

UNIVERSITI TEKNOLOGI MARA

**REVERSIBLE REACTION KINETIC
OF TETRAESTER FORMATION
SIMULATION FROM SECONDARY
DATA: EFFECT OF TEMPERATURE**

**FATIN NABILA BINTI MOHD
ARIPIN**

B. Eng. (Hons) Chemical

July 2019

ABSTRACT

Polyol ester synthesized from palm oil methyl ester (POME) are environmentally friendly, biodegradable and non-toxic bio-lubricants. A kinetic model that describe chemical transesterification of palm oil-based methyl esters (POMEs) with pentaerythritol (PE) has been developed. The reaction is believed to be a series reaction whereby POME and PE reacted to form an intermediates of PE monoester, PE diester, PE triester and a designed product of PE tetraester. However, the data that were key in in the Matlab is based on overall reversible transesterification reaction. The model considers the transesterification reaction to take place in both forward and reverse directions. The resulting kinetic equations were solved using ode45 solver function in MATLAB. The obtained results were comparing the simulated curve with experimental data. From the results, a good reaction rate was observed only for temperature up to 170°C. The kinetic reaction rate equation used able to predict the value of rate constant with accurate as temperature increase up to 170°C while temperature at 180°C indicated at higher temperature tends to reverse the reaction.

TABLE OF CONTENTS

| | |
|--|-----------|
| AUTHOR’S DECLARATION | 1 |
| SUPERVISOR’S CERTIFICATION | 2 |
| COORDINATOR’S CERTIFICATION | 3 |
| ABSTRACT..... | 4 |
| ACKNOWLEDGEMENT..... | 5 |
| TABLE OF CONTENTS..... | 6 |
| LIST OF TABLES..... | 8 |
| LIST OF FIGURES | 9 |
| LIST OF ABBREVIATIONS / NOMENCLATURE | 10 |
| CHAPTER ONE..... | 11 |
| INTRODUCTION | 11 |
| 1.1 Research Background..... | 11 |
| 1.2 Problem Statement..... | 12 |
| 1.3 Research Objective | 13 |
| 1.4 Scope and Limitation of Work..... | 13 |
| CHAPTER TWO | 14 |
| LITERATURE REVIEW | 14 |
| 2.1 Vegetable Oil-Based Lubricant | 14 |
| 2.1.1 Bio-lubricant from Palm Oil..... | 15 |
| 2.2 Tetra ester..... | 17 |
| 2.3 Process of Transesterification Process | 18 |
| 2.3.1 Transesterification of Acid Catalyzed | 18 |

| | | |
|-------|---|----|
| 2.3.2 | Transesterification of Base-Catalyzed | 19 |
| 2.4 | Factors of Transesterification Process | 20 |
| 2.4.1 | Reaction Temperature | 20 |
| 2.4.2 | Molar Ratio of Reactant to Substrate..... | 21 |
| 2.4.3 | Catalyst | 22 |
| 2.4.4 | Agitator Speed..... | 23 |
| 2.5 | Simulation Methodology..... | 24 |
| | CHAPTER THREE | 26 |
| | SIMULATION METHODOLOGY..... | 26 |
| 3.1 | Kinetic Mechanism and Assumptions..... | 26 |
| 3.2 | Procedures | 27 |
| 3.2.1 | Kinetic model equation | 27 |
| 3.2.2 | Matlab Simulation | 29 |
| | CHAPTER FOUR..... | 30 |
| | RESULTS AND DISCUSSIONS..... | 30 |
| 4.1 | Effect of Temperature on Transesterification Process..... | 30 |
| 4.2 | Effect of Reaction Time at Various Temperature | 31 |
| 4.3 | Effect of Rate Constant, k at Various Temperature..... | 32 |
| | CHAPTER FIVE | 37 |
| | CONCLUSION AND RECOMMENDATIONS | 37 |
| 5. 1 | Conclusion | 37 |
| 5. 2 | Recommendation..... | 37 |
| | REFERENCES | 38 |
| | APPENDICES | 41 |

CHAPTER ONE

INTRODUCTION

1.1 Research Background

Renewable resources such as animal fats and plant oils can produce bio-lubricants that are also known as oil-based lubricants whereas these products are environmentally friendly, biodegradable and non-toxic lubricants (Chan, et al., 2018). In lubricant production, plant-based oil is one of the potentials to replace the mineral oils since their structure is similar and comes along with the characteristics of being renewables, economic, environmentally friendly and non-toxic (Heikal, et al., 2017).

Regarding to European standards, bio-based carbon content and biodegradability that are required for a certified bio-lubricant at least 25% and 60% respectively. There are factors affecting the market demand which are government directives, global demand and consumer environmental awareness for lubricants. Bio-lubricant is an alternative way that researchers found to overcome the increasingly worse issue that provides hazardous conditions that require high environmental cost and non-degradable lubricant entering the environment.

Process of transesterification is the main process in bio-lubricant production. The functions of bio-lubricant are to prevent heat loss and reduce wear resulting from contact of moving surfaces, to prevent corrosion and to reduce oxidation (Cerón, et al., 2018). Bio-lubricant can be described as liquid oils produced from renewable or biomass feed stock that can provide the oil easily biodegradable and harmless to human beings or aquatic habitat due to toxicity.

Other than transesterification process, hydrogenation and epoxidation process also can be applied for lubricant production. This process is the chemical modification due to the production of bio-lubricant have limitations of plant oil. This modification is to produce synthetic ester by enhance the bio-lubricant thermal stability (Resul, et al., 2012).