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**Effect of Different Catalysts for Biodiesel Production via
Aspen Plus® Simulation**

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the degree of Bachelor of Applied Science (Bioindustrial
Technology) with Honours**

FACULTY OF BIOENGINEERING AND TECHNOLOGY

UMK

2024

DECLARATION

I declare that this thesis entitled “Effect of Different Catalyst for Biodiesel Production via Aspen Plus® Simulation” is the results of my own research except as cited in the references.

Signature : _____

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Effect of Different Catalyst for Biodiesel Production via Aspen Plus® Simulation

ABSTRACT

The study addresses the challenge of optimizing biodiesel production methods, considering the time, cost, and resource-intensive nature of conventional testing techniques. The deficiency in a cost-effective and comprehensive approach prompts the exploration of Aspen Plus® simulation as a tool to enhance biodiesel production techniques. The objective is to develop an online environment for researching and optimizing the process parameters, catalysts, and operational conditions, with the aim of improving efficiency, reducing expenses, and expediting the discovery of environmentally friendly and profitable biodiesel production approaches. The research employs Aspen Plus® simulation software to simulate biodiesel production from waste cooking oil using various heterogenous catalysts such as crab shell and plantain peel, tungsten and activated charcoal. The efficiency of these heterogeneous catalysts is evaluated by comparing biodiesel yield and purity. Additionally, the performance of bifunctional heterogeneous catalysts is compared with other catalysts commonly used in biodiesel production. The methodology involves Aspen Plus® simulation and transesterification as the primary process, utilizing waste cooking oil, methanol, and catalysts. The viability of the suggested base case study is assessed through process simulation, emphasizing glycerol management and optimizing transesterification conditions for the production of 80000 tonnes per year of biodiesel. The outcomes of this study proven that heterogenous bifunctional catalyst has produced highest yield and purity compared to others. They also contribute to a more sustainable and economically viable biodiesel production process.

Keywords: Biodiesel production, waste cooking oil, Aspen Plus®, simulation, heterogenous catalyst

Kesan Katalis Berbeza untuk Pengeluaran Biodiesel melalui Simulasi

Aspen Plus®.

ABSTRAK

Kajian ini mengatasi cabaran dalam mengoptimumkan kaedah pengeluaran biodiesel, dengan mempertimbangkan masa, kos, dan sifat yang memerlukan banyak sumber teknik pengujian konvensional. Kekurangan dalam pendekatan yang berkesan dari segi kos dan menyeluruh mendorong penyelidikan simulasi Aspen Plus® sebagai alat untuk meningkatkan teknik pengeluaran biodiesel. Objektifnya adalah untuk membangunkan persekitaran dalam talian untuk penyelidikan dan mengoptimumkan parameter proses, katalis, dan keadaan operasi, dengan tujuan untuk meningkatkan kecekapan, mengurangkan perbelanjaan, dan mempercepatkan penemuan pendekatan pengeluaran biodiesel yang mesra alam dan menguntungkan. Kajian ini menggunakan perisian simulasi Aspen Plus® untuk mensimulasikan pengeluaran biodiesel dari minyak masak terpakai menggunakan pelbagai katalis heterogen seperti kulit ketam dan kulit pisang, tungsten dan arang aktif. Kecekapan katalis heterogen ini dinilai dengan membandingkan hasil dan kemurnian biodiesel. Selain itu, prestasi katalis heterogen bifungsional dibandingkan dengan katalis lain yang biasa digunakan dalam pengeluaran biodiesel. Metodologi ini melibatkan simulasi Aspen Plus® dan transesterifikasi sebagai proses utama, menggunakan minyak masak terpakai, metanol, dan katalis. Kekadarans kes asas yang dicadangkan dinilai melalui simulasi proses, dengan menekankan pengurusan gliserol dan mengoptimumkan keadaan transesterifikasi untuk pengeluaran 40000 tan setahun biodiesel. Keputusan kajian ini membuktikan bahawa katalis heterogen bifungsional menghasilkan hasil dan kemurnian tertinggi berbanding dengan yang lain. Mereka juga menyumbang kepada proses pengeluaran biodiesel yang lebih mampan dan ekonomi.

Kata kunci: Pengeluaran Biodiesel, Minyak Masak Terpakai, Aspen Plus®, Simulasi, Katalis Heterogen.

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LIST OF ABBREVIATIONS

C	Carbon	5
O	Oxygen	10
K	Potassium	3
Na	Sodium	3
H	Hydrogen	6
Cl	Chlorine	1

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LIST OF SYMBOLS

®	Registered trademark	26
%	Percentage	56
\$	Dollar sign	1
°C	Celsius	3

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

The level of thought spent on the manufacturing of biodiesel as a replacement for petroleum has increased significantly during the last few years. It is better for the environment than natural gas and crude oil since it is made out of resources that can be replaced (Brahma et al., 2022). Biodiesel is made through a process called transesterification. Lipids are substances from plants or animal-based fats that are mixed with alcohol, usually ethanol or methanol, and a chemical called a catalyst. The choice of catalyst has a big effect on the rate of the chemical reaction, as well as the amount produced and the properties of the resulting biodiesel that comes out of the process. During this time, different types of catalysts, which include homogeneous (alkali and acid) and heterogeneous (solid bases and acids, enzymes, and immobilised catalysts), have been investigated to make biodiesel (Zik et al., 2020). During the entire procedure of making biodiesel, a byproduct called glycerol is made. Glycerol is used in numerous fields, especially in cosmetics and medical treatment businesses. It is also used to make a broad spectrum of various chemicals (Chilakamarry et al., 2021). While manufacturing biodiesel, it has several distinct types of fuels that can be utilised. There are enzymatic catalysts, homogeneous catalysts, and mixed catalysts. The focus of this work is on employing different types of heterogeneous catalysts to turn cooking oil into biodiesel (Sarno & Iuliano, 2019).

By employing Aspen Plus® simulation software, the purpose of this investigation is to determine the impact that various catalysts have on the amount of biodiesel produced as well as its overall quality. The three different types of catalysts that were utilized in this research were a heterogenous bifunctional catalyst (crab shell and plantain peel) (Amenaghawon et al., 2022), a heterogenous acid catalyst that using tungsten (W) (Yusuff & Owolabi, 2019) and a heterogenous alkali catalyst (activated charcoal) (Marwaha et al., 2018). Since these types of catalysts are produced using discarded products in order it makes them a good fit for the idea of converting trash become treasure, that contributed to their selection. This investigation made utilise waste cooking oil has its source material; waste cooking oil is an unwanted by product of the food production industry (Sahar et al., 2018). The recycling of used cooking oil into a feedstock in for manufacturing of biodiesel is a strategy that is beneficial to for the natural world because it results in less waste and less releases of atmospheric greenhouse gases (Masahiro Matsuura et al., 2018). In combination with this, it serves as an affordable substitute to utilising virgin oils, that are pricey as could end up in a shift in land usage.

The Aspen Plus® simulation software can be used to efficiently simulate and optimise operations (José Luis Valverde et al., 2022). This makes it possible to conduct studies and research on chemical processes that can later be put into use, including the production of biodiesel. The software programme can simulate the kinetics of reactions and forecast the characteristics of the final product, with the goal of aiding in procedure parameter optimisation (Zik et al., 2020). By analysing the yield and quality of the biodiesel that is produced, this study aims to assess the three catalysts' performance. The amount produced in biodiesel is determined by the transformation of triglyceride to

methyl ester, and this conversion rate is influenced by the type and amount of catalyst used. Additionally, the chemical and physical properties of biodiesel that have an impact on the fuel's quality as a whole include the fuel's viscosity, density, flash point, and acid value. The features of the final biodiesel output are influenced by the type of catalyst used and the conditions of the reaction that occur (Soria-Figueroa et al., 2020).

In conclusion, the use of waste cooking oil as a feedstock and waste materials as catalysts for the creation of biodiesel is a strategy that shows promise for the generation of environmentally friendly energy. The Aspen Plus® simulation software can be utilised to assist in the optimisation of the process parameters and the evaluation of the effectiveness of various catalysts. The findings of this research could aid in the formulation of a method for the manufacturing of biodiesel that is both more environmentally friendly and more productive.

1.2 Problem Statement

The problem statement of this study is improving the Aspen Plus simulation variables in order to achieve maximum biodiesel yield and process efficiency while utilising waste cooking oil as the feedstock for biodiesel production. Conventional testing techniques for optimizing biodiesel production take quite a bit of time and money, as well as a lot of resources. Due to this, there currently needs to be a better way to examine the parameters of the process, catalysts, and operational conditions that will also be cheaper. The intention of this project is to use Aspen Plus® simulation as a tool to solve the aforementioned issue while developing an online environment for researching and enhancing the techniques of making biodiesel. By using Aspen Plus® modelling, the present research hopes to improve the effectiveness of the production process, lower

expenses, and speed up the discovery of approaches to making biodiesel that are both environmentally friendly and profitable.

