CHAPTER II
THEORETICAL BACKGROUND AND LITERATURE REVIEW

In this chapter, background information related to this research is described. Also, the related works in deoxygenation reaction of oxygenated compound is summarized.

2.1 Diesel fuel

Diesel fuel refers to fuel oils which are intended for compression ignition engines or diesel engines. Diesel fuel can be divided into petroleum-based diesel and alternative non-petroleum-based diesel (biodiesel or diesel that derived from biomass).

2.1.1 Petroleum-based Diesel

Petroleum-based diesel is a mixture of hydrocarbons, including paraffins, naphthenes, olefins, and aromatics, in the range of carbon numbers from 12 to 18. The petroleum-based diesel is obtained from the fractional distillation of crude oil in the boiling range of 200 to 350°C at atmospheric pressure. Normally, it is composed of about 75% saturated hydrocarbons, and 25% aromatic hydrocarbons. Petroleum-based diesel is immiscible in water. It has the density of about 850 g/dm^3 and typically releases about 40.9 MJ/ dm^3 when it is burnt.

2.1.2 Biodiesel

Biodiesel refers to any diesel-equivalent bio-fuel derived from vegetable oils or animal fats and other biomass-derived oils. Normally, biodiesel is defined as mono-alkyl ester. However, renewable diesel (bio-alkanes) is also available.

2.1.2.1 Raw Materials for Biodiesel Production

Vegetable oils and animal fats are considered as raw materials for biodiesel production because they are broadly available from a variety of sources, and they are renewable. The example of vegetable oils use for biodiesel production are palm oil, sunflower oil, corn oil, coconut oil, jatropha oil, olive oil, canola oil, cottonseed oil, castor oil, soybean oil, etc. As well, animal fats, recycled cooking oil, trap grease (from restaurant grease traps), and float grease (from waste water treatment plants), are also available as raw materials for biodiesel production.

Both oils and fats are composed of molecules called triglycerides. Fat generally refers to the triglycerides in solid form at room temperature, whereas oils are liquid at room temperature. The molecule of triglyceride is composed of three long-chain fatty acids of 8 to 22 carbons attached to a glycerol backbone. The chemical structure of a triglyceride is shown in Figure 2.1 where R_1, R_2, and R_3, which may be the same or different, represent long chain fatty acids which are mostly palmitic, stearic, oleic, linoleic, and linolenic acids.
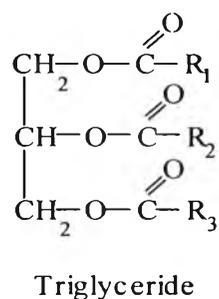
Triglyceride

Figure 2.1 A Chemical Structure of Triglyceride.

2.1.2.2 Biodiesel Production

The production of biodiesel from renewable sources is mainly done via a chemical reaction called transesterification. However, it can as well be done via the deoxygenation reaction.

2.1.2.2.1 Transesterification of Triglyceride

Normally, mono-alkyl ester is produced via the trans-esterification of vegetable oils or animal fats (triglycerides). In this process, triglycerides react with alcohols, generally methanol or ethanol, in the presence of a catalyst to produce mono-alkyl esters (biodiesel) and glycerin. (Jon Van Gerpen *et al.*, 2004). The transesterification reaction can be catalyzed by bases, acids, or enzymes. The most common catalysts used are strong bases, such as sodium hydroxide, potassium hydroxide, and sodium methoxide. The typical transesterification process is shown in Figure 2.2.
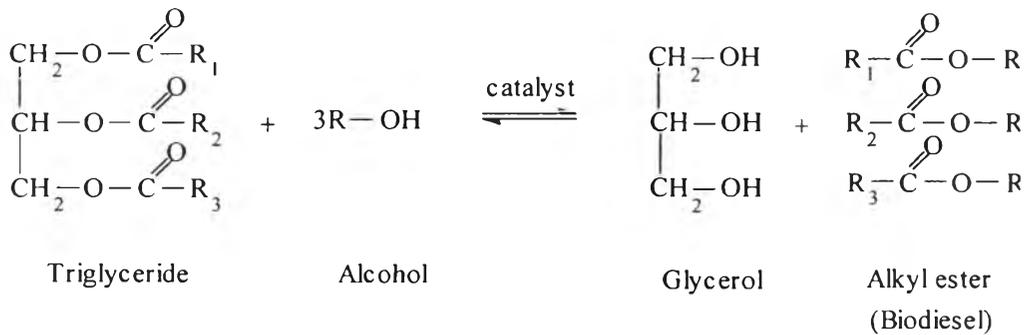
Figure 2.2 The production of biodiesel via transesterification of triglyceride.

