

Property estimation of palmitoylethanolamide and sucrose palmitate for process  
design from methyl palmitate



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เมทิลปาล์มไมเตท เป็นองค์ประกอบหลักในไบโอดีเซลที่ผลิตได้จากน้ำมันปาล์ม และเป็น  
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 ประสิทธิภาพของธุรกิจไบโอดีเซล ด้วยเหตุผลดังกล่าว จึงทำให้ผู้ประกอบการหันมาสนใจที่จะนำไบ  
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 เนื่องจากปาล์มไมโทอิลเอทานอลาไมด์ และซูโครสปาล์มไมเตท ไม่มีอยู่ในฐานข้อมูลของโปรแกรม  
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Methyl palmitate is the primary component of palm oil-based biodiesel. It is a saturated fatty acid methyl ester which has a high melting point that results in low cold flow properties of biodiesel. Besides, lack of government support may affect the revenue of biodiesel business. For that reason, the producers turn attention to using biodiesel as a raw material for the production of value-added chemicals. Initially, we selected the studied products based on the gross profit margin, production process, market demand and application. This work simulated the production of palmitoylethanolamide, sucrose palmitate and normal alkanes from methyl palmitate using Aspen Plus V11. Because palmitoylethanolamide and sucrose palmitate were not available in Aspen Plus's databases, so we need to estimate the property parameters required in the process simulation, including parameters for mass and energy balance and parameters for thermodynamic reference state. Then, the economic analysis was performed. This study founded that the production of sucrose palmitate was the most profitable, followed by the production of palmitoylethanolamide and normal alkanes. This research indicated that the production of value-added chemicals from methyl palmitate was an attractive alternative to biodiesel producers because these production processes could be profitable even without government support.

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## CHAPTER 1

### INTRODUCTION

#### 1.1. Background and problem statement

Nowadays, the world's energy consumption mostly comes from fossil fuels such as petroleum, coal and natural gas. However, population growth and industrial development cause the depletion of these non-renewable resources. Besides, the burning of fossil fuels leads to environmental impacts such as air pollution and global warming [1]. For these two reasons, it is necessary to find renewable energy sources. Biodiesel is a good alternative for substituting petroleum-based diesel because it has similar properties to petrodiesel and we can use it in diesel engines without any modifications. Moreover, it produces less polluting and greenhouse gas emissions [2].

In 2017, Thailand had 13 biodiesel producers that had a total production capacity of 6.62 million litres per day. Crude palm oil is a primary raw material for biodiesel production. From a total of 2.63 million tonnes of crude palm oil, 0.97 million were used to produce biodiesel. The profitability of biodiesel industry depends on 1) costs of raw materials (which account for 70% of total production costs), 2) biodiesel proportion in the blends 3) the government's policies and supports, and 4) profit margins [3]. The lack of government supports can negatively impact business profits. Therefore, the producers pay attention to use biodiesel as a raw material for value-added chemicals production instead of selling as fuels.

Palm oil-based biodiesel is mainly rich in methyl palmitate (44.3%) and methyl oleate (39.1%) [4]. The high amount of methyl palmitate, which is saturated fatty acid methyl esters (FAMES), results in low cold flow properties due to its high melting point. Fractionation is one of the methods used to improve the cold flow properties of biodiesel. This method reduces saturated FAMES concentration by cooling down to the temperature between the cloud point and pour point. After that, the formed crystals of saturated FAMES are separated by filtration [5].

Methyl palmitate which separated from biodiesel can be used as raw material to produce value-added chemicals. Figure 1 presents the potential chemical products converted from methyl palmitate. These products are consumed in various industries such as cosmetic, food, pharmaceutical and lubricant industries. Furthermore, they are used as chemical intermediates to produce other chemicals and as solvents. Initially, we calculated the gross profit margin of each alternative, as present in Appendix A. From the analysis results, there are six processes with negative profit margins. They are butyl palmitate, cetyl alcohol, cetyl palmitate, ethyl palmitate, isopropyl palmitate, and palmitic acid. A negative value indicates that the process will not be profitable, so we did not further investigate these production processes in this work [6].

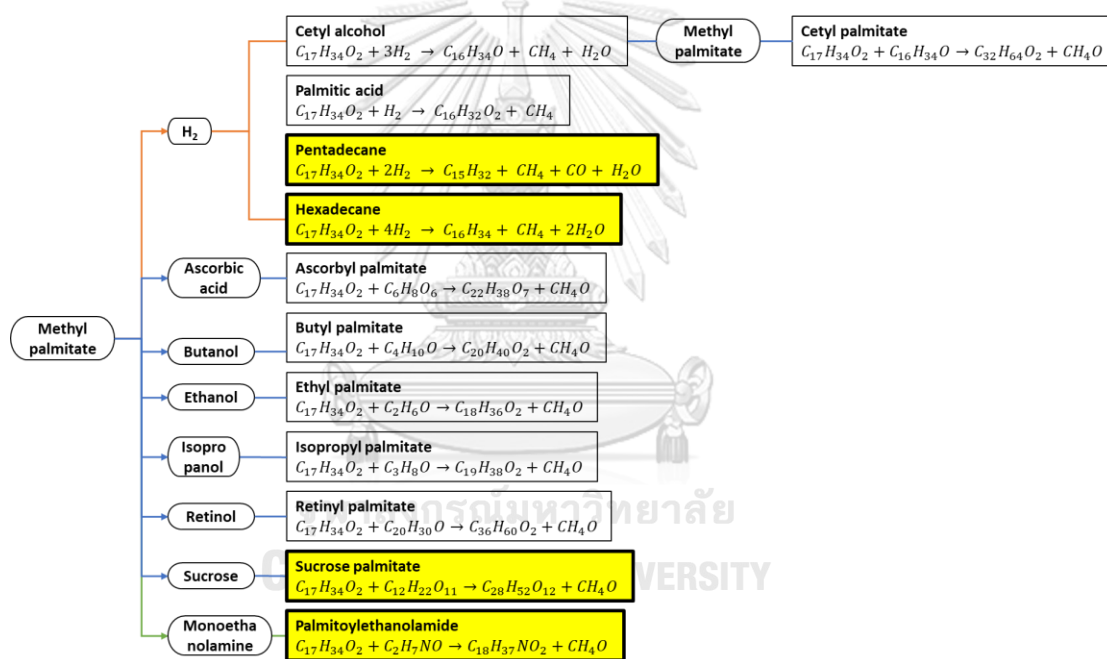


Figure 1 Reaction pathways from methyl palmitate.

