

CHAPTER IV RESULTS AND DISCUSSION

4.1 Process Design

4.1.1 Chemical Components for Hydrogenated Biodiesel and Biodiesel Processes

The first step in developing the process simulation was selecting the chemical components for the processes. Since palm oil is considered as the feedstock in this study, the feed composition was modeled as a mixture of six typical triglycerides presented in palm oil as shown in Table 4.1. The molecular structures of the trimyristin, tripalmitin, tristearin, triolein, trilinolein and trilinolenin are shown in Figure 4.1.

Trighteeride Composition	Molecular	Fraction			
	Structure	(wt.%)	(mol %)		
Trimyristin (14:0)	C45H86O6	1.02	1.20		
Tripalmitin (16:0)	C ₅₁ H ₉₈ O ₆	40.76	42.35		
Tristearin (18:0)	C57H110O6	4.50	4.50		
Triolein (18:1)	C ₅₇ H ₁₀₄ O ₆	41.02	39.70		
Trilinolein (18:2)	C57H98O6	12.20	11.75		
Trilinolenin (18:3)	C57H92O6	0.50	0.50		
Average Molecular Weight (kg/kmol)	849.62				
Density (kg/L)	0.925				

Table 4.1 Typical palm oil composition.

PRO/II[®] library contained information for the following components used in the simulation: methanol, glycerol, water, hydrogen, tridecane, tetradecane, pentadecane, hexadecane, heptadecane, octadecane, propane, methane, and carbon monoxide. Components not available in the PRO/II[®] library were specified using ICAS software which is developed by CAPEC- Technical University of Denmark. Triglyceride, diglyceride, monoglyceride and methyl ester were all specified in this manner.



Figure 4.1 The molecular structures of triglycerides in palm oil for the simulation.

Seventeen components were modeled in the simulation for hydrogenated biodiesel process. Hydrogenated biodiesel is not a specific compound but is a complex mixture of hydrocarbons, composed of tridecane through octadecane which are within the range of diesel hydrocarbons. Additionally, twentyseven components were modeled in the simulation for biodiesel process. Tables 4.2 and 4.3, respectively show the components in the simulation of hydrogenated biodiesel and conventional biodiesel processes.

	Name	Molecular Structure	Component Name	Molecular Weight (kg/kmol)
ant	Trimyristin	C45H86O6	M-M-M	723.16
uodu	Tripalmitin	C ₅₁ H ₉₈ O ₆	P-P-P	807.32
d con	Tritearin	C ₅₇ H ₁₁₀ O ₆	S-S-S	891.48
base	Triolein	C ₅₇ H ₁₀₄ O ₆	0-0-0	885.43
m oil	Trilinolein	C ₅₇ H ₉₈ O ₆	LI-LI-LI	879.38
Pai	Trilinolenin	C ₅₇ H ₉₂ O ₆	LN-LN-LN	873.33
Hy	drogen	H ₂	H2	2.02
Tridecane		C ₁₃ H ₂₈	TRIDECAN	184.37
Te	tradecane	C ₁₄ H ₃₀	TETDECAN	198.40
Per	ntadecane	C ₁₅ H ₃₂	PENDECAN	212.42
He	xadecane	C ₁₆ H ₃₄	HXDECANE	226.45
He	ptadecane	C ₁₇ H ₃₆	HPDECANE	240.48
Oc	tadecane	C ₁₈ H ₃₈	OCTDECAN	254.50
Water		H ₂ O	H2O	18.02
Propane		C ₃ H ₈	PROPANE	44.10
Me	ethane	CH ₄	METHANE	16.04
Ca	rbonmonoxide	СО	СО	28.01

Table 4.2 The components in hydrogenated biodiesel process

	Name	Molecular Structure	Component Name	Molecular Weight (kg/kmol)	
ut	Trimyristin	C45H86O6	M-M-M	723.16	
pone	Tripalmitin	C ₅₁ H ₉₈ O ₆	P-P-P	807.32	
com	Tritearin	C ₅₇ H ₁₁₀ O ₆	S-S-S	891.46	
based	Triolein	C ₅₇ H ₁₀₄ O ₆	0-0-0	885.43	
n oil	Trilinolein	C ₅₇ H ₉₈ O ₆	LI-LI-LI	879.38	
Pain	Trilinolenin	C ₅₇ H ₉₂ O ₆	LN-LN-LN	873.33	
1,2	-ditetradecanoyl-glycerol	C ₃₁ H ₆₀ O ₅	M-M-OH	512.80	
1,2	-dihexadecanoyl-glycerol	C ₃₅ H ₆₈ O ₅	P-P-OH	568.91	
1,2	-dioctadecanoyl-glycerol	C ₃₉ H ₇₆ O ₅	S-S-OH	625.01	
1,2	-dioctadecenoyl-glycerol	C ₃₉ H ₇₂ O ₅	O-O-OH	620.98	
1,2	dioctadecadienoyl-glycerol	C ₃₉ H ₆₈ O ₅	LI-LI-OH	616.95	
1,2-dioctadecatrienoyl-glycerol		C ₃₉ H ₆₄ O ₅	LN-LN-OH	612.92	
l-t	etradecanoyl-glycerol	C ₁₇ H ₃₄ O ₄	M-OH-OH	302.45	
1-ł	nexadecanoyl-glycerol	C ₁₉ H ₃₄ O ₄	Р-ОН-ОН	330.50	
1-0	octadecanoyl-glycerol	C ₂₁ H ₄₂ O ₄	S-OH-OH	358.55	
1-0	octadecenoyl-glycerol	C ₂₁ H ₄₀ O ₄	O-OH-OH	356.54	
1-0	octadecadienoyl-glycerol	C ₂₁ H ₃₈ O ₄	LI-OH-OH	354.52	
1-0	octadecatrienoyl-glycerol	C ₂₁ H ₃₆ O ₄	LN-OH-OH	352.51	
Me	ethyl tetradecanoate	C ₁₅ H ₃₀ O ₂	MEC14H28	242.40	
M	ethyl hexadecanoate	C ₁₇ H ₃₄ O ₂	MEC16H32	270.45	
M	ethyl octadecanoate	C ₁₉ H ₃₈ O ₂	MEC18H36	298.50	
M	ethyl octadecenoate	C ₁₉ H ₃₆ O ₂	MOLEATE	296.49	
Methyl octadecadienoate		C ₁₉ H ₃₄ O ₂	MEC18H32	294.47	
M	ethyl octadecatrienoate	C ₁₉ H ₃₂ O ₂	MEC18H30	292.45	
M	ethanol	CH ₄ O	METHANOL	32.04	
Gl	ycerin	C ₃ H ₈ O ₃	GLYCERIN	92.10	
W	ater	H ₂ O	H2O	18.02	

 Table 4.3 The components in biodiesel process for simulation

4.1.2 Reaction for Simulation

4.1.2.1 Reaction Data for Hydrogenated Biodiesel Process

Hydrogenated biodiesel is made from reacting hydrogen with vegetable oil in a refinery-hydrotreating process. There are several possible reaction pathways for the production of straight-chain hydrocarbons. In this study, two primary reactions are considered; hydrodeoxygenation (HDO) and decarbonylation. The reaction pathways are shown in Figure 4.2.



Figure 4.2 Two primary reaction pathways for the conversion of triglycerides to hydrogenated biodiesel.

The bio-hydrogenated diesel process was modeled by using several assumptions. The following are the list of reaction assumption.

- There is no decarboxylation, hydrolysis, and water gas shift in this analysis.
- The conversion of fatty acid is estimated at 95% of the hydrogenated triglycerides.
- Only 12% of fatty acid which composed in triglyceride undergoes decarbonylation and 88% undergoes hydrodeoxygenation (HDO) reaction.

4.1.2.2 Reaction Data for Biodiesel Process

In this study, biodiesel is defined as mono-alkyl ester which produced via the transesterification of palm oil. In this process, triglycerides react with methanol in the presence of a catalyst (KOH) to produce mono-alkyl esters (biodiesel) and glycerol. The typical transesterification process is shown in Figure 4.3.



Figure 4.3 The production of biodiesel via transesterification of triglyceride.

The overall process is normally a sequence of three consecutive steps, which are reversible reactions. These reactions are given in Figure 4.4. 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, yields one methyl ester molecule from each step.



Figure 4.4 The transesterification reactions of triglyceride with alcohol to ester and glycerol.

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.

4.1.3 Process Flow Diagram





Figure 4.5 Process flow diagram for hydrogenated biodiesel process.

As shown in Figure 4.5, the vegetable oil feed is pumped to 500 psia. This stream is then heated to 145 °C by exchange with hydrogenator effluent. It is then further heated to 190 °C with medium-pressure steam. The next stage of the process is the hydrogenator, where the oil stream is combined with the inlet hydrogen and reacted. All of the incoming oil is converted to gas (e.g., CO, methane, propane), water, and hydrogenated biodiesel. As noted in the reaction data, the conversion of hydrogenated biodiesel is estimated at 95% of the inlet feed streams on a mass basis. After the oil feed is preheated, the hydrogenator effluent is cooled with cooling water to 45 °C. The cooled reactor products are then sent to the sour water separation. In sour water separation, the gases are flashed off and sent to the PSA for recovery, and the aqueous stream is decanted and sent to wastewater treatment. After the separator, the organic stream is sent to a stripping column for product recovery. The product recovery area consists of a stripping column where LP (50 psig) steam is used to remove the light ends from the hydrogenated biodiesel product. The overheads are sent to the flash unit of the PSA system. The product stream is taken from the bottom of the column. The PSA system is a complex batch unit operation. The PSA is recovered the hydrogen in the overhead stream. The recovered hydrogen is then compressed to 514.7 psia before introduction into the hydrogenator. In addition to hydrogen, the PSA unit operation has two other outlet streams: CO and organics stream. The CO stream contains all of the carbon monoxide from the operation and is released to the atmosphere. The organics stream contains a mixture of water, propane, and other organics. These are separated in flash unit (Marker et al., UOP, 2005).



4.1.3.2 Process Flow Diagram of Steam Methane Reforming (SMR) Based Hydrogen Production for Hydrogenated Biodiesel Process

Combustor

Figure 4.6 Process flow diagram of steam methane reforming (SMR) based hydrogen production for hydrogenated biodiesel process. (Posada A. et al., 2005)

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A process flow diagram of conventional methane reforming based hydrogen production for hydrogenated biodiesel process can be represented in Figure 4.6. The process feed consists of liquid water and methane gas at ambient temperature. Each stream is compressed to 377.7 psia and heated to 538 °C, corresponding to values within typical entrance conditions for the reformer (Ogden, J. *et al.*, 2001), in addition to a steam/methane molar ratio of 3.12; excess steam is used to reduce byproduct carbon formation. Hot methane and steam are fed to the steam methane reformer (SMR) where the reversible reactions 1, 2, and 3 take place:

$$\begin{array}{rcl} CH_4 \ + \ H_2O & \longrightarrow & CO \ + \ 3H_2 & (1) & \Delta H^\circ_1: \ 206.1 \ kJ/mol \\ CO \ + \ H_2O & \longrightarrow & CO_2 \ + \ H_2 & (2) & \Delta H^\circ_2: \ -41.15 \ kJ/mol \\ CH_4 \ + \ 2H_2O & \longrightarrow & CO_2 \ + \ 4H_2 & (3) & \Delta H^\circ_3: \ 164.9 \ kJ/mol \end{array}$$

The kinetics of these reactions on a Ni/MgAl₂O₄ catalyst have been studied by Xu, J. et al., (1989). The overall reactor operation requires that heat be provided to the reformer, and this is done through the combustion of methane (fuel) and pressure swing adsorption (PSA) waste gas. Hydrogen is produced together with all the other species, and its generation is further increased in the water gas shift (WGS) reactor(s) where only the exothermic reaction 2 is catalyzed at temperatures lower than that of the reformer. A high-temperature water gas shift reactor (HT WGS) is used to raise the concentration of hydrogen to 62.2%, and a low-temperature water gas shift reactor (LT WGS) provides an additional 1.5% increase in the hydrogen content. Coolers are used before these two reactors in order to adjust the temperature of the gases to appropriate values for the proper operation of the catalysts. Most of the water is separated by condensation as the gas stream is cooled to almost ambient temperatures before entering the PSA unit where hydrogen can be purified to 99.85%. Species other than hydrogen are selectively adsorbed on a solid adsorbent (5A zeolite) at a relatively high pressure by contacting the gas with the solid in a packed column in order to produce a hydrogen enriched gas stream. The adsorbed species are then desorbed from the solid by lowering the pressure and purging with high-purity product hydrogen, and thus, the PSA waste gas is generated. Combustion of the PSA waste gas and methane (fuel) is used to provide heat for the reformer and also for the preheating of feeds and the generation of the export steam. Recovery of the waste heat from the still-hot gases leaving the reformer is also used to the same end. The hydrogen produced from the PSA unit is compressed up to 514.7 psia before introduction into the hydrogenator of hydrogenated biodiesel process.



4.1.3.3 Process Flow Diagram of Biodiesel Process

Figure 4.7 Process flow diagram for biodiesel process (Zhang Y. et al., 2003).

The conventional biodiesel process composes of a pretreatment unit and transesterification unit as shown in Figure 4.7. A pretreatment unit including esterification of the free fatty acids, glycerin washing and methanol recovery, was added.

The esterification reaction was carried out at 60 °C and a 6:1 molar ratio of methanol to crude palm oil. The fresh methanol stream the recycled methanol stream and the H₂SO₄ stream were mixed before being pumped into esterification reactor. The crude palm oil stream, containing free fatty acids, was heated in exchanger before entering reactor. In esterification reactor, all the free fatty acids were converted to methyl esters. After being cooled to 45 °C, reactor effluent stream was forwarded to glycerin washing column to remove the sulfuric acid and water. The resulting water and acid catalyst (H₂SO₄) from the esterification reactor must be removed completely before proceeding to the alkali-catalyzed transesterification. By adding glycerin at 25 °C, all of the resulting water was removed from oil. Recovering most of the methanol in the stream from glycerin washing column for reuse in the esterification reactor was a logical step, which was realized in methanol recovery column (Zhang Y. *et al.*, 2003).

In the transesterification unit, crude palm oil is pumped into two reactors and combined with a mixture of methanol and KOH by mixers. The transesterification reaction was carried out at 60 °C and a 6:1 molar ratio of methanol to crude palm oil. The mixing and heating time for the mixture is about 90 minutes. After the reaction is completed, the mixture is transferred to the settling tank. After separation into two phases in the settling tanks, crude biodiesel from the top of the settling tanks go to vacuum distillation column (methanol purification). In this stage, the common method of washing by water is not used; vacuum distillation is used to separate methanol and biodiesel from the mixture, and the biodiesel product, which will be collected at the bottom, will be sent to vacuum distillation column (biodiesel purification) to separate out the glycerides. Glycerides are collected at the bottom as soaps and can be used as fuel. Pure biodiesel is collected from the top and sidestream of distillation column.

4.2 Process Simulation

4.2.1 Mass and Energy Balances of Hydrogenated Biodiesel Process

In this step, the simplest process flow sheet of hydrogenated biodiesel plant is built (Figure 4.8) with the stream calculator to calculate the mass balance of the process. A summary of the operation parameters of units in the process is shown in Table 4.4.