1.3 Objectives

The objectives are:

1. To simulate the production of biodiesel from waste cooking oil using the different catalyst such as crab shell and plantain peel, tungsten and activated charcoal catalysts via Aspen Plus® simulation software.
2. To evaluate the efficiency of the heterogeneous catalysts in converting waste cooking oil to biodiesel by comparing the yield and purity of biodiesel produced using the three different catalysts.
3. To compare the performance of the bifunctional heterogeneous catalysts with other catalysts used in biodiesel production.

1.4 Scope of Study

The study can investigate and compare the efficiency of the three catalysts in terms of biodiesel yield. This can be done by analysing the impact of the different catalysts on the conversion of waste cooking oil to biodiesel, and comparing the yields obtained from each catalyst (Smith, et al., 2020). In the proposed research, the effect of biodiesel production on the surrounding ecosystem will be examined utilising a variety of catalysts (Johnson & Brown, 2018). It will take into account things like the amount of trash produced, the emissions of greenhouse gases, and the general sustainability of the

operation. In order to determine which method of producing biodiesel is the least harmful to the surrounding ecosystem, comparisons between the various catalysts will be conducted. The scope of study can be to optimize the process conditions for each of the catalysts with the aim of maximizing the yield of biodiesel (Garcia, et al., 2020). This can involve varying parameters such as temperature, pressure and reactant concentrations to determine the optimal conditions for each catalyst.

1.5 Significances of Study

According to Smith et al. (2019), the manufacturing of biodiesel using used cooking oil has garnered a lot of media coverage over the past decade because of the fact that it possesses a chance to be a healthier for the environment option to petroleum and natural gas. According to Chen et al.'s research from 2020, the kind of catalyst that is utilised has a significant impact on how effective the biodiesel synthesis procedure is. Developing environmentally friendly energy sources requires an in-depth comprehension of how the performance of different catalysts influences the amount of biodiesel that may be produced. Through applying the capabilities of the Aspen Plus® modelling programme, the goal of this investigation is to offer a few fresh perspectives through the catalyst that is highly efficient for manufacturing biodiesel using waste cooking oil. The amount of biodiesel that can be produced is going to be considered evaluated as an important factor in the research. Additionally, according to Yang et al. (2022), the usage of catalysts that are created from discarded materials can bring considerable benefits, both economically and environmentally, and is consistent alongside the ideas underlying the so-called circular economy. It is possible to regard waste products is an expensive commodity that may be regenerated to make use of waste products in the creation of catalysts.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

As an eco-friendly substitute for petroleum diesel, biodiesel has attracted a lot of interest (Pasha et al., 2021). There is evidence that biodiesel has several positive characteristics. It may be utilised in previously current generators without requiring major changes because the material is sustainable, harmless, renewable, has intrinsic lubrication, carries very little or no sulphur, and has excellent environmental properties (Singh et al., 2020). Due to its high incompatibility with gasoline and diesel, it can be mixed in various gasoline and diesel ratios.

2.2 Current Trends in Biodiesel

Although governments throughout the globe search for alternative sources of energy, biodiesel manufacturing has seen a rise in market share. Grand View Research predicts that by 2027, the worldwide biodiesel marketplace will be worth \$54.8 billion due to rising worries about the natural world and regulatory requirements encouraging the use of alternative biofuels (Grand View Research Reports, 2019).

In the United States, sodium hydroxide (NaOH) and potassium hydroxide (KOH) are the two types of hydroxides that are utilised the most frequently as a catalyst for the

manufacture of biodiesel. Both sodium hydroxide (NaOH) and potassium hydroxide (KOH) are powerful alkali catalysts that have a high level of catalytic activity. This results in accelerated transesterification processes and increased biodiesel yields. (National Biodiesel Board, 2021) Problems can arise, however, due to the corrosive nature of these substances and the possibility for difficulties in the disposal of waste. Research is being done to produce heterogeneous catalysts such solid acids and enzymes that give benefits in terms of the recovery and reusability of the catalyst. Aspen Plus® modelling experiments have showed the efficacy of solid acid catalysts such as Amberlyst-15 and sulfonated graphene oxide in increasing biodiesel output and quality. These catalysts have greater selectivity and stability, reducing the generation of soap and other undesirable by-products. Furthermore, enzyme catalysts such as lipases have demonstrated encouraging outcomes by providing softer reaction conditions and lowering energy needs.

In Europe, methanol in conjunction with sodium or potassium hydroxide is the most commonly used catalyst for biodiesel generation. However, as a result of environmental concerns and a desire for a more sustainable approach, the emphasis is turning to other catalysts. Acid catalysts, such as sulfuric acid and hydrochloric acid, are gaining popularity because they allow for the utilization of low-cost feedstocks such as waste frying oil and animal fats. Aspen Plus® simulations show that using acid catalysts improves the esterification of free fatty acids, resulting in better biodiesel yields. The selection of acid concentration and reaction parameters is critical in attaining optimal conversion rates while minimising undesirable side reactions. Furthermore, solid acid catalysts such as sulfated zirconia and zeolites have been investigated as possible alternatives to liquid acids due to their ease of separation and low waste production (Ennetta et al., 2022).

Biodiesel production in Asia is quickly expanding due to rising energy demands and environmental concerns. Sodium or potassium hydroxide in conjunction with methanol is a common catalyst. To minimize competing with food crops, researchers are working on inventing catalysts that can utilize non-edible oils such as jatropha, pongamia, and waste vegetable oils (Syafiuddin et al., 2020). Alkali metal catalysts paired with low-cost feedstocks can result in high biodiesel yields, according to Aspen Plus® simulations. Furthermore, heterogeneous catalysts such as calcium oxide and hydrotalcites have shown promise in biodiesel synthesis, providing economic benefits while lowering environmental effect. In addition, research on enzyme catalysts, particularly immobilised lipases, is gaining traction because to their capacity to convert non-edible oils into biodiesel at greater conversion rates and with enhanced fuel characteristics.

Over the past few years, the worldwide biodiesel business has grown a lot, and manufacturing and utilization are expected to grow a lot more in 2008. Biofuels, like petroleum, have become a good alternative to fossil fuels as worries regarding warming temperatures and the demand for sources of clean energy keep growing. The research presented here looks at the patterns and estimates of biofuel production around the world. It focuses on information collected in 2008 and gives predictions for the expansion of the renewable energy sector up to 2025 (Ali et al., 2022).

As can be seen in Figure 2.1, global production and sales of biodiesel have increased in the past few years as countries attempt to reduce their reliance on petroleum and diesel and lessen the environmental effect of transportation. Biodiesel is an environmentally friendly fuel that comes from vegetable oil-based products, livestock

fats, and recycled cooking oils. It is a viable alternative to regular diesel fuel since it may be utilised by diesel engines without modification. Biodiesel manufacturing requires numerous phases, including feedstock cultivation and gathering, extraction and refining, as well as processing. Soybean oil, rapeseed oil, palm oil, and leftover cooking oil are the most often utilised feedstocks for biodiesel manufacturing. Biodiesel, once produced, can be utilised locally or traded abroad.

A multitude of variables will influence the regional distribution of global biodiesel production and consumption in 2025, including policy from governments, source availability, technological advancements, and market demand. It is impossible to calculate exact numbers for 2025, however it is anticipated that the following sectors will continue to be important for the extraction and use of biodiesel. The distribution within a region of biodiesel production and use worldwide in 2025 will be influenced by a wide range of factors, such as consumer demand, technological advancements, source availability, and governmental choices. Even though it is hard to make exact forecasts for 2025, it is projected that the following sectors will continue to play crucial parts in the gathering and utilisation of biodiesel.

Brazil and Argentina are the two countries that produce the most biodiesel in South America. Brazil, known for its sugarcane ethanol industry, has expanded its production of biodiesel from soybean oil. Argentina, a large producer of soybeans, sells a significant amount of biodiesel to markets across the world. In the Asia-Pacific region, biodiesel production is rising quickly. Indonesia and Malaysia are significant rivals in the biodiesel market due to their massive production of palm oil. To increase domestic

consumption, biodiesel blending is required in both countries. Moreover, countries like Vietnam, Thailand, as well as the Philippines are growing their biodiesel sector.

Some regions, including parts of the Middle East and Africa, are starting to look into the production of biodiesel. Programmes to produce biodiesel have been started in South Africa, Nigeria, and Egypt in an effort to reduce reliance on fossil fuels and promote agricultural development. It is critical to keep in mind that market circumstances, resource availability, and legislative changes can all affect regional distributions. In addition, future developments in technology, such advanced biofuels or electric vehicles, might impact the use and distribution of biodiesel.