However, considering the production routes of ascorbyl palmitate and retinyl palmitate, they are commercially produced through the esterification of palmitic acid with acid catalysts. Palmitic acid has a lower price and is preferable feedstock than methyl palmitate. Thus, we did not consider these two products in this study.

The remaining products are considered in terms of application and market demand. Palmitoylethanolamide (PEA) is used as a wetting agent and foam booster in

cosmetics and personal care products. High purity PEA can be used as a pain killer and anti-inflammatory agent [7]. Moreover, it is used as a corrosion inhibitor and lubricant additive. Global demand for alkanolamides is 90,000 ton per year [8]. Sucrose palmitate can be used as an emulsifier, emollient and skin conditioning agent in cosmetics, food additive, fruit preservation and stabilizer for drug delivery system. Global demand for sucrose esters is 15,000 ton per year [9]. Pentadecane and hexadecane are used as feedstocks for other chemicals production, solvents and phase change material (PCM) for thermal energy storage applications [10].

Based on the above considerations, the promising chemicals produced from methyl palmitate are palmitoylethanolamide, sucrose palmitate and normal alkanes. Thus, this work proposed the conceptual process design of these chemicals production processes using Aspen Plus V11. Unfortunately, palmitoylethanolamide and sucrose palmitate are not available in Aspen database. Consequently, we needed to study the suitable property estimation methods to assess their properties. After that, process simulation and economic analysis were performed to find the optimal processing route to produce value-added chemicals from methyl palmitate.

## 1.2. Research objective

This work aimed to perform property estimation of palmitoylethanolamide and sucrose palmitate including the conceptual process design of value-added chemicals production, which are palmitoylethanolamide, sucrose palmitate and normal alkanes (C15 and C16), from methyl palmitate.

## 1.3. Scope of research

- 1.3.1. Estimate the properties of palmitoylethanolamide and sucrose palmitate using property estimation methods available in Aspen Plus V11.
- 1.3.2. Perform conceptual process design of palmitoylethanolamide production using Aspen Plus V11 based on the work of Wang et al. [11]. The conversion of PEA

was 100% under reaction conditions of 20:1 molar ratio of monoethanolamine to methyl palmitate, 60 °C reaction temperature, 3%wt sodium methoxide as a catalyst and 1.5 h reaction time.

- 1.3.3. Perform conceptual process design of sucrose palmitate production using Aspen Plus V11 based on the work of Gutierrez et al. [12]. The optimal sucrose esters content was 22.86%wt under reaction conditions of 2.5:1 molar ratio of methyl palmitate to sucrose, 136 °C reaction temperature, 0.334 bar reaction pressure, 5%wt potassium carbonate as a catalyst, 16.15%wt sucrose ester as a surfactant and 3.92 h reaction time.
- 1.3.4. Perform conceptual process design of normal alkanes production using Aspen Plus V11 based on the work of Yan et al. [13]. The optimal yield of pentadecane and hexadecane were 70.0% and 28.3% under reaction conditions of 220 °C reaction temperature, 10 bar reaction pressure, 3%wt Mo-Ni@PSi and 2.5 h reaction time.
- 1.3.5. Compare economic performance between the three production processes in terms of discounted present value (DPV), discounted payback period (DPP) and discounted cash flow rate of return (DCFROR).

#### Design basis

- The feedstock is methyl palmitate with 100,000 tonnes per year.
- The desired purities of chemical products are  $\geq 98\%$ wt.
- The design pressure is specified as 10% of maximum operating pressure, and the design temperature is typically plus 30 °C.

#### **1.4. Expected outputs**

Property parameters estimated by Aspen Plus's built-in estimation methods were expected. After that, these parameters were used to perform the conceptual process design for palmitoylethanolamide, sucrose palmitate and normal alkanes production processes from methyl palmitate.

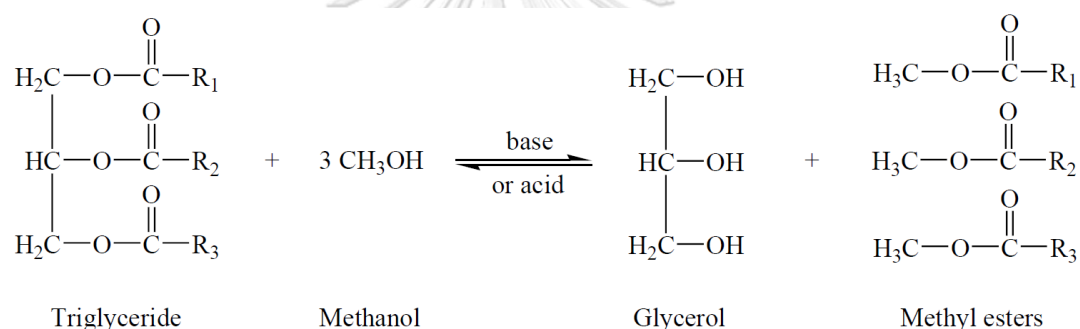
## CHAPTER 2

### FUNDAMENTAL THEORY AND LITERATURE REVIEWS

#### 2.1. Fundamentals

##### 2.1.1. Biodiesel

Biodiesel is commonly produced by transesterification of vegetable oils, animal fats or waste cooking oils with methanol in the presence of a catalyst, as illustrated in Figure 2. The mixture of fatty acid methyl esters (biodiesel) is obtained with glycerol as a by-product. Biodiesel has many advantages compared to petrodiesel such as sulphur-free, low emissions, high cetane number and high lubricity [14].



**Figure 2** Transesterification of triglyceride with methanol to produce biodiesel [15].

Table 1 presents the major FAMES composition of biodiesel obtained from crude palm oil. It contains high amounts of saturated FAMES which have high melting points. Saturated FAMES tend to solidify at low temperature. These solid crystals clog the fuel lines, filters and injectors, resulting in fuel starvation and operational problems in vehicle engines. According to the work of Dunn [16], biodiesel has poor cold flow properties when saturated FAMES is more than 20%wt. Cold flow properties can be improved by adding chemical additives such as pour point depressants and crystalline wax modifiers, blending with petrodiesel or biodiesel with high unsaturated or shorter-chain FAMES, using the longer chain ( $C_3$  to  $C_8$ ) or branched alcohols instead of methanol in transesterification process, reducing total saturated FAMES by fractionation such as winterization, solvent fractionation and vacuum distillation [17].

