



شبكة المعلومات الجامعية  
التوثيق الإلكتروني والميكرو فيلم

# بسم الله الرحمن الرحيم



**HANAA ALY**



شبكة المعلومات الجامعية  
التوثيق الإلكتروني والميكروفيلم



# شبكة المعلومات الجامعية التوثيق الإلكتروني والميكروفيلم



**HANAA ALY**



شبكة المعلومات الجامعية  
التوثيق الإلكتروني والميكروفيلم

# جامعة عين شمس

## التوثيق الإلكتروني والميكروفيلم

### قسم

نقسم بالله العظيم أن المادة التي تم توثيقها وتسجيلها  
علي هذه الأقراص المدمجة قد أعدت دون أية تغييرات



### يجب أن

تحفظ هذه الأقراص المدمجة بعيدا عن الغبار



**HANAA ALY**



Cairo University

# **MODELING AND SIMULATION OF ALKALINE ETHANOL-AIR FUEL CELL STACK**

By

**Shimaa Mohamed Ali Abdela Obaid**

A Thesis Submitted to the  
Faculty of Engineering at Cairo University  
in Partial Fulfillment of the  
Requirements for the Degree of  
**MASTER OF SCIENCE**  
in  
**Chemical Engineering**

FACULTY OF ENGINEERING, CAIRO UNIVERSITY  
GIZA, EGYPT  
2020

# **MODELING AND SIMULATION OF ALKALINE ETHANOL-AIR FUEL CELL STACK**

By

**Shimaa Mohamed Ali Abdela Obaid**

A Thesis Submitted to the  
Faculty of Engineering at Cairo University  
in Partial Fulfillment of the  
Requirements for the Degree of  
**MASTER OF SCIENCE**  
in  
**Chemical Engineering**

Under the Supervision of

**Prof. Dr. Omar El farouk Abdel  
Salam**

**Prof. Dr. Ibrahim Mohamed  
Ahmed Mahmoud Ismail**

.....

.....

Professor of  
Chemical Engineering department  
Faculty of Engineering, Cairo University

Associate Professor  
Chemical Engineering department  
Faculty of Engineering, Cairo University

**Asc.Prof. Fatma Ibrahim Sayed**

.....

Associate Professor  
Chemical engineering department  
Faculty of Engineering, Cairo University

**FACULTY OF ENGINEERING, CAIRO UNIVERSITY  
GIZA, EGYPT  
2020**

# MODELING AND SIMULATION OF ALKALINE ETHANOL-AIR FUEL CELL STACK

By

**Shimaa Mohamed Ali Abdela Obaid**

A Thesis Submitted to the  
Faculty of Engineering at Cairo University  
in Partial Fulfillment of the  
Requirements for the Degree of  
**MASTER OF SCIENCE**  
in  
**Chemical Engineering**

Approved by the  
Examining Committee

.....

**Prof. Dr. Omar El farouk Abdel Salam**, Thesis Main Advisor

.....

**Prof. Dr. Ibrahim Mohamed Ahmed Mahmoud**, Advisor

.....

**Prof. Dr. Mohamed Hanafy Mahmoud Sayed**, Internal Examiner

.....

**Prof. Dr. Ahmed Mohamed Awad Abouelata**, External Examiner

- Chemical engineering and pilot plant department at National Research center (NRC)

FACULTY OF ENGINEERING, CAIRO UNIVERSITY  
GIZA, EGYPT  
2020

**Engineer's Name:** Shima Mohamed ali abdela obaid  
**Date of Birth:** 11/04/1991  
**Nationality:** Egyptian  
**E-mail:** Shimaamohamed\_60@yahoo.com  
**Phone:** 01122341699-01011195179  
**Address:** Newcairo. 5th settlement. 1st neighborhood. 5th area.  
Street 41. Villa 114  
**Registration Date:** 1/10/2014  
**Awarding Date:** ....../....../2020  
**Degree:** Master of Science  
**Department:** Chemical Engineering



**Supervisors:**

Prof. Dr.Omar El Farouk Abdel Salam  
Prof. Dr.Ibrahim Mohamed Ahmed Mahmoud  
Asc.Prof. Fatma Ibrahim Sayed

**Examiners:**

Prof. Dr. Ahmed Mohamed Awad (External examiner)  
Chemical engineering and pilot plant department at  
National Research center (NRC)  
Prof. Dr.Mohamed Hanafy (Internal examiner)  
Prof. Dr.Omar El Farouk (Thesis main advisor)  
Prof. Dr.Ibrahim Mohamed Ahmed mahmoud (advisor)

**Title of Thesis:**

Modeling and simulation of alkaline ethanol-air fuel cell stack.

**Key Words:**

Modeling of fuel cell; ethanol-air fuel cell stack ; alkaline alcohol fuel cell .

