UNDERGRADUATE RESEARCH PROJECT 2 THESIS

3D DESIGN OF HETEROGENEOUS CATALYTIC BIODIESEL REACTOR USING AVEVA PDMS

MUHAMAD AKMAL BIN MUHAMAD YUSUF (KA09174)

A proposal is submitted in fulfillment of the

requirement in completing the assessment of Final Year Project (URP2)

Supervise by:

Dr. -Ing. Mohamad Rizza bin Othman

Faculty of Chemical Engineering and Natural Resources

Universiti Malaysia Pahang

January 2013

3D DESIGN OF HETEROGENEOUS CATALYTIC BIODIESEL REACTOR AND ITS PLANT USING AVEVA PDMS

MUHAMAD AKMAL BIN MUHAMAD YUSUF (KA09174)

Thesis submitted in fulfillment of the requirements
for the award of degree of
Bachelor in Chemical Engineering

Faculty of Chemical Engineering and Natural Resources

Universiti Malaysia Pahang

JANUARY 2013

TABLE OF CONTENTS

LIST OF FIGURES

ACKNOWLEDGEMENT

It gives me immense pleasure to express my gratitude to my supervisor **Dr. Mohamad Rizza Bin Othman** for his guidance, motivation, constant inspiration and above all for his co-operating attitude that enables me in bringing up this thesis in the present form.

I express my sincere gratitude to the Chemical Engineering and Natural Resource faculty staff for providing the necessary facilities in the computer laboratory.

I also wanted to say thank you to my fellow friends that given me a lot of support especially Taufik Abu Bakar who co-operate with me in developing the 3D design during the research.

ABSTRACT

The research focuses on how to design a 3D model of the heterogeneous catalytic biodiesel reactor and its plant by using AVEVA PDMS software. The scope of the research firstly was to model the heterogeneous catalytic biodiesel plant for production of biodiesel according to F3 factory concept. Then, produce a detail piping and instrumentation diagram (P&ID) of the plant and lastly simulate the design of the plant in 3D drawing by using AVEVA PDMS software. In this research, batch system is chosen due to its flexibility and follows F3 factory concept and the plant was built on the container truck. The methodology of the research was designing according to the piping and instrumentation diagram (P&ID). Then, sizing of the equipment and mechanical design and lastly involve 3D simulation. For the result a 3D design of heterogeneous catalytic biodiesel reactor and its conceptual design of the biodiesel plant are by using AVEVA PDMS was achieved. Lastly, the importance of the research is to fulfill the industrial demand on 3D design and showing it to be as the best way to review the plant layout and how to manage the plant because it contains all specification such as measurement, material selection and already visualize. Meanwhile, 3D design is also used for pipe checking to avoid clash of pipe.

ABSTRAK

Penyelidikan ini memberi tumpuan bagaimana hendak mereka bentuk model reaktor biodiesel pemangkin heterogen beserta lojinya berdasarkan 3D dengan menggunakan perisian AVEVA PDMS. Skop kajian ini adalah untuk memodelkan loji biodiesel pemangkin heterogen bagi pengeluaran biodiesel mengikut konsep kilang F3. Kemudian, untuk menghasilkan paip terperinci dan instrumentasi gambarajah (P & ID) loji dan akhir sekali mereka bentuk loji dalam lukisan 3D dengan menggunakan perisian AVEVA PDMS. Dalam kajian ini, sistem kelompok dipilih kerana fleksibiliti dan mengikuti konsep kilang F3 dan kilang tersebut dibina di atas trak kontena. Metodologi penyelidikan adalah mereka bentuk berdasarkan diagram paip dan instrumentasi (P & ID). Kemudian, mengira saiz peralatan dan reka bentuk mekanikal. Akhir sekali, simulasi 3D dijalankan. Untuk mernghasilkan reka bentuk 3D reaktor biodiesel pemangkin heterogen dan reka bentuk konsep loji biodiesel dengan menggunakan AVEVA PDMS telah dicapai. Akhir sekali, kepentingan kajian adalah untuk memenuhi permintaan industri dalam mereka bentuk 3D dan supaya ia menjadi sebagai cara yang terbaik untuk menguruskan loji dari segi system perpaipan, meletakkan peralatan, struktur kilang dan sitem pendawaian elektrik. Ia juga membantu dalam pengurusan sistem seperti pengukuran, pemilihan bahan dan mudah digambarkan. Sementara itu, reka bentuk 3D juga digunakan untuk memeriksa paip untuk mengelakkan pertembungan paip.