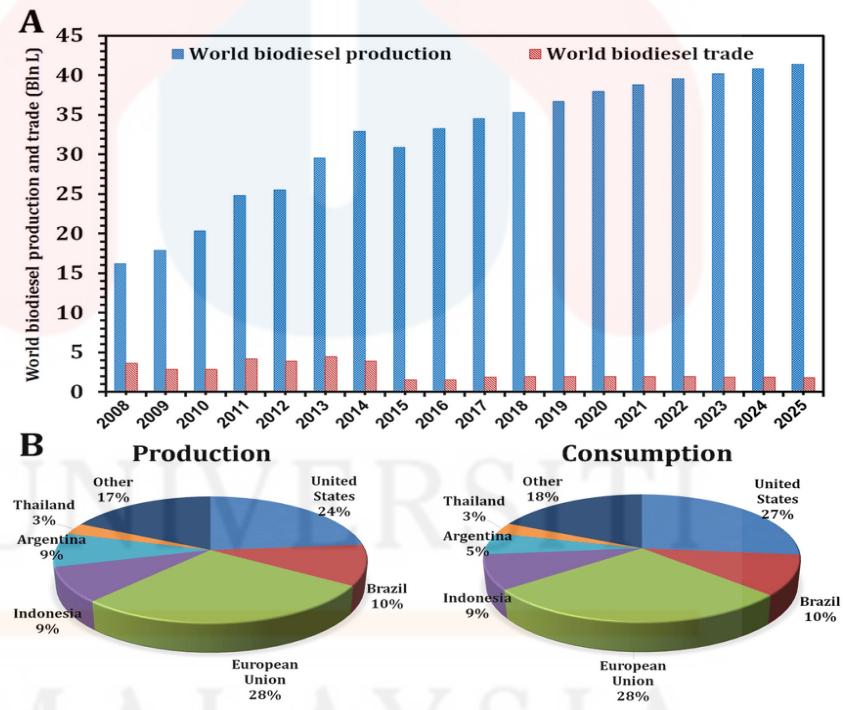


Figure 2.1: Worldwide production and exports of biodiesel (A). Geographical distributions of the production and use of biodiesel globally in 2025 (B).

(Source: Ali et al., 2022)

2.3 Properties of Biodiesel

Biodiesel is an environmentally friendly substitute to standard diesel fuel that has various specific qualities that allow it a potential choice for the automobile sector. Viscosity, flash point, heating value, and water content are among the characteristics that have a significant impact on how well biodiesel performs and works with diesel engines.

2.3.1 Viscosity

The viscosity of biodiesel is an essential feature that influences its performance as a fuel. Waste cooking oil has recently attracted more attention as a potential fuel for biodiesel generation. The impact of reaction conditions on the viscosity of biodiesel made from used cooking oil has been examined in a number of research. Zarei et al. (2020) performed a techno-economic analysis of the manufacture of biodiesel from used cooking oil. The study discovered that employing this approach to produce biodiesel was more expensive than using standard diesel fuel. However, the study also discovered that using used cooking oil as a feedstock for making biodiesel can have considerable environmental advantages, including decreased greenhouse gas emissions and lower costs associated with waste disposal. Choi et al. (2018) studied the influence of reaction temperature and pressure on the viscosity of biodiesel generated from waste cooking oil. According to the study, lowering the reaction temperature and pressure caused the biodiesel's viscosity to drop. This is because quicker reaction rates brought on by greater temperatures and pressures cause a more thorough conversion of triglycerides to biodiesel, which has a lower viscosity.

2.3.2 Flash Point

The flash point is the lowest temperature at which a fuel can create enough vapour to ignite in the presence of air. In this examination of the literature, can see at the connection between the quantity of biodiesel made from used cooking oil at high pressures and temperatures and its flash point. Numerous research has looked at how high pressure and temperature affect the production of biodiesel from waste oil. For instance, research by Wang et al. (2018) found that using supercritical methanolysis at a pressure of 20 MPa and a temperature of 280°C can boost biodiesel output by up to 95%. The study also shown that the biodiesel generated under these circumstances had a greater flash point than biodiesel produced using conventional transesterification techniques.

2.3.3 Heating Value

The quantity of heat energy generated by the burning of a unit volume or mass of biodiesel is referred to as the heating value. A precise evaluation of the thermal energy content of the generated biodiesel is possible by virtue of the ability to estimate the thermal efficiency of biodiesel synthesis using Aspen Plus® simulation. Biodiesel is a sustainable fuel made from diverse feedstocks that include vegetable fats as well as animal fats that may be used in place of traditional diesel fuel. The process simulation programme Aspen Plus® provides sophisticated capabilities for modelling and analysing the transesterification process in biodiesel synthesis. Aspen Plus® can compute the heating value of the produced biodiesel by inputting important data such as feedstock composition, reaction kinetics, and operating conditions. Aspen Plus® evaluates the molecular content of the biodiesel, including the presence of fatty acid methyl esters (FAMEs) in the product, during the simulation. It uses thermodynamic equations and sources to calculate the biodiesel's lower heating value (LHV) or higher heating value

(HHV). The heating value is the quantity of heat energy emitted when the biodiesel is completely burned. It is an important quantity since it shows the fuel's possible energy amount as well as combustion efficiency. Greater heating values take into consideration the heat produced by the water created through the ignition process, whilst lower heating values do not. The simulation results demonstrated that the suggested procedure may produce a significant amount of biodiesel while using little energy (Salehi et al., 2019).

2.3.4 Water Content

The amount of water in biodiesel can significantly affect its viscosity, density, flash point, and oxidative stability. Increased water content in biodiesel can result in a decrease in the flash point and oxidative stability while increasing viscosity and density. These characteristics may have an impact on how well and how long biodiesel will last in storage. According to research, the quantity of water in biodiesel is affected by a variety of factors, including the feedstock utilised, the kind of catalyst employed, the reaction conditions, and the separation methods used. According to a review of the production of biodiesel from waste oil at high pressure and temperature by Sheng et al. (2021), the amount of water in biodiesel may be decreased by raising the reaction's temperature and pressure. The study also demonstrated that the amount of water in biodiesel may be greatly reduced by using heterogeneous catalysts.

2.4 Biodiesel Production from Transesterification Process

Biodiesel manufacturing from used cooking oil has grown in popularity due to its ability to reduce greenhouse gas emissions and waste. One of the most widely utilised processes for producing biodiesel is transesterification. In recent years, the

transesterification procedure for producing biodiesel from spent cooking oil has been designed and optimised using Aspen Plus® modelling. Using Aspen Plus® modelling, we will examine the most recent developments in the synthesis of biodiesel in this literature review, with an emphasis on the utilisation of membrane reactors. Transesterification is a chemical process that includes the exchange of an ester group in a triglyceride with an alcohol, often methanol or ethanol, to generate fatty acid methyl esters (FAMEs) or fatty acid ethyl esters (FAEEs), with glycerol as a byproduct. The following equation can be used to illustrate the entire transesterification reaction.

FAME and glycerol are created through the transesterification process of lipids derived vegetable oils with alcohols in with the assistance of a catalyst, as shown in Figure 2.2. The aforementioned alcohols can be manufactured by fermentation, which makes them accessible and affordable. It also makes homogenous catalysts easier to dissolve (Mukhtar et al., 2022). Methanol and ethanol are among the majority prevalent alcohols used in the aforementioned procedures. Because of the chemical reaction's complete bidirectionality, a significant amount of alcohol is needed to tilt the balance in favour of the desired outcomes. A triglyceride first combines with alcohol to produce a fatty acid methyl ester and a diglyceride. In order to create an additional molecule of the fatty acid methyl ester with a monoglyceride, this molecule reacts with a distinct molecular form of alcohol. The exact same thing occurs once more. Stoichiometry therefore shows that three molecules of alcohol and three molecules of triglyceride can be converted into three molecules of FAME and one molecule of glycerol (Ketzer et al., 2022). The transesterification process is typically sped up in a factory setting by the addition of a powerful basic catalyst, such as NaOH or KOH. However, other methods include the use of enzymes like lipases, strong acids like H_2SO_4 and HCl, and heterogeneous catalysts

(Bunushree Behera et al., 2020). Following the procedure, there are going to be two phases: glycerol on the bottom and biodiesel (FAME) on top. Water, organic compounds that gave the oil its colour and flavour, inorganic salts, alcohol, glycerides, and a catalyst are all components of the final step, which was also present in the vegetable oil. In order to be employed as a raw material in other operations, this waste product can therefore be cleaned and sorted.