During transesterification, three consecutives and reversible reactions are believed to occur. These reactions are given below:
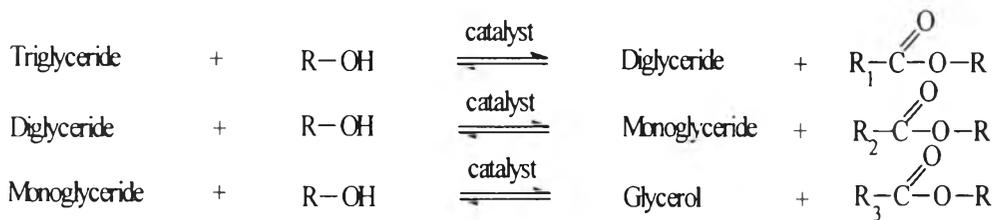
The first step is the conversion of triglycerides to diglycerides, followed by the conversion of diglycerides to monoglycerides. In the last step, the conversion of monoglycerides to glycerol, yielding one methyl ester molecule from each step (Srivastava A. *et al.*, 2000).

The stoichiometric relation between triglyceride and alcohol is a one mole of triglyceride reacts with three moles of alcohol. However, for the transesterification to occur, usually 6 moles of alcohol are used for every mole of triglyceride, which is more than the equation indicates. The reason is that the equilibrium of the reaction needs to be shifted toward the right side of the equation. To force the equilibrium in the direction of the desired products, one or more parameter(s) of the reaction may need to be changed such as the molar ratio, temperature, pressure, and catalyst type.

The most popular mono-alkyl ester is methyl esters, resulting from the reaction of triglyceride with methanol, shown as Fig. 2.3.
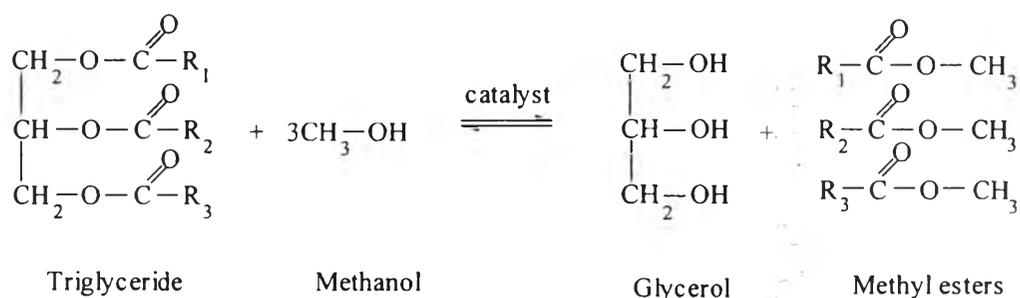
Figure 2.3 A chemical reaction of triglyceride with methanol.

The conversion of triglycerides into mono-alkyl esters through the transesterication reaction reduces the molecular weight to one-third that of the triglyceride and slightly increases the volatility.

An example of basic schemes for biodiesel production is shown in Figure 2.4.

Recycled   Sulphur + methanol

Vegetable oils

Dilute acid esterification

Methanol + KOH

Transesterification

Methanol Recovery

Crude Glycerin

Crude Biodiesel

Glycerin Refining

Refining

Residue

Glycerin
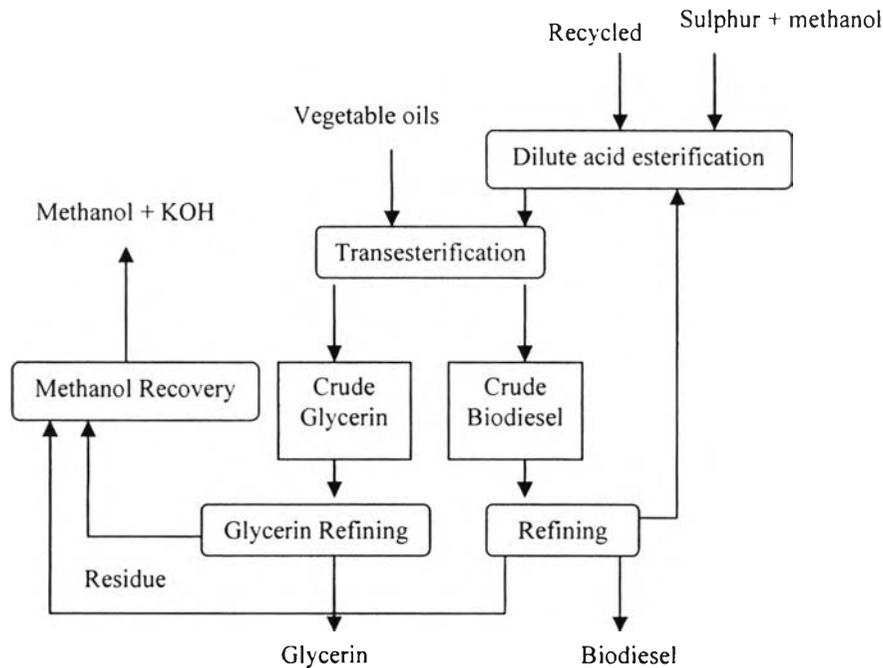
Biodiesel

Figure 2.4 A basic schemes for biodiesel production.