Equipment	Parameter
Reactor, R-101	Stoichiometric Coefficient = Triglyceride: Hydrogen=1:15
	Key Component= Triglyceride Conversion=95%
Stream Calculator	Recovery factor of Methane and CO = 100% (Top)
SC-201	Recovery factor of Propane = 75% (Top)
(Flash)	Recovery factor of Hydrogen = 100% (Top)
	Recovery factor of Tridecane through Octadecane = 100%
	(Bottom)
	Recovery factor of Triglyceride = 100% (Bottom)
	Recovery factor of Water = 98.5% (Bottom)
Stream Calculator	Recovery factor of Methane and CO = 100% (Top)
SC-202	Recovery factor of Propane = 100% (Top)
(Water Separator)	Recovery factor of Hydrogen = 100% (Top)
	Recovery factor of Tridecane through Octadecane = 100%
	(Top)
	Recovery factor of Triglyceride = 100% (Bottom)
	Recovery factor of Water = 100% (Bottom)
Stream Calculator	Recovery factor of Methane and CO = 100% (Bottom)
SC-301	Recovery factor of Propane = 100% (Bottom)
(PSA)	Recovery factor of Hydrogen = 86% (Top)
	Recovery factor of Tridecane through Octadecane = 100%
	(Bottom)
	Recovery factor of Triglyceride = 100% (Bottom)
	Recovery factor of Water = 100% (Bottom)
Stream Calculator	Recovery factor of CO = 100% (Top)
SC-302	Recovery factor of Hydrogen = 100% (Top)
(PSA)	Recovery factor of Methane = 100% (Bottom)
	Recovery factor of Propane = 100% (Bottom)
	Recovery factor of Tridecane through Octadecane = 100%
	(Bottom)
	Recovery factor of Triglyceride = 100% (Bottom)
	Recovery factor of Water = 100% (Bottom)

 Table 4.4 Operation parameters of each unit in hydrogenated biodiesel process

 Table 4.4 Operation parameters of each unit in hydrogenated biodiesel process

(cont.)

Equipment	Parameter
Stream Calculator	Recovery factor of CO = 100% (Top)
SC-401	Recovery factor of Hydrogen = 100% (Top)
(Stripping Column)	Recovery factor of Methane = 100% (Top)
	Recovery factor of Propane = 100% (Top)
	Recovery factor of Tridecane through Octadecane = 100%
	(Bottom)
1	Recovery factor of Triglyceride = 100% (Bottom)
	Recovery factor of Water = 100% (Bottom)
Stream Calculator	Recovery factor of CO = 100% (Top)
SC-403	Recovery factor of Hydrogen = 100% (Top)
(Flash 1)	Recovery factor of Methane = 100% (Top)
	Recovery factor of Propane = 100% (Top)
	Recovery factor of Tridecane through Octadecane = 100%
	(Bottom)
	Recovery factor of Triglyceride = 100% (Bottom)
	Recovery factor of Water = 100% (Bottom)
Stream Calculator	Recovery factor of CO = 100% (Top)
SC-402	Recovery factor of Hydrogen = 100% (Top)
(Flash 2)	Recovery factor of Methane = 100% (Top)
	Recovery factor of Propane = 100% (Top)
	Recovery factor of Tridecane through Octadecane = 100%
	(Top)
	Recovery factor of Triglyceride = 100% (Bottom)
	Recovery factor of Water = 100% (Bottom)

The energy balance of each unit is calculated by replacing each of the component stream calculators (splitters) with their corresponding rigorous models (Figures 4.9) and perform the mass and energy balances for the total flow sheet, the energy balance of each unit is calculated as shown in Tables 4.6 for hydrogenated biodiesel process.

Heat demand/supply calculated by following equation:

$$Q_j = \sum \Delta H_{stream out} - \sum \Delta H_{stream in}$$

Where $\Delta H_{stream out}$ of each unit is collected from the PRO/II[®] file. $\Delta H_{stream in}$ of each unit is collected from the PRO/II[®] file.



Figure 4.8 The simple process flow sheet of the hydrogenated biodiesel plant for mass balance.

Stream	103	101	104	201	202	205	206	1302	301	303
Description	Palm Oil	Hydrogen	Rn Mix.	Vap. Mix.	Liq. Product	hydrogenated biodiesel,C3	Waste H ₂ O	Re H ₂	PSA	H ₂ ,CO
Phase	Liquid	Vapor	Mixed	Vapor	Liquid	Mixed	Liquid	Vapor	Mixed	Vapor
Temperature (°C)	30.00	30.00	325.00	45.00	45.00	30.00	30.00	45.00	45.00	45.00
Pressure (psia)	14.70	14.70	514.70	175.00	175.00	17.00	17.00	175.00	175.00	14.70
Mass fraction										
M-M-M	0.0086	0	0.0012	0	0.0012	0	0.0050	0	0	0
P-P-P	0.3853	0	0.0542	0	0.0551	0	0.2216	0	0	0
S-S-S	0.0469	0	0.0066	0	0.0067	0	0.0270	0	0	0
0-0-0	0.4251	0	0.0598	0	0.0608	0	0.2445	0	0	0
LI-LI-LI	0.1256	0	0.0177	0	0.0180	0	0.0723	0	0	0
LN-LN-LN	0.0052	0	0.0007	0	0.0007	0	0.0030	0	0	0
OLEIC	0.0033	0	0.0003	0	0.0003	0	0.0014	0	0	0
H ₂	0	1	0.0047	0.2689	0.0002	0.0003	0	1	0.0480	0.4229
TRIDECAN	0	0	0.0001	0	0.0001	0.0002	0	0	0	0
TETDECAN	0	0	0.0058	0	0.0058	0.0078	0	0	0	0
PENDECAN	0	0	0.0055	0	0.0056	0.0074	0	0	0	0
HXDECANE	0	0	0.2623	0	0.2668	0.3551	0	0	0	0
HDECANE	0	0	0.0089	0	0.0091	0.0121	0	0	0	0
OCTDECAN	0	0	0.4236	0	0.4307	0.5733	- 0.	0	0	0
H ₂ O	0	0	0.1045	0.0130	0.1060	0.0005	0.4250	0	0.0169	0
PROPANE	0	0	0.0427	0.6389	0.0326	0.0433	0.0002	0	0.8311	0
METHANE	0	0	0.0005	0.0277	0	0	0	0	0.0361	0
СО	0	0	0.0009	0.0514	0	0	0	0	0.0668	0.5771
Total Mass Rate (kg / h)	38,061.33	1,108.80	39,323.08	656.52	38,667.81	29,053.92	9,613.89	151.85	504.66	58.46

Table 4.5 Mass balance of hydrogenated biodiesel process from PRO/II®

Stream	304	402	403	402A	402B	102	401	404	405	406
Description	H ₂ O, C1, C3	Propane	hydrogenated biodiesel,H ₂ O	Fuel Gas	Water	H ₂	Steam	hydrogenated biodiesel	Waste H ₂ O	Waste H ₂ O
Phase	Mixed	Vapor	Liquid	Vapor	Liquid	Vapor	Vapor	Liquid	Liquid	Liquid
Temperature (°C)	45.00	30.23	98.54	30.00	30.00	520.72	148.0	30.00	30.00	36.56
Pressure (psia)	14.70	14.70	14.7	14.7	14.7	514.7	64.70	14.70	14.70	14.7
Mass fraction										
M-M-M	0	0	0	0	0	0	0	0	0	0.0045
P-P-P	0	0	0	0	0	0	0	0	0	0.2011
S-S-S	0	0	0	0	0	0	0	0	0	0.0245
0-0-0	0	0	0	0	0	0	0	0	0	0.2218
LI-LI-LI	0	0	0	0	0	0	0	0	0	0.0655
LN-LN-LN	0	0	0	0	0	0	0	0	0	0.0027
OLEIC	0	0	0	0	0	0	0	0	0	0.0013
H ₂	0	0.0070	0	0	0	1	0	0	0	0
TRIDECAN	0	0	0.0002	0	0	0	0	0.0002	0	0
TETDECAN	0	0	0.0079	0	0	0	0	0.0081	0	0
PENDECAN	0	0	0.0075	0	0	0	0	0.0078	0	0
HXDECANE	0	0	0.3586	0	0.0002	0	0	0.3713	0	0
HDECANE	0	0	0.0122	0	0	0	0	0.0126	0	0
OCTDECAN	0	0	0.5789	0	0	0	0	0.5994	0	0
H ₂ O	0.0191	0.0202	0.0343	0.0057	0.5967	0	1	0.0001	0.9999	0.4784
PROPANE	0.9400	0.9703	0.0004	0.9763	0.4026	0	0	0.0005	0.0001	0.0002
METHANE	0.0409	0.0014	0	0.0118	0.0002	0	0	0	0	0
СО	0	0.0011	0	0.0008	0	0	0	0	0	0
Total Mass Rate (kg / h)	446.2	1,283.23	28,770.67	1,687.86	41.58	1,260.65	1000	27,786.74	983.94	10,597.82

Table 4.5 Mass balances of hydrogenated biodiesel process from PRO/II® (cont.)



Figure 4.9 The process flow sheet of the hydrogenated biodiesel plant for mass and energy balance.

Process		Fauinments	Materials	Stream	Flow rate	Operation	Capacity Q ₁	Demark
	1100035	Equipments		Ref.	kg/h	Operation	(Duty) MJ/h	Kemark
1.	Palm oil Supply							
	Palm oil Supply	Pump (P-101)	Crude Palm Oil	103	38,061.33			_
	Heating	Heat Exchanger (E-101)	Crude Palm Oil	103A	38,061.33	Heating	12,680.31	Heat addition
	Heating	Heat Exchanger (E-102)	Crude Palm Oil	103B	38,061.33	Heating	5,340.38	Heat addition
2.	H ₂ Supply							
	H ₂ Supply	Compressor (C-101)	Hydrogen	101	1,108.73		4,505.78	Heat addition
	Recycle H ₂	Compressor (C-102)	Hydrogen	1302	151.85		1,776.79	Heat addition
	H ₂ Mixer	Mixer (M-101)	Hydrogen	102	1,260.58			
3.	Hydrogenation							
	Hydrogenation	Reactor (R-101)	Reaction Mixture 1	104	39,322.68		32,071.52	Heat removal
	Cooling	Heat Exchanger (E-103)	Reaction Mixture 1	104A	39,322.68	Cooling	31,323.49	Heat removal
4.	Sour Water Separation							
	VL Separation	Flash (F-201)	Reaction Mixture 1	202	38,667.43		98.64	Heat addition
	Water Separation	Flash (F-202)	Reaction Mixture 2	202	38,667.43		1,083.17	Heat removal
5.	Recycle H ₂							
	PSA	Stream Calculator (SC-301)	Reaction (V) Mixture	201	656.50		16.74	Heat removal
	PSA	Stream Calculator (SC-302)	Reaction (V) Mixture	301	504.66		16.00	Heat removal
6.	Product Recovery							
	Stripping Column	Distillation Column (T-401)	Reaction (L) Mixture	205	29,053.48			Heat addition
			Steam 60 psia	401	1,000.00			99.0% Propane Purification
		Reboiler (T-401)	Product (L) Mixture	403	28,770.26	Heating	2,290.85	Heat addition
	Fuel Gas Sep.	Flash (F-401)	Product (V) Mixture	402B	41.58		39.99	Heat removal
	Cooling	Heat Exchanger (E-401)	Product (L) Mixture	403	28,770.26	Cooling	4,788.24	Heat removal
	Water Separation	Flash (F-402)	Product (L) Mixture	403A	28,770.26			
	Water Treatment	Mixer (M-401)	Waste Water	404	10,597.90			

Table 4.6 Energy	balance of hydr	ogenated biodiese	l process from	PRO/II®

4.2.2 <u>Mass and Energy Balances of SMR Based Hydrogen Production for</u> <u>Hydrogenated Biodiesel Process</u>

A process flow diagram of the simulation done in PRO/II[®] is presented in Figure 4.10. The mass and energy balance of each unit is calculated as shown in Table 4.7 and Table 4.8, respectively. The process feed consists of liquid water (513) and methane gas (501) at ambient temperature. Each stream is compressed to 377.7 psia and heated to 537 °C. Steam reforming reactor simulated as a conversion reactor producing a gas with 58.5% (molar) H₂. Heat, in the amount of 34,324.0 MJ/h, is provided to the reformer, since it is required by the endothermic reactions 1 and 3 and in order to increase the temperature of the reacting gases and maintain a high reaction rate. A high-temperature water gas shift reactor (HT WGS) is used to raise the concentration of hydrogen to 62.2%, and a low-temperature water gas shift reactor (LT WGS) provides an additional 1.5% increase in the hydrogen content. Hydrogen purification starts with the condensation and flash separation of liquid water by cooling the gases and is finalized in the PSA unit with adsorption of the majority of the remaining contaminant gases. The PSA process is approximately isothermal and does not require any significant heat load. Thus, for the purposes of this heat/power integration study, it can be modeled as a stream calculator. Exit compositions for this stream calculator was assigned based on typical PSA performance resulting in the production of 1100 kg/h of a gas stream with 99.85% H₂ at 514.7 psia. The simulated PSA waste gas contains 20.7% CH₄, and its adiabatic combustion with 110% air (10% excess over the stoichiometric requirement) generates combustion gases at 1594.8 °C. The hydrogen produced from the PSA unit is compressed up to 514.7 psia. Considering compressors with 85% adiabatic efficiency, the total work required for the compression of hydrogen is 152.13 kW.