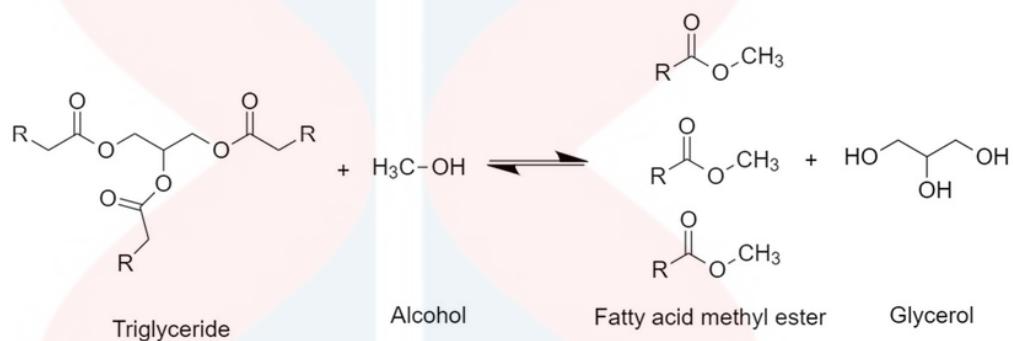


Figure 2.2: Transesterification reaction from triglyceride

(Source: Suárez-Torielle, 2021)

2.4.1 Bifunctional Heterogenous Catalyst

The production of biodiesel using waste oil from cooking is a cost-effective solution for minimising waste while simultaneously providing an additional source of energy. The application of standard chemical catalysts, on the other hand, can make the manufacturing process expensive and environmentally destructive. As a more environmentally friendly and cost-effective option, researchers have investigated the utilisation of renewable resource catalysts, particularly ones created from waste products. Nwosu et al. (2020) studied the use of a natural catalyst in the production of biodiesel, used crab shell and plantain peel, two waste materials, to create a bifunctional catalyst to facilitate the transesterification of wasted cooking oil into biodiesel. The crab shell and plantain peel were initially treated with a solution of sulfuric and nitric acids by the

researchers, who then calcined the material as a means of preparing the catalyst. In order to maximize the biodiesel output, they then utilized the catalyst in the transesterification of spent cooking oil with methanol under varied reaction conditions. The outcomes demonstrated the effectiveness of the bifunctional catalyst in accelerating the transesterification reaction, with a maximum biodiesel yield of 97.6% being attained at a catalyst loading of 3 weight percent and a methanol/oil molar ratio of 12:1 respectively. The catalyst may be employed up to three times without significantly losing activity, the researchers discovered.

2.4.2 Heterogenous Acid Catalyst

The use of tungsten catalyst (W) as an acid catalyst in the generation of biodiesel from waste cooking oil has shown excellent results. The conditions for transesterifying used cooking oil with the tungsten catalyst were optimized in a study by Almeida et al., (2021). This study aimed to produce the most biodiesel possible. The reaction conditions for the tungsten catalyst's transesterification of waste cooking oil were improved by the authors utilising a factorial design technique. The catalyst loading, methanol to oil molar ratio, reaction duration, and reaction temperature are among the reaction parameters that were investigated. The scientists discovered that a catalyst loading of 2.5 weight percent, a methanol to oil molar ratio of 3:1, a reaction period of 120 minutes, and a reaction temperature of 65°C were the ideal conditions for maximal biodiesel output.

2.4.3 Heterogenous Alkali Catalyst

An appealing option to cut waste and produce a green fuel source is to make biodiesel from used cooking oil. Using an activated charcoal bio-based heterogeneous catalyst which has a number of benefits over conventional homogeneous catalysts is one

intriguing strategy. Wang et al. (2021) optimised the generation of biodiesel from used cooking oil by utilising a functionalized bio-based heterogeneous catalyst made of activated charcoal in recent research. By using only 0.5 weight percent of the catalyst, the scientists showed that this catalyst could produce large yields of FAME (up to 97.5%) and maintain good conversion rates even at low temperatures (50°C).

2.5 Advantages and Disadvantages of using Biodiesel as Fuel

Getting a lot of interest as a potential replacement for traditional petroleum-based fuels is biodiesel, a sustainable biofuel produced using plant-based materials like vegetable oils or animal-based fats. There are a lot of benefits throughout conventional fuel that is made from petroleum-based substances. But, like any other fuel, biodiesel has both pros and cons.

One of the key benefits of biodiesel is its ability to minimise greenhouse gas emissions. When burned, biodiesel emits less carbon dioxide, particulate matter, and sulphur compounds due to its less carbon content than diesel fuel made from petroleum. According to research by Knothe et al. (2020), biodiesel made from soybean oil can cut carbon dioxide emissions from diesel fuel by up to 78%. A higher oxygen level in biodiesel also encourages more thorough combustion, which produces less emissions of carbon monoxide and unaltered hydrocarbons.

The biodiesel's suitability with current diesel-powered vehicles and infrastructure is another benefit. Without requiring considerable adjustments, diesel engines may run on pure biodiesel or a combination of it with petroleum-based diesel. This adaptability

makes the switch to biodiesel simpler and avoids the need for substantial expenditures in new infrastructure or vehicle fleets. According to Zhu et al. (2019), biodiesel blends up to 20% (B20) may be utilised without modifying the engine, illustrating how biodiesel can be seamlessly incorporated into current diesel systems.

Biodiesel is also a renewable energy source, as it can be produced from various feedstocks such as soybeans, rapeseed, palm oil, and used cooking oil. Unlike fossil fuels, which are finite resources, the production of biodiesel can be sustained through ongoing cultivation and recycling of waste oils. This aspect makes biodiesel a potentially more sustainable option in the long term. Demirbas (2021) highlighted the importance of biodiesel production from waste vegetable oils and animal fats, emphasizing the potential to reduce waste and promote circular economy principles.

However, there are several downsides to using biodiesel that should be addressed. The struggle for feedstock between the extraction of fuel and food is a big obstacle. Given that biodiesel is predominantly produced from crops, there is fear that the growth in biodiesel production may result in a rise in the need for agricultural land, displacing possible food crops and spiking food prices. According to research by Searchinger et al. (2018), it is essential to carefully manage land use and use environmentally friendly feedstocks in order to reduce these hazards and guarantee that the production of biodiesel does not jeopardise food security.

The potential effect of biodiesel on the loss of biodiversity and deforestation is another drawback. In places like Southeast Asia and South America, the manufacturing of biodiesel from some crops such as palm oil has been linked to deforestation.

Threatening biodiversity, this deforestation may result in the eradication of significant ecosystems and habitats. To reduce the environmental effect of biodiesel production, it is critical to encourage sustainable practises, such as obtaining feedstocks from producers that have earned certification as sustainable and encouraging the utilisation of waste oils (Yusoff et al., 2020).

To sum up, there are a number of benefits to using biodiesel, including decreased emissions of greenhouse gases, compatibility with current diesel infrastructure, and possibility for renewable production. The possibility of deforestation and biodiversity loss, as well as the rivalry for feedstock with food production, are drawbacks. Promoting ecological feedstock options, supporting circular economy theories, and implementing responsible land-use planning are essential to maximising the advantages of biodiesel and minimising its disadvantages. To overcome these difficulties and increase the long-term viability and effectiveness of biodiesel as a fuel source, continuous study and development initiatives are crucial.

2.6 Simulation of Biodiesel Production

Aspen Plus software simulates the synthesis of biodiesel by modelling every step of the process and optimising different parameters. To improve the effectiveness of following reactions, contaminants are first removed from the waste cooking oil during pretreatment. Biodiesel and glycerol are produced during the transesterification process when the oil combines with an alcohol (such as methanol or ethanol) in amid the presence of a catalyst. Solid acids and bases are examples of heterogeneous catalysts that are frequently used because of their effectiveness and simplicity in separation. In order to guarantee adequate mixing, the reaction usually takes place in a reactor vessel with

agitation. The biodiesel is separated by removing glycerol and unreacted reactants using separation equipment such distillation columns or separators. In order to fulfil quality standards, the biodiesel is finally put through purification processes, which may include drying and washing with water. Aspen Plus enables the modelling and optimisation of every unit activity to reduce production costs and maximise the yield of biodiesel.

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CHAPTER 3

MATERIALS AND METHODS

3.1 Introduction

The main method used in the manufacturing process of biodiesel is transesterification, in which triglycerides from waste cooking oil (WCO) react with an alcohol usually methanol in the presence of a catalyst to create biodiesel, which is fatty acid methyl esters with a byproduct known as glycerol (Miyuranga et al., 2023). The suggested base case study's viability was evaluated by a process simulation using Aspen Plus® version 14 while taking into account the management of the byproduct glycerol and the optimisation of the transesterification conditions for effective biodiesel generation for producing 8000 tonnes per year biodiesel.

3.2 Base Case Study: Bifunctional Heterogenous Catalyst

The present research was only about simulating the responses as well as the procedure separation for making biodiesel from used cooking oil using Aspen Plus® version 14 process model software. Current simulation tools like Aspen Plus and Aspen HYSYS can tell the user how a process works thanks to their sophisticated computational methods, large thermodynamics packages, and large element collections. Biodiesel is usually made by transesterifying waste cooking oil in a bioreactor. The resulting biodiesel

will pass through several multiple-phase distillation columns to get rid of extra methanol and divide the biodiesel and glycerol.