Although mono-alkyl ester is considered as a potential sustainable alternative fuel but there are still disadvantages associated with its use. There are several properties of mono-alkyl ester that limit their uses. First, mono-alkyl ester has cloud point and pour point higher than conventional diesel, the performance of biodiesel in cold conditions is poorer than petroleum diesel, which might be caused engine problems and increased nitrogen oxide emissions. Second, mono-alkyl ester is a good solvent, it can dissolve rubber and some plastics, remove paint, and oxidize the metals. Third, the hydrophilic property of mono-alkyl ester might cause the corrosion of the engine. Lastly, mono-alkyl ester contains oxygen which may be undesirable for certain applications. The presence of oxygen lowers the heat content as shown by the volumetric heating values of it, which are 9-13% lower than conventional diesel (Tyson, K.S. *et al.*, 2006) . Therefore, the deoxygenation of triglyceride becomes an alternative process of diesel production because there are a lot of advantages of this process over transesterification, including compatibil-

ity with infrastructure of conventional oil refineries, compatibility with engines and fuel standards, lower processing costs, and raw materials flexibility. (Stumborg *et al.*, 1996). Moreover, the obtained products from this reaction have high quality and similar properties to conventional diesel fuel. The comparison of properties of diesel (ULSD), biodiesel (FAME), and renewable diesel (green diesel) are shown in Table 2.1.

Table 2.1 Physical and chemical properties of diesel (ULSD), biodiesel (FAME), and renewable diesel (green diesel) (Marker, T.L., 2005)

Properties	Diesel	Biodiesel	Renewable Diesel
Oxygen content by wt%	0	11	0
Specific gravity g/ml	0.84	0.88	0.78
Sulfur content, ppm	<10	<1	<1
Heating Value (lower) MJ/kg	43	38	44
% change in NOx emission	-	+10	0 to -10
Cloud Point °C	-5	-5 to +15	-20 to +20
Cetane	40	50-65	70-90
Stability	Good	Marginal	Good

2.1.2.2.2 Deoxygenation of Fatty Acid

Diesel fuel can be produced via deoxygenation reaction, the hydrocarbon chain is broken and undesired oxygen is removed, leading to a production of straight-chain hydrocarbons suitable for diesel fuel. The deoxygenation reaction may be carried out in the presence of homogeneous or heterogeneous catalysts under controlled hydroprocessing conditions, known as hydrotreating or hydrocracking processes.

There are several possible reaction pathways for a production of straight-chain hydrocarbons, shown as Fig. 2.5. Fatty acids can be di-

rectly decarboxylated or decarbonylated. Direct decarboxylation removes the undesired oxygen by releasing carbon dioxide and producing aliphatic hydrocarbon chains with one carbon atom less than in the original feed, while direct decarbonylation removes the undesired oxygen by forming carbon monoxide and water, as explained by reactions I and II. Moreover, the fatty acid can be deoxygenated by adding hydrogen leading to a production of straight-chain hydrocarbons and undesired oxygen will be removed through formation of water, as explained by reactions III. (Murzin D.Yu. *et al.*, 2006)

$$(\text{I})\ \text{Decarboxylation}\quad R-\overset{\displaystyle O}{\underset{}{C}}-OH \longrightarrow R-H\ +\ CO_2$$

$$(\text{II})\ \text{Decarbonylation}\quad R-\overset{\displaystyle O}{\underset{}{C}}-OH \longrightarrow R-H\ +\ CO\ +\ H_2O$$

$$R-\overset{\displaystyle O}{\underset{}{C}}-OH\ +\ H_2 \longrightarrow R-H\ +\ CO\ +\ H_2O$$

$$(\text{III})\ \text{Hydrogenation}\quad R-\overset{\displaystyle O}{\underset{}{C}}-OH\ +\ 3\,H_2 \longrightarrow R-CH_3\ +\ 3\,H_2O$$
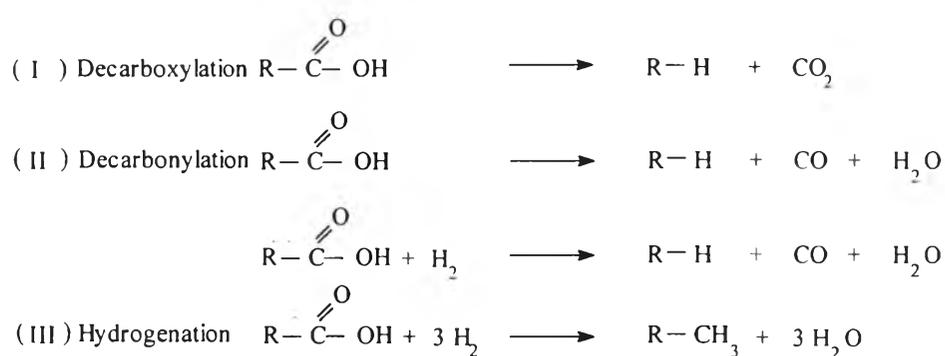
Figure 2.5 The possible liquid-phase reaction pathways for production of straight-chain hydrocarbons from fatty acids.