**Table 1** Major fatty acid methyl esters composition of palm-oil based biodiesel.

Composition	Melting point (°C) [18]	Percentage of total FAME [4]
Methyl palmitate (16:0)	28.5	44.3%
Methyl stearate (18:0)	37.7	5.0%
Methyl oleate (18:1)	-20.2	39.1%
Methyl linoleate (18:2)	-43.1	10.1%

Biodiesel can directly be used as transportation fuel, fuel for power generation, heating oil, solvent, lubricity additive, fuel additive, pesticide and fertilizer carriers [19]. Besides, individual methyl ester can be used to produce other chemical products.

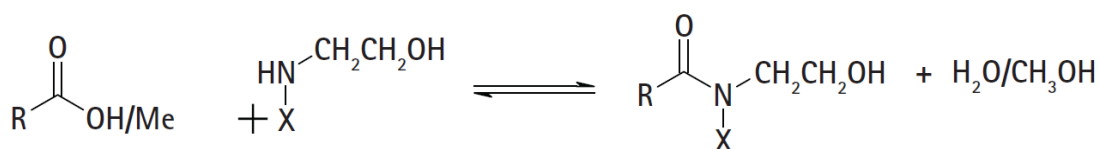
### 2.1.2. Palmitoylethanolamide

Palmitoylethanolamide is one of the fatty acid amides produced via amidation of acyl donors with monoethanolamine in the presence of a base catalyst (typically sodium methoxide). The feasible acyl donors are free fatty acids, fatty acid methyl esters, fatty acid chlorides, triglyceride oils and fatty acid vinyl esters. The comparison between each acyl donor is presented in Table 2.

**Table 2** Advantage and disadvantage of each acyl donor [20].

Acyl donor	Advantage	Disadvantage
Free fatty acids	- Commercially available	- High amount of by-product impurities
Fatty acid methyl esters	- Higher yield than FAs - Commercially available	
Fatty acid chlorides	- Most effective	- Most expensive - Corrosive and toxic
Triglyceride oils	- Safe and cheap - No ion pairs formed	- Not suitable for medicinal use
Fatty acid vinyl esters	- Effective	- Less available

In this work, fatty acid methyl ester is used as raw material for fatty acid amide synthesis. The reaction takes place at around 100 °C and 4 kPa or less using sodium methoxide as a catalyst. Vacuum pressure is used to remove the produced methanol [8]. Figure 3 illustrates the reaction scheme of the fatty acid amide synthesis.



**Figure 3** Amidation of FAME with ethanolamine to produce fatty acid amide [8].

(methyl palmitate: R = C<sub>15</sub>H<sub>31</sub>, monoethanolamine: X = H)

### 2.1.3. Sucrose palmitate

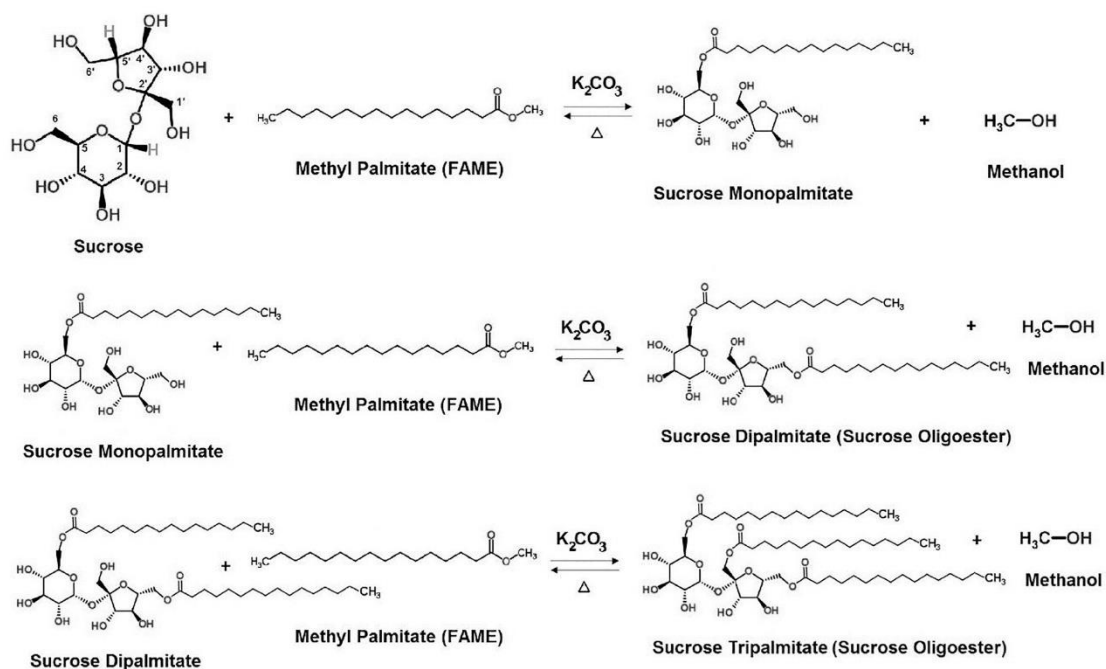
Sucrose palmitate is non-ionic surfactant obtained from reacting sucrose with acyl donors such as free fatty acids, fatty acid methyl esters and fatty acid chlorides. According to sucrose chemical structure, it has the three primary hydroxyl groups (6, 1' and 6') and five secondary hydroxyl groups. Consequently, sucrose monoesters up to sucrose octa-esters can be produced. Most commercial products contain at least 80%wt of sucrose monoesters and diesters [12].

In general, sucrose esters are produced by transesterification of sucrose with fatty acid methyl esters using a base catalyst (typically potassium carbonate). Direct esterification of sucrose with fatty acids is impractical because a base catalyst can promote the neutralization of fatty acids, resulting in reactant depletion and low yield [9]. Sucrose palmitate synthesised by transesterification process is shown in Figure 4.

Considering the nature of raw materials, sucrose is highly polar solid and methyl palmitate is highly non-polar liquid. Thus, the reactants are immiscible with each other. There are many routes to improve the compatibility between reactants. The first is the solvent process, dimethylformamide (DMF) or dimethyl sulfoxide (DMSO) are used to dissolve the two reactants, resulting in a homogeneous mixture. The disadvantages of this route are the high amount of solvent required (60%wt) and high energy required to remove a solvent from the product. The second route is the solvent-free process,



surfactants, such as alkaline soaps, multivalent fatty acid soaps, sucrose esters, mono- and diacyl-glycerol esters, are used to disperse sucrose in methyl palmitate. In this route, the amount of used surfactant is 1-30%wt [12].