3.3 Process Simulation of Biodiesel Production using Aspen Plus®

The simulation was carried out with Aspen Plus® Version 14 software. Based on Sagar Ban's study (2022), the simulation of processes for the procedure known as transesterification, which is necessary for the generation of biodiesel, primarily involves indicated the chemical elements, determined a thermodynamic model, decided the capacity of the plant, decided upon appropriate operating units, and established and set up input parameters included rate of flow, pressure, temperature, and various other conditions. Biodiesel, additionally referred to as methyl oleate ($C_{19}H_{36}O_2$) is going to be characterized as the outcome of a simultaneous reaction including the processes of esterification and transesterification. The primary processing units consist of CSTR reactor set to 65°C and 1 bar, a continuous solid catalysed reaction will be carried out.

Figure 3.1 to 3.6 were the simulation procedures for the base case simulation of biodiesel production namely transesterification process.

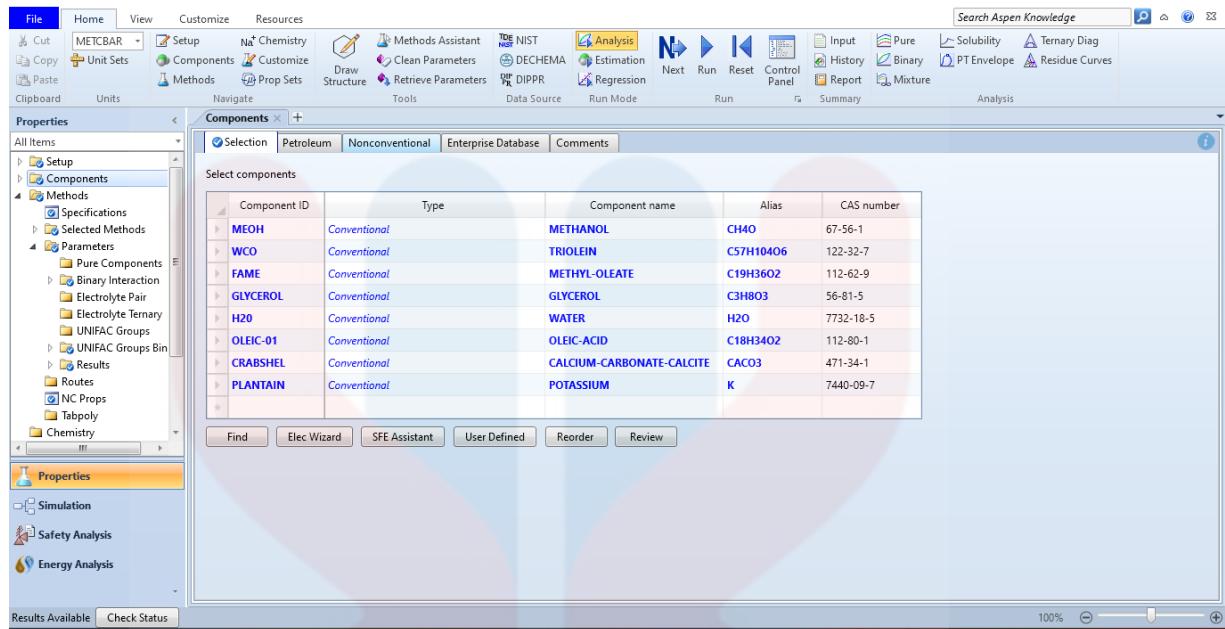


Figure 3.1: Selection of unit operation

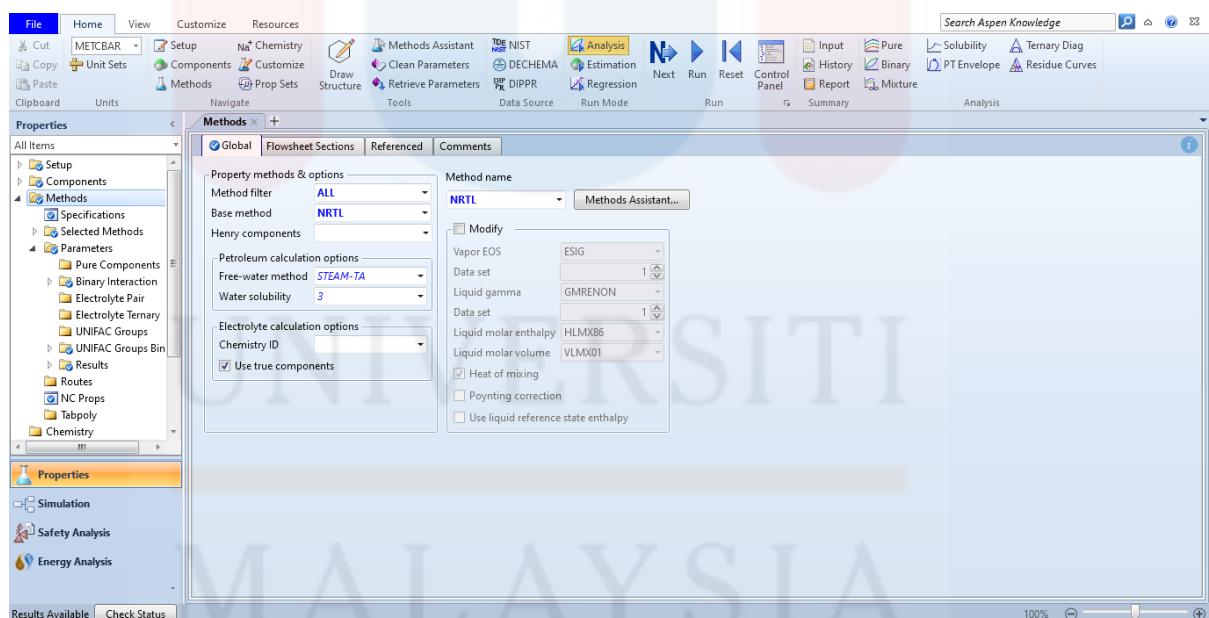


Figure 3.2: Selection of property method (fluid packages)