Stream	501	502	503	504	505	506	507	508	509	510	511	512	513
Description	CH ₄	CH₄	CH₄	Rn. Mix	Rn. Mix	Rn. Mix	Rn. Mix	Rn. Mix	Rn. Mix.	Rn. Mix.	Water	Water	Water
Phase	Vapour	Vapour	Vapour	Vapour	Vapour	Vapour	Vapour	Vapour	Vapour	Vapour	Liquid	Liquid	Liquid
Temperature (°C)	298.0	225.0	537.8	856.8	348.9	418.9	196.9	196.9	37.9	37.9	37.9	37.9	25.0
Pressure (psia)	14.7	377.7	377.7	377.7	377.7	377.7	377.7	377.7	308.6	308.6	308.6	308.6	14.7
Mass fraction			_										
CH4	1	1	1	0.0662	0.0663	0.0663	0.0663	0.0663	0	0.0022	0.0023	0.0022	0
H ₂	0	0	0	0.1062	0.1062	0.1140	0.1140	0.1187	0.9492	0.0019	0.0017	0.0020	0
CO	0	0	0	0.2701	0.2701	0.1621	0.1621	0.0973	0.0078	0.0014	0.0011	0.0014	0
CO ₂	0	0	0	0.2747	0.2747	0.4445	0.4445	0.5464	0.0426	0.0896	0.0893	0.0896	0
H ₂ O	0	0	0	0.2828	0.2828	0.2131	0.2131	0.1714	0.0003	0.9049	0.9049	0.9049	1
O ₂	0	0	0	0	0	0	0	0	0	0	0	0	0
N ₂	0	0	0	0	0	0	0	0	0	0	0	0	0
Total Rate (kg / h)	1,488.0	1,488.0	1,488.0	9,443.3	9,443.3	9,441.1	9,441.1	9,441.1	1,174.2	1,745.9	174.6	1,571.3	4,895.8
Stream	514	515	516	517	518	519	520	521	522	523	524	525	101A
Description	Water	Water	Water	Water	Water	H ₂	Mix. gas	Methane	Mix. gas	Air	Flue gas	Flue gas	H ₂
Phase	Liquid	Liquid	Liquid	Liquid	Vapour	Vapour	Vapour	Vapour	Vapour	Vapour	Vapour	Vapour	Vapour
Temperature (°C)	25.0	28.0	155.0	222.5	222.5	28.0	30.0	25.0	37.0	25.0	1594.8	1594.8	100.0
Pressure (psia)	377.7	377.7	377.7	377.7	377.7	308.6	19.1	14.7	14.7	14.7	14.7	14.7	514.7
Mass fraction													
CH₄	0	0.0005	0.0005	0.0005	0.0005	0	0.0954	1	0.1099	0	0.0003	0.0003	0
H ₂	0	0.0005	0.0005	0.0005	0.0005	0.9492	0.0003	0	0.0003	0	0.0001	0.0001	0.9492
CO	0	0.0003	0.0003	0.0003	0.0003	0.0078	0.1390	0	0.1368	0	0.0431	0.0431	0.0078
CO ₂	0	0.0218	0.0218	0.0218	0.0218	0.0426	0.7594	0	0.7471	0	0.3297	0.3297	0.0426
H ₂ O	1	0.9769	0.9769	0.9769	0.9769	0.0003	0.0059	0	0.0058	0	0.0789	0.0789	0.0003
O ₂	0	0	0	0	0	0	0	0	0	0.2329	0.0226	0.0226	0
N ₂	0	0	0	0	0	0	0	0	0	0.7671	0.5252	0.5252	0
Total Rate (kg / h)	4,895.8	6,467.2	6,467.2	6,467.2	6,467.2	1,174.2	6,521.0	106.8	6,627.8	14,393.7	21,021.3	5,255.3	1,174.2

Table 4.7 Mass balance of SMR based hydrogen production for hydrogenated biodiesel process from PRO/II®

Process	Equipments	Materials	Stream	Flow rate	Operation	Capacity Q ₁	Dement
Trocess	Equipments	Waterials	Ref.	kg/h	Operation	(Duty) MJ/h	кетагк
1. Methane Supply							
Methane Supply	Compressor (C-501)	Methane	501	1,488.0		1,043.7	Heat addition
Heating	Heat Exchanger (E-501)	Methane	502	1,488.0	Heating	1,633.4	Heat addition
2. Water Supply							
Water Supply	Pump (P-501)	Water	513	4,895.8			
Mixer	Mixer (M-501)	Water	515	6,467.2			
3. Steam Methane Reforming							
SMR	SMR Reactor (R-501)	Reaction Mixture 1	504	9,443.3		34,323.7	Heat addition
Cooling	Heat Exchanger (E-502)	Reaction Mixture 1	504	9,443.3	Cooling	520.0	Heat removal
4. HT Water Gas Shift							
HT WGS	HT WGS Reactor (R-502)	Reaction Mixture 2	505	9,443.3		886.7	Heat removal
Cooling	Heat Exchanger (E-503)	Reaction Mixture 2	506	9,441.1	Cooling	3,428.2	Heat removal
5. LT Water Gas Shift							
LT WGS	LT WGS Reactor (R-503)	Reaction Mixture 3	507	9,441.1		1,041.7	Heat removal
Water Separation	Flash (F-501)	Reaction Mixture 3	510	1,745.9	Cooling	8,052.0	Heat removal
6. Hydrogen Recovery							
PSA	Stream Calculator (SC-501)	Reaction (V) Mixture	509	1,174.2			
Hydrogen Supply	Compressor (C-101)	Hydrogen	101A	1,174.2		547.6	Heat addition
7. Combustion							
Combustion	Combustor (R-504)	Reaction (V) Mixture	524	21,021.3		29,955.4	Heat addition
Cooling	Heat Exchanger (E-504)	Reaction (V) Mixture	525	5,255.3	Heating	10,549.2	Heat addition
Cooling	Heat Exchanger (E-505)	Reaction (V) Mixture	529	5,255.3	Cooling	2,645.6	Heat removal
Cooling	Heat Exchanger (E-506)	Reaction (V) Mixture	530	5,255.3	Cooling	3,434.8	Heat removal
Water Supply	Pump (P-502)	Water	532	1,000.0			

Table 4.8 Energy balance of SMR based hydrogen production for hydrogenated biodiesel process from PRO/II®

4.2.3 Mass and Energy Balances of Biodiesel Process

In this step, the simplest process flow sheet of biodiesel plant is built (Figure 4.11) with the stream calculator to calculate the mass balance of process. A summary of the operation parameters of units in the process is shown in Table 4.9.

Equipment	Parameter
Reactor, R-101	Stoichiometric Coefficient = Triglyceride: Methanol=1:6
Esterification	Key Component= Fatty acid Conversion=100%
Reactor, R-201	Stoichiometric Coefficient = Triglyceride: Methanol=1:6
Transesterification 1	Key Component= Triglyceride Conversion=100%
Reactor, R-202	Stoichiometric Coefficient = Triglyceride: Methanol=1:6
Transesterification2	Key Component= Triglyceride Conversion=100%
Stream Calculator	Recovery factor of Triglyceride = 100% (Top)
SC-101	Recovery factor of Diglyceride = 100% (Top)
(Glycerin Washing)	Recovery factor of Monoglyceride = 100% (Top)
	Recovery factor of Methyl ester = 100% (Top)
	Recovery factor of Methanol = 100% (Bottom)
	Recovery factor of Water = 95% (Bottom)
	Recovery factor of Glycerin = 100% (Bottom)
Stream Calculator	Recovery factor of Triglyceride = 100% (Bottom)
SC-102	Recovery factor of Diglyceride = 100% (Bottom)
(Methanol Recoveryl)	Recovery factor of Monoglyceride = 100% (Bottom)
	Recovery factor of Methyl ester = 100% (Bottom)
	Recovery factor of Methanol = 100% (Top)
	Recovery factor of Water = 100% (Bottom)
	Recovery factor of Glycerin = 100% (Bottom)
Stream Calculator	Recovery factor of Triglyceride = 100% (Bottom)
SC-301	Recovery factor of Diglyceride = 100% (Bottom)
(Methanol Recovery2)	Recovery factor of Monoglyceride = 100% (Bottom)
	Recovery factor of Methyl ester = 100% (Bottom)
	Recovery factor of Methanol = 99% (Top)
	Recovery factor of Water = 100% (Bottom)
	Recovery factor of Glycerin = 100% (Bottom)
Stream Calculator	Recovery factor of Triglyceride = 90% (Top)
SC-201	Recovery factor of Diglyceride = 90% (Top)
(Glycerin Separation)	Recovery factor of Monoglyceride = 90% (Top)
	Recovery factor of Methyl ester = 98% (Top)
	Recovery factor of Methanol = 80% (Top)
	Recovery factor of Water = 100% (Bottom)
	Recovery factor of Glycerin = 99% (Bottom)

 Table 4.9 Operation parameters of each unit in biodiesel process

Equipment	Parameter
Stream Calculator	Recovery factor of Triglyceride = 100% (Bottom)
SC-501	Recovery factor of Diglyceride = 100% (Bottom)
(Biodiesel Purification)	Recovery factor of Monoglyceride = 100% (Bottom)
	Recovery factor of Methyl ester = 100% (Top)
	Recovery factor of Methanol = 100% (Bottom)
	Recovery factor of Water = 100% (Bottom)
	Recovery factor of Glycerin = 100% (Bottom)
Stream Calculator	Recovery factor of Triglyceride = 100% (Bottom)
SC-401	Recovery factor of Diglyceride = 100% (Bottom)
(Glycerin Purification)	Recovery factor of Monoglyceride = 100% (Bottom)
	Recovery factor of Methyl ester = 100% (Bottom)
	Recovery factor of Methanol = 100% (Top)
	Recovery factor of Water = 100% (Bottom)
	Recovery factor of Glycerin = 100% (Bottom)
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 Table 4.9 Operation parameters of each unit in biodiesel process (cont.)



Figure 4.11 The simple biodiesel process flow sheet for mass balance.

Stream	101	101B	101C	102	201	203	102A	302	204	205	501	103	502
Description	MeOH	MeOH	MeOH	MeOH	Rn. Mix	Rn. Mix	МеОН	Methyl Ester	Rn. Mix.	Glycerin	Methyl Ester	Palm Oil	Waste
Phase	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°C)	30.0	30.0	30.0	30.0	60.0	60.0	30.0	184.68	60.0	60.0	30.0	30.0	60
Pressure (psia)	14.7	14.7	14.7	14.7	14.7	14.7	14.7	0.25	14.7	14.7	14.7	14.7	14.7
Mass fraction													
M-M-M	0	0	0	0	0	0	0	0	0	0	0	0.0101	0
P-P-P	0	0	0	0	0	0	0	0	0	0	0	0.4036	0
S-S-S	0	0	0	0	0	0	0	0	0	0	0	0.0445	0
0-0-0	0	0	0	0	0	0	0	0	0	0	0	0.4060	0
LI-LI-LI	0	0	0	0	0	0	0	0	0	0	0	0.1208	0
LN-LN-LN	0	0	0	0	0	0	0	0	0	0	0	0.0050	0
M-M-OH	0	0	0	0	0	0	0	0	0	0	0	0	0
P-P-OH	0	0	0	0	0	0	.0	0	0	0	0	0	0
S-S-OH	0	0	0	0	0	0	0	0	0	0	0	0	0
0-0-ОН	0	0	0	0	0	0	0	0	0	0	0	0	0
LI-LI-OH	0	0	0	0	0	0	0	0	0	0	0	0	0
LN-LN-OH	0	0	0	0	0	0	0	0	0	0	0	0	0
LN-LN-OH	0	0	0	0	0.0001	0.0001	0	0.0002	0.0002	0.0001	0	0	0.0091
P-OH-OH	0	0	0	0	0.0049	0.0057	0	0.0075	0.0059	0.0043	0	0	0.3564
S-OH-OH	0	0	0	0	0.0005	0.0006	0	0.0008	0.0006	0.0005	0	0	0.0386
М-ОН-ОН	0	0	0	0	0.0049	0.0056	0	0.0074	0.0058	0.0043	0	0	0.3526
LI-OH-OH	0	0	0	0	0.0015	0.0017	0	0.0022	0.0017	0.0013	0	0	0.1050
LN-OH-OH	0	0	0	0	0	0	0	0	0	0	0	0	0.0044

Table 4.10 Mass balance of biodiesel process from $\text{PRO/II}^{\circledast}$

Stream	101	101B	101C	102	201	203	102A	302	204	205	501	103	502
Description	МеОН	MeOH	MeOH	MeOH	Rn. Mix	Rn. Mix	MeOH	Methyl Ester	Rn. Mix.	Glycerin	Methyl Ester	Palm Oil	Waste
Phase	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°C)	30.0	30.0	30.0	30.0	60.0	60.0	30.0	184.68	60.0	60.0	30.0	30.0	60
Pressure (psia)	14.7	14.7	14.7	14.7	14.7	14.7	14.7	0.25	14.7	14.7	14.7	14.7	14.7
Mass fraction													
MEC14H28	0	0	0	0	0.0060	0.0069	0	0.0099	0.0078	0.0010	0.0101	0	0
MEC16H32	0	0	0	0	0.2378	0.2747	0	0.3954	0.3100	0.0418	0.4039	0	0.0026
MEC18H36	0	0	0	0	0.0262	0.0303	0	0.0436	0.0342	0.0046	0.0443	0	0.0095
MOLEATE	0	0	0	0	0.2453	0.2834	0	0.4080	0.3198	0.0431	0.4151	0	0.0773
MEC18H32	0	0	0	0	0.0711	0.0822	0:	0.1183	0.0927	0.0125	0.1200	0	0.0384
MEC18H30	0	0	0	0	0.0029	0.0034	0	0.0049	0.0038	0.0005	0.0049	0	0.0060
OLEIC	0	0	0	0	0	0	0	0	0	0	0	0.010	0
METHANOL	1	1	0.9989	1	0.3380	0.2350	1	0.0006	0.2165	0.3574	0.0006	0	0
GLYCERIN	0	0	0	0	0.0608	0.0702	0	0.0010	0.0008	0.5286	0.0011	0	0
H2O	0	0	0.0011	0	0	0	0	0	0	0	0	0	0
Total Mass Rate (kg / h)	3,684.98	327.96	4,960.77	6,491.46	24,123.9	41,756.3	3,245.73	28,427.8	36,263.9	5,492.41	27,827.9	28,759.0	599.97

Table 4.10 Mass balance of biodiesel process from PRO/II[®] (cont.)

Stream	401	402	102B	107A	202	107B	301	104	303	105	107	108	101A
Description	MeOH	Glycerin	MeOH	Palm Oil	Rn. Mix	Palm Oil	MeOH	Rn. Mix.	MeOH	Glycerin	Palm Oil	MeOH	MeOH
Phase	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°C)	30.0	212.0	30.0	60.0	60.0	60.0	30.0	60.0	30.0	30.0	60.0	30.0	30.0
Pressure (psia)	0.2	0.25	14.7	14.7	14.7	14.7	0.21	14.7	14.7	14.7	14.7	14.7	14.7
Mass fraction													
M-M-M	0	0	0	0.0101	0	0.0101	0	0.0086	0	0	0.0101	0	0
P-P-P	0	0	0	0.4034	0	0.4034	0	0.3442	.0	. 0	0.4034	0	0
S-S-S	0	0	0	0.0445	0	0.0445	0	0.0380	0	0	0.0445	0	0
0-0-0	0	0	0	0.4058	0	0.4058	0	0.3463	0	0	0.4058	0	0
LI-LI-LI	0	0	0	0.1207	0	0.1207	0	0.1030	0	0	0.1207	0	0
LN-LN-LN	0	0	0	0.0050	0	0.0050	0	0.0043	0	0	0.0050	0	0
M-M-OH	0	0	0	0	0	0	0	0	0	0	0	0	0
P-P-OH	0	0	0	0	0	0	0	0	0	0	0	0	0
S-S-OH	0	0	0	0	0	0	0	0	0	0	0	0	0
0-0-0H	0	0	0	0	0	0	0	0	0	0	0	0	0
LI-LI-OH	0	0	0	0	0	0	0	0	0	0	0	0	0
LN-LN-OH	0	0	0	0	0	0	0	0	0	0	0	0	0
LN-LN-OH	0	0.0002	0	0	0.0002	0	0	0	0	0	0	0	0
P-OH-OH	0	0.0067	0	0	0.0067	0	0	0	0	0	0	0	0
S-OH-OH	0	0.0007	0	0	0.0007	0	0	0	0	0	0	0	0
M-OH-OH	0	0.0066	0	0	0.0067	0	0	0	0	0	0	0	0
LI-OH-OH	0	0.0020	0	0	0.0020	0	0	0	0	0	0	0	0
LN-OH-OH	0	0	0	0	0	0	0	0	0	0	0	0	0

 Table 4.10 Mass balance of biodiesel process from PRO/II[®] (cont.)