**Summary:**

- Ethanol-air fuel cell is a new technology for energy-conversion which provide high efficiency with pollution –free operation. The performance of alkaline ethanol-air fuel cell stacks was simulated using simple model based on thermodynamics, kinetics and mass transfer considerations. The mathematical model is tested by experimental data used in a previously published paper.
- In mathematical model, the increase in concentration of electrolyte with constant concentration of the fuel, the cell performance increases initially then decrease. This result is close to the experimental data. In mathematical model, the increase in concentration of fuel with constant concentration of the electrolyte, the cell performance slightly changes because of the consumption of fuel with increase in current density isn't taken into consideration .The result in experimental paper, the maximum power density =50mW/cm<sup>2</sup> at current density at 17 mA/cm<sup>2</sup> but The result in mathematical model, the maximum power density =46.5mW/cm<sup>2</sup> at current density at 20 mA/cm<sup>2</sup>



# **DISCLAIMER**

I hereby declare that this thesis is my own original work and that no part of it has been submitted for a degree qualification at any other university or institute.

I further declare that I have appropriately acknowledged all sources used and have cited them in reference section.

Name:

Signature:

Date: .../.... /**2020**



## ACKNOWLEDGEMENT

First, I would like to thank my supervisor, Professor **DR. OMAR EL FAROUK**, whose expertise was extremely valuable in formulating the research questions and methodology. His insightful feedback pushed me to sharpen my thinking and brought my work to a higher level. He has provided me with constant encouragement, patience, and guidance at different stages of my research, and his enthusiasm for research combined with his wonderful work ethic have taught me to greatly appreciate his depth of knowledge.

I would also like to thank my tutors, **ASC.PROF Dr. FATMA IBRAHIM**, for her valuable guidance throughout my studies. She provided me with the tools that I needed to choose the right Path and successfully complete my dissertation. Her guidance helped me in all the time of research and writing of this thesis.

I would like to express my very great appreciation to Professor **DR. IBRAHIM MOHAMED** for his valuable and constructive suggestions during the planning and development of this research work. His willingness to give his time so generously has been very much appreciated.

In addition, I would like to thank my family and my husband for their wise counsel sympathetic ear, providing the required atmosphere for my study, and for their total support. Mainly, I'd like to give the credit of this work to my parents as they provide everything whether in their abilities or over in order for this work to come to light.

# TABLE OF CONTENTS

<b>DISCLAMIR</b>	<b>I</b>
<b>ACKNOWLEDGEMENT</b>	<b>VI</b>
<b>TABLE OF CONTENT</b>	<b>III</b>
<b>LIST OF TABLES</b>	<b>V</b>
<b>LIST OF FIGURES</b>	<b>VI</b>
<b>NOMENCLATURE</b>	<b>VII</b>
<b>ABSTRACT</b>	<b>VIII</b>
<b>CHAPTER 1: INTRODUCTION</b>	<b>1</b>
<b>CHAPTER 2: LITERATURE REVIEW</b>	<b>3</b>
2.1 Introduction .....	3
2.2 Electricity Generation Methods .....	3
2.2.1 Combustion Engine .....	3
2.2.2 Batteries .....	4
2.2.3 Fuel Cell .....	5
2.2.3.1 The History Of The Fuel Cell.....	5
2.2.3.2 Classification Of The Fuel Cell.....	6
1. Alkaline Fuel Cell.....	6
2. Phosphoric Acid Fuel Cell.....	8
3. Molten Carbonate Fuel Cell .....	9
4. Solid Oxide Fuel Cell.....	10
5. Polymer Electrolyte Membrane Fuel Cell .....	11
2.2.3.3 Types Of Fuels.....	12
I. Hydrogen.....	12
Ii. Methanol.....	13
Iii. Ethanol.....	13
Iv. Ethylene Glycol.....	13
2.2.3.4 Advantage Of Fuel Cell.....	14
2.2.3.5 Disadvantage.....	14
2.3 Why Alkaline Fuel Cell? .....	16
2.4 Previous Work In Modeling And Simulation Of Fuel Cell .....	16

<b>CHAPTER 3: CONCEPT OF MODELING</b>	<b>19</b>
3.1 INTRODUCTION .....	19
3.2 FUEL CELL PERFORMANCE: .....	19
3.2.1 Ideal Voltage At Variable Concentration (Nerset Equation).....	19
3.2.2 Kinetics Of Alkaline Fuel Cell.....	20
3.3 EXPERIMENTAL PAPER .....	21
3.3.1 Experimental Data.....	21
3.3.2 Operation Of The Fuel Cell.....	22
<b>CHAPTER 4: RESULT AND DISCUSSION</b>	<b>23</b>
4.1 INTRODUCTION.....	23
4.1.1 Assumptions.....	23
4.1.2 Thermodynamics Voltage.....	23
4.1.3 Ohmic Over Potential.....	25
4.1.4 Concentration Over Potential.....	26
4.1.5 Activation Over Potential.....	29
4.1.6 Undesired Losses At Electrode.....	30
4.2 STUDYING THE EFFECT OF EACH PARAMETER ON THE REAL VOLTAGE FUEL CELL .....	30
4.2.1 Concentration Of Potassium Hydroxide.....	30
4.2.2 Concentration Of Ethanol.....	32
4.2.3 Temperature.....	32
<b>CHAPTER 5: CONCLUSION AND RECOMMENDATION</b>	<b>33</b>
<b>REFERENCES.....</b>	<b>36</b>
<b>APPENDIX A: RESULT TABLES.....</b>	<b>39</b>