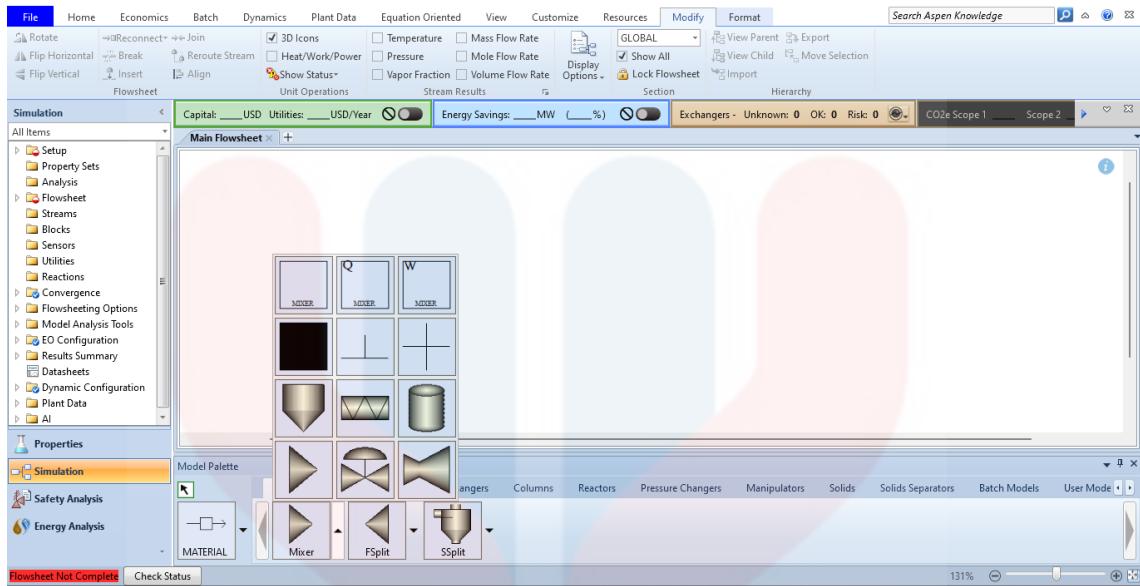


Figure 3.3: Selection of unit operation

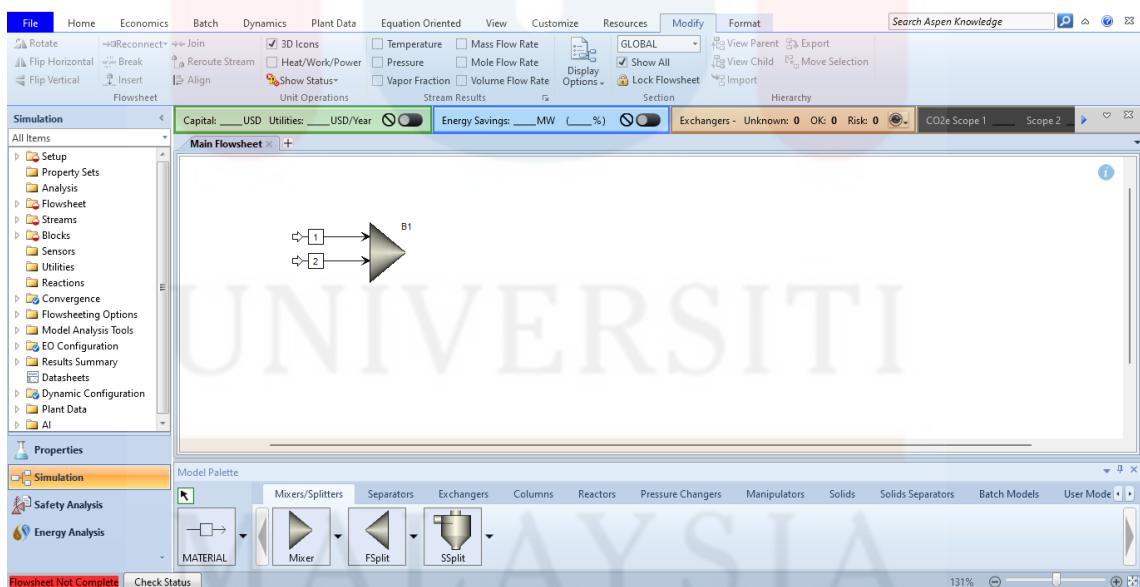


Figure 3.4: Stream added to unit operation

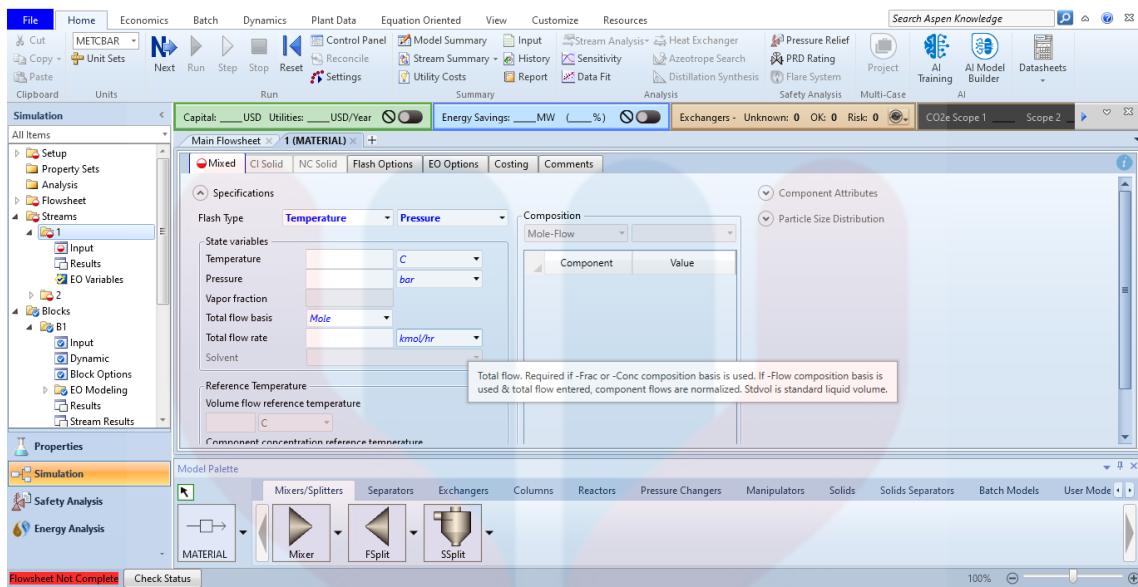


Figure 3.5: Specifications for stream properties

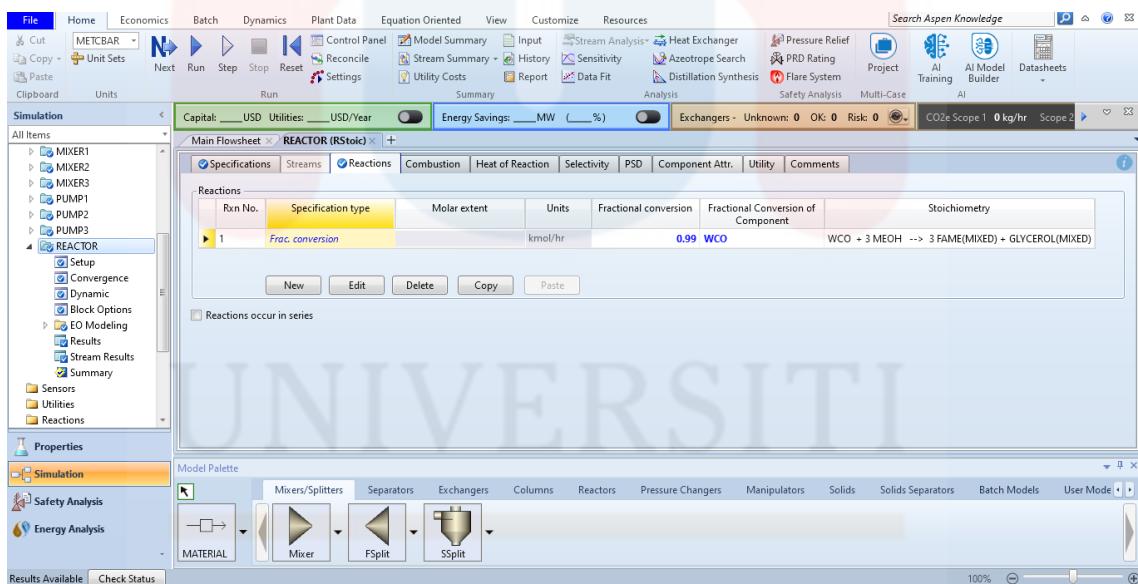


Figure 3.6: Reaction for simulation process

3.4 Thermodynamics and Kinetic Parameters

According to Souza, Hirata, and Batista (2020), the Dortmund enhanced UNIFAC (functional group activity coefficients), UNIF-DMD, will be used for thermodynamic analyses in 2020. Despite the fact that the non-random two-liquid (NRTL) thermodynamic package has already been utilized for modeling fatty acid systems, the UNIF-DMD package is projected to function superiorly in the water-based wash part. Pacheco et al. (2022) demonstrated better separating efficiency in the washing phase utilizing the UNIQUAC (universal quasi-chemical, the foundation of the UNIFAC model) program in contrast to the NRTL package. Through applying the required quantity of water to the water rinse part, which is a multiple-phase fluid-liquid extraction system, it is expected to achieve nearly complete separation of FAME and glycerol. As a result, the UNIF-DMD thermodynamic package will be used in the simulation for this investigation. It is worth mentioning that the simulation results of other unit operations, such as reactors and multi-stage distillation columns, should not differ much depending on the model selected.

The transesterification reaction is depicted in the illustration following (Gebremariam and Marchetti, 2021). In conjunction with the current research on the manufacture of biodiesel from waste cooking oil using bifunctional heterogenous catalyst with different temperatures (40–65 °C) and a methanol to oil molar ratio of 10:1 (Woo et al., 2021; Sim et al., 2021), the first-order reaction model has been employed to get the kinetic parameters required for the simulation to be performed. Equation 3.1 can be used to express the rate of response for the initial-order model:

$$\text{Reaction rate} = -\frac{d[TG]}{dt} = k[TG] \quad \text{Equation 3.1}$$

When equation (1) is integrated, it results in,

$$\ln \left[\frac{TG_t}{TG_0} \right] = -kt \quad \text{Equation 3.2}$$

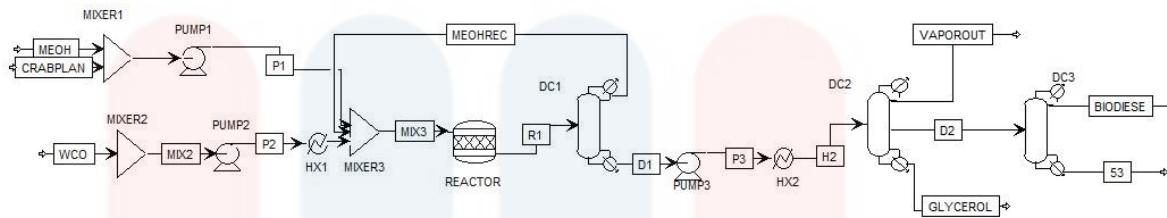
When TG_t and TG_0 are the oil concentrations at time t and $t = 0$. Equation 3.2 could be simplified more thoroughly to

$$\frac{TG_t}{TG_0} = e^{-kt} \quad \text{Equation 3.3}$$

$$1-x_t = e^{-kt} \quad \text{Equation 3.4}$$

As reported by Silva et al. (2022), the aforementioned reaction is predicated on the premise that intermediary products of the reaction such as diglycerides and monoglycerides can be ignored. Transesterification reactions are typically carried out at a larger alcohol to oil molar ratio, so that the pace of reaction is solely determined by the concentration of oil. As a result, the first order reaction model is commonly used to investigate the kinetics of the transesterification reaction (Haryanto et al., 2020).