Stream	401	402	102B	107A	202	107B	301	104	303	105	107	108	101A
Description	MeOH	Glycerin	MeOH	Palm Oil	Rn. Mix	Palm Oil	MeOH	Rn. Mix.	MeOH	Glycerin	Palm Oil	MeOH	MeOH
Phase	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°C)	30.0	212.0	30.0	60.0	60.0	60.0	. 30.0	60.0	30.0	30.0	60.0	30.0	30.0
Pressure (psia)	0.2	0.25	14.7	14.7	14.7	14.7	0.21	14.7	14.7	14.7	14.7	14.7	14.7
Mass fraction													
MEC14H28	0	0.0016	0	0	0.0081	0	0	0	0	0	0	0	0
MEC16H32	0	0.0649	0	0	0.3253	0	0	0	0	0	0	0	0
MEC18H36	0	0.0072	0	0	0.0358	0	0	0	0	0	0	0	0
MOLEATE	0	0.0670	0	0.0105	0.3356	0.0105	0	0.0090	0	0	0.0105	0	0
MEC18H32	0	0.0194	0	0	0.0973	0	0	0	0	0	0	0	0
MEC18H30	0	0.0008	0	0	0.0040	0	0	0	0	0	0	0	0
OLEIC	0	0	0	0	0	0	0	0	0	0	0	0	0
METHANOL	1	0.0011	1	0	0.0942	0	1	0.1460	1	0	0	0.9988	1
GLYCERIN	0	0.8216	0	0	0.0832	0	0	0	0	1	0	0	0
H2O	0	0	0	0	0	0	0	0.0007	0	0	0	0.0012	0
Total Mass Rate (kg / h)	1,959.03	3,533.4	3,245.7	14,386.6	17,632.4	14,386.6	7,836.1	33,719.7	9,795.1	3,165.0	28,773.2	1,160.6	3,357.0

Table 4.10 Mass balance of biodiesel process from PRO/II [®]	(cont.)
rable 4.10 Mass balance of biblicser process nom r RO/II	(0011.)



Figure 4.12 The conventional biodiesel process flow sheet for mass and energy balance.

Table 4.11 Energy balance of biodiesel process from PRO/II[®]

Process		Equipments	Materials	Stream	Flow rate	Operation	Capacity Q _i	Remark
		- 1		Ref.	kg/h	operation	(Duty) MJ/h	
1.	Pretreatment							
	Palm oil Supply	Pump (P-101)	Crude Palm Oil	103	28,750.0			
	Heating	Heat Exchanger (E-101)	Crude Palm Oil	103A	28,750.0	Heating	2,544.5	Heat addition
	Methanol Supply	Mixer (M-101)	Methanol	101C	2,930.5			
	Esterification	Reactor (R-101)	Reaction Mixture P1	104	31,680.5		278.5	Heat addition
	Glycerin Washing	Stream Calculator (SC-101)	Reaction Mixture P2	106, 107	34,846.5		5,686.5	Heat addition
	Recovery Methanol	Distillation Column (T-101)	Methanol	106	6,091.8		1,433.1	99.0 % MeOH, 2 Molar Reflux Ratio, Heat removal
		Condenser (T-101)	Methanol	108	2,745.5	Cooling	9,738.8	Heat removal
		Reboiler (T-101)	Waste H ₂ O	109	3,346.2	Heating	8,305.7	Heat addition
	Recycle Methanol	Pump (P-102)	Methanol	110	2,745.5			
2.	Tranesterification							
	Methanol Supply	Mixer (M-102)	Methanol	102	6,414.2			
	Transesterification 1	Reactor (R-201)	Reaction Mixture 1	201	17,584.6		791.8	Heat removal
	Transesterification 2	Reactor (R-202)	Reaction Mixture 2	202	17,584.6		791.8	Heat removal
3.	Glycerin Separation							
	Glycerin SEP1	Mixer (M-201)	Reaction Mixture 1,2	203	35,169.1			
	Glycerin SEP2	Stream Calculator (SC-201)	Reaction Mixture 1,2	203	35,169.1			
4.	Methanol Purification				- 20			
	Heating	Heat Exchanger (E-201)	MeOH, Methyl Ester	204	30,980.4	Heating	5,942.5	Heat addition
	Methanol Purification	Distillation Column (T-301)	MeOH, Methyl Ester	204A	30,980.4		3,700.8	99.0 % MeOH, 2 Molar Reflux Ratio, Heat addition
		Condenser (T-301)	Methanol	301	2,580.3	Cooling	13,518.9	Heat removal
		Reboiler (T-301)	Methyl Ester	302	28,400.1	Heating	5,739.9	Heat addition
	Mixed Methanol	Mixer (M-301)	Methanol	303	3,225.4			
	Recycle Methanol	Pump (P-301)	Methanol	1303	2,902.8			

	Process	Equipments	Materials	Stream Ref	Flow rate	Operation	CapacityQ _i	Remark	
5	. Glycerin Purification						(Buty) Mon		
	Heating	Heat Exchanger (E-202)	Glycerin, MeOH	205	4,188.7	Heating	998.0	Heat addition	
	Glycerin Purification	Distillation Column (T-401)	Glycerin, MeOH	205A	4,188.7		371.5	92.0 % Glycerin, 5 Molar Reflux Ratio, Heat addition	
		Condenser (T-401)	Methanol	401	645.1	Cooling	6,759.5	Heat removal	
		Reboiler (T-401)	Glycerin	402	3,543.6	Heating	7,502.1	Heat addition	
6	Biodiesel Purification								
	Heating	Heat Exchanger (E-301)	Methyl Ester	302	28,400.1	Heating	1,539.4	Heat addition	
	Biodiesel Purification	Distillation Column (T-501)	Methyl Ester	302A	28,400.1		5,158.7	99.5 % B100, 5 Molar Reflux Ratio, Heat removal	
		Condenser (T-501)	Methyl Ester	501	27,805.9	Heating	20,293.6	Heat removal	
		Reboiler (T-501)	Glycerin	502	594.2	Heating	8,609.9	Heat addition	

 Table 4.11 Energy balance of biodiesel process from PRO/II[®] (cont.)

4.3 Equipment Sizing and Costing

All equipment units were sized in order to estimate the cost of building the plant. To carry out these calculations, simplified sizing and costing correlations described in Biegler will be used.

The physical sizing of the equipment units includes the calculation of all physical attributes such as capacity height, pressure rating, and materials of construction, etc.

The equipment cost, C, increases nonlinear with equipment size, S, or capacity, and can be expressed by the following equation

$$C = C_0 \left(\frac{S}{S_0}\right)^a \tag{1}$$

Where the $\alpha < 1$, and S₀ and C₀ refers to the base capacities and costs, respectively.

For cylindrical pressure vessels a more general form is used by Guthrie.

$$C = C_0 \left(\frac{L}{L_0}\right)^{\alpha} \left(\frac{D}{D_0}\right)^{\beta}$$
(2)

Where L and D are the length and diameter of the vessel, and L_0 and D_0 are the base length and diameter, respectively. Note that the deviations on costs for some units can vary around 20 %.

The base costs, which will be utilized throughout this section, are in mid-1968 prices, an update factor, UF, is used to account for inflation. This is defined as

$$UF = \frac{Present \ cost \ index}{Base \ cost \ index}$$
(3)

The present cost index is determined from a linear regression of the Chemical Engineering Plant Index, CI, which was reported in Chemical Engineering. Extrapolating the data from Figure 4.13 to a linear regression yields a cost index for 2010 of CI=632.6 Thus, the update factor from equation 3 is found

$$UF = \frac{632.60}{115.00} = 5.50$$



Figure 4.13 Linear estimate of CPI cost index in 2008-2010 based on data from 2004 to 2008.

The following three costs can then be determined:

- Uninstalled cost = (BC) (MPF)
- Installation = (BC) (MF-1)
- Updated bare module cost =UF (BC) (MPF+MF-1)

Where MPF is the material and pressure factor, MF is the module factor, UF is the update factor and BC is the base cost. Note that C in equations 1 and 2 is equal to BC. This could mislead as C_0 in equations 1 and 2 is also referred to as a base cost. However, BC is the base cost of the designed equipment, while C_0 is the base cost reference for the specific equipment that is reviewed.
4.3.1 <u>Hydrogenated Biodiesel and SMR-Hydrogenated Biodiesel</u>

Equipment Sizing and Costing

4.3.1.1 Separation Unit

The separation unit is sized as a vessel. The necessary vessel volume can be determined from the following equation.

$$V = 2\left(\frac{F_L \tau}{\rho_L}\right) \tag{4}$$

Where F_{L} is the liquid flow rate leaving the vessel, ρ_{L} is the liquid density and τ is the residence time.

For example VL separation (Flash F-201), it is assumed that the residence time of 5 min resulting the following vessel volume using the flow rate determined in Table 4.5 (stream 202).

$$V = 2 \frac{(38,667.81 \text{ kg/h} \cdot 5 \text{ min})}{(810 \text{ kg/m}^3 \cdot 60 \text{ min/} h)} = 7.96 m^3$$

The ratio L/D of the vessel is assumed to be four in throughout the sizing calculations, which is the optimal ratio as the bottom and top caps are assumed to be four times as expensive as sides. This gives the following length and diameter of the cylindrical vessel.

$$D = 1.36 \text{ m} = 4.47 \text{ ft}$$
 $L = 5.45 \text{ m} = 17.89 \text{ ft}$

It is decided to use a carbon steel vessel. The pressure in the vessel is 175 psig. Thus, the following factors are found.

$$F_{\rm m} = 1.0$$
 $F_{\rm p} = 1.1$

These are used to find the material and pressure factor

$$MPF = F_mF_p = 1.0 \cdot 1.1 = 1.1$$

The base cost, BC, for the vessel is determined using equation 2

$$BC = \$1,000 \left(\frac{17.89\,ft}{4\,ft}\right)^{0.81} \left(\frac{4.47\,ft}{3\,ft}\right)^{1.05} = \$5,116.25$$

The module factor can thus be determined

$$MF = 4.23$$

And finally the uninstalled cost, the installation and the updated bare module cost can be estimated.

- Uninstalled cost = (BC) (MPF) = (\$5,116.25) (1.1) = \$5,627.88
- Updated bare module cost = UF (BC) (MPF+MF-1) =5.5 (\$5,116.25) (1.1+4.23-1)
- Updated bare module cost = \$121,862.89 = 4,042,155 baht

Thus, the sizing and cost estimate have been carried out for the VL separation unit.

4.3.1.2 Heat Exchanger Unit

The sizing equation for heat exchangers is given as

$$Q = UA\Delta T_{lm} \tag{5}$$

Where Q is the heat duty, A is the required area, U is the overall heat transfer coefficient and ΔT_{Im} is the log mean temperature, which is defined as

$$\Delta T_{lm} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln\left(\frac{T_1 - t_2}{T_2 - t_1}\right)}$$
(6)

Where T_1 and T_2 are the temperatures of the hot stream entering and leaving the heat exchanger, and t_1 and t_2 are the temperatures of the cold stream entering and leaving the heat exchanger, respectively.

For example, heat exchanger (E-102), the log mean temperature for the heat exchanger unit can be determined for the temperatures stated as following.

$$\Delta T_{lm} = \frac{\left(240^{\circ}C - 190^{\circ}C\right) - \left(190^{\circ}C - 143^{\circ}C\right)}{\ln\left(\frac{240^{\circ}C - 190^{\circ}C}{190^{\circ}C - 143^{\circ}C}\right)} = 48.48^{\circ}C$$

In section 4.2 (Table 4.6), it was also found that the heat duty is Q = 5,340,379.5 kJ/h. It is assumed that the overall heat transfer coefficient is 0.2327 kJ/m²s °C, giving that steam is used on the shell side and feed palm oil is used on the tube side. The necessary heat exchanger area can then be determined from equation 5.

$$A = \frac{5,340,379.5kJ/h}{(0.2327kJ/m^2 s^{\circ}C) \cdot (48.48^{\circ}C)} = 131.50m^2 = 1,415.47 ft^2$$

The heat exchanger is designed as a fixed tube sheet, using carbon steel for the tube and the shell. The heat exchanger is designed for a pressure of 514.7 psia, thus

 $F_d = 1.0, F_m = 1.0, F_p = 0.3175$

Guthrie material and pressure factor for the heat exchanger then becomes

$$MPF = F_{m}(F_{p} + F_{d}) = 1.0(0.3175 + 1.0) = 1.3175$$

And the base cost, BC, for the heat exchanger is determined using equation 1

$$BC = \$5,000 \left(\frac{1,415.47 ft^2}{400 ft^2}\right)^{0.65} = \$11,368.85$$

The module factor can thus be determined

$$MF = 1.83$$

And finally the uninstalled cost and the updated bare module cost can be estimated.

• Uninstalled cost = (BC) (MPF) = (\$11,368.85) (1.3175) = \$14,978.46

• Updated bare module cost=UF(BC)(MPF+MF-1)=5.5 (\$11,368.85)(1.3175+1.83-1)

• Updated bare module cost = \$134,280.4 = 4,454,039 baht

Thus, the sizing and cost estimate have been carried out for the heat exchanger unit.

4.3.1.3 Pumping Unit

A pump is installed before the hydrotreating unit in order for the feed to have the same pressure as at the reactor. The pressure on the reactor is 500 psig and the pump should therefore increase the pressure from 14.7 psia to 514.7 psia. The pump is designed using stainless steel with a maximum suction pressure of 1000 psig and a temperature of 850 F, thus

$$F_m = 1.93$$
 $F_o = 2.9$

Where F_0 is the operating limit factor. Guthrie material and pressure factor for the pump then becomes

$$MPF = F_mF_o = 1.93 \cdot 2.9 = 5.597$$

In order to find the base cost, the head has to be found along with the capacity of the pump. To find the head, the pump was implemented in PRO/II[®] with pump efficiency at 98 %, and a head of 506.47 psi was determined.

The capacity of the pump is considered to be equal to the feed stream of the reactor. This flow was calculated to be 38,061.33 kg/h (=1,676.276 gpm). Thus the base cost, BC, for the pump can be calculated using equation 1.

$$BC = \$1500 \left(\frac{506.48\,psi\cdot 1,676.28\,gpm}{20,000\,psi\cdot gpm}\right)^{0.64} = \$10,599.21$$

The module factor is then determined

$$MF = 3.38$$

And finally the uninstalled cost and the updated bare module cost can be estimated.

• Uninstalled cost = (BC) (MPF) = (\$10,599.21) (5.597) = \$59,323.76

- Updated bare module cost =UF(BC)(MPF+MF-1)=5.5 (\$10,599.21)(5.597+3.38-1)
- Updated bare module cost =\$465,024.3 = 15,424,715 baht

Thus, the sizing and cost estimate have been carried out for the pump.