CHAPTER ONE

INTRODUCTION

1.1 Background of the Proposed Study

Generally, drawing of reactor design specifically is needed so that every people that see it can understand. The drawing can be done by using two dimensional (2D) or three dimensional (3D). Two dimensional (2D) means the drawing only involve length and width of the object. It usually use in drafting. Meanwhile, for three dimensional (3D), it involves length, width and height of the object. The 3D usually use in designing of object. In this research, 3D is required to design the alkali based heterogeneous catalytic reactor for the production of biodiesel. The 3D is chosen because the model provides much more detail so that designers and engineers can communicate the product information and visualize complex parts and assemblies more clearly. Since 3D model data can be transferred to analysis and validation tools and used for Computer

Aided Manufacturing (CAM) as well, it increases the accuracy of results and saves time by eliminating the need to re-create data. Many 3D modeling programs offer features that increase productivity by automating aspects of the design process, for example, by enabling the reuse of existing designs or the quick creation of part families. The main goal of 3D design is to reduce the time needed to get new products to market. Other objectives include meeting consumer demand for new products, improving product performance, enhancing product quality, and addressing increasingly complex customer requests. In many cases, companies are driven to 3D just to keep up with the competition. The key area for this research is based on AVEVA PDMS software to model an alkali based heterogeneous catalytic reactor for the production of biodiesel using pure cooking oil. AVEVA PDMS (Plant Design Management System) is software that provides a fully interactive, easy-to-use 3D environment and supported by Microsoft Office-style user interface to design a plant. It is customizable software, which means it is a multi-user and multi-discipline, engineer controlled design software package for engineering, designing and project construction. The software is also used in offshore and onshore oil & gas industry, chemical & process plants, mining, pharmaceutical, food industry, power generation and paper industries.

1.2 Problem Statement

Two dimensional, 2D designs of the alkaline based catalytic reactor and the plant only shows the draft of all the equipment which only provide information about the measurement of the equipment. From this, the model didn't provide much more detail such as visualization of complex parts and assemblies of the equipment. Due to the problem, 3D design is introduced where 3D design has ability to increase plant development performance and quality because of its full information on the specification of the plant.

1.2 Research Objective

Designing a conceptual alkali based heterogeneous catalytic biodiesel reactor and biodiesel plant based on 3D design by using AVEVA PDMS software.

1.4 Research Questions

1.4.1 What is the importance of 3D design in designing the alkali based heterogeneous catalytic biodiesel reactor and the conceptual 3D design of biodiesel plant?

1.4.2 How to design the alkali based heterogeneous catalytic reactor and a conceptual design of biodiesel plant by using AVEVA PDMS software?

1.5 Scope of the Proposed Study

1.5.1 To model an alkali based heterogeneous catalytic reactor.

1.5.2 To draw a detail piping and instrumentation diagram (P&ID) of the biodiesel reactor and plant.

1.5.3 To develop a 3D drawing of the biodiesel reactor and plant* using AVEVA PDMS software.

* The detail on the pipe size and structure is not included in this work.

1.6 Expected outcome:

3D design of heterogeneous catalytic biodiesel reactor and the conceptual design of the biodiesel plant will be produce by using AVEVA PDMS.

1.7 Significant of proposed study:

In fulfilling industries demand, the new 3D design is the best way to review the product because it contains all specification such as measurement, material selection and already visualize. This causes it to become more convincing rather than 2D design.

1.8 Thesis overview

In the next chapter, the part that will be highlight first is to gather the information by reviewing on the biodiesel process, batch reactor design, and type of heterogeneous catalyst and AVEVA PDMS software. Secondly, the methodologies on how to conduct the research on 3D design.