3.5 Process Flow Diagram of Biodiesel Production via Transesterification Process



During the initial mixing phase, methanol, the catalyst for the mixture is combined in a mixer. After that, this mixture is moved to another mixer. The leftover cooking oil is then added to another mixer and blended with the mixture that remains from the previous stage. After this combination, a new mixture is produced, which is heated in a heat exchanger (HX1) to raise its temperature. The transesterification process takes place in a stoichiometry reactor once the mixture has been heated. Glycerol and biodiesel are produced during transesterification, which is the process by which the mixture's molecules reorganize itself with the aid of the catalyst. The mixture that emerges from the reactor is then sent to a distillation column where the glycerol and biodiesel are separated. In a second distillation column, the biodiesel is further purified to remove any last traces of contaminants. At last, the separated glycerol is also collected for potential uses, and the refined biodiesel is collected as the end product. This all-inclusive procedure makes it easier to turn leftover cooking oil and plant-based materials into a sustainable fuel source, reducing our dependency on fossil fuels and helping to preserve the environment.

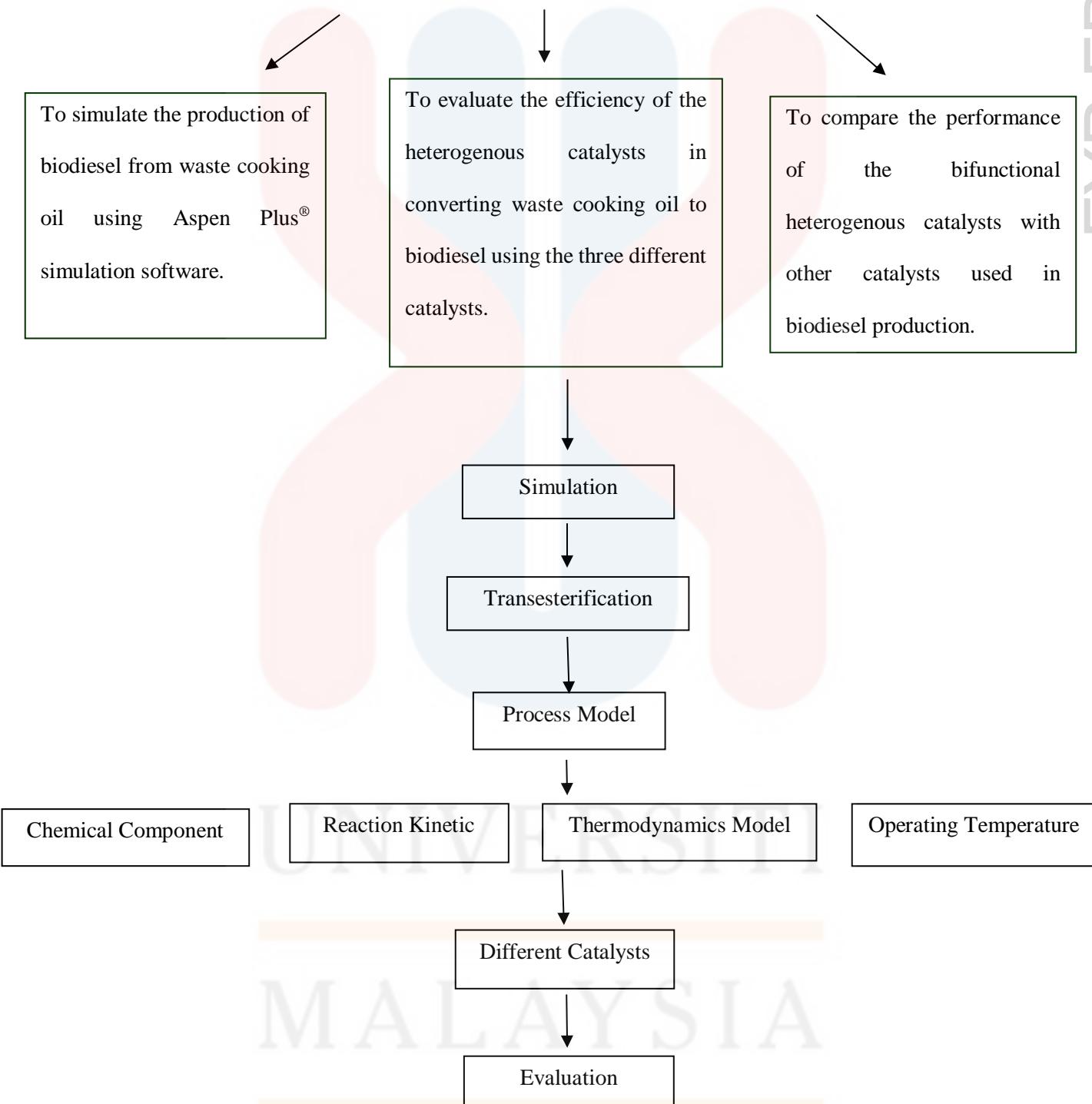
3.6 Methodology Development

Figure 3.7 summarized the flow chart for the production of biodiesel using waste cooking oil via Aspen Plus simulation. Three stages were categorized namely stage 1 for gathering the important data. Stage 2 for flow sheeting the transesterification process using Aspen Plus software version 14. Finally, stage 3 for analyze the process which based on economic and energy analysis.

Figure 3.7: Flow chart for the production of biodiesel using waste cooking oil
via Aspen Plus® simulation

EFFECT OF DIFFERENT CATALYSTS FOR BIODIESEL PRODUCTION VIA

ASPEN PLUS® SIMULATION



CHAPTER 4

RESULTS AND DISCUSSION

4.1 Operating Mode

The decision about the type of operating mode is crucial when examining how various catalysts affect the generation of biodiesel using Aspen Plus simulation. According to Sandhya et al. (2020), when comparing batch versus continuous processes, continuous processes were chosen for their efficiency and scalability. Constant input and output flows are made possible by continuous processes, which provide a more automated and efficient method. Lower labour costs, increased control over reaction parameters, and faster production speeds are the outcomes of this.

The aim for a more affordable and environmentally friendly approach has led to the decision to use Aspen Plus to imitate a continuous process in biodiesel manufacturing. Enhanced catalyst utilisation and overall procedure productivity are the results of enhanced reaction condition optimisation made possible by continuous processes (Boukhalkhal et al., 2019). Continuous operations' steady-state character also makes monitoring and controlling processes and supervision of varied feedstock quality easier.

The catalyst performance may be evaluated under standard settings with the use of the continuous Aspen Plus simulation, which offers significant information into

efficiency and reliability over the long run. This operational decision emphasises the value of effectiveness and environmental responsibility in the manufacture of biodiesel and is consistent with contemporary manufacturing procedures.

4.2 Fluid Packages

The selection of fluid packages in the Aspen Plus® biodiesel production simulation is essential for precisely modelling and forecasting the dynamics of the constituent parts. The NRTL (Non-Random Two-Liquid) fluid package is used in this work because it can be applied to model non-ideal liquid phase performance, which is an important part of the manufacturing of biodiesel. In biodiesel synthesis, triglycerides react with alcohol and catalysts in combinations that involve polar and non-polar components. In these types of systems, NRTL is especially suitable (Ban et al., 2022). The NRTL model takes interactions between various molecular species into consideration when accounting for non-idealities in liquid mixtures. This is essential for capturing the intricate phase equilibria and precisely forecasting the reaction mixture's thermodynamic characteristics during the biodiesel manufacturing process.

There are several reasons why Aspen Plus® chose to include NRTL as a dynamic package. First of all, it makes it possible to mimic phase equilibria that occur during transesterification processes, guaranteeing that the simulation takes into consideration the production of glycerol, biodiesel, and other byproducts. Second, NRTL helps forecast how catalysts will affect reaction kinetics, which is important when assessing how various catalysts would affect the production and quality of biodiesel (Albuquerque et al., 2020).