**Figure 4** Transesterification of sucrose with methyl palmitate to produce sucrose palmitate [12].

Sucrose esters have a wide range of applications depending on the degree of substitution, as presented in Figure 5. Hydrophilic-lipophilic balance (HLB) is calculated by multiplying the ratio of molecular weight of hydrophilic groups to the molecular weight of the whole molecule by 20. Accordingly, sucrose esters with high monoesters possess high HLB value or vice versa [21].

#### 2.1.4. Pentadecane and hexadecane

Green diesel consists of saturated hydrocarbons with 15 to 18 carbon atoms, including pentadecane and hexadecane. Normal alkanes are obtained from hydro-processing of fatty acids, fatty acid esters and triglyceride oils. The reaction takes place at mild temperatures between 280 °C and 450 °C and pressure of 1–5 MPa. The mostly used catalysts are Ni-Mo, Co-Mo and Ni-W on the alumina ( $Al_2O_3$ ) support [22].

Fatty acyl group	HLB									
	1	2	3	5	7	9	11	15	16	
C12	Fats & oils chocolate				Powdered milk		Detergent			
C14									Ice cream	
C16	Tablet				Curry roux		Wheat products dough		Milk beverage Frozen dough	
C18										
C18	W/O emulsion				Chewing gum			Cake batter		
C18:1	Shortening chocolate				Beverage			O/W emulsion		
C22:1									Sauce, dressing	
C22:1					Seasoning		Ice cream			
C22										

Figure 5 Applications of sucrose esters [21].

When fatty acid esters and triglyceride oils are used as feedstocks, the C=C double bonds are saturated by hydrogenation. Then, they are hydrogenated to fatty acids [23]. Finally, the oxygens are removed by deoxygenation, and normal alkanes are obtained. This reaction consists of three pathways: (1) Decarboxylation (DCO<sub>2</sub>) and (2) Decarbonylation (DCO) and Hydrodeoxygenation (HDO), as shown in Figure 6.

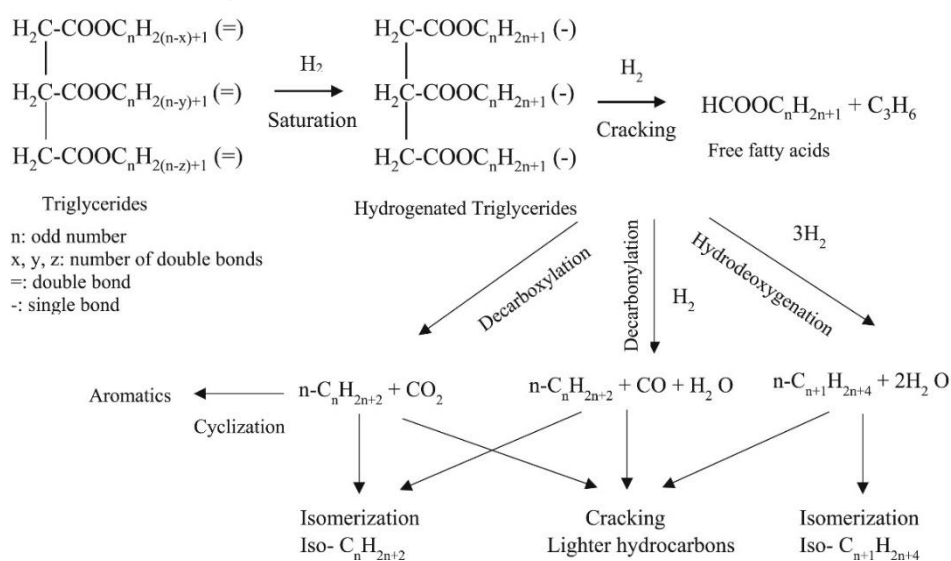


Figure 6 Hydro-processing of triglycerides to produce normal alkanes [24].

DCO and DCO<sub>2</sub> pathways yield the normal alkanes with one less carbon atom than the starting fatty acids, whereas the HDO pathway yields the normal alkanes with the same carbon atom.

### 2.1.5. Property estimation methods

Property estimation methods are used to estimate the missing properties of compounds which are not available in literature, online database and simulator databanks. The estimation methods help to reduce the time-consuming and costs of experimental measurements. The property parameters used in process simulation are divided into two parts [25].

- **Parameter requirements for mass and energy balance simulations:**  
molecular weight (MW), ideal gas heat capacity (CPIG), vapor pressure (PL) and heat of vaporization (DHVL)
- **Parameter requirements for thermodynamic reference state:**  
critical temperature (TC), critical pressure (PC), critical volume (VC), critical compressibility factor (ZC) and standard heat of formation (DHFORM)

In Aspen Plus software, the minimum information required to estimate property parameters is the normal boiling point, molecular weight and molecular structure. Aspen Plus's built-in estimation methods and their equation for each property are summarized in Table 3 to 9. For compressibility factor (ZC), it calculated by definition, as shown in Equation 1.

$$Z_c = \frac{P_c V_c}{RT_c} \quad (1)$$

Where:

$P_c$	=	Critical pressure
$V_c$	=	Critical volume
$R$	=	Universal gas constant
$T_c$	=	Critical temperature

**Table 3** Aspen Plus's built-in estimation methods for estimating critical temperature.

Method	Information required	Equation	Average relative error (%)	Reference
(1) Joback	Structure, TB	$T_c \text{ (K)} = T_b \left[ 0.584 + 0.965 \sum N_i \cdot T_{c_i} - \left( \sum N_i \cdot T_{c_i} \right)^2 \right]^{-1}$	0.8 (NC = 400)	[25], [26]
(2) Lydersen	Structure, TB	$T_c \text{ (K)} = T_b \left[ 0.567 + \sum N_i \cdot T_{c_i} - \left( \sum N_i \cdot T_{c_i} \right)^2 \right]^{-1}$	2 – 5	[25], [27]
(3) Ambrose	Structure, TB	$T_c \text{ (K)} = T_b \left[ 1 + \left( 1.242 + \sum N_i \cdot T_{c_i} \right)^{-1} \right]$	0.7 (NC = 400)	[25], [28]
(4) Fedors	Structure	$T_c \text{ (K)} = 535 \log \left( \sum N_i \cdot T_{c_i} \right)$	4 (NC = 199)	[25], [28]
(5) Simple	MW, TB	$T_c \text{ (K)} = b + m \log \text{ (MW)}$	2.3 (NC = 200)	[25], [29]
(6) Gani	Structure	$T_c \text{ (K)} = 181.128 \ln \left[ \sum N_{1,i} \cdot T_{c_{1,i}} + W \sum N_{2,i} \cdot T_{c_{2,i}} \right]$	0.85 (NC = 400)	[25], [28]