CHAPTER 2

LITERATURE REVIEW

2.1 The Background of Biodiesel Process.

Chemically biodiesel is defined as monoalkyl esters of long chain fatty acids derived from renewable feed stock like vegetable oils and animal fats. It is produced by transesterification in which, oil or fat is reacted with a monohydric alcohol in presence of a catalyst (Meher, Vidya Sagar, & Naik, 2006). According to Meher, Vidya Sagar & Naik, (2006), transesterification or alcoholysis is the displacement of alcohol from an ester by another in a process. The reaction requires a catalyst, usually a strong base, such as sodium or potassium hydroxide, and produces new chemical compounds called methyl esters (Gerpen, 2005). This process has been widely used to reduce the high viscosity of triglycerides. The transesterification reaction is represented by the general equation:

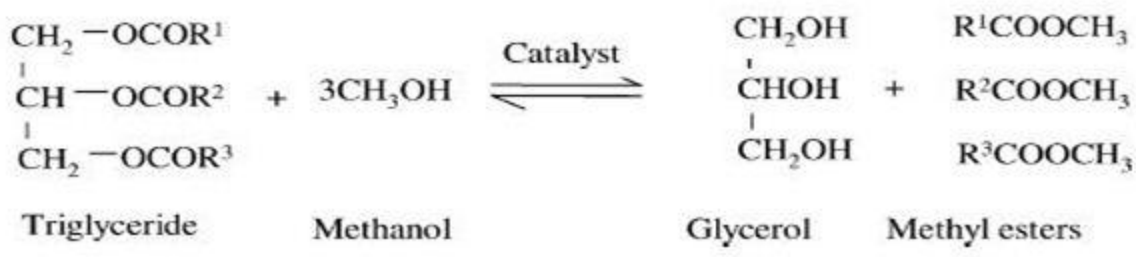

Figure 2.1.1: General equation for transesterification of FAME (Meher, et al., 2006)

Transesterification consists of three consecutive reversible reactions; conversion of triglyceride to diglyceride, diglyceride to mono glyceride and monoglyceride to fatty ester and glycerol. The reaction mechanism that takes place is according to this chemical equation:

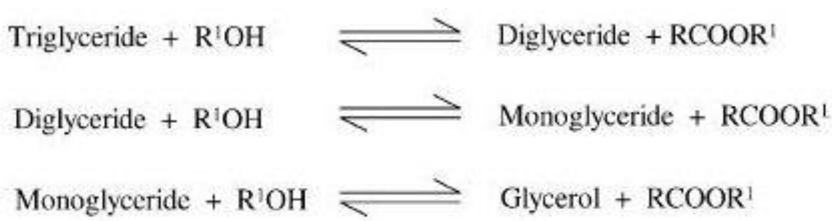

Figure 2.1.2: Mechanism for transesterification of triglyceride to FAME and glycerol (Meher, et al., 2006)

The reaction is facilitated with a suitable catalyst. If the catalyst remains in the same (liquid) phase to that of the reactants during transesterification, it is homogeneous catalytic transesterification. On the other hand, if the catalyst remains in different phase (i.e. solid, immiscible liquid or gaseous) to that of the reactants the process is called heterogeneous catalytic transesterification (Chouhan & Sarma, 2011) .In conclusion, the process of transesterification is affected by the mode of reaction condition, molar ratio of alcohol to oil, type of alcohol, type and amount of catalysts, reaction time and temperature and purity of reactants (Narasimharao, Lee, & Wilson, 2007).

