been noted on the 3 Bar. That means the highest cell performance can be achieved on the 3 Bar working temperature. Consequently, the main finding of this study can be summarized as follows (proper operating pressure of PEM Fuel cells around 3-4 bar).

5.1. RECOMMENDATION

PEM Fuel cells topics have wide knowledge gaps that need to fill, one of their, strong attention is to cool PEM Fuel cells by using Nano-fluids, thereby improving the cell thermal conductivity. other, recommendations are to utilize nanoparticles in

the catalyst layer, take into account water management and membrane dehydration because they're play a vital importance in PEM Fuel cells , and have a significant impact on the PEM Fuel cells performance.

REFERENCE

- 1. S. Bertrand., "Climate, Environmental, and Health Impacts of Fossil Fuels Fact Sheet," *Environ. Energy Study Inst.*, pp. 1–3, (2021).
- S. G. Eriksson and A. K. Azad, "Nanomaterials for solid oxide fuel cells: A review," *Renew. Sustain. Energy Rev.*, vol. 82, no. February, pp. 353–368, (2018.)
- 3. M. Safiuddin and R. Finton, "Global renewable energy grid project-integrating renewables via high-voltage direct current and centralized storage," *Mediu. Direct Curr. Grid Resilient Oper. Control Prot.*, no. August, pp. 85–99, (2019).
- 4. J. Ness and B. Moghtaderi, "Biomass and bio-energy," *Fuel Energy Abstr.*, vol. 44, no. 3, p. 158, (2003.).
- H. S. Sachdev, A. K. Akella, and N. Kumar, "Analysis and evaluation of small hydropower plants: A bibliographical survey," *Renew. Sustain. Energy Rev.*, vol. 51, pp. 1013–1022, (2015).
- E. B. Agyekum, C. Nutakor, A. M. Agwa, and S. Kamel, "A Critical Review of Renewable Hydrogen Production Methods: Factors Affecting Their Scale-Up and Its Role in Future Energy Generation," *Membranes (Basel)*., vol. 12, no. 2, (2022).
- 7. O. Alhadethi and S. Saraoglu, "Numerical investigations of the effect of operation tempreture and relative humidity on the pem fuel cell mechanical engineering," Yüksek Lisans Tezi, *Karabük Üniversitesi Fen Bilimleri Enstitüsü*, *Karabük*, (2020).
- T. Wilberforce, A. Alaswad, A. Palumbo, M. Dassisti, and A. G. Olabi, "Advances in stationary and portable fuel cell applications," *Int. J. Hydrogen Energy*, vol. 41, no. 37, pp. 16509–16522, (2016).
- 9. Y. Wang, K. S. Chen, J. Mishler, S. C. Cho, and X. C. Adroher, "A review of polymer electrolyte membrane fuel cells: Technology, applications, and needs on fundamental research," *Appl. Energy*, vol. 88, no. 4, pp. 981–1007, (2011).
- E. Ogungbemi, J. Thompson, and O. Ijaodola, "Review of operating condition, design parameters and material properties for proton exchange membrane fuel cells," *Energy Researh*, pp. 1–19, (2020)
- 11. E. H. Ehite, "Study of two-phase flow pressure drop characteristics in Proton Exchange Membrane (PEM) fuel cell flow channels of different geometries," *Diss. Master's Theses Master's Reports*, (2016).

- D. Paul, A. Fraser, J. Pearce, and K. Karan, "Understanding the Ionomer Structure and the Proton Conduction Mechanism in PEFC Catalyst Layer: Adsorbed Nafion on Model Substrate," *ECS Trans.*, vol. 41, no. 1, pp. 1393– 1406, (2011).
- S. S. Dihrab, K. Sopian, and A. Zaharim, "Review on the unitized regenerative fuel cells materials," *WSEAS Trans. Environ. Dev.*, vol. 4, no. 12, pp. 1151– 1160, (2008).
- S. Park, J. W. Lee, and B. N. Popov, "A review of gas diffusion layer in PEM fuel cells: Materials and designs," *Int. J. Hydrogen Energy*, vol. 37, no. 7, pp. 5850–5865, (2012).
- 15. S. O. Obayopo, T. Bello-Ochende, and J. P. Meyer, "Thermodynamic optimization of PEM fuel cell stack gas channel for optimal thermal performance," *2010 14th Int. Heat Transf. Conf. IHTC 14*, vol. 5, no. January, pp. 29–35, (2010).
- 16. S. Litster and G. McLean, "PEM fuel cell electrodes," *J. Power Sources*, vol. 130, no. 1–2, pp. 61–76, (2004).
- 17. F. Barbir, *PEM fuel cells: theory and practice*. Academic Press, (2012).
- 18. N. Jain, A. Roy, R. Jain, N. C. Karmakar, and I. D. D. Student, "Polymer Electrolyte Membrane Fuel Cells: Alternative to fossil fuels for power supply to Heavy Earth Moving and Allied Machinery in Mining and Civil Engineering Industry Hydraulic Fracturing and fracture modelling of Indian Shale reserve View project Tri," *Conference Paper · December* (2013)
- M. M. Saleh, T. Okajima, M. Hayase, F. Kitamura, and T. Ohsaka, "Exploring the effects of symmetrical and asymmetrical relative humidity on the performance of H2/air PEM fuel cell at different temperatures," *J. Power Sources*, vol. 164, no. 2, pp. 503–509, (2007).
- 20. Ö. EKİCİ, "Modelling of Thermal and Water Management in Automotive Polymer Electrolyte Membrane Fuel Cell Systems/OtomotivPolimer Membran Elektrolit Yakit HücresSistemlerinin Isil Ve Yönetiminin Modelenmesi" Abdulrazzak Akroot," Yüksek Lisans Tezi, *Hacettepe Üniversitesi Fen Bilimleri Enstitüsü*, Ankara, (2014).
- 21. F. Barbir, Fuel Cell Operating Conditions. Book (2013).
- 22. B. Wang *et al.*, "Numerical analysis of operating conditions effects on PEM fuel-cells with anode recirculation," *Energy*, vol. 173, pp. 844–856, (2019).
- 23. J. Zhang, H. Zhang, J. Wu, and J. Zhang, "Pressure Effects on PEM Fuel Cell Performance," *Pem Fuel Cell Test. Diagnosis*, pp. 225–241, (2013).