**Table 4** Aspen Plus's built-in estimation methods for estimating critical pressure.

Method	Information required	Equation	Average relative error (%)	Reference
(1) Joback	Structure	$P_c \text{ (bar)} = \left[ 0.113 + 0.0032 N_{\text{atoms}} - \sum N_i \cdot P_{c_i} \right]^{-2}$	5.2 (NC = 390)	[25], [26]
(2) Lydersen	Structure, MW	$P_c \text{ (bar)} = \text{MW} \left[ 0.34 + \sum N_i \cdot P_{c_i} \right]^{-2}$	4	[25], [27]
(3) Ambrose	Structure, MW	$P_c \text{ (bar)} = \text{MW} \left[ 0.339 + \sum N_i \cdot P_{c_i} \right]^{-2}$	4.6 (NC = 390)	[25], [28]
(4) Gani	Structure	$P_c \text{ (bar)} = \left[ \sum N_{1,i} \cdot P_{c_{1,i}} + W \sum N_{2,i} \cdot P_{c_{2,i}} + 0.10022 \right]^{-2} + 1.3705$	2.89 (NC = 390)	[25], [28]

**Table 5** Aspen Plus's built-in estimation methods for estimating critical volume.

Method	Information required	Equation	Average relative error (%)	Reference
(1) Joback	Structure	$V_c \text{ (cc/mol)} = 17.5 + \sum N_i \cdot V_{c_i}$	2.3 (NC = 310)	[25], [26]
(2) Lydersen	Structure	$V_c \text{ (cc/mol)} = 40 + \sum N_i \cdot V_{c_i}$	4	[25], [27]
(3) Ambrose	Structure	$V_c \text{ (cc/mol)} = 40 + \sum N_i \cdot V_{c_i}$	2.8 (NC = 310)	[25], [28]
(4) Riedel	TB, TC, PC	$V_c \text{ (cc/mol)} = \frac{RT_c}{P_c} [3.72 + 0.26(\alpha - 7.0)]^{-1}$	-	[30]
(5) Fedors	Structure	$V_c \text{ (cc/mol)} = \sum N_i \cdot V_{c_i}$	4 (NC = 310)	[25], [30]
(6) Gani	Structure	$V_c \text{ (cc/mol)} = -0.00435 + \left[ \sum N_{1,i} \cdot V_{c_{1,i}} + W \sum N_{2,i} \cdot V_{c_{2,i}} \right]$	1.79 (NC = 310)	[25], [28]

**Table 6** Aspen Plus's built-in estimation methods for estimating standard heat of formation.

Method	Information required	Equation	Average error (kJ/mol)	Reference
(1) Benson	Structure	$\Delta H_f^\circ \text{ (kJ/mol)} = \sum N_i \cdot \Delta H_{f_i}^\circ$	3.7	[25], [26]
(2) Joback	Structure	$\Delta H_f^\circ \text{ (kJ/mol)} = 68.29 + \sum N_i \cdot \Delta H_{f_i}^\circ$	8.9	[25], [26]
(3) BensonR8	Structure	$\Delta H_f^\circ \text{ (kJ/mol)} = \sum N_i \cdot \Delta H_{f_i}^\circ$	-	[26]
(4) Gani	Structure	$\Delta H_f^\circ \text{ (kJ/mol)} = 10.835 + \left[ \sum N_{1,i} \cdot \Delta H_{f_{1,i}}^\circ + W \sum N_{2,i} \cdot \Delta H_{f_{2,i}}^\circ \right]$	3.71	[25], [26]

**Table 7** Aspen Plus's built-in estimation methods for estimating ideal gas heat capacity.

Method	Information required	Equation	Average relative error (%)	Reference
(1) Benson	Structure	$C_p^\circ(T) \left( \frac{J}{\text{mol} \cdot K} \right) = \sum N_i \cdot C_{p,i}^\circ$	1.1% (NC = 27)	[25], [26]
(2) Joback	Structure	$C_p^\circ(T) \left( \frac{J}{\text{mol} \cdot K} \right) = \left\{ \sum N_i \cdot C_{pA,i} - 37.93 \right\} + \left\{ \sum N_i \cdot C_{pB,i} + 0.201 \right\} T + \left\{ \sum N_i \cdot C_{pC,i} - 3.91E-04 \right\} T^2 + \left\{ \sum N_i \cdot C_{pD,i} + 2.06E-07 \right\} T^3$	1.4% (NC = 28)	[25], [26]
(3) BensonR8	Structure	$C_p^\circ(T) \left( \frac{J}{\text{mol} \cdot K} \right) = \sum N_i \cdot C_{p,i}^\circ$	-	[26]

**Table 8** Aspen Plus's built-in estimation methods for estimating vapor pressure.

Method	Information required	Equation	Average relative error (%)	Reference
(1) Riedel	TB, TC, PC	$\ln(P_L) \text{ (bar)} = A - B/T_r + C \ln(T_r) + DT_r^6$	-	[26]
(2) Li-Ma	Structure, TB	$P_L = 101.325 \ln T_b \left[ b_1 + b_2 \sum N_i \cdot P_{L,i} + b_3 \left( \sum N_i \cdot P_{L,i} \right)^2 + b_4 \left( \sum N_i \cdot P_{L,i} \right)^3 \right]^{-1}$	0.61% (NC = 28)	[26]