In addition to the liquid-phase reactions, the water gas shift and methanation reaction are occurred with a number of carbon monoxide, carbon dioxide, hydrogen, and water formed during decarbonylation/decarboxylation reaction. The water-gas-shift reaction may balance the concentrations of CO and CO_2, while methanation reaction of fatty acids gives methane and water, shown as Fig. 2.6.

$$\text{Methanation}\quad CO_2\ +\ 4\,H_2 \rightleftharpoons CH_4\ +\ 2\,H_2O$$

$$\text{Methanation}\quad CO\ +\ 3\,H_2 \rightleftharpoons CH_4\ +\ H_2O$$

$$\text{Water-gas-shift}\quad CO\ +\ H_2O \rightleftharpoons H_2\ +\ CO_2$$
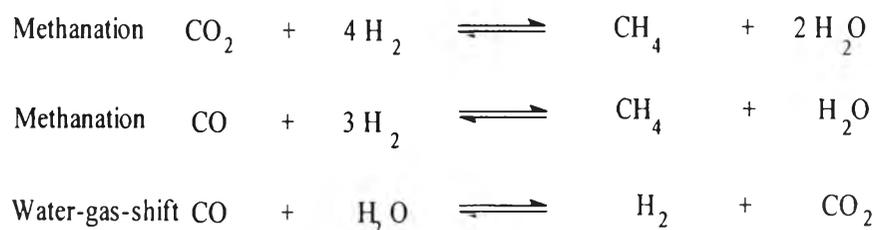
Figure 2.6 Gas phase reactions of CO or CO_2 with H_2 or H_2O.

2.2 Neste Technology (NExBTL technology)

Neste Oil Corporation has developed a technology called NExBTL technology that uses to produce high quality biodiesel. The product obtained from this technology is called NExBTL renewable diesel or Green diesel.

Chemically, NExBTL renewable diesel is produced via direct catalytic hydrogenation of vegetable oil, which is triglyceride, into the corresponding alkane. The glycerol chain of the triglyceride is hydrogenated to propane, the corresponding C3 alkane. This process removes oxygen from the oil; the product is not an oxygenate like traditional biodiesel. The product is a clear and colorless paraffin, with a high cetane number (85 to 95) and better properties than even petroleum-based diesel.

NExBTL renewable diesel is an advanced fuel that performs more efficiently and has a lower level of environmental impact than petroleum-based diesel or FAME biodiesel. Using NExBTL also helps improve overall air quality, as it generates significantly less nitrogen oxide and particulate emissions as well. The reaction of NExBTL renewable diesel production is shown as Fig 2.7.
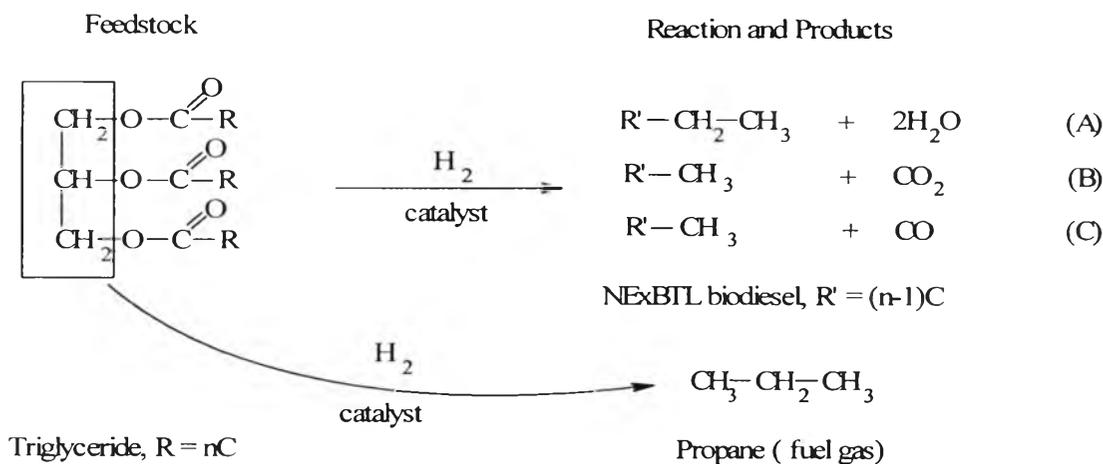
Figure 2.7 The reaction of NExBTL renewable diesel production.

The schemes for NExBTL process is shown in Figure 2.8.