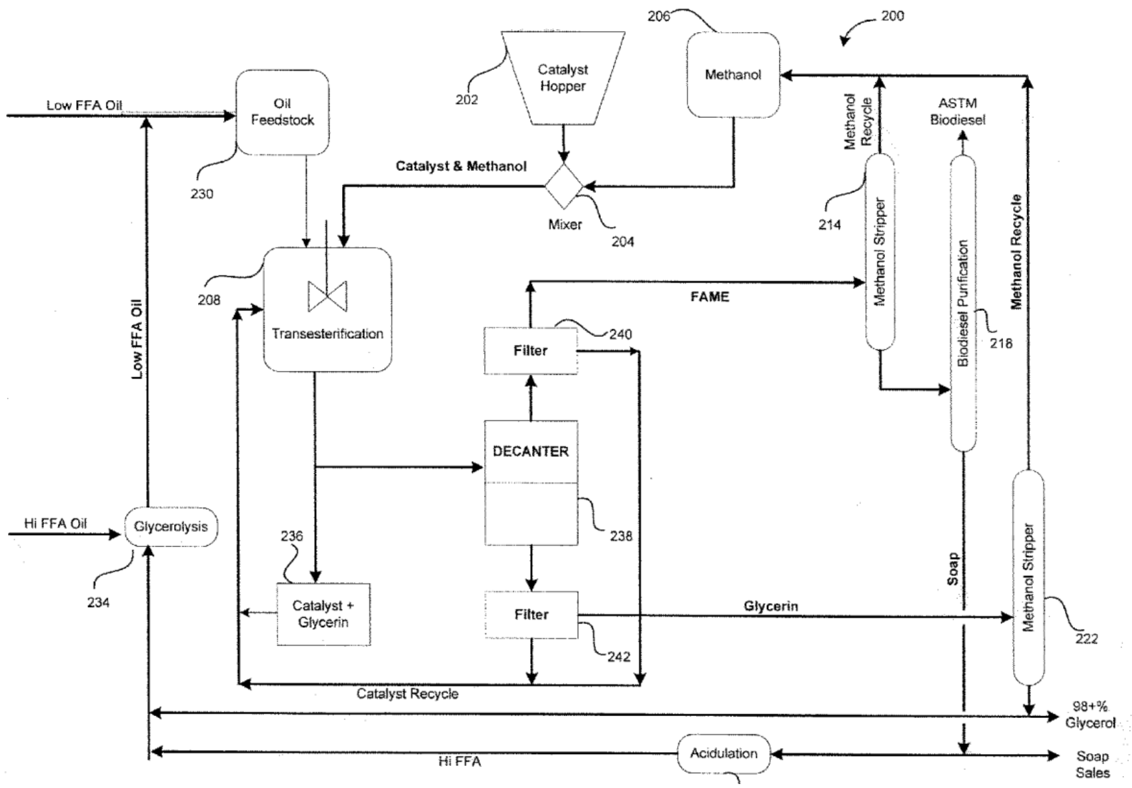

Figure 2.1.3: The process flow diagram for biodiesel production (Cai, Nieweg, Turner, & Wilkinson, 2010)

Meanwhile, the biodiesel process plant is separated into five sections as follows: section 1: feedstock treatment, section 2: methanol and catalyst feed, section 3: transesterification process, section 4: glycerin and catalyst separation, section 5: methanol separation and section 6; FAME purification and waste by product recycling.

Section 1 involve the feedstock treatment, in this process, the oil is being convert to become low free fatty acid, FFA oil. For the soap that recycle back from biodiesel purification separation, it will undergoes acidulation process. Then, it and high free fatty acid oil will be sent to glycerolysis to create low free fatty acid oil . Next, the FFA oil is sent to the oil feedstock.

Section 2 involve methanol and catalyst feed. The catalyst consist of solid metal oxide powder and is inserted into the catalyst hopper. Then, the methanol is placed into the methanol storage tank from the recycle. Both of them will be mixed throughly in mixer before entering the reactor.

Section 3 involve transesterification process. In transesterification process, the methanol and FFA oil will undergoes transesterification to produce fatty acid methyl ester and glycerin. The reaction is carried out in batch manner at 25 ^{o}C and 1atm. Meanwhile, the catalyst is in mobilized manner.

Section 4 involves the glycerin and catalyst separation. In this section, the glycerin and catalyst will be separated by using decanter. FAME and methanol will go upward because of their less density (lighter weight) and glycerin and catalyst will go downward because it is heavier.

Section 5: methanol separation. Methanol is separate by using evaporator at its boiling point, 82^{o}C and at 0.09 atm (Cai, et al., 2010).

Section 6 consist of FAME purification and waste by product recycling. The FAME is purified by using distillation column at 159 ^{o}C and 30 kPa. FAME will be top product and oil will be the bottom product because it has boiling point of 318 ^{o}C (Gurski, Kazim, Cheung, & Obeid, 2009).

2.2 Types of Heterogeneous Catalyst.

Heterogeneous catalyst is widely used in production of biodiesel because of its advantages: it has relatively faster reaction rate than acid-catalyzed transesterification, the reaction can occur at mild reaction condition and the catalyst do not mix thoroughly with the product because the catalyst exists in solid phase while the product is in liquid form. The heterogeneous catalyst for biodiesel production mainly consists of metal oxides. Different metal oxides have different specification and performance. Catalyst is use to decrease the activation energy and fastened the reaction.