**Table 9** Aspen Plus's built-in estimation methods for estimating heat of vaporization.

Method	Information required	Equation	Average relative error (%)	Reference
(1) Definition	TC, PC, PL	$\Delta H_{U298}(\text{kJ/mol}) = (1.99) \frac{T_2 T_1}{(T_2 - T_1)} 2.30 \log \frac{P_2}{P_1}$	1.8% (NC = 94)	[26]
(2) Vetere	MW, TB	$\Delta H_{U298}(\text{kJ/mol}) = RT_b \left( A + B \ln T_b + \frac{CT_b^{1.72}}{M_i} \right)$	1.6%	[25], [26]
(3) Gani	Structure	$\Delta H_{U298}(\text{kJ/mol}) = 6.829 + \sum N_{1,i} \cdot h_{U,1,i} + W \sum N_{2,i} \cdot h_{U,2,i}$	-	[26]
(4) Ducros	Structure	$\Delta H_{U298}(\text{kJ/mol}) = \sum N_{1,i} \cdot h_{U,i}$	-	[31]
(5) Li-Ma	Structure, TB	$\Delta H_{U298}(\text{kJ/mol}) = \sum N_{1,i} \cdot h_{U,i} \left( \frac{1-T_r}{1-T_{br}} \right)^q$	1.05% (NC = 400)	[26], [32]

For temperature-dependent properties, the estimation results are presented in terms of coefficients of the equations as follows.

Aspen Ideal Gas Heat Capacity Polynomial (CPIG)

$$C_p^{*,ig} = C_{1i} + C_{2i}T + C_{3i}T^2 + C_{4i}T^3 + C_{5i}T^4 + C_{6i}T^5 \quad \text{for } C_{7i} \leq T \leq C_{8i}$$

$$C_p^{*,ig} = C_{9i} + C_{10i}T^{C_{11i}} \quad \text{for } T < C_{7i} \quad (2)$$

Extended Antoine Equation (PL)

$$\ln p_i^{*,l} = C_{1i} + \frac{C_{2i}}{T+C_{3i}} + C_{4i}T + C_{5i}\ln T + C_{6i}T^{C_{7i}} \quad \text{for } C_{8i} \leq T \leq C_{9i} \quad (3)$$

Watson heat of vaporization equation (DHVL)

$$\Delta_{\text{vap}} H_i^*(T) = \Delta_{\text{vap}} H_i^*(T_1) \left( \frac{1-T/T_{ci}}{1-T_1/T_{ci}} \right)^{a_i+b_i(1-T/T_{ci})} \quad \text{for } T > T_{\text{min}} \quad (4)$$

Where:  $C_{1i} = \Delta_{\text{vap}} H_i^*(T)$ ,  $C_{2i} = T_1$ ,  $C_{3i} = a_i$ ,  $C_{4i} = b_i$  and  $C_{5i} = T_{\text{min}}$



## 2.2. Literature reviews

### 2.2.1. Synthesis of fatty acid amides

In 2012, Wang et al. studied the synthesis of palmitoylethanolamide (PEA) using vinyl palmitate as acyl donor. The results showed that 3% sodium methoxide exhibit the highest catalytic activity with the 98% yield of PEA at temperature 60 °C with 1: 20 molar ratio of vinyl palmitate to monoethanolamine for 1.5 h. After that, the reaction product was washed with water to remove excess ethanolamine [11].

In the following year, they used methyl linoleate as acyl donor to synthesize of linoleoyl ethanolamide (LEA). 97.2% yield of LEA was obtained when the optimal conditions were: 1:10 molar ratio of methyl linoleate to monoethanolamine, 15  $\mu\text{L}$ , 5.4 mol·L<sup>-1</sup> sodium methoxide in methanol, 30 °C temperature and 1 h reaction time. This study provides a higher yield and conversion than the work of Platina et al [33]. which used linoleic acid as acyl donor. The lower effectiveness when using FAs due to the formation of ion pairs with ethanolamine [20].

In 2016, they investigated the amidation of sunflower oil (87.5% oleic acid) with monoethanolamine in a solvent and solvent-free system. The reactions were carried out using 1:10 molar ratio of sunflower oil to monoethanolamine and 1%wt of sodium methoxide at 250 rpm for 3 h. The used solvents were hexane, ethane, acetone and 1:1 (v/v) of hexane/ethanol. Among these solvents, the mixed hexane/ethanol solvent provided the highest yield (90.1%) while 57.6% yield of fatty acid amide was obtained in a solvent-free system. Then, the effect of solvent volume, catalyst amount and reaction time were considered. 90.2% yield of fatty acid amide and 91.8% conversion were obtained at 1 mL solvent volume, 1.5% catalyst concentration and 4 h reaction time. The reaction product was a mixture of fatty acid amides, so it was not suitable for medicinal purposes. Finally, crystallization was used to purify the product and then high-purities of oleoyl ethanolamide (OEA) with 70.3% yield was achieved [34].

### 2.2.2. Synthesis of sucrose esters

In 2018, Gutierrez et al. studied the transesterification of sucrose with methyl palmitate for sucrose palmitate production. Various surfactants were used to enhance the compatibility of reactants. Experiments were carried out using 2.5:1 molar ratio of methyl palmitate to sucrose and 5%wt potassium carbonate as a catalyst at 33.4 kPa with a stirring speed of 700 rpm. The used surfactants were potassium palmitate (water-soluble, HLB = 20), glycerol monostearate (oil-soluble, HLB = 4) and sucrose ester (water-soluble, HLB = 15). They found that high HLB surfactants provided the final product with a high proportion of sucrose monoesters. Nevertheless, the surfactant removal process was not needed when using sucrose ester as a surfactant. In this case, the 22.86 %wt of sucrose esters (52.50%wt of monoesters in total SE) with 43.09% conversion of methyl palmitate were obtained at 409 K, 16.15%wt surfactant and 3.92 h reaction time [12].

In 2019, Chen et al. synthesized sucrose esters by transesterification of sucrose and methyl stearate in solvent-free process. The results showed that 88.2% yield of sucrose esters (selectivity: 10.4% mono, 27.1% di, 62.5% tri) and 91.4% conversion of methyl stearate were obtained when performed milling pretreatment before reaction. Reaction conditions were fixed as 1:2:0.15:0.22 molar ratio of sucrose: methyl stearate: potassium carbonate: potassium stearate (surfactant), 135 °C reaction temperature, 0.5 kPa reaction pressure, 3 h reaction time and 500 rpm stirring rate [35].