4.3 Flowsheet Balance

Table 4.1: Mass and energy balance of biodiesel production using crab shell and plantain peel

Conventional Components (kmol/hr)	In	Out	Generation	Relative Difference
MEOH	2.95798	0.318629	-2.64337	-0.136103e-02
WCO	0.890025	0.200803e-01	-0.881125	-0.125615e-01
FAME	0.00000	14.6515	2.664337	-0.819584
GLYCEROL	0.00000	7.08004	0.881125	-0.875548
H2O	0.00000	0.00000	0.00000	0.00000
OLEIC-01	0.697491	2.36570	0.00000	-0.705165
CRABSHELL	0.244787e-01	0.552260e-01	0.00000	-0.556755
PLANTAIN PEEL	0.6266626e-01	0.141419	0.00000	-0.556902
Total Balance				
Mole (kmol/hr)	4.63264	24.6326	0.195156e-15	-0.811931
Mass (kg/hr)	1084.77	5703.40	-	-0.809803
Enthalpy (cal/sec)	-207265	-929267	-	0.776959

Table 4.2: Mass and energy balance of biodiesel production using tungsten

Conventional Components (kmol/hr)	In	Out	Generation	Relative Difference
MEOH	3.78932	0.409679	-3.37964	0.978578e-14
WCO	1.18584	0.592919e-01	-1.12655	0.193098e-15
FAME	0.00000	3.37964	3.37964	0.144541e-14
GLYCEROL	0.00000	1.12655	0.12655	0.00000
H2O	0.00000	0.00000	0.00000	0.00000
OLEIC-01	0.00000	0.00000	0.00000	0.00000
TUNGSTEN	0.215658	0.215658	0.00000	0.167312e-14
H3PO4	0.00000	0.00000	0.00000	0.00000
Total Balance				
Mole (kmol/hr)	5.19082	5.19082	0.195156e-15	0.804197e-14
Mass (kg/hr)	1221.42	1221.42	-	0.223387e-14
Enthalpy (cal/sec)	-222540	-180815	-	-0.187496

Table 4.3: Mass and energy balance of biodiesel production using activated charcoal

Conventional Components (kmol/hr)	In	Out	Generation	Relative Difference
MEOH	3.37992	0.363731e-01	-3.34407	0.978578e-14
WCO	1.18584	0.151571	-1.11469	0.193098e-15
FAME	0.00000	13.1087	3.34407	0.144541e-14
GLYCEROL	0.00000	10.2772	-1.11469	0.00000
H2O	0.00000	0.00000	0.00000	0.00000
OLEIC-01	0.00000	0.00000	0.00000	0.00000
ACTIVATED CHARCOAL	0.877529	1.86936	0.00000	0.167312e-14
Total Balance				
Mole (kmol/hr)	5.44329	25.4433	0.00000	-0.786062
Mass (kg/hr)	1168.84	4990.96	-	-0.765809
Enthalpy (cal/sec)	-179522	-828370	-	0.783284

The given mass and energy balance statements show three distinct chemical process scenarios, each with varying input, output, generation, and relative differences of important components. These balances are essential instruments for assessing the chemical system's overall performance, yields, and efficiency.

The mass and energy balance of the first scenario shows a notable creation of glycerol and fatty acid methyl esters (FAME) together with a large drop in methanol (MEOH) and waste cooking oil (WCO) from input to output (Ban et al., 2022). The effective utilisation of MEOH and WCO is shown by their negative relative differences, which probably result from transesterification processes that produce biodiesel (FAME). The exothermic process suggested by the net mass drop and the adverse enthalpy balance highlights the release of energy linked to the synthesis of biodiesel.

A similar tendency may be seen in the second case, where glycerol and FAME show a notable generation while MEOH and WCO decrease. The effectiveness of the biodiesel manufacturing process is once again highlighted by the negative relative discrepancies. It's interesting to note that the presence of actichar, a carbon-based substance, in this case suggests the possibility of a side reaction or the synthesis of additional products. The process's exothermic character is reaffirmed by the negative enthalpy balance.

New elements including phosphoric acid (H₃PO₄) and tungsten are added to the equilibrium in the third scenario. Notably, glycerol and FAME exhibit production, although MEOH and WCO continue to decline. The addition of tungsten and H₃PO₄ implies an alteration to the initial system or a new procedure. The almost zero mass and

mole total balances and the tiny enthalpy balance point to a steady-state situation with no variation in compositional or energy content. The minimal relative variations for important constituents demonstrate a carefully preserved equilibrium in the system (Ennetta et al., 2022).

To sum up, the three scenarios highlight the effectiveness of producing biodiesel from leftover cooking oil and offer an understanding of the constantly changing dynamics of the chemical process. Negative relative differences show that the feedstock was successfully used, while variances in other components point to possible improvements or changes to the initial procedure (Mukhtar et al., 2022). To properly determine the processes and mechanisms causing the noticed energy and mass balances in each scenario, more in-depth research as well as experimentation would be required.

4.4 Biodiesel Experiments

Table 4.4: Yield distribution of biodiesel and glycerol from biodiesel production

Mass Composition (%) / Catalysts	Crab shell and Plantain peel	Tungsten	Activated charcoal
Biodiesel	98	96	97
Glycerol	92	94	93

The biodiesel and glycerol yield distribution that is displayed, based on the results of the Aspen Plus simulation, is obtained by employing several catalysts, including plantain peel, crab shell, and tungsten and activated charcoal. The catalysts exhibit differences in yield distribution, which may be explained by their unique surface characteristics, catalytic activity, and reactions with the feed in this case is waste cooking oil.

Plantain peel and crab shell are naturally abundant and have intrinsic catalytic qualities, which may explain their employment as catalysts. These substances may include alkaline elements that function as catalytic in transesterification processes, enabling the conversion of cooking oil waste's triglycerides into glycerol and biodiesel. The yield distribution of glycerol is around 92% and biodiesel is approximately 98% according to published data, indicating a reasonably good performance.

Since tungsten is a transition metal, it has special catalytic qualities (Mukhtar et al., 2022). Its application as a catalyst in the synthesis of biodiesel may include particular reactions with the feed that alter the reaction pathways. The biodiesel and glycerol yield

distributions, which are 96% and 94%, respectively, show how well tungsten works as a catalyst and may even provide selectivity for particular processes.

The adsorption qualities of activated charcoal may affect the reaction kinetics differently. It is possible that activated charcoal might serve as an efficient interface for the process of reaction to take place and produce the necessary products, based on the observed yield distribution of glycerol and biodiesel (93% and 97% respectively).

Selecting the right catalyst is crucial for producing biodiesel, as seen by the variations in yield distribution between catalysts. Process efficiency is affected by selectivity, reaction kinetics, and catalyst selection. The idea of "waste to wealth" is especially applicable in this case as using used cooking oil as a feedstock is in line with sustainable methods, which take resource usage and environmental issues into considerations (Albuquerque et al., 2021).

The generation of biodiesel from waste cooking oil has the potential to mitigate greenhouse gas emissions. By recycling waste materials, the waste-to-wealth idea further boosts the environmental advantages of biodiesel, which is seen to be an environmentally friendly substitute to traditional fossil fuels. Such procedures are essential to a viable and circular economic system as they significantly reduce greenhouse gas emissions, which is a major factor in the fight against climate change.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusion

In summary, the study "Effect of Different Catalysts for Biodiesel Production via Aspen Plus® Simulation" has shed light on the viability of using used cooking oil as a feedstock for the manufacture of biodiesel. The research investigated the effectiveness of many heterogeneous catalysts, including tungsten, activated charcoal, plantain and crab shell peels. This approach adopted the waste to wealth idea. By using waste cooking oil as a feedstock, we can reduce the pollution that enters the environment from inappropriate disposal of used cooking oil. This is in line with sustainable practices (Yusuff & Owolabi, 2019). The utilisation of several catalysts, including plantain and crab shell peel, tungsten, and activated charcoal, emphasises the need of utilising economical and environmentally sustainable options for the production of biodiesel.

This study was made possible by the Aspen Plus® simulation programme, which was essential in enabling a thorough examination of the biodiesel synthesis process. The software's capacity to model intricate chemical reactions, forecast reaction kinetics, and enhance operational parameters greatly facilitated the comprehension of the effects of various catalysts on the yield of biodiesel and the synthesis of glycerol. The outcomes indicate the mass percentage of glycerol and biodiesel produced by each catalyst (Albuquerque et al., 2021). Variations in selectivity and activity of the catalysts are shown

by variances in yields of glycerol and biodiesel. The maximum biodiesel production 98% was obtained via the employment of plantain peel and crab shell catalysts, while tungsten and activated charcoal catalysts showed competitive results with yields of 96% and 97%, respectively. The results of the glycerol production show how crucial catalyst selection is in influencing the creation of byproducts as well as the biodiesel yield, with values that range from 92% to 94%.

Overall, this work highlights the importance of choosing the right catalysts to get desired results and optimises the generation of biodiesel from leftover cooking oil. Combining the waste to wealth idea with the potent simulation programme Aspen Plus strengthens the feasibility of using waste materials for both economic and environmental advantages and advances the advancement of biodiesel production methods in a sustainable manner.

5.2 Recommendations

The research "Effect of Different Catalysts for Biodiesel Production via Aspen Plus Simulation" identifies a number of important topics that warrant future development and investigation. The optimisation of catalyst composition is one important factor. Further studies with different catalyst compositions are advised in order to maximise biodiesel output while reducing glycerol generation. To find the best effective catalyst blend, this entails altering the ratios of tungsten, activated charcoal, and plantain and crab shell peel.

A scale-up investigation is recommended in light of the optimised biodiesel manufacturing process's potential industrial applications. This entails determining if the procedure can be applied more widely and industrially (Tadesse Anbessie Degfie et al., 2019). It's also advised to carry out a techno-economic study to assess the economic feasibility, accounting for elements like catalyst costs, equipment needs, and overall process effectiveness.

A thorough environmental impact study is needed to determine the long-term viability of the biodiesel manufacturing process. An examination of the energy use, greenhouse gas emissions, and other environmental factors related to various catalysts and production processes should be part of this review.

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