Oils/Fats

Acid
Caustic
Water

Pretreatment
Impurities removal

Solids

Water

Triglycerides

Hydrogen

NExBTL-process
Conversion of fatty acids
to paraffins and iso
parafins

Water

Bio fuel gas

Bio gasoline

NExBTL Diesel
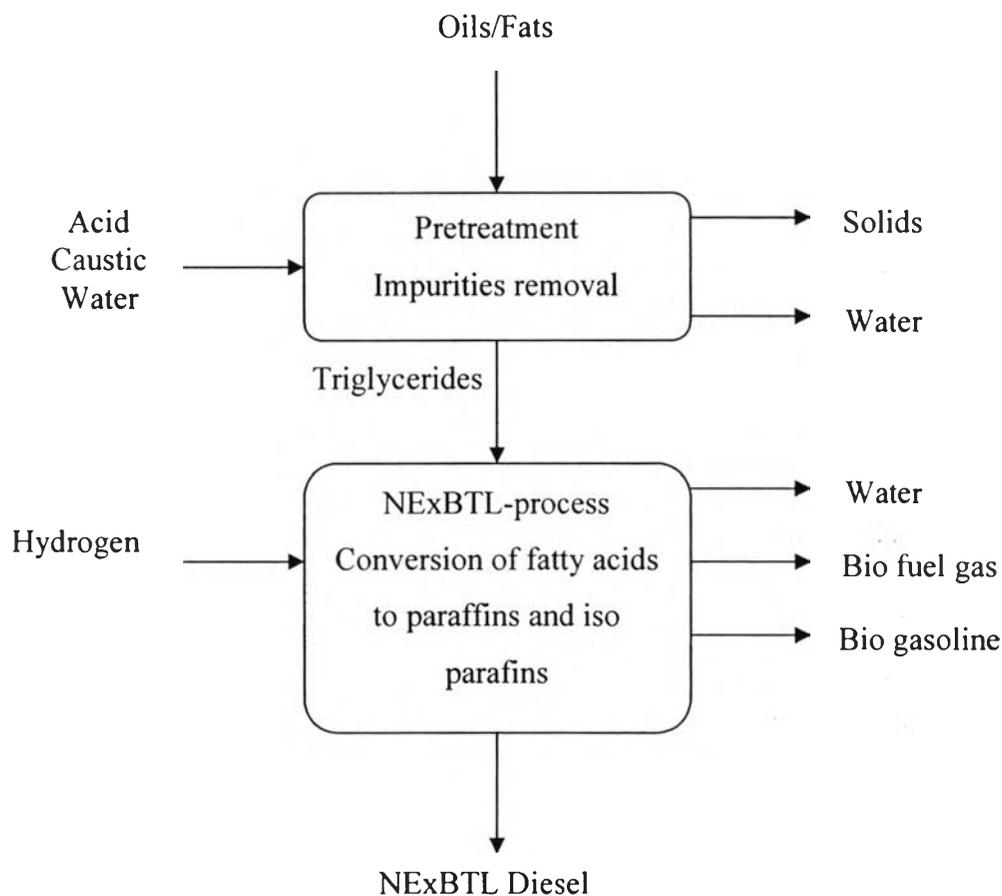
Figure 2.8 The schemes for NExBTL process.

Literature review

More than 80 years ago, a study of homogeneous catalyst reaction was investigated that, only 50% yield of paraffin over selenium catalyst was observed (Betram *et al.*, 1936).

The deoxygenation of vegetable based feeds over the heterogeneous catalysts have been studied barely in the past. The decarboxylation of heptanoic acid to octane was studied by Maier W. F. *et al.*, (1982). The reaction was carried out in the gas phase over Pd/SiO_2 and Ni/Al_2O_3 catalysts. The results showed that the decar-

boxylation of heptanoic acid over Pd/SiO_2 yielded 98% octane at 330°C, whereas over the Ni/Al_2O_3 catalyst, the yield of octane was 64% at 180°C. In 1985, a production of straight-chain olefins from saturated fatty acid ester over nickel based catalyst with either tin, germanium, or lead was a subject to U.S. patent by Stern R. *et al.* (Dmitry Yu. Murzin *et al.*, 2006)

A model triglycerides, including trilaurin, tripalmitin, and tristearin, have been pyrolyzed to determine reaction products and elucidate thermal decomposition pathways. Typical reaction products, included hydrocarbons, ketones, esters, carboxylic acids, and acrolein. (Bressler D.C. *et al.*, 2007)

Catalytic deoxygenation of heavy gas oil was researched. The extent of oxygen removal during catalytic hydrotreatment of heavy gas oils depends on the chemical composition of catalysts. Deoxygenation increases with the concentration of MoO_3 (6 wt%) on the alumina support. Further increase in the MoO_3 concentration do not appreciably increase the oxygen removal. The deoxygenation reaction is also improved by the addition of cobalt and nickel oxides to the molybdate catalysts. Independent acidity measurements on the liquid products suggest the presence of phenols (Edward Furimsky., 1977).

Seringa and ucuuba oils were cracked using a $NiMo/\gamma-Al_2O_3$ catalyst at 360°C and 14 MPa. The results showed that conversions of nearly 100% were obtained and the primary reaction products were alkanes and cycloalkanes. (Da Rocha Filho G.N. *et al.*, 1992). In a similar study (Da Rocha Filho G.N. *et al.*, 1993), catalytic hydrocracking of vegetable oils in the presence of $NiMo/\gamma-Al_2O_3$ catalyst sulfided with element sulfur under hydrogen pressure was studied. For hydrocracking experiments, vegetable oils, catalyst precursor $NiMo/\gamma-Al_2O_3$, and element sulfur were added to a batch micro reactor. The initial hydrogen pressure at room temperature and the heating rate were 7 to14 MPa, and 300 Kh^{-1}, respectively. The reactor was maintained for 1 to 2 h at the final temperature, 300, 330, 360, 390, or 450°C, before cooling and analysis products by GC. The main liquid product was n-alkanes with carbon number equal to or one less than the original acids. The selectivity to alkanes increased with the reaction temperature, then decreasing with a future rise in temperature above 360°C. The gas phase products were CO (small amounts),

H_2O, and CO_2 (70–80 wt% of gas phase). The yields of CO_2 and H_2O suggest that the decarbonylation and the reduction of carboxylic groups are the major reactions in the cracking of triglyceride over $NiMo/\gamma-Al_2O_3$ sulfided catalyst.