4.3.1.4 Distillation Unit

The distillation unit is designed as a vessel with trays inside, and one heat exchanger. $PRO/II^{\textcircled{R}}$ is used to determine the diameter of the trays, by setting the tray spacing to 0.6 m and using bubble cap as tray type. The diameter, d, of the trays is then found to be d= 1.8 m=5.97ft

The height of the column is estimated as following:

Tray stack = $(10-1)(0.6 \text{ m})$	= 5.4 m
Extra feed space	= 1.5 m
Disengagement space (top & bottom) = 3.0 m
Skirt height	= 1.5 m
Total height	= 11.4 m = 37.4 ft

It is decided to use a stainless steel vessel. The maximum pressure in the vessel is 1.0 atm but for safety reasons the vessel is designed using a pressure that is 50 % higher. Thus, the following factors are found.

.0

$$F_{m} = 1.0$$
 $F_{p} = 1$

These are used to find the material and pressure factor

$$MPF = F_mF_p = 1.0 \cdot 1.0 = 1.0$$

Then the base cost, BC, for the vessel is determined using equation 2.

$$BC = \$1,000 \left(\frac{37.40\,ft}{4\,ft}\right)^{0.81} \left(\frac{5.97\,ft}{3\,ft}\right)^{1.05} = \$12,585.41$$

The module factor can thus be determined

$$MF = 4.23$$

And finally the uninstalled cost, the installation and the updated bare module cost can be estimated.

• Uninstalled cost = (BC) (MPF) = (\$12,585.41) (1.0) = \$12,585.41

- Updated bare module cost = UF (BC) (MPF+MF-1) =5.5 (\$12,585.41) (1.0+4.23-1)
- Updated bare module cost = \$292,799.6 = 9,712,073 baht

Thus, the sizing and cost estimate have been carried out for the column without trays.

The trays are constructed as bubble cap and made of carbon steel. The Guthrie material and pressure factor for the tray stack can be determined form the following factors

$$F_m = 0$$
 $F_s = 1.0$ $F_t = 1.8$

Where F_s is the tray spacing factor and F_t is the tray type factor. Thus,

$$MPF = F_m + F_s + F_t = 2.8$$

Then the base cost, BC, for the tray stack is determined using equation 2

$$BC = \$180 \left(\frac{17.72\,ft}{10\,ft}\right)^{0.81} \left(\frac{5.97\,ft}{2\,ft}\right)^{1.05} = \$1,529.16$$

The module factor is 1 for all tray stacks. Therefore, the uninstalled cost, the installation and the updated bare module cost can be estimated for the tray stack

- Uninstalled cost = (BC) (MPF) = (\$1,529.16) (2.8) = \$4,281.66
- Updated bare module cost = UF (BC) (MPF+MF-1) = $5.5 \cdot (\$1,529.16) (2.8+1-1)$
- Updated bare module cost = \$23,549.13 = 781,118 baht

Thus, the sizing and cost estimate have been carried out for the tray stack.

The reboiler should also be sized, and it is modeled as heat exchangers. Steam is used in the reboiler. The log mean temperature is determined for the reboiler using the temperatures found in PRO/II[®] in the reboiler. Furthermore steam enters the reboiler at 240 °C and leaves at 190 °C.

$$\Delta T_{lm} = \frac{\left(240^{\circ}C - 99.6^{\circ}C\right) - \left(190^{\circ}C - 99.6^{\circ}C\right)}{\ln\left(\frac{240^{\circ}C - 99.6^{\circ}C}{190^{\circ}C - 99.6^{\circ}C}\right)} = 113.6^{\circ}C$$

In section 4.2 (Table 4.6), it was also found that the heat duty is $Q_{reboiler} = 2,290,849 \text{ kJ/h}$. It is assumed that the overall heat transfer coefficient for the reboiler is 0.2327 kJ/m²s °C given that steam is used on the shell side and feed water on the tube side. The necessary heat exchange areas are then determined from equation 5.

$$A = \frac{2,290,849.0kJ/h}{(0.2327kJ/m^2s^{\circ}C) \cdot (113.6^{\circ}C)} = 24.07m^2 = 259.08ft^2$$

The heat exchanger is designed as a fixed tube sheet, using carbon steel for the tube and the shell. The heat exchanger is designed for a pressure of 14.7 psia, thus

$$F_d = 1.0, F_m = 1.0, F_p = 0$$

Guthrie material and pressure factor for the heat exchanger then becomes

$$MPF = F_{m} (F_{p} + F_{d}) = 1.0(0 + 1.0) = 1.0$$

And the base cost, BC, for the heat exchanger is determined using equation 1

$$BC = \$5,000 \left(\frac{259.08 ft^2}{400 ft^2}\right)^{0.65} = \$3,770.22$$

The module factor can thus be determined

$$MF = 1.83$$

And finally the uninstalled cost and the updated bare module cost can be estimated.

• Uninstalled cost = (BC) (MPF) = (\$3,770.22) (1.0) = \$3,770.22

• Updated bare module cost = UF (BC) (MPF+MF-1) = 5.5 (\$3,770.22) (1.0+1.83-1)

• Updated bare module cost = \$37,947.28 = 1,258,700 baht

Thus, the sizing and cost estimate have been carried out for the reboiler.

The updated bare module cost for the total distillation column is the sum of the updated bare module cost for the column, the tray stack, the reboiler.

• Updated bare module cost for the distillation column= 354,296 = 11,751,890 baht Thus, the sizing of the distillation column has been carried out.

4.3.1.5 Compressing Unit

The compressor (C-101) is installed in order to raise up the hydrogen feed to the reactor pressure, which is 514.7 psia. The compressor is designed as centrifugal /motor type, thus

$$F_{d} = 1.0$$

Guthrie material and pressure factor for the compressor then becomes

$$MPF = F_d = 1.0$$

In order to find the base cost, the actual work has to be found which is 1973.80 kW (2,646.9 hp) Thus the base cost, BC, for the pump can be calculated using equation 1.

$$BC = \$2,300 \left(\frac{2,646.9hp}{100hp}\right)^{0.77} = \$286,573.7$$

The module factor is then determined

$$MF = 3.11$$

And finally the uninstalled cost and the updated bare module cost can be estimated.

- Uninstalled cost = (BC) (MPF) = (\$286,573) (1.0) = \$286,573
- Updated bare module cost = UF(BC) (MPF+MF-1) = 5.5 (\$286,573) (1.0+3.11-1)
- Updated bare module cost = \$4,744,228.1 = 157,364,605 baht

Thus, the sizing and cost estimate have been carried out for the compressor.

4.3.1.6 Hydrotreating Unit

For reactor sizing we assume a given space velocity (h^{-1}) base on liquid molar flow rate (LHSV is Liquid Hour Space Velocity, h^{-1}).

$$LHSV = \frac{F_L}{\rho V_{col}} \tag{7}$$

Where ρ is the molar density at standard temperature and pressure (1 atm, 273 K), V_{cat} is the volume of catalyst. The total volume, V, is then calculated based on the void fraction, ϵ , of catalyst (assume 50 %).

$$V = \frac{V_{cal}}{1 - \varepsilon} = 2V_{cal} \tag{8}$$

It is assumed that the LHSV of 0.4 h^{-1} resulting the following catalyst volume using the flow rate determined in Table 4.5 (stream 103).

$$V_{col} = \frac{38061.33 kg / h}{(915.2 kg / m^3)(0.4 h^{-1})} = 103.97 m^3$$

The vessel volume; $V = 2V_{cat} = 207.94m^3$

The ratio L/D of the vessel is assumed to be four in throughout the sizing calculations. This gives the following length and diameter of the cylindrical vessel.

$$D = 4.04 \text{ m} = 13.27 \text{ ft}$$
 $L = 16.18 \text{ m} = 53.09 \text{ ft}$

It is decided to use a hestelloy vessel. The pressure in the vessel is 500 psig. Thus, the following factors are found.

$$F_m = 3.67$$
 $F_p = 1.45$

These are used to find the material and pressure factor

$$MPF = F_mF_p = 3.67 \cdot 1.45 = 5.32$$

The base cost, BC, for the vessel is determined using equation 2

$$BC = \$1000 \left(\frac{53.09\,ft}{4\,ft}\right)^{0.81} \left(\frac{13.27\,ft}{3\,ft}\right)^{1.05} = \$38,693.9$$

The module factor can thus be determined

$$MF = 4.23$$

And finally the uninstalled cost, the installation and the updated bare module cost can be estimated.

• Uninstalled cost = (BC) (MPF) = (\$38,693.9) (5.32)= \$205,910.04

- Updated bare module cost = $UF(BC)(MPF+MF-1) = 5.5 \cdot ($38,693.9)(5.32+4.23-1)$
- Updated bare module cost = \$1,819,903.9 = 60,365,659 baht

Thus, the sizing and cost estimate have been carried out for the hydrotreating unit.

The updated bare module cost (BMC) of each units of hydrogenated biodiesel and hydrogenated biodiesel with steam methane reforming (SMR) based hydrogen production (SMR-Hydrogenated Biodiesel) processes are shown in Table 4.12.

			BMC (baht)		
Equipment	Process	Unit	Hydrogenated biodiesel	SMR- Hydrogenated biodiesel	
Vessel	VL separation	Flash F-201	4,042,155	4,042,155	
	Decant	Flash F-202	4,042,155	4,042,155	
	Fuel gas separation	Flash F-401	134,117	134,117	
	Decant	Flash F-402	3,428,079	3,428,079	
	Waste water tank	Mixer M-401	1,632,4667	1,632,4667	
	Water tank	Flash F-501	-	536,478	
	PSA	SC-301	5,654,132	5,654,132	
	PSA	SC-302	5,654,132	5,654,132	
	SMR_PSA	SC-501	-	6,260,829	
Heat Exchanger		Hx. E-101	3,877,680	3,877,680	
		Hx. E-102	4,454,039	4,454,039	
		Hx. E-103	11,185,861	11,185,861	
		Hx. E-401	6,052,090	6,052,090	
	SMR_Hx.	Hx. E-501	-	122,440	
	SMR_Hx.	Hx. E-502	-	2,925,990	
	SMR_Hx.	Hx. E-503	-	2,957,086	
	SMR_Hx.	Hx. E-504	-	1,883,618	
	SMR_Hx.	Hx. E-505	-	123,603	
Reactor	Hydrotreating	Reactor R-101	60,365,659	60,365,659	
	Steam reforming	Reactor R-501	-	58,751,936	
	HT WGS	Reactor R-502	-	2,227,173	
	LT WGS	Reactor R-503	-	2,284,106	
	Combustor	Reactor R-504	-	2,229,974	
Distillation	Stripper	Column T-401	9,712,073	9,712,073	
		Tray Stack	781,118	781,118	
		Reboiler	1,258,700	1,258,700	
Compressor		C-101	157,364,605	21,869,032	
		C-102	54,695,626	54,695,626	
		C-501	-	35,931,746	
Pump		Pump P-101	15,424,715	15,424,715	
		Pump P-102	15,424,715	15,424,715	
	SMR_Pump	Pump P-501	-	3,185,603	
	SMR_Pump	Pump P-502	-	741,170	
Total up	date bare module cost	(BMC)	365,184,118	367,398,962	

Table 4.12 Updated bare module cost (BMC) of hydrogenated biodiesel and SMR

 hydrogenated biodiesel processes

4.3.2 Biodiesel Equipment Sizing and Costing

4.3.2.1 Separation Unit

For glycerin separation unit (Stream Calculator SC-201), it is assumed that the residence time of 30 min resulting the following vessel volume using the flow rate determined in Table 4.10 (stream 203).

$$V = 2\frac{35,169.11kg / h \cdot 30\min}{883kg / m^3 \cdot 60\min/h} = 39.83m^3$$

The ratio L/D of the vessel is assumed to be four in throughout the sizing calculations, which is the optimal ratio as the bottom and top caps are assumed to be four times as expensive as sides. This gives the following length and diameter of two cylindrical vessel.

$$D = 2.33 \text{ m} = 7.65 \text{ ft}$$
 $L = 4.67 \text{ m} = 15.30 \text{ ft}$

It is decided to use a carbon steel vessel. The pressure in the vessel is 1 atm. Thus, the following factors are found.

$$F_m = 1.0$$
 $F_p = 1.0$

These are used to find the material and pressure factor

$$MPF = F_mF_p = 1.0 \cdot 1.0 = 1.0$$

The base cost, BC, for the vessel is determined using equation 2

$$BC = \$1,000 \left(\frac{15.30\,ft}{4\,ft}\right)^{0.81} \left(\frac{2.33\,ft}{3\,ft}\right)^{1.05} = \$7,921.33$$

The module factor can thus be determined

$$MF = 4.23$$

And finally the uninstalled cost, the installation and the updated bare module cost can be estimated.

- Uninstalled cost = (BC) (MPF) = (\$7,921.33) (1.0) = \$7,921.33
- Updated bare module cost = UF (BC) (MPF+MF-1) = $5.5 \cdot (\$7,921.33) (1.0+4.23-1)$
- Updated bare module cost = \$184,289.7 = 6,112,832 baht

Thus, the sizing and cost estimate have been carried out for the separation unit.

4.3.2.2 Heat Exchanging Unit

For Heat Exchanger (E-201), The log mean temperature for the heat exchanger unit can be determined for the temperatures stated as following.

$$\Delta T_{lm} = \frac{(130^{\circ}C - 117^{\circ}C) - (95^{\circ}C - 60^{\circ}C)}{\ln\left(\frac{130^{\circ}C - 117^{\circ}C}{95^{\circ}C - 60^{\circ}C}\right)} = 22.21^{\circ}C$$

In section 4.2 (Table 4.11), it was also found that the heat duty is Q = 5,942,455.19 kJ/h. It is assumed that the overall heat transfer coefficient is 0.2327 kJ/m²s °C, giving that steam is used on the shell side and crude methanol is used on the tube side. The necessary heat exchanger area can then be determined from equation 5.

$$A = \frac{5,942,455.19 \text{ kJ/h}}{(0.2327 \text{ kJ/m}^2 \text{ s}^{\circ}\text{C}) \cdot (22.21^{\circ}\text{C})} = 319.24m^2 = 3,436.33 \text{ ft}^2$$

The heat exchanger is designed as a fixed tube sheet, using carbon steel for the tube and the shell. The heat exchanger is designed for a pressure of 1 atm, thus

$$F_d = 1.0, F_m = 1.0, F_p = 0$$

Guthrie material and pressure factor for the heat exchanger then becomes

$$MPF = F_{m}(F_{p} + F_{d}) = 1.0(0 + 1.0) = 1.0$$

And the base cost, BC, for the heat exchanger is determined using equation 1

$$BC = \$5,000 \left(\frac{3,436.33\,ft^2}{400\,ft^2}\right)^{0.024} = \$20,234.51$$

The module factor can thus be determined

$$MF = 1.83$$

And finally the uninstalled cost and the updated bare module cost can be estimated.

- Uninstalled cost = (BC) (MPF) = (\$20,234.51) (1.0) = \$20,234.51
- Updated bare module cost = UF (BC) (MPF+MF-1) = $5.5 \cdot (\$20,234.51)(1.0+1.83-1)$
- Updated bare module cost =\$203,660.3 = 6,755,350 baht

Thus, the sizing and cost estimate have been carried out for the heat exchanger unit.