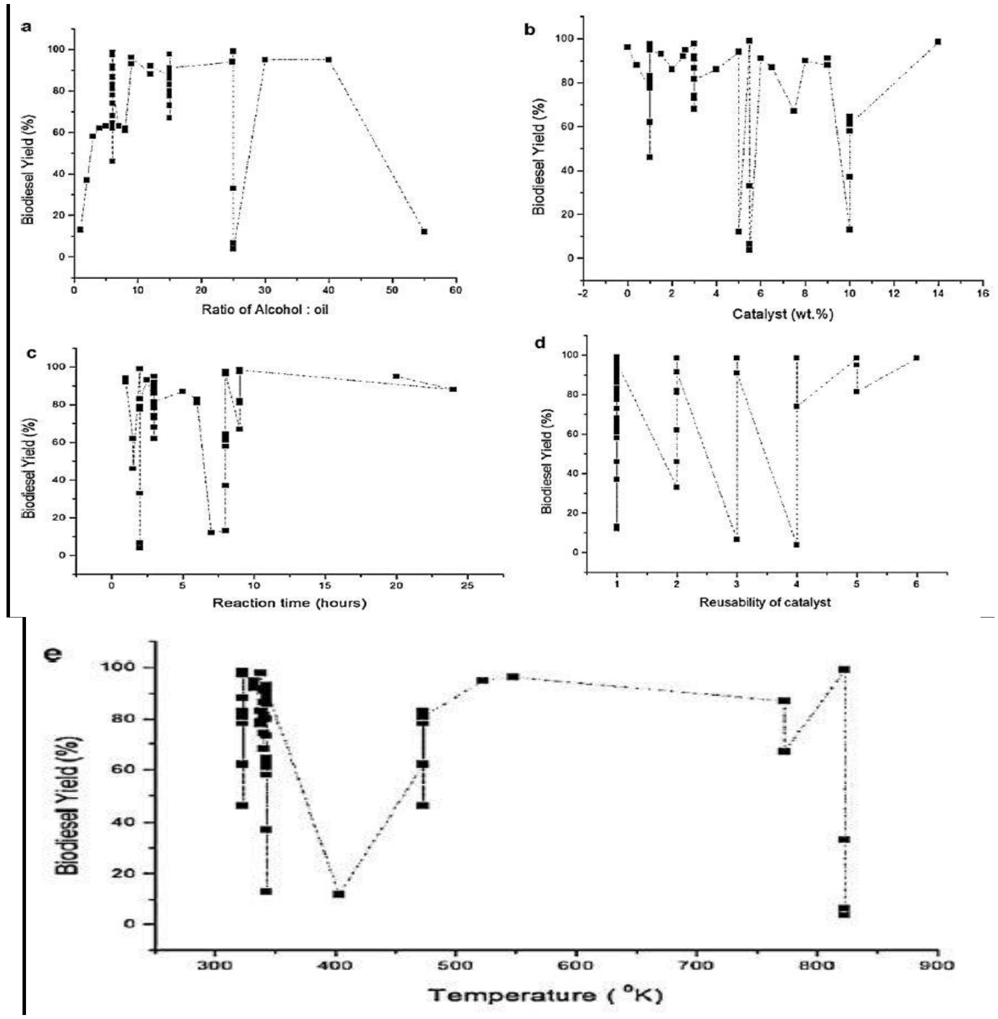

Figure 2.2.1: Effect of earth metal oxide based heterogeneous catalyst,(a) effect of alcohol: oil on biodiesel yield, (b) effect of catalyst on biodiesel yield, (c) effect of reaction time with biodiesel yield, (d) reusability of catalyst on catalyst production and effect of temperature on biodiesel.(Chouhan & Sarma, 2011)

Catalyst	Catalyst characterizations	Catalyst preparation	Feedstock	Operation conditions	Results	Ref.
Nano MgO solid base	Particle size = 60 nm	Not reported	Soybean oil	P = 24 MPa, T = 250 °C, t = 10 min, alcohol/oil = 36:1, catalyst content = 3%	Conversion = 99%	[33]
CaO solid base	SSA[a] = 32 m^2/g, MPS[b] = 25–30 nm	CaO powder was calcined at 1000 °C.	Sunflower oil	T = 60 °C, t = 100 min, alcohol/oil = 13:1, catalyst content = 3%	Conversion = 94%	[32]
CaO solid base	SSA = 56 m^2/g	Not reported	Soybean oil	T = 65 °C, t = 3 h, alcohol/oil = 12:1, catalyst content = 8%	Conversion = 95%	[45]
$Ca(C_2H_3O_2)_2$/SBA-15 solid base	SSA = 7.4 m^2/g, pore volume = 0.019 cm^3/g	The catalyst was prepared by an impregnation method of aqueous solution of calcium acetate on the support followed by calcination at 900 °C for 4 h.	Sunflower oil	T = 60 °C, t = 5 h, methanol/oil = 12:1, catalyst content = 1%	Conversion = 95%	[67]
$Ca(OCH_3)_2$ solid base	SSA = 19 m^2/g, pore size = 40 nm	Calcium methoxide was synthesized by a direct reaction of calcium and methanol at 65 °C for 4 h.	Soybean oil	T = 65 °C, t = 2 h, alcohol/oil = 1:1, catalyst content = 2%	Conversion = 98%	[71]
SrO solid base	SSA = 1.05 m^2/g	SrO was prepared from calcination of strontium carbonate in a muffle furnace at 1200 °C for 5 h.	Soybean oil	T = 65 °C, t = 30 min, alcohol/oil = 12:1, catalyst content = 3%	Conversion = 95%	[21]
ZnO/$Sr(NO_3)_2$ solid base	Basicity = 10.8 mmol/g	The aqueous solution of Sr $(NO_3)_2$ was loaded on ZnO by impregnation method and calcined at 600 °C for 5 h.	Soybean oil	T = 65 °C, t = 5 h, methanol/oil = 12:1, catalyst content = 5%	Conversion = 93%	[66]