### 2.2.3. Synthesis of normal alkanes (C15 and C16)

In 2017, Yan et al. investigated the catalytic deoxygenation process of methyl palmitate over molybdenum oxide doping nickel phyllosilicate catalyst. 10%wt Methyl palmitate in hexane with excess hydrogen was fed into the reactor which was operated at 220 °C and 10 bar for 2.5 h. The results showed that 3% Mo-Ni@PSi provided full conversion of methyl palmitate with 70.0% yield of pentadecane and 28.3% yield of hexadecane. They reported that no CO<sub>2</sub> was detected in the gas-phase product; therefore, decarboxylation did not occur under this condition [13].

#### 2.2.4. Property estimation

In 2019, Sousa et al. evaluated the temperature nondependent properties of 16 fatty acids ( $C_8$  to  $C_{24}$ ) which are components of biomasses. Estimation methods for each property are presented in Table 10.

**Table 10** Method for the temperature nondependent properties estimation [36].

Property	Methods
Normal boiling point	(1) Joback and Reid, (2) Constantinou and Gani, (3) Marrero-Marejon and Pardillo-Fontdevila, (4) Marrero and Gani, (5) Nannoolal et al.
Normal melting point	(1) Joback and Reid, (2) Constantinou and Gani, (3) Marrero and Gani
Critical parameter (TC, PC and VC)	(1) Joback and Reid, (2) Constantinou and Gani, (3) Wilson and Jasperson, (4) Marrero-Marejon and Pardillo-Fontdevila, (4) Marrero and Gani, (5) Nannoolal et al.
Acentric factor	(1) Pitzer et al., (2) Lee and Kesler, (3) Watanasiri et al., (4) Ambrose and Walton, (5) Chen et al., (6) Constantinou et al.

The estimated parameters obtained from different estimation methods were compared with the values from the NIST database. From the results, the bold methods in Table 10 provide the minimum average absolute relative deviation, which means that they are the most accurate estimation methods for each property.

## CHAPTER 3

### METHODOLOGY

#### 3.1. Property estimation of palmitoylethanolamide and sucrose palmitate using Aspen Plus's built-in estimation methods

**Task 1A:** Searching for compounds which chemically similar to palmitoylethanolamide, sucrose monopalmitate and sucrose dipalmitate

Due to the lack of properties data of palmitoylethanolamide and sucrose palmitate in experimental and literature data, we could not examine the accuracy of estimation results. Thus, we needed to find similar compounds having experimental properties data to find out which estimation method provides estimation results close to the experimental data. Table 11 presents similar compounds to the three estimating compounds, and Figure 7 presents their molecular structures.

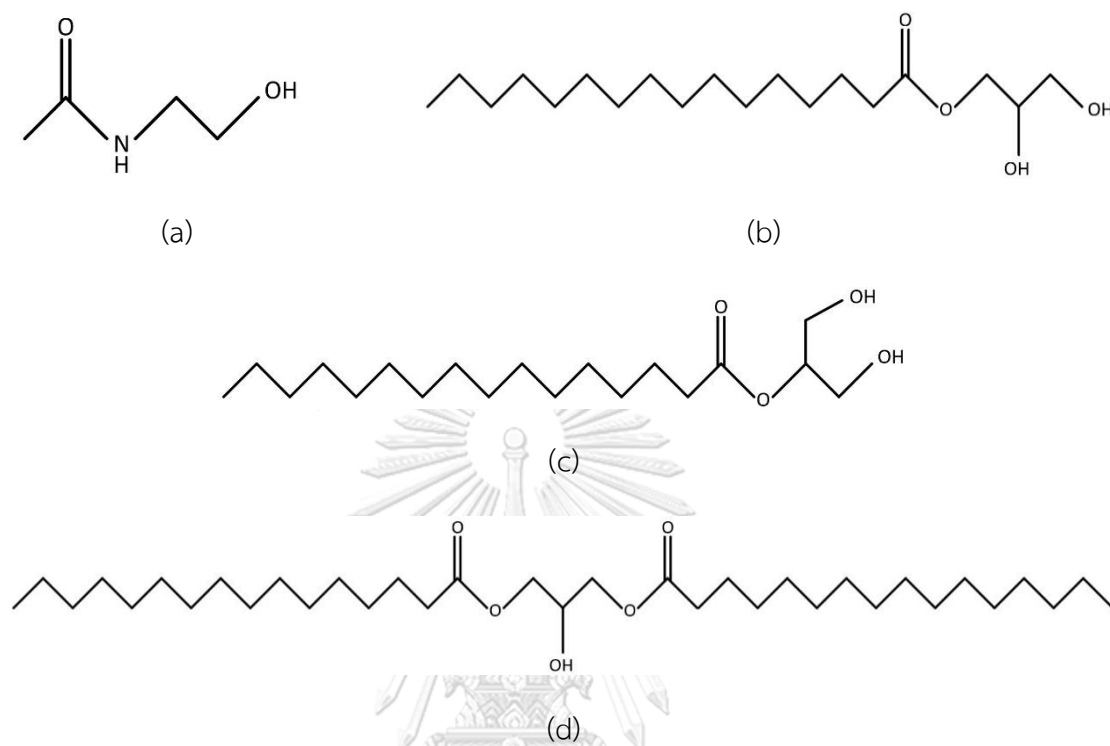
**Table 11** Similar compounds to palmitoylethanolamide and sucrose palmitate.

Estimating compound	Similar compound	Formula	M.W.	NBP (°C)
(1) Palmitoylethanolamide	2-Acetamidoethanol	C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>	103.12	296.09
(2) Sucrose monopalmitate	1-Monopalmitin	C <sub>19</sub> H <sub>38</sub> O <sub>4</sub>	330.51	421.20
	2-Monopalmitin	C <sub>19</sub> H <sub>38</sub> O <sub>4</sub>	330.51	426.17
(3) Sucrose dipalmitate	1,3-Dipalmitin	C <sub>35</sub> H <sub>68</sub> O <sub>5</sub>	568.92	543.66

**Task 2A:** Property parameters estimation of similar compounds using Aspen Plus's built-in estimation methods

In “Components” | “Specifications” | “Selection” tab, clicked on the “User Defined” button. The “User-Defined Component Wizard” window would show up as Figure 8. First, we entered the component ID and selected the type of component as the conventional type. Next, we entered the molecular structure, molecular weight and normal boiling point from Table 11. For molecular structure, we could draw the structures by ourselves or import .mol file from online databases such as ChemSpider, NIST, SciFinder<sup>n</sup>, etc., as shown in Figure 9. After that, the added components would

show up under “Molecular Structure” folder. Went to the “Structure and Functional Group” tab and clicked on “Calculate Bonds” button, as shown in Figure 10.