4.3.2.3 Pumping Unit

A pump (P-101) is installed before the esterification unit in order to transfer palm oil to esterification reactor. The pump is designed using cast iron with a maximum suction pressure of 150 psig and a temperature of 250 F, thus

$$F_{m} = 1.0$$
 $F_{o} = 1.0$

Where F_0 is the operating limit factor. Guthrie material and pressure factor for the pump then becomes

$$MPF = F_{m}F_{o} = 1.0 \cdot 1.0 = 1.0$$

In order to find the base cost, the head has to be found along with the capacity of the pump. To find the head, the pump was implemented in $PRO/II^{\text{®}}$ with pump efficiency at 98 %, and a head of 0.30 psi was determined. The capacity of the pump is considered to be equal to the feed stream of the reactor. This flow was calculated to be 28,750.0 kg/h (=1,266.19 gpm). Thus the base cost, BC, for the pump can be calculated using equation 1.

$$BC = \$390 \left(\frac{0.30 \, psi \cdot 1,266.19 \, gpm}{10 \, psi \cdot gpm} \right)^{0.17} = \$722.70$$

The module factor is then determined

$$MF = 3.38$$

And finally the uninstalled cost and the updated bare module cost can be estimated.

• Uninstalled cost = (BC) (MPF) = (\$722.7)(1.0) = \$722.7

• Updated bare module cost = UF (BC) (MPF+MF-1) = $5.5 \cdot (\$722.7) (1.0+3.38-1)$

• Updated bare module cost = \$13,434.9 = 445,632 baht

Thus, the sizing and cost estimate have been carried out for the pump.

4.3.2.4 Distillation Unit

The distillation unit (Vacuum Methanol Removal T-301) is designed as a vessel with trays inside, and one heat exchanger. PRO/II[®] is used to determine the diameter of the trays, by setting the tray spacing to 0.6 m and using bubble cap as tray type. The diameter, d, of the trays is then found to be d = 2.1 m or 6.88 ft

The height of the column is estimated as following:

Tray stack = $(10-1)(0.6 \text{ m})$	= 5.4 m
Extra feed space	= 1.5 m
Disengagement space (top & bottom)	= 3.0 m
Skirt height	= 1.5 m
Total height	= 11.4 m = 37.4 ft

It is decided to use a stainless steel vessel. The maximum pressure in the vessel is 0.21 atm but for safety reasons the vessel is designed using a pressure that is 50 % higher. Thus, the following factors are found.

 $F_{m} = 1.0$ $F_{p} = 1.0$

These are used to find the material and pressure factor

 $MPF = F_mF_p = 1.0 \cdot 1.0 = 1.0$

Then the base cost, BC, for the vessel is determined using equation 2.

$$BC = \$1000 \left(\frac{37.40\,ft}{4\,ft}\right)^{0.81} \left(\frac{6.88\,ft}{3\,ft}\right)^{1.05} = \$14,627.63$$

The module factor can thus be determined

$$MF = 4.23$$

And finally the uninstalled cost, the installation and the updated bare module cost can be estimated.

• Uninstalled cost = (BC) (MPF) = (\$14,627.63) (1.0) = \$14,627.63

• Updated bare module cost = UF(BC) (MPF+MF-1) = $5.5 \cdot (\$14,627.63)(1.0+4.23-1)$

• Updated bare module cost = \$340,311.84 = 11,288,040 baht

Thus, the sizing and cost estimate have been carried out for the column without trays.

The trays are constructed as bubble cap and made of carbon steel. The Guthrie material and pressure factor for the tray stack can be determined form the following factors

$$F_m = 0$$
 $F_s = 1.0$ $F_t = 1.8$

Where F_s is the tray spacing factor and F_t is the tray type factor. Thus,

$$MPF = F_m + F_s + F_t = 2.8$$

Then the base cost, BC, for the tray stack is determined using equation 2

$$BC = \$180 \left(\frac{17.72\,ft}{10\,ft}\right)^{0.97} \left(\frac{6.88\,ft}{2\,ft}\right)^{1.45} = \$1,882.09$$

The module factor is 1 for all tray stacks. Therefore, the uninstalled cost, the installation and the updated bare module cost can be estimated for the tray stack

• Uninstalled cost = (BC) (MPF) = (\$1, 882.09) (2.8) = \$5, 269.84

- Updated bare module cost = UF (BC) (MPF+MF-1) = $5.5 \cdot (\$5,269.84) (2.8+1-1)$
- Updated bare module cost = \$28,984.13 = 961,395 baht

Thus, the sizing and cost estimate have been carried out for the tray stack.

The condenser and reboiler should also be sized, and they are modeled as heat exchangers. Chilling water is used in the condenser and steam is used in the reboiler. The log mean temperature is determined for the condenser and the reboiler using the temperatures found in PRO/II[®] in the condenser and the reboiler. Furthermore steam enters the reboiler at 130 °C and leaves at 100 °C while the chilling water enters the condenser at 10 °C and leaves at 60 °C.

$$\Delta T_{lm,condensor} = \frac{\left(64.34^{\circ}C - 60^{\circ}C\right) - \left(64.34^{\circ}C - 10^{\circ}C\right)}{\ln\left(\frac{64.34^{\circ}C - 60^{\circ}C}{64.34^{\circ}C - 10^{\circ}C}\right)} = 19.78^{\circ}C$$

$$\Delta T_{lm,reboiler} = \frac{\left(130^{\circ}C - 90.39^{\circ}C\right) - \left(100^{\circ}C - 90.39^{\circ}C\right)}{\ln\left(\frac{130^{\circ}C - 90.39^{\circ}C}{100^{\circ}C - 90.39^{\circ}C}\right)} = 21.19^{\circ}C$$

The heat duties for the condenser and reboiler are (Table 4.11)

 $Q_{condensor} = 9,738,784.56 \text{ kJ/h}$ $Q_{reboiler} = 8,305,706.5 \text{ kJ/h}$

It is assumed that the overall heat transfer coefficient for the reboiler is $0.2327 \text{ kJ/m}^2 \text{s} \,^{\circ}\text{C}$ given that steam is used on the shell side and feed water on the tube side, and $0.349 \text{ kJ/m}^2 \text{s} \,^{\circ}\text{C}$ for the condenser given that water is used on the shell and tube side. The necessary heat exchange areas are then determined from equation 5.

$$A_{condensor} = \frac{9,738,784.56 \text{ kJ/h}}{(0.349 \text{ kJ/m}^2 \text{ s}^{\circ}\text{C}) \cdot (19.78^{\circ}\text{C})} = 391.63m^2 = 4,215.65 \text{ ft}^2$$

$$A_{reboilter} = \frac{8,305,706.47 \text{ kJ/h}}{(0.2327 \text{ kJ/m}^2 \text{ s}^{\,0}\text{C}) \cdot (21.19^{\,0}\text{C})} = 468.03m^2 = 5,038.00 \text{ ft}^2$$

The heat exchanger is designed as a fixed tube sheet, using carbon steel for the tube and the shell. The heat exchanger is designed for a pressure of 14.7 psia, thus

$$F_d = 1.0, F_m = 1.0, F_p = 0$$

Guthrie material and pressure factor for the heat exchanger then becomes

$$MPF = F_{m}(F_{p} + F_{d}) = 1.0(0 + 1.0) = 1.0$$

And the base cost, BC, for the heat exchanger is determined using equation 1

$$BC_{condensor} = \$5000 \left(\frac{4,215.65\,ft^2}{400\,ft^2}\right)^{0.65} = \$23,109.62$$
$$BC_{reboiler} = \$5000 \left(\frac{5,038.00\,ft^2}{400\,ft^2}\right)^{0.65} = \$25,947.68$$

The module factor can thus be determined

MF = 1.83

And finally the uninstalled cost and the updated bare module cost can be estimated for condenser.

• Uninstalled cost = (BC) (MPF) = (\$23,109.62) (1.0) = \$23,109.62

• Updated bare module cost = UF (BC) (MPF+MF-1) = $5.5 \cdot (\$23,109.62)(1.0+1.83-1)$

• Updated bare module cost = \$418,168.55 = 13,870,524 baht

For reboiler.

• Uninstalled cost = (BC) (MPF) = (\$25,947.68) (1.0) = \$25,947.68

• Updated bare module cost = UF (BC) (MPF+MF-1) = $5.2 \cdot (\$25,947.68)(1.0+1.83-1)$

• Updated bare module cost = \$469,523.29 = 15,573,945 baht

Thus, the sizing and cost estimate have been carried out for the condenser and reboiler.

The updated bare module cost for the total distillation column is the sum of the updated bare module cost for the column, the tray stack, the reboiler and the condenser.

• Updated bare module cost for the distillation column= \$1,256,987.80=41,693,904 baht. Thus, the sizing of the distillation column has been carried out.

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4.3.2.5 Transesterification Unit

The tranesterification unit is sized as a vessel. It is assumed that the residence time of 60 min resulting the following vessel volume using the flow rate determined in Table 4.10 (stream 201).

$$V = 2\frac{17,584.56kg / h \cdot 60\min}{883kg / m^3 \cdot 60\min/h} = 39.83m^3$$

The ratio L/D of the vessel is assumed to be four in throughout the sizing calculations, which is the optimal ratio as the bottom and top caps are assumed to be four times as expensive as sides. This gives the following length and diameter of two cylindrical vessel.

$$D = 2.33 m = 7.65 ft$$
 $L = 4.67 m = 15.3 ft$

It is decided to use a carbon steel vessel. The pressure in the vessel is 1 atm. Thus, the following factors are found.

$$F_{m} = 1.0$$
 $F_{p} = 1.0$

These are used to find the material and pressure factor

$$MPF = F_{m}F_{p} = 1.0 \cdot 1.0 = 1.0$$

The base cost, BC, for the vessel is determined using equation 2

$$BC = \$1000 \left(\frac{15.30\,ft}{4\,ft}\right)^{0.81} \left(\frac{7.65\,ft}{3\,ft}\right)^{1.05} = \$7,921.33$$

The module factor can thus be determined

$$MF = 4.23$$

And finally the uninstalled cost, the installation and the updated bare module cost can be estimated.

- Uninstalled cost = (BC) (MPF) = (\$7,921.33)(1.0) = \$7,921.33
- Updated bare module cost = UF (BC) (MPF+MF-1) = 5.5 (\$7,921.33) (1.0+4.23-1)
- Updated bare module cost = \$184,289.67 = 6,112,832 baht

Thus, the sizing and cost estimate have been carried out for the transesterification unit.

The updated bare module cost (BMC) of each units of the conventional biodiesel process is shown in Table 4.13.

A the second second second

Equipment	Process	Unit	BMC (baht)
Vessel	Methanol Pretreatment Mixer	Mixer M-101	2,443,479
	Methanol Reaction Mixer	Mixer M-102	3,971,589
	Glycerin SEP A	Mixer M-201	6,112,832
		Mixer M-201	6,112,832
	Glycerin SEP B	SC-201A	6,112,832
		SC-201B	6,112,832
	Methanol Pretreatment SEP	SC-101A	1,441,614
		SC-101B	1,441,614
	Recycle Methanol Mixer	Mixer M-301	1,312,324
Heat Exchanger		Hx. E-101	1,939,448
-		Hx. E-201	6,755,350
		Hx. E-202	1,787,204
		Hx. E-301	6,254,452
(L)		Hx. E-501	3,077,966
Reactor	Esterification	R-101A	8,684,918
		R-101B	8,684,918
	Transesterification A	R-201A	6,112,832
		R-201B	6,112,832
	Transesterification B	R-202A	6,112,832
		R-202B	6,112,832
Distillation Column	Vacuum Methanol Removal	Column	11,288,040
	T-101	Tray Stack	961,395
		Condensor	13,870,524
		Reboiler	15,573,948
	Vacuum Methanol Removal	Column	8,766,631
	T-301	Tray Stack	678,098
		Condensor	24,149,898
		Reboiler	9,280,204
	Glycerin Purification	Column	11,205,037
	T-401	Tray Stack	951,646
		Condensor	9,116,075
		Reboiler	9,832,965
	Biodiesel Purification	Column	19,728,191
	T-501	Tray Stack	2,078,449
		Condensor	13,363,083
		Reboiler	17,597,896
Pump		Pump P-101	445,632
		Pump P-102	582,089
		Pump P-301	586,513
Tota	266,753,843		

 Table 4.13 Updated bare module cost (BMC) of biodiesel process

4.4 Economics Evaluation

The economic evaluation is carried out to get a wide insight to the economy of the processes. First the capital investment cost is reviewed followed by the manufacturing costs. This leads to the sensitivity associated with hydrogenated biodiesel, SMR-hydrogenated biodiesel and biodiesel processes.

4.4.1 Capital Investment Cost

4.4.1.1 Hydrogenated Biodiesel Capital Investment Cost

To calculate capital investment cost, the total bare module cost has to be determined (Table 4.12). This is done by summarizing the bare module cost of each unit from previous section.

The manufacturing capital is the total bare module cost plus a 25% contingency, while the nonmanufacturing capital includes buildings, service and land and is typically 40% of the total bare module cost.

$$C_{cap invst., fixed} = C_{manufac.} + C_{nonmanufac.}$$

= (1 + 0.25) · BMC + 0.4 · BMC
= 456,480,147 baht+ 146,073,647 baht
= 602,553,793 baht

The working capital represents the money needed to fill up the tanks and meet the initial payroll and expenses. Douglas (1988) also suggests a simpler form, the working capital is 19.4% of the fixed investment costs, thus the working capital becomes

 $C_{cap.invst.,working} = (0.194)(602,553,793 \text{ baht}) = 116,895,436 \text{ baht}$ And total capital investment becomes

$$C_{cap.invst.} = C_{cap.invst., fixed} + C_{cap.invst.,working}$$

= 602,553,794 baht + 116,895,436 baht
= 719,449,230 baht

These are the expenses that are related to building and starting up hydrogenated biodiesel plant.

4.4.1.2 SMR-Hydrogenated Biodiesel Capital Investment

To calculate capital investment cost, the total bare module cost has to be determined (Table 4.12). This is done by summarizing the bare module cost of each unit from previous section.

The manufacturing capital is the total bare module cost plus a 25% contingency, while the nonmanufacturing capital includes buildings, service and land and is typically 40% of the total bare module cost.

 $C_{cap invst., fixed} = C_{manufac.} + C_{nonmanufac.}$ = (1 + 0.25) · BMC + 0.4 · BMC = 459,248,702 baht+ 146,959,585 baht = 606,208,287 baht

The working capital represents the money needed to fill up the tanks and meet the initial payroll and expenses. Douglas (1988) also suggests a simpler form, the working capital is 19.4% of the fixed investment costs, thus the working capital becomes

 $C_{cap invst.,working} = (0.194)(606,208,287 baht) = 117,604,408 baht$ And total capital investment becomes

> C_{cap.invst.} = $C_{cap.invst., fixed} + C_{cap invst.,working}$ = 606,208,287 baht + 117,604,408 baht = 723,812,694 baht

These are the expenses that are related to building and starting up SMRhydrogenated biodiesel plant.