Figure 2.2.2: Different type of catalyst and its performance at different feedstock.(Lam, Lee, & Mohamed, 2010)

2.3 Batch Reactor Design Equation.

A batch reactor is a chemical reactor in which the reactants and catalyst are introduced in the desired quantities and the vessel is then closed to the delivery of additional material. In this reactor, there is no inflow and outflow of reactant and product. A typical batch reactor consists of a tank with an agitator and integral heating and cooling system. Products within batch reactors usually liberate or absorb heat during processing. Even the action of stirring stored liquids generates heat. In order to hold the reactor contents at the desired temperature, heat has to be added or removed by a cooling jacket or cooling pipe. Heating or cooling coils or external jackets are used for heating and cooling batch reactors. Heat transfer fluid passes through the jacket or coils to add or remove heat. The main part of batch reactor is the residence time. Residence time is a time taken to complete one batch. The batch reactor has many advantages. Firstly, it has high conversion that can be obtained by leaving the reactant in the reactor for a long period of time (Fogler, 2006).Then, the batch reactor has the flexibility of operation-same reactor can produce one product one time and a different product the next. Lastly, it is easy to be clean up. While reaction is carried out in this reactor, flow in and flow out is equal to zero.

(F_{in} = F_{out} = 0). Therefore, according to the resulting mole balance is: input + generation = output + accumulation (Fogler, 2006)

$$F_{jo} + \int_{V_o}^{V} r_j \, \partial V = F_j + \frac{\partial N_j}{\partial t}$$

Where,

Input, F_{jo} = output, $F_j = 0$

Therefore,

$$\int_{V_o}^{V} r_j \, \partial V = \frac{\partial N_j}{\partial t}$$

$$\partial t = \frac{\partial N_j}{r_j V}$$

Then, integrating limits that at $t = 0$, $N_j = N_{jo}$ and at $t = t_1$, $N_j = N_{j1}$, therefore:

$$\mathbf{t = \int_{N_{j1}}^{N_{j0}} \frac{\partial N_j}{r_j V}}$$

Where,

t = residence time (time taken to complete one batch)

The solid catalyst used for the reaction is Calcium oxide, CaO. This is because CaO produce conversion at range from 90% to 99% at time from 1 hour to 5 hours for reaction temperature of 60^{o}C to 80^{o}C(Gurski, et al., 2009). Concerning the transesterification of oil with methanol using solid CaO catalyst, abstraction of proton from methanol by the basic sites to form methoxide anion is the first step of the reaction. The methoxide anion attacks carbonyl carbon

in a molecule of the triglyceride, which leading to formation of the alkoxycarbonyl intermediate. Then, the alkoxycarbonyl intermediate divides into two molecules: FAME and anion of diglyceride.