**Figure 7** Molecular structures of 2-Acetamidoethanol (a), 1-Monopalmitin (b), 2-Monopalmitin (c) and 1,3-Dipalmitin (d).

Figure 8 shows two screenshots of the User-Defined Component Wizard window. The left screenshot is the initial step, titled "User-Defined Component Wizard". It contains a welcome message and a form with "Component ID: 2-ACETAM" and "Type: Conventional" selected. Below this, it lists "Required properties for conventional components include: Molecular weight, normal boiling point, molecular structure, vapor pressure and ideal gas heat capacity". The right screenshot is the "Basic data for conventional component" step. It shows "Component ID: 2-ACETAM" and "Alias" fields. Under "Enter molecular structure", there are buttons for "Draw/Import/Edit structure" and "Define molecule by its connectivity". The "Enter available property data" section includes input fields for "Molecular weight" (296.09), "Normal boiling point" (103.14) with a unit dropdown set to "C", and "Ideal gas enthalpy of formation" and "Ideal gas Gibbs energy of formation" both with unit dropdowns set to "cal/mol".

**Figure 8** User-Defined Component Wizard window.

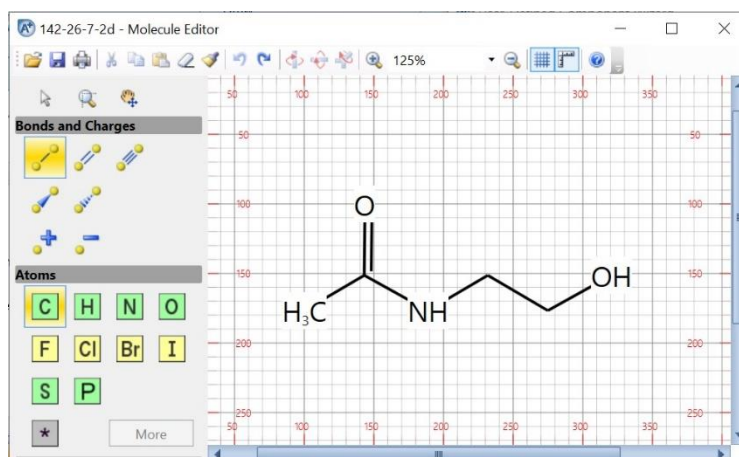


Figure 9 Molecule Editor window.

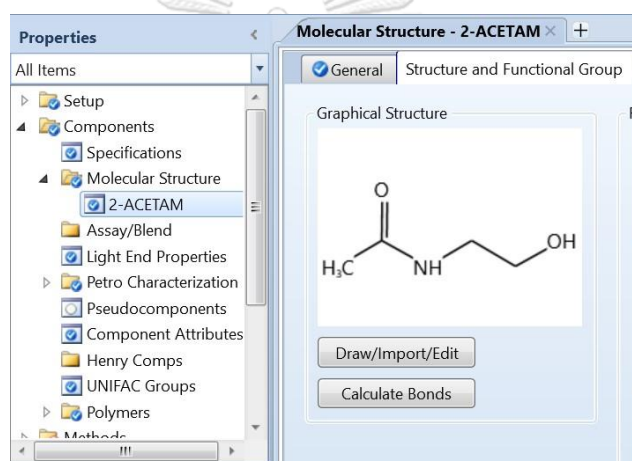


Figure 10 Molecular structure window.

Then, we switched the run mode to “Estimation”. In “Estimation” | “Input” | “Setup” tab, we chose “Estimate only the selected parameters” option and selected “Pure component scalar parameters” and “Pure component temperature-dependent property correlation parameters” in the check box. For “Pure component” and “T-Dependent” tabs, selected similar compound and all Aspen Plus's built-in estimation methods for each property parameter, as discussed in Chapter 2. Finally, clicked run the property estimation. The estimation results would display on the “Estimation” | “Results” tab sheet. Figure 11 and 12 show the example of estimating the critical temperature of 2-Acetamidoethanol.

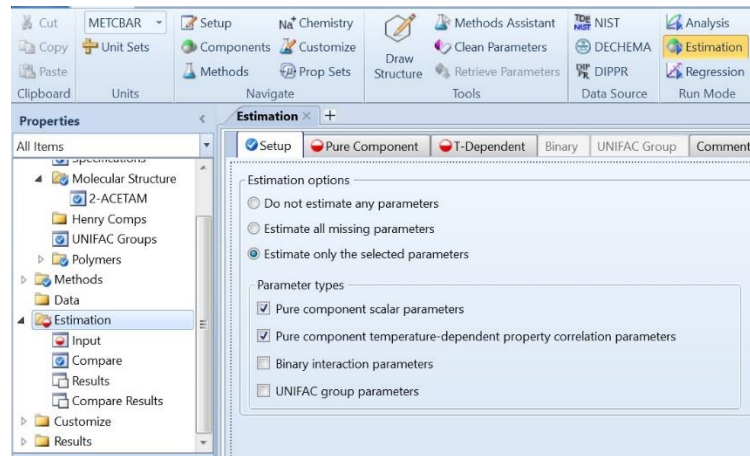


Figure 11 Estimation window.

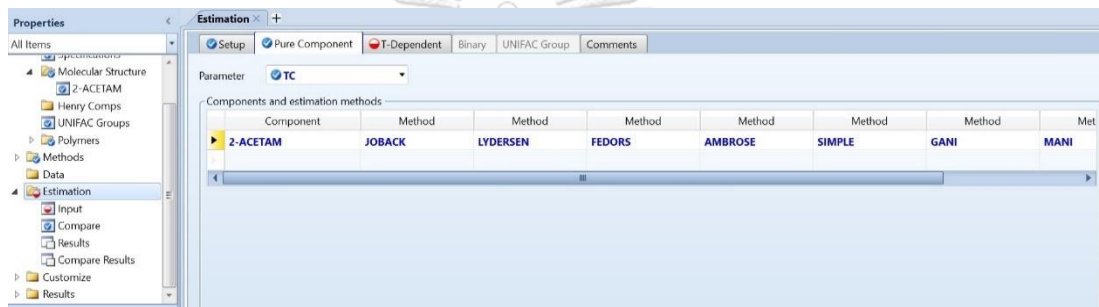


Figure 12 Estimating critical temperature of 2- Acetamidoethanol.

**Task 3A:** Comparing the estimation results to the experimental data of each property