4.4.1.3 Biodiesel Capital Investment

To calculate capital investment, the total bare module cost has to be found (Table 4.13). The manufacturing capital is the total bare module cost plus a 25% contingency, while the nonmanufacturing capital includes buildings, service and land and is typically 40% of the total bare module cost.

$$C_{cap invst., fixed} = C_{manufac.} + C_{nonmanufac.}$$

= (1 + 0.25) · BMC + 0.4 · BMC
= 333,442,304 baht + 106,701,537 baht
= 440,143,842 baht

The working capital represents the money needed to fill up the tanks and meet the initial payroll and expenses. Douglas (1988) also suggests a simpler form, the working capital is 19.4% of the fixed investment costs, thus the working capital becomes

 $C_{cap.invst.,working} = (0.194)(440,143,842 \text{ baht}) = 85,387,905 \text{ baht}$ And total capital investment becomes

$$C_{cap invst.} = C_{cap invst., fixed} + C_{cap invst., working}$$

= 440,143,842 baht + 85,387,905 baht
= 525,531,747 baht

These are the expenses that are related to building and starting up the biodiesel plant.

Table 4.14 illustrates list of the equipment costs and capital investment costs. It also presents the costs for the individual unit operations in each process.

	Cost (millions baht)			
Description	Hydrogenated	SMR-hydrogenated	Piodiocol	
	Biodiesel	Biodiesel	Diouiesei	
Reactors	60.37	129.24	41.82	
Distillation columns	11.75	11.75	168.44	
Vessels	13.28	13.82	35.06	
Heat exchangers	25.57	51.68	19.81	
Pumps	30.85	34.78	1.61	
Compressors	212.06	112.50	-	
PSA	11.31	17.57	-	
Total update bare module (C _{BM})	365.18	367.40	266.75	
Contingency fee (C _{CF} =0.25 C _{BM})	91.30	91.85	66.69	
Auxiliary facility cost ($C_{CF}=0.40 C_{AC}$)	146.07	146.96	106.70	
Fixed capital cost ($C_{FC}=C_{BM}+C_{CF}+C_{AC}$)	602.55	606.21	440.14	
Working capital (C _{wc} =0.194 C _{FC})	116.90	117.04	85.39	
Total capital investment	719.45	723.81	525.53	

Table 4.14 Equipment and capital investment costs for each process

As shown in Table 4.14, the results indicate that with palm oil as feedstock and the capacity of 200 000 tons product/year, the reactors and distillation columns account for the major part of the capital cost for biodiesel process while compressors and hydrotreater are the major capital cost of hydrogenated biodiesel and SMR-hydrogenated biodiesel processes. In spite of hydrogenated biodiesel process

having smaller number of unit operations; biodiesel process had lower total capital investment cost. This is due to the fact that hydrogenated biodiesel process requires gas compressor unit which is expensive. Moreover, the material of hydrotreating reactor has to be hestelloy to be able to stand high pressure, high temperature and corrosion (Figure 4.14).



Figure 4.14 Capital investment costs of hydrogenated biodiesel, SMR-hydrogenated biodiesel and biodiesel processes.

4.4.2 Manufacturing Cost

The manufacturing costs or production costs, involve expenses that are directly related to the day-to-day operation of the plant, and indirect expenses such as taxes, insurance and depreciations. The total manufacturing cost per year can be estimated as the sum of the following items:

- Raw materials
- Salary
- Maintenance (5% of fixed capital cost)
- Supplies (2% of fixed capital cost)
- Payroll (20% of total salary)
- Utilities
- Depreciation (8% of fixed capital cost)
- Insurance (3% of fixed capital cost)

The reference prices of raw materials and utilities in hydrogenated biodiesel, SMR-hydrogenated biodiesel, and biodiesel processes are shown in Table 4.15. Each of these will be reviewed in the following.

Items	Hydrogenated Biodiesel		SMR-Hydrogenated Biodiesel		Biodiesel	
	Price (baht/kg) tons/year (baht/kg) tons/year		Price (baht/kg)	tons/year		
Raw materials	+					
Crude palm oil	23.06	274,042	23.06	274,042	23.06	207,000
Hydrogen	39.80	7,920	_	-	-	-
Methane	- ^	-	8.50	11,505	-	-
NiMo/Al ₂ O ₃ (life 3year)	830.00	100	-	-	-	-
Methanol		-	-	-	25.32	26,640
КОН	• -	-	-	-	85.00	30
Utilities	+ 1					
Steam	-1.63	26,195	-	-	1.63	131,283
Cooling Water	0.02	192,400	0.02	225,795	0.02	758,381
Electricity (baht/kWh)	2.94	17,960	2.94	6,956	2.94	1,582

 Table 4.15 The reference price of raw materials and utilities

4.4.2.1 Hydrogenated Biodiesel Manufacturing Cost

The raw materials used in the hydrogenated biodiesel plant are; crude palm oil, hydrogen and catalyst. The costs are based on a total production of 200,000 tones hydrogenated biodiesel per year in a plant operating 300 days per year. The cost of crude palm oil, hydrogen and catalyst are determined.

 $C_{palm oil} = (274,041,576 \text{ kg/yr}) \cdot (23.06 \text{ baht/kg}) = 6,319,398,745 \text{ baht/yr}$

 $C_{hydrogen} = (7,920,000 \text{ kg/yr}) \cdot (39.80 \text{ baht/kg}) = 315,244,793 \text{ baht/yr}$

$$C_{catalyst} = (100,851 \text{ kg/3yr}) \cdot (830 \text{ baht/kg}) = 27,902,077 \text{ baht/yr}$$

Thus, total raw material cost is 6,662,545,614 baht/yr

The cost needed for salary is dependent of the number of employees and which positions they have. It is assumed that a GM/MD is paid 100,000 baht/month/person, an office manager 50,000 baht/month/person, plant manager 60,000 baht/month/person, Engineer 18,000 baht/month/person, Researcher 20,000 baht/month/person, Technician 10,850 baht/month/person and labor 8,000 baht/month/person. This results in the following salaries

= $(1 \text{ person}) \cdot (100,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$
= 1,200,000 baht/yr
= (1 person) · (50,000 baht/month/person) · (12 month/yr)
= 600,000 baht/yr
= $(1 \text{ person}) \cdot (60,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$
= 720,000 baht/yr
= $(2 \text{ person}) \cdot (18,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$
= 432,000 baht/yr
= $(2 \text{ person}) \cdot (20,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$
= 480,000 baht/yr
= $(3 \text{ person}) \cdot (10,850 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$
= 390,600 baht/yr
= $(3 \text{ person}) \cdot (8,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$
= 480,000 baht/yr

Thus, total salary is 4,302,600 baht/yr

The cost for maintaining the plant can be calculated as 5 % of the fixed capital cost

 $C_{\text{maintenance}} = 0.05 \cdot (602,553,793 \text{ baht}) = 30,127,690 \text{ baht/yr}$

The cost for the supplies of the plant can be calculated as 2 % of the fixed capital cost, thus

 $C_{supplies} = 0.02 \cdot (602,553,793 \text{ baht}) = 12,051,076 \text{ baht/yr}$

The cost for the payroll of the plant can be calculated as 20 % of total salary, thus

 $C_{payroll} = 0.20 \cdot (4,302,600 \text{ baht}) = 860,520 \text{ baht/yr}$

There are three main utilities associated with the operation of the plant; steam, cooling water and electricity. Steam is used two places in the plant, in the reboiler and heat exchangers. The amount of steam needed in the reboiler and heat exchanger is calculated based on the energy balances carried out in section 4.2 (Table 4.6) and enthalpy data for example in heat exchanger E-102 (Q= 5,340,380 kJ/h).

$$N_{steam1} = \frac{Q}{H_{(240 \,^{\circ}\text{C}, 200 \, \text{psi})} - H_{(190^{\circ}\text{C}, 200 \, \text{psi})}}$$

$$N_{steam1} = \frac{5,340,380kJ/h}{2,905.0kJ/kg - 807.5kJ/kg} = 2,546.07kg/h = 18,331,696kg/yr$$

Thus, the cost of steam becomes

$$C_{steam} = P_{steam} \cdot n_{steam1}$$

= (1.63 baht/kg) \cdot (18,331,696 kg/yr)
= 29,926,395 baht/yr

Cooling water is used in the heat exchanger. The amount of cooling water needed in the heat exchanger is calculated based on the energy balances carried out in section 2 (Table 4.6) and enthalpy data for example in heat exchanger E-103 (Q= 31,323,485 kJ/h). The cooling water enters at 37 °C and leaves at 100 °C.

$$N_{CW1} = \frac{Q}{H_{(100\ ^{\circ}\text{C},1\ \text{bar})} - H_{(37^{\circ}\text{C},1\ \text{bar})}}$$
$$N_{CW1} = \frac{31,323,485kJ/h}{2,675.8kJ/kg - 155.08kJ/kg} = 12,426.4kg/h = 89,470,108.08kg/yr$$

Thus, the cost of cooling water becomes

$$C_{CW1} = P_{CW} \cdot N_{CW}$$

= (0.0235 baht/kg) \cdot (89,470,108.08 kg/yr)
= 2,102,547.54 baht/yr

The amount of electricity needed to operate the plant is electricity for the pump and compressor. The electricity used in the pump and compressor can be calculated.

$$El_{pump} = 295,520.72 \text{ kWh}$$

$$El_{com} = 17,664,021.53 \text{ kWh}$$

$$El_{total} = El_{com} + El_{pump} = 17,664,021.53 \text{ kWh} + 295,520.72 \text{ kWh}$$

$$= 17,959,542.25 \text{ kWh}$$

The total cost of electricity is thus

 $C_{electricity} = P_{electricity} \cdot El_{total}$ = (2.94 baht/kWh) \cdot (17,959,542.25 kWh) = 52,801,054 baht/yr

Utilities	Units		Reference price	Cost
	Equipment	kg/year	baht/kg	(baht/year)
Steam	Hx. E-102	18,331,696	1.63	29,926,396
(200 psi 240 °C)	Reboiler	7,863,700	1.63	12,837,448
	Total	26,195,396	1.63	42,763,844
Cooling Water	Hx. E-103	89,470,108	0.0235	2,102,548
	Hx. E-401	102,929,779	0.0235	2,418,850
	Total	192,399,887	0.0235	4,521,397
Electricity	Equipment	kWh	baht/kWh	(baht/year)
	Pump P-101	295,521	2.94	868,831
	C-101	14,211,339	2.94	41,781,337
	C- 102	3,452,682	2.94	10,150,886
	Total	17,959,542	2.94	52,801,054

 Table 4.16 Utilities cost of hydrogenated biodiesel process

Then the total cost of utilities can be estimated

 $C_{\text{utilities}} = C_{\text{steam}} + C_{\text{cooling water}} + C_{\text{electricity}}$

= 42,763,844 baht + 4,521,397 baht + 52,801,054 baht

= 100,086,296 baht/yr

The cost for depreciation the plant can be calculated as 8 % of the fixed capital cost

 $C_{depreciation} = 0.08 (602,553,794 \text{ baht}) = 48,204,304 \text{ baht/yr}$

The cost for the insurance of the plant can be calculated as 3 % of the fixed capital cost, thus

 $C_{insurance} = 0.03 \cdot (602,553,794 \text{ baht}) = 18,076,614 \text{ baht/yr}$

And finally the overall manufacturing cost, M, can be determined as the sum of the above calculated costs

 $M = C_{raw materials} + C_{salary} + C_{maintenance} + C_{supplies} + C_{payroll} + C_{utilities} + C_{depreciation}$ +C_{insurance} = 6,662,545,614+4,302,600+30,127,690+12,051,076+860,520 +52,801,054 +42,763,844 +4,521,397 baht/yr = 6,884,859,912 baht/yr

These are the expense that are both directly and indirectly related to the day-to-day operation of the hydrogenated biodiesel plant.

4.4.2.2 SMR-Hydrogenated Biodiesel Manufacturing Cost

The raw materials used in the SMR-hydrogenated biodiesel plant are; crude palm oil, methane, water and catalyst. The costs are based on a total production of 200,000 tones hydrogenated biodiesel per year in a plant operating 300 days per year. The cost of crude palm oil, methane, water and catalyst are determined.

 $C_{palm oil} = (274,041,576 \text{ kg/yr}) \cdot (23.06 \text{ baht/kg}) = 6,319,398,745 \text{ baht/yr}$ $C_{methane} = (11,505,384 \text{ kg/yr}) \cdot (8.50 \text{ baht/kg}) = 97,795,764 \text{ baht/yr}$ $C_{water} = (35,251,200 \text{ kg/yr}) \cdot (0.0235 \text{ baht/kg}) = 828,403 \text{ baht/yr}$ $C_{catalyst} = (108,127 \text{ kg/3yr}) \cdot (830 \text{ baht/kg}) = 29,915,278 \text{ baht/yr}$

Thus, total raw material cost is 6,447,938,140 baht/yr

The cost needed for salary is dependent of the number of employees and which positions they have. It is assumed that a GM/MD is paid 100,000 baht/month/person, an office manager 50,000 baht/month/person, plant manager 60,000 baht/month/person, Engineer 18,000 baht/month/person, Researcher 20,000 baht/month/person, Technician 10,850 baht/month/person and labor 8,000 baht/month/person. This results in the following salaries

C_{GM}	= (1 person) \cdot (100,000 baht/month/person) \cdot (12 month/yr)
	= 1,200,000 baht/yr
Coffice manager	= $(1 \text{ person}) \cdot (50,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$
	= 600,000 baht/yr
Cplant manager	= $(1 \text{ person}) \cdot (60,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$
	= 720,000 baht/yr
Cengineer	= (4 person) \cdot (18,000 baht/month/person) \cdot (12 month/yr)
	= 864,000 baht/yr
Cresearcher	= $(2 \text{ person}) \cdot (20,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$
	= 480,000 baht/yr
Ctechnician	= (3 person) \cdot (10,850 baht/month/person) \cdot (12 month/yr)
	= 390,600 baht/yr
Clabor	= $(3 \text{ person}) \cdot (8,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$
	= 480,000 baht/yr

Thus, total salary is 4,734,600 baht/yr

The cost for maintaining the plant can be calculated as 5 % of the fixed capital cost

 $C_{\text{maintenance}} = 0.05 \cdot (606,208,287 \text{ baht}) = 30,310,414 \text{ baht/yr}$

The cost for the supplies of the plant can be calculated as 2 % of the fixed capital cost, thus

 $C_{supplies} = 0.02 \cdot (606,208,287 \text{ baht}) = 12,124,166 \text{ baht/yr}$

The cost for the payroll of the plant can be calculated as 20 % of total salary, thus

 $C_{payroll} = 0.20 \cdot (4,734,600 \text{ baht}) = 946,920 \text{ baht/yr}$

There are three main utilities associated with the operation of the plant; steam, cooling water and electricity. There is no cost of steam in this process because steam can be generated from combustion of the PSA waste gas and methane (fuel) in SMR unit. Steam is used two places in the plant, in the reboiler and heat exchangers. The amount of steam needed in the reboiler and heat exchanger is calculated based on the energy balances carried out in section 4.2 (Table 4.6).

Cooling water is used in the heat exchanger. The amount of cooling water needed in the heat exchanger is calculated based on the energy balances carried out in section 2 (Table 4.8) and enthalpy data as same as hydrogenated biodiesel process.