Influences of hydrogen sulfide partial pressure and nitrogen compound on the hydrodeoxygenation activity of a CoMo/Carbon catalyst was studied by Maria Ferrari *et al.* The experiments were carried out in a hydrogen sulfide atmosphere (as a partial pressure 10–150 kPa), under a total pressure of 7 MPa, at 200 and 270°C in the fixed bed continuous flow tubular reactor. The transformation of a mixture of re-actants, guaiacol, ethyldecanoate, and 4-methylacetophenone in *p*-xylene was likely three different active sites were responsible for hydrogenolysis, hydrogenation, and acid-catalyzed reactions. The activity of sulfided CoMo/C catalyst was rarely af-fected by additions of the hydrogen sulfide partial pressure. Hydrogen sulfide did not affect to the activity and conversion of guaiacol on the CoMo/Carbon catalyst. For ethyldecanoate, the conversion was not influenced by hydrogen sulfide and the selec-tivity in hydrogenated and decarboxylated products was slightly changed. Methy-lacetophenone was the only reactant molecule whose conversion was inhibited by the H_2S (Maria Ferrari *et al.*, 2001).

The pyrolysis reactions of soybean, palm, and castor oils were carried out at temperature ranging from 350 to 400°C in stainless still batch reactor. The vapor feed left the reactor enters a water cooled heat exchanger. Two liquid fractions were obtained, aqueous and organic fraction. Alternatively, the vapor feed was passed through H-ZMS5 zeolite plug bedded in a filled bottom glass tube in the catalytic deoxygenating reactor, which was placed between the pyrolysis reactor and the heat exchanger. This reactor was heated to maintain temperature feed at approximately 400°C. The heavy fractions of pyrolysis and pyrolysis catalytic deoxygenating prod-ucts were analyzed by GC and FTIR. For pyrolysis products, hydrocarbons and oxy-genated organic compounds, such as alkanes, alkenes, and carboxylic acids were identified. For pyrolysis catalytic deoxygenating products, peak corresponding to carboxylic acids diminished, and new peak corresponding to hydrocarbon products emerged. This result indicated that the deoxygenation of pyrolyzed vegetable oil ob-tained an enriched diesel like fuel. (Daniela G. Lima *et al.*, 2004)

The influence of hydrogen partial pressure on the conversion and products distribution on the deoxygenation of stearic acid, ethyl stearate, and tristearine, over palladium supported on activated carbon to produce diesel fuel-like hydrocarbons was studied. The experiments were done at temperature ranging from 300 to 360°C and overall pressure 17–40 bar in a conventional Parr autoclave (300 ml) operating in a semi-batch mode. Different reaction atmospheres, e.g. helium (He), hydrogen (H_2), hydrogen (5 vol%) -argon (H_2-Ar) mixture, were applied. The results showed that all the three reactants were converted to the same final products, n-heptadecane, with high selectivity. The presence of hydrogen in the reaction atmosphere particularly diminished the undesired products such as unsaturated C17 and aromatic hydrocarbons. (Dmitry Yu. Murzin *et al.*, 2005)

The hydrodeoxygenation of methyl esters, methyl heptanoate and methyl hexanoate, on sulphided NiMo/γ-Al_2O_3 and sulphided CoMo/γ-Al_2O_3 catalysts was studied. The reactions were carried out in a tubular continuous flow reactor under isothermal conditions at 250°C. The products obtained were analyzed by GC. The results showed that both methyl esters yielded a number of alkanes, alkenes, alcohols, and carboxylic acids. The oxide NiMo catalyst showed more activity for the reaction of aliphatic methyl ester than the oxide CoMo catalyst. However, oxide NiMo yieled mainly the alkenes. For sulphided catalysts, sulphidation greatly increased the selectivity of the catalyst. The sulphided NiMo/γ-Al_2O_3 catalyst is more active than the sulphided CoMo/γ-Al_2O_3. Moreover, the aliphatic methyl esters are converted to hydrocarbons via three paths as shown in Figure 2.9. The first path gave alcohols followed by dehydration to alkenes with the same number of carbon atoms as in the acyl group of the ester. Deesterification yielded and alcohol and carboxylic acid in the second path. Carboxylic acid was further converted to hydrocarbons either directly or with an alcohol intermediate. Decarboxylation of the esters led to alkenes with on carbon atom less than in the acyl group in the third path. The hydrogenation of the formed alkenes takes place following this deoxygenation. The major formation of alkanes on the sulphided NiMo catalyst is consistent with its higher hydrogenation activity. The most alkanes formed from methyl heptanoate is n-heptane and from methyl hexanoate is n-hexane under all conditions (O.I. Enol *et al.*, 2005).