## List of Tables

Table 1 The Comparison Between The Four Types of Fuel .....	14
Table 2 The Comparison Between Combustion Engine , Batteries and Fuel cell .....	16
Table 3 the design of the fuel cell .....	21
Table 4 Gibbs Free Energy Of Some Substance And Number Of Moles .....	23
Table 5 The Constants In Conductivity Equation .....	26
Table 6 The Constants In Density of Ethanol Equation .....	27
Table 7 The Constants In Viscosity of Water Equation .....	27
Table 8 The Parameters In Concentration Over Potential Equation .....	27
Table 9 The Parameters In Binary diffusion coefficient equation .....	28
Table 10 The Parameters In activation over potential equation .....	29

## List of Figures

Fig. 1 The Components of The Hydrogen-Oxygen Fuel Cell.....	1
Fig. 2 Internal and External combustion engine .....	4
Fig. 3 Battery Elements .....	4
Fig. 4 Representatives of a Fuel Cell and It's Operation.....	5
Fig. 5 Mobile Electrolyte AFC's.....	7
Fig. 6 Static electrolyte AFC'S .....	7
Fig. 7 Dissolved fuel AFC's.....	8
Fig. 8 Operation of Alkaline Fuel Cell.....	8
Fig. 9 The Operation of PFC .....	9
Fig. 10 The CO <sub>2</sub> Recycling Process in MCFC.....	10
Fig. 11 The Operation of MCFC .....	10
Fig. 12 The Operation of SOFC .....	11
Fig. 13 The Operation of PEMFC .....	12
Fig. 14 Specific Energy and Energy Density vs. Pressure for Hydrogen Gas Tank .....	13
Fig. 15 Comparison Between Heat Engine , Battery and Fuel cell.....	15
Fig. 16 The Relation Between Voltage And Current Density.....	19
Fig. 17 Mass Transport Develops At The Anode Of An Operating H <sub>2</sub> -O <sub>2</sub> Fuel Cell. ..	21
Fig. 18 Schematic of direct alcohol alkaline fuel cell stack of four cells. ....	22
Fig. 19 The Effect Of Concentration Of Potassium Hydroxide At Constant Concentration Of Ethanol = 1M .....	31
Fig. 20 The Effect Of Concentration Of Potassium Hydroxide At Constant Concentration Of Ethanol = 2M .....	31
Fig. 21 The Effect Of Concentration Of Potassium Hydroxide At Constant Concentration Of Ethanol = 4M .....	32
Fig. 22 The Effect Of temperature at Concentration Of Potassium Hydroxide =3M At Constant Concentration Of Ethanol = 2M.....	32
Fig. 23 Comparison Between Modelling And Experimental .....	34

# Nomenclature

Symbol	Quantity
$V$	Real voltage
$E$	Ideal Voltage
$A_p, A_R$	Activity of products , Activity of reactant
$n$	Number of electrons
$F$	Faraday Number
$P_i, P_t$	Partial Pressure Of substance (i), where i=Water, Carbon Dioxide and oxygen, Total pressure.
$X_i$	Mole Fraction Of substance (i), where i=Water, Carbon Dioxide and oxygen
$C_i$	Concentration Of substance (i), where i=Water, Carbon Dioxide , oxygen and Ethanol
$\eta_{Act}$	Activation over potential
$\eta_{Conc}$	Concentration over potential
$\eta_{Ohmic}$	Ohmic over potential
AFC	Alkaline fuel cell
PEMFC	Polymer electrolyte membrane fuel cell
MCFC	Molten carbonate fuel cell
SOFC	Solid oxide fuel cell
PAFC	Phosphoric acid fuel cell (PAFC)
PTFE	Poly tetra Fluoro Ethylene

## **Abstract**

Ethanol-air fuel cells are emerging new technologies for energy-conversion which provide high efficiency, modular structure and pollution –free operation. The performance of alkaline ethanol-air fuel cell stacks was simulated using simple model based on thermodynamics, kinetics and mass transfer considerations ,and the model was tested using published experimental data " Development of a Direct Alkaline Fuel Cell Stack"[1]. The effects of ethanol concentration, potassium hydroxide concentration, current density and temperature, on cell stack voltage and power density were studied. The calculated cell potentials and power densities match well with experimental data within reasonable accuracy in spite of the simplicity of the model. The model can be used for both design, optimization and process control. The model in spite being simple and taking into consideration the experimental error and the model assumption, it can be used within reasonable accuracy for estimation of optimum operating condition and maximum power output.