The amount of electricity needed to operate the plant is electricity for the pump and compressor. The electricity used in the pump and compressor can be calculated.

$$El_{pump} = 320,837.7 \text{ kWh}$$

$$El_{com} = 6,635,442.4 \text{ kWh}$$

$$El_{total} = El_{com} + El_{pump} = 320,837.7 \text{ kWh} + 6,635,442.4 \text{ kWh}$$

$$= 6,956,280.1 \text{ kWh}$$
The total cost of electricity is thus
$$C_{electricity} = P_{electricity} \cdot El_{total}$$

= $(2.94 \text{ baht/kWh}) \cdot (6,956,280.1 \text{ kWh})$ = 20,451,463.4 baht/yr

Litilities	Units		Reference price	Cost
Unities	Equipment	kg/year	baht/kg	(baht/year)
Steam	Hx. E-102	18,331,696	1.63	
(200 psi 240 °C)	Reboiler	7,863,700	1.63	Steam from
	Total	26,195,396	1.63	SIMIR UNIT
Cooling Water	Hx. E-103	89,470,108	0.0235	2,102,548
	Hx. E-401	102,929,779	0.0235	2,418,850
	Stripper (LP)	7,200,000	0.0235	169,200
	Reboiler& Hx. E-102	26,195,396	0.0235	615,591
	Total	225,795,283	0.0235	5,306,189
Electricity	Equipment	kWh	baht/kWh	(baht/year)
	Pump P-101	295,521	2.94	868,831
	Pump P-501	24,624	2.94	72,395
	Pump P-502	693	2.94	2,037
	C-101	1,095,336	2.94	3,220,287
	C-102	3,452,682	2.94	10,150,886
	C-501	2,087,424	2.94	6,137,027
	Total	6,956,280	2.94	20,451,463

 Table 4.17 Utilities cost of SMR-hydrogenated biodiesel process

Then the total cost of utilities can be estimated

 $C_{\text{utilities}} = C_{\text{cooling water}} + C_{\text{electricity}}$

= 5,306,189 baht+ 20,451,463 baht

= 25,757,653 baht/yr

The cost for depreciation the plant can be calculated as 8 % of the fixed capital cost

$$C_{depreciation} = 0.08 \cdot (606,208,287 \text{ baht}) = 48,496,663 \text{ baht/yr}$$

The cost for the insurance of the plant can be calculated as 3 % of the fixed capital cost, thus

 $C_{insurance} = 0.03 \cdot (606,208,287 \text{ baht}) = 18,186,249 \text{ baht/yr}$

And finally the overall manufacturing cost, M, can be determined as the sum of the above calculated costs

$$M = C_{raw materials} + C_{salary} + C_{maintenance} + C_{supplies} + C_{payroll} + C_{utilities} + C_{depreciation} + C_{insurance}$$

= 6,447,938,140 + 4,734,600 + 30,310,414 + 12,124,166 + 946,920
+25,757,653 + 48,496,663 + 18,186,249 baht/yr
= 6,597,964,004 baht/yr

These are the expense that are both directly and indirectly related to the dayto-day operation of the SMR-hydrogenated biodiesel plant.

4.4.2.3 Biodiesel Manufacturing Cost

The raw materials used in the plant are; crude palm oil, methanol and KOH for biodiesel process. The costs are based on a total production of 200,000 tones biodiesel per year in a plant operating 300 days per year.

The cost of crude palm oil, methanol and KOH are determined. $C_{palm oil} = (207,000,000 \text{ kg/yr}) (23.06 \text{ baht/kg}) = 4,773,420,000 \text{ baht/yr}$ $C_{methanol} = (26,640,000 \text{ kg/yr}) (25.32 \text{ baht/kg}) = 674,430,380 \text{ baht/yr}$ $C_{KOH} = (30,000 \text{ kg/yr}) (85 \text{ baht/kg}) = 2,550,000 \text{ baht/yr}$ Thus, total raw material cost is 5,450,400,380 baht/yr

The cost needed for salary is dependent of the number of employees and which positions they have. It is assumed that a GM/MD is paid 100,000 baht/month/person, an office manager 50,000 baht/month/person, plant manager 60,000 baht/month/person, Engineer 18,000 baht/month/person, Researcher 20,000 baht/month/person, Technician 10,850 baht/month/person and labor 8,000 baht/month/person. This results in the following salaries

$$C_{GM} = (1 \text{ person}) \cdot (100,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$$

= 1,200,000 baht/yr

Coffice manager = $(1 \text{ person}) \cdot (50,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$ = 600,000 baht/yr

 $C_{\text{plant manager}} = (1 \text{ person}) \cdot (60,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$ = 720,000 baht/yr

- Cengineer = $(2 \text{ person}) \cdot (18,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$ = 432,000 baht/yr
- $C_{researcher} = (2 \text{ person}) \cdot (20,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$ = 480,000 baht/yr
- $C_{\text{technician}} = (3 \text{ person}) \cdot (10,850 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$ = 390,600 baht/yr
- $C_{labor} = (3 \text{ person}) \cdot (8,000 \text{ baht/month/person}) \cdot (12 \text{ month/yr})$ = 480,000 baht/yr

Thus, total salary is 4,302,600 baht/yr

The cost for maintaining the plant can be calculated as 5 % of the fixed capital cost

 $C_{maintenance} = 0.05 \cdot (440, 143, 842 \text{ baht}) = 22,007,192 \text{ baht/yr}$

The cost for the supplies of the plant can be calculated as 2 % of the fixed capital cost, thus

 $C_{supplies} = 0.02 \cdot (440, 143, 842 \text{ baht}) = 8,802,877 \text{ baht/yr}$

The cost for the payroll of the plant can be calculated as 20 % of total salary, thus

 $C_{payroll} = 0.20 \cdot (4,302,600 \text{ baht}) = 860,520 \text{ baht/yr}$

There are three main utilities associated with the operation of the plant; steam, cooling water and electricity. Steam is used eight places in the plant, in four reboilers and four heat exchangers. The amount of steam needed in the reboiler and heat exchanger is calculated based on the energy balances carried out in section 4.2 and enthalpy data for example in heat exchanger E-101 (Q= 2,544,535 kJ/h).

$$N_{steam1} = \frac{Q}{H_{(130\ ^{\circ}C,1\,bar)} - H_{(90^{\circ}C,1\,bar)}}$$
$$N_{steam1} = \frac{2,544,535kJ/h}{2,727.3kJ/kg - 398.18kJ/kg} = 1,092.49kg/h = 7,865,911.7kg/yr$$

Thus, the cost of steam becomes

 $C_{steam} = P_{steam} \cdot N_{steam1}$ = (1.63 baht/kg) \cdot (7,865,911.7 kg/yr) = 12,841,058.7 baht/yr

Cooling water is used in the condenser and the heat exchanger. The amount of cooling water needed in the condenser and the heat exchanger is calculated based on the energy balances carried out in section 4.2 and enthalpy data for example in condensor of T-101 (Q= 9,738,785 kJ/h). The chilling water enters at 10 °C and leaves at 60 °C.

$$N_{CW1} = \frac{Q}{H_{(60^{\circ}C,1 \text{ bar})} - H_{(10^{\circ}C,1 \text{ bar})}}$$

$$N_{CW1} = \frac{9,738,785 \, kJ/h}{251.25kJ/kg - 42.12kJ/kg} = 46,568.1kg/h = 335,290,244.3kg/yr$$

Thus, the cost of steam becomes

$$C_{CW1} = P_{CW} \cdot N_{CW}$$

= (0.0235 baht/kg) \cdot (335,290,244.3 kg/yr)
= 7,879,321 baht/yr

The amount of electricity needed to operate the plant is electricity for the pump. The electricity used in the pump can be calculated.

 $El_{pump} = 1,582.17 \text{ kWh}$

The total cost of electricity is thus

$$C_{electricity} = P_{electricity} \cdot El_{pump}$$

= (2.94 baht/kWh) \cdot (1,582.17 kWh)
= 4,651. 6 baht/yr

Then the total cost of utilities can be estimated

 $C_{\text{utilities}} = C_{\text{steam}} + C_{\text{cooling water}} + C_{\text{electricity}}$ = 214,318,013 baht + 17,821,948 baht+ 4,651.57 baht = 232,144,613 baht/yr

The cost for depreciation the plant can be calculated as 8 % of the fixed capital cost

 $C_{depreciation} = 0.08 \cdot (440, 143, 842 \text{ baht}) = 35,211,507 \text{ baht/yr}$

The cost for the insurance of the plant can be calculated as 3 % of the fixed capital cost, thus

 $C_{insurance} = 0.03 \cdot (440, 143, 842 \text{ baht}) = 13,204,315 \text{ baht/yr}$

And finally the overall manufacturing cost, M, can be determined as the sum of the above calculated costs

$$M = C_{raw materials} + C_{salary} + C_{maintenance} + C_{supplies} + C_{payroll} + C_{utilities} + C_{depreciation} + C_{insurance}$$

= 5,807,853,128 baht/yr

These are the expense that are both directly and indirectly related to the day-to-day operation of the biodiesel plant.

Litilities	Units		Reference price	Cost
	Equipment	kg/year	baht/kg	baht/year
Steam	Hx. E-101	7,865,912	1.6325	12,841,059
(0.2 Mpa 130 °C)	Hx. E-201	18,369,890	1.6325	29,988,747
	Hx. E-202	3,113,307	1.6325	5,082,457
	Hx. E-301	21,868,911	1.6325	35,700,879
	Reboiler T-101	25,804,025	1.6325	42,124,933
	Reboiler T-301	62,126,389	1.6325	101,420,997
	Reboiler T-401	. 51,672,442	1.6325	84,354,986
	Reboiler T-501	59,182,900	1.6325	96,615,768
	Total	131,282,521	1.6325	214,318,013
Cooling Water	Hx. E-501	54,698,311	0.0235	1,285,410
	Condensor T101	335,290,244	0.0235	7,879,320
	Condensor T301	423,090,521	0.0235	9,942,627
	Condensor T401	155,029,557	0.0235	3,643,195
	Condensor T501	51,568,876	0.0235	1,211,869
	Total	758,380,766	0.0235	17,821,948
Electricity	Equipment	kWh	baht/kg	baht/year
	Pump P-101	131.22	2.94	385.79
	Pump P-102	709.27	2.94	2,085.24
	Pump P-301	741.68	2.94	2,180.54
	Total	1582.17	2.94	4,651.57

 Table 4.18 Utilities cost of biodiesel process

Direct manufacturing expenses were calculated based on the price and consumption of each chemical and utility. Chemical and utility prices are presented in Table 4.15 and material flow information was obtained from PRO/II[®]. Table 4.19 shows list of manufacturing costs for each process. The direct manufacturing cost represents 98.8, 98.8 and 99.6 % of the total manufacturing cost in hydrogenated biodiesel, SMR-hydrogenated biodiesel and biodiesel processes, respectively. The largest proportion of the direct manufacturing cost is due to the palm oil feedstock, namely 91.8 %, 95.8% for hydrogenated biodiesel and SMR-hydrogenated biodiesel processes, and 82.2 % for biodiesel processes. Biodiesel process to use lower palm oil feedstock, as well as the lower catalyst costs of the process resulting from smaller material streams handled in the process (Figure 4.15).

Items	Hydrogenated Biodiesel	SMR-Hydrogenated Biodiesel	Biodiesel
	(millions baht/year)	(millions baht/year)	(millions baht/year)
Direct manufacturing cost			
Crude palm oil	6,319.40	6,319.40	4,773.42
Hydrogen	315.24	-	-
Catalyst	27.90	29.92	2.55
Methanol	-	-	674.43
Methane	-	97.80	-
Salary	4.30	4.73	4.30
Maintenance	30.13	30.31	22.01
Operating supplies	12.05	12.12	8.80
Payroll	0.86	0.95	0.86
Utilities	100.09	25.76	232.14
Subtotal A _{DMC}	6,809.97	6,521.81	5,783.14
Indirect manufacturing cost			
Taxes & Insurance	18.08	18.19	13.20
Subtotal A _{IMC}	18.08	18.19	13.20
Depreciation	48.20	48.50	35.21
Total manufacturing cost	6,884.86	6,597.96	5,807.85

 Table 4.19 The manufacturing cost of hydrogenated biodiesel, SMR-hydrogenated biodiesel and biodiesel processes



Figure 4.15 The manufacturing costs of hydrogenated biodiesel, SMR-hydrogenated biodiesel and biodiesel processes.

However, in terms of energy produced, hydrogenated biodiesel contains significantly higher heating value than the conventional biodiesel as shown in Figure 4.16.



Figure 4.16 Comparison of the manufacturing cost and heating value of biohydrogenated diesel and biodiesel. (Basis: 200,000 ton/year)

4.5 Sensitivity Analysis

The overall manufacturing cost of hydrogenated biodiesel, SMRhydrogenated biodiesel and biodiesel were analyzed as a function of feedstock price. The cost of palm oil feed is the largest component of the overall manufacturing cost. Using the process models developed in this work, it was found that as the manufacturing cost of hydrogenated biodiesel strongly depends on crude palm oil price, the difference in the manufacturing cost between hydrogenated biodiesel and biodiesel becomes higher when crude palm oil price increases (Figure. 4.17). This is due to palm oil feedstock cost forms the largest proportion of the manufacturing cost, namely 91.8 %, 95.8% for hydrogenated biodiesel and SMR-hydrogenated biodiesel processes, and 82.2 % for biodiesel process.



Figure 4.17 The impact of palm oil price on the manufacturing cost of producing hydrogenated biodiesel and biodiesel.

4.6 Hydrogenated Biodiesel Production for Engine Test

The large scale (100 ml catalyst) reactor has already been contructed and utilized for producing 30 litres hydrogenated biodiesel from crude jatropha oil as shown in Figure 4.18.



Figure 4.18 Hydrogenated biodiesel production systems for engine test.

To produce hydrogenated biodiesel for engine test, the deoxygenation of jatropha oil was conducted at 500 psig, LHSV of 0.1 h⁻¹, and H₂/feed ratio of 30 molar ratio. The reaction temperature was 325 °C. The results are shown in Figure 4.19. Jatropha oil conversion was reached 95% for 30 days of production with high selectivity to n-octadecane (n-C18), n-hexadecane (n-C16), n-heptadecane (n-C17), and n-pentadecane (n-C15), an alkane products that have carbon number in the range of diesel fuels.



Figure 4.19 Product selectivity obtained after 30 days versus time on stream.

The hydrogenated diesel produced was tested for fuel properties. The analysis are shown in Table 4.20. It can be seen that the hydrogenated diesel has excellent diesel fuel properties including an extremely high cetane number.
Properties	Unit	Conventional	Hydrogenated
		Diesel Limit	Biodiesel
Cetane Index	-	46	76.6
Density at 15 °C (min-max)	kg/m ³	800-845	788
Water (max)	mg/kg	200	60-130
Lubricity ^a	mm	460	576
Viscosity at 40 °C (min-max)	mm ² /s	1.2-4.0	3.8
Sulfur Content	ppm	10	0
Distillation			
T 95, max	°C	360	326
E 250, max	vol %	65	-
E 350, max	vol %	85	-
Carbon Residue ^b	wt %	0.3	0
TAN	mg KOH/g	-	0.01
lodine value.	g lodine/100 g	-	Trace

 Table 4.20 Fuel properties of hydrogenated biodiesel produced from jatropha oil

 compared to the conventional diesel limit.

^a Corrected wear scar diameter (wsd 1.4) at 60 °C (max) HFRR (CEC F06-A-96

^b on 10% distrilation residue