$$CH_3-OH + HO-C_{n+1}-H_{2n+3} \xrightarrow{[-H_2O]} C_{n+1}-H_{2n+2} \xrightarrow{[+H_2]} C_{n+1}-H_{2n+4}$$

$[+2H_2]$ I

$[+2H_2, -H_2O]$

$$CH_3-O-\overset{O}{\overset{\|}{C}}-C_nH_{2n+1} \underset{[-H_2O]}{\overset{[+H_2O]}{\rightleftharpoons}} \;^{II}\; CH_3-OH + HO-\overset{O}{\overset{\|}{C}}-C_nH_{2n-1} \xrightarrow{[-CO_2, -H_2]} C_nH_{2n} \xrightarrow{[+H_2]} C_nH_{2n+2}$$

III $[-CH_4, -CO_2]$
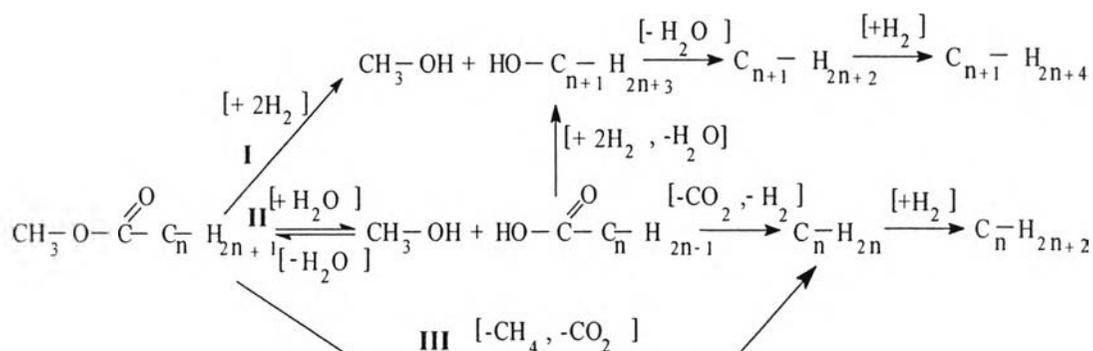
Figure 2.9 The hydrodeoxygenation reaction scheme of aliphatic methyl esters (n=6) for methyl heptanoate and n=5 for methyl hexanoate).

The deoxygenation of stearic acid over the heterogeneous catalysts for production of biodiesel was investigated by Dmitry Yu. Murzin *et al.*, (2006). A variety of metal (Pd, Pt, Ru, Mo, Ni, Rh, Ir, and Os) supported on Al_2O_3, Cr_2O_3, MgO, and SiO_2, as well as activated carbons were studied. The deoxygenation experiment were carried out in a semi batch reactor under constant overall pressure and temperature at 600 kPa and 300°C, respectively. In case of noncatalytic deoxygenation, it was found that less than 5% of stearic acid was converted within 6 h of reaction and the main products formed were linear C17 hydrocarbons. In the heterogeneous catalytic deoxygenation of stearic acid achieved with high activity and selectivity to n-heptadecane (n-C17), desired product. The catalyst screening showed that the reaction can be effectively performed over palladium and platinum supported on activated carbons. Furthermore, the gas phase analysis indicated that the decarboxylation reaction was more preferably over the Pd/C catalyst, as the decarbonylation was more preferably over the Pt/C catalyst.

Hydrotreating of pure sunflower oil were performed in a fixed bed reactor with a sulfided NiMo/γ-Al_2O_3 catalyst. The reaction were done at temperature ranging from 300 to 450°C, pressure of 50 bar, LHSV 4.97 h^{-1} and H_2 to feed ratio of 1600 ml H_2 /ml liquid feed. The gas inlet was 91% H_2 with the balanced with Ar. The products obtained were analyzed by GC. It was found that the fraction distillated