- 24. M. A. Salam *et al.*, "Effect of Temperature on the Performance Factors and Durability of Proton Exchange Membrane of Hydrogen Fuel Cell: A Narrative Review," *Mater. Sci. Res. India*, vol. 17, no. 2, pp. 179–191, (2020).
- 25. A. A. Hayder Dhahad, A. H. Wissam Alawee, and E. Ali Eh Sheet, "Experimental Study Of The Operating Temperature Effect On The Performance of PEM Fuel Cell," *World Res. Innov. Conv. Eng. Technol.*, no. October, pp. 24–25, (2016).
- Q. Yan, H. Toghiani, and H. Causey, "Steady state and dynamic performance of proton exchange membrane fuel cells (PEM Fuel-cells) under various operating conditions and load changes," *J. Power Sources*, vol. 161, no. 1, pp. 492–502, (2006).
- Y. Liu, S. Bai, P. Wei, P. Pei, S. Yao, and H. Sun, "Numerical and Experimental Investigation of the Asymmetric Humidification and Dynamic Temperature in Proton Exchange Membrane Fuel Cell," *Fuel Cells*, vol. 20, no. 1, pp. 48–59, (2020).
- 28. B. ÖZSAN, "Effect of relative humidity of reactant gases effect of relative humidity of reactant gases on proton exchange membrane fuel cell," no. May, (2012).
- 29. T. Wilberforce *et al.*, "Effect of humidification of reactive gases on the performance of a proton exchange membrane fuel cell," *Sci. Total Environ.*, vol. 688, pp. 1016–1035, (2019).
- Y. Xu, G. Chang, J. Zhang, Y. Li, and S. Xu, "Investigation of inlet gas relative humidity on performance characteristics of PEM Fuel-cells operating at elevated temperature," *World Electr. Veh. J.*, vol. 12, no. 3, pp. 1–11, (2021).
- 31. I. Taymaz, "Numerical Investigation of the Effects of Operating Conditions on Counter- Flow Pem Fuel Cell Performance Numerical Investigation of the Effects of Operating Conditions on Counter-Flow Pem Fuel Cell Performance," no. January, (2020).
- 32. O. Alhadethi and S. Sağiroğlu, "The Effect of Operating Temperature and inlet gases relative humidity on Proton Exchange Membrane Fuel Cell Performance-CFD study," *Uluslararası Demir Çelik Sempozyumu (UDCS'21)*, (2021).
- 33. F. Barbir, PEM Fuel Cells, Book. (2005).
- 34. Y. Amadane, H. Mounir, A. El Marjani, E. M. Karim, and A. Awan, "Numerical investigation of hydrogen consumption in Proton Exchange Membrane Fuel Cell by using computational fluid dynamics (CFD) simulation," *Mediterr. J. Chem.*, vol. 7, no. 6, pp. 396–415, (2019).

- P. Choopanya and Z. Yang, "An effective mesh strategy for CFD modelling of polymer electrolyte membrane fuel cells," *Int. J. Hydrogen Energy*, vol. 41, no. 15, pp. 6445–6456, (2016).
- 36. T. D. Canonsburg, "ANSYS FLUENT Fuel Cell Modules Manual," *Knowl. Creat. Diffus. Util.*, vol. 15317, no. October, pp. 724–746, (2012).
- 37. Adam avery, "Proton exchange membrane fuel cell modeling and simulation using Ansys Fluent 12.1." *Arizona state university* (2012).

RESUME

Sarah Suhail Gatea ALHUSAINI finished first and elementary education in Baghdad city. She completed high school education in ALFAROQ High School, and after that. She started the undergraduate program in the MIDDLE TECHNICAL UNIVERSITY Department Refrigeration and air conditioning engineering in 2011-2015. To complete their M. Sc. education, she moved to KARABUK UNIVERSITY, where she is still working as M. Sc. from 2020-2022.