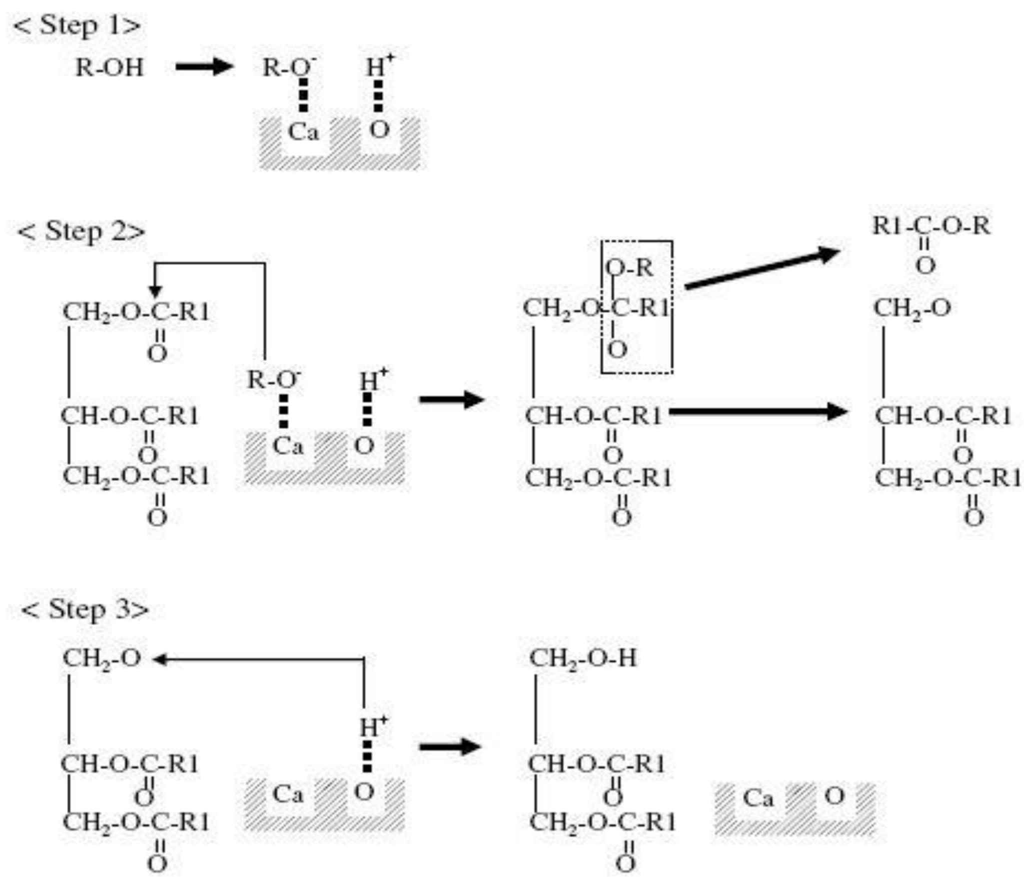

Figure 2.3.1: Mechanism on the catalyzed transesterification using CaO (Kouzu, et al., 2008)

Meanwhile, the raw material use for the production is vegetables oil and methanol. Both of the material has different physical properties. The physical properties for triglycerides mainly triolein are it has flash point of 327^{o}C, boiling point of above

400^{o}C, density of 950 kg/m^3 , viscosity of 0.039884 Pa.s and it exist as yellowish liquid at room temperature. Meanwhile, methanol has molar mass of 32.04 g mol−1, density of 0.7918 g cm−3, melting point of −98^{o}C to -97 °C, flash point from 11^{o}C to 12^{o}C, viscosity of 5.9×10−4 Pa s and boiling point of 65 °C. Methanol exists as colorless liquid at room temperature. Furthermore, the product consists of the Fatty Acid Methyl Ester, FAME or biodiesel and glycerol. The physical properties of Biodiesel (FAME) are it has flash point of 164^{o}C, density of 871 kg/m3, viscosity of 0.0044 kg/ms and boiling point at 360^{o}C. Then, glycerol has molar mass of 92.09 g mol−1, flash point of 204.5oC, density of 1.261 g/cm3, boiling point at 290 °C, melting point at 17.8 °C, viscosity of 1.412 Pa s and it exist as clear colorless solid at room temperature.

2.4 Why 3D CAD is needed instead of 2D CAD?

3D CAD is needed because it has several advantages. The advantages are saving time & money, more detail information; helps identify errors early and enhance communication. The 3D CAD has proved that it can save time and money because it is more accurate than 2D CAD drawings. Thus, the product produce is better, optimized in size and weight, better performance and no faults in the design. Then, the 3D CAD has more detail information than 2D CAD because it contain the total weight, width, height, length and volume very often can be crucial elements in a design, especially when performing a structural analysis and when meeting legal requirement.

There're many kinds of information should be treated while in 3-d review, including graphic information, topological information and attribute information.