from 250 to 350°C was the major distillation fraction. This fraction is mostly n-C15, n-C16, n-C17, and n-C18. The maximum in this fraction occurred at reaction temperature of 350°C. The reaction pathways involves hydrogenation of the C=C bonds of the vegetable oils followed by alkane production by three different pathways: decarbonylation, decarboxylation and hydrodeoxygenation as shown in Figure 2.10. Moreover, the straight chain alkanes can undergo isomerization and cracking to produce lighter and isomerized alkanes. In addition, they proposed that the catalyst and reaction condition play an important role to determine the yield of the decarbonylation, decarboxylation and hydrodeoxygenation pathways. (Avelino Corma *et al.*, 2007).
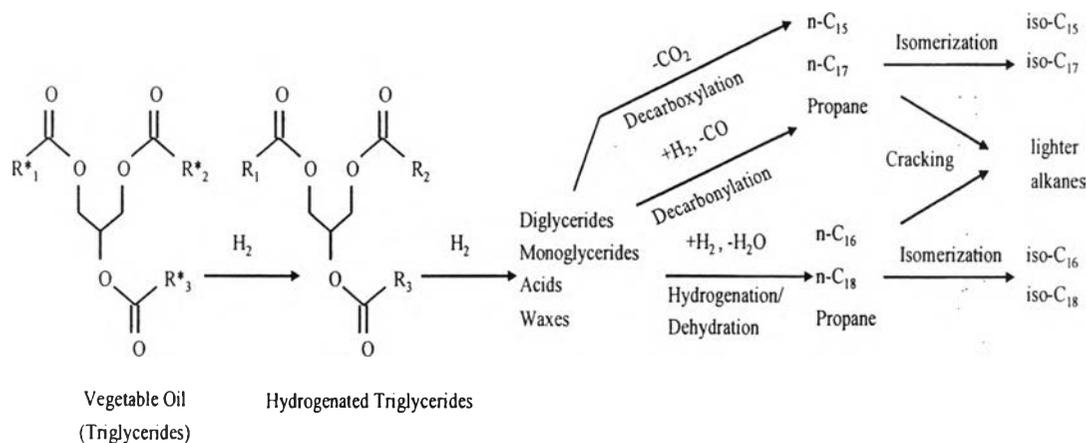
Figure 2.10 The reaction pathway for conversion of triglycerides to alkanes.

The catalytic decarboxylation of fatty acids and there derivatives for production of linear hydrocarbons has been studied by Dmitry Yu. Murzin *et al.*, (2007). The reaction has been investigated over Pd/C catalyst in a semibatch reactor under temperature and pressure range at 300–320°C and 6–17.5 bars. The reaction atmosphere was either helium, nitrogen, argon, hydrogen, and a mixture thereof. The results showed that there are different reaction pathways for the catalytic transformations of stearic acid and ethyl stearate. Decarboxylation is the main path for the catalytic transformations of stearic acid, whereas ethyl stearate, the main reaction path under inert gas mixtures is decarbonylation over alkaline catalysts forming n-heptadecane as main product, while over the acidic catalyst, decarboxylation is the

main path and yieled mainly stearic acid. Moreover, the main reaction path of the catalytic transformations of ethyl stearate under hydrogen-rich conditions over acidic catalysts is decarbonylation, forming n-heptadecane as a main product. The effect of the gas mixture, in the presence of hydrogen, decarboxylation proceeded faster, higher conversions, and higher yields of desired product, n-heptadecane was obtained. The conversion level was the highest after 360 min for stearic acid. The decarboxylation (catalytic transformation) of unsaturated fatty acids leaded to hydrogenated products that reacted further to hydrocarbons.

The potential for using bio-renewable feedstock in oil refineries was studied. The study considered the production of biodiesel and green diesel from vegetable oils and greases. The results showed that green diesel produced from hydrotreating vegetable oil and grease was identified as one of the best options for refiners, agricultural producers, and forest products producers. Green diesel has superior product properties, requires less capital investment to produce, and has a lower environmental impact than biodiesel. Green diesel hydrocarbons do not contain oxygen in their molecular structure. The experiments performed in this project showed that both hydrodeoxygenation and decarboxylation occur, with the results summarized in Table 2.2. Decarboxylation is favored at lower pressures and hydrodeoxygenation increased with increasing pressure. Decarboxylation results in odd number paraffin production and CO_2 formation whereas hydrodeoxygenation results in even carbon number paraffin production; therefore the ratio of n-C17 to n-C18 is a measure of the $DeCO_2$ /HDO ratio. Standard hydrotreating catalysts of NiMo, CoMo and Pd all showed activity for both reactions. Furthermore it was demonstrated that the process could be run at lower temperatures than cited in the Arbokem patent and heavy material boiling above diesel range, which Arbokem produced, could be eliminated or reduced with proper choice of catalyst and conditions. Also, most experiments were done at 500 psi which is well below the pressures cited in the Arbokem patent. (Marker, T.L., 2005).

Table 2.2 Green diesel experimental summary (Marker, T.L., 2005)

	524	531	1316-C3	1316-C4
Feed	Vegetable oil	Vegetable oil	Vegetable oil	Vegetable oil
Catalyst	HCT (NiMo)	N200 (CoMo)	HCT (NiMo)	HCT (NiMo)
Test Unit	Autoclave	Autoclave	Plt 1316-B1	Plt 313-B1
WHSV (h^{-1})	1.9	1.7	0.8	0.3
Temperature (°C)	300-350	300-350	325	310
Pressure (psia)	500	500	500	500
Products				
% water	1.7	1.2	4.9	9.9
% CO_2+ CO	12.7	13.4	2.6	1.9
% Light HC	7.0	5.2	3.4	3.9
% diesel +	79	80	88.3	84
% heavy	0	3.2	0.3	0.3
% deoxygenation	90+	91+	85	99
n-C17/ n-C18	3.0	2.1	0.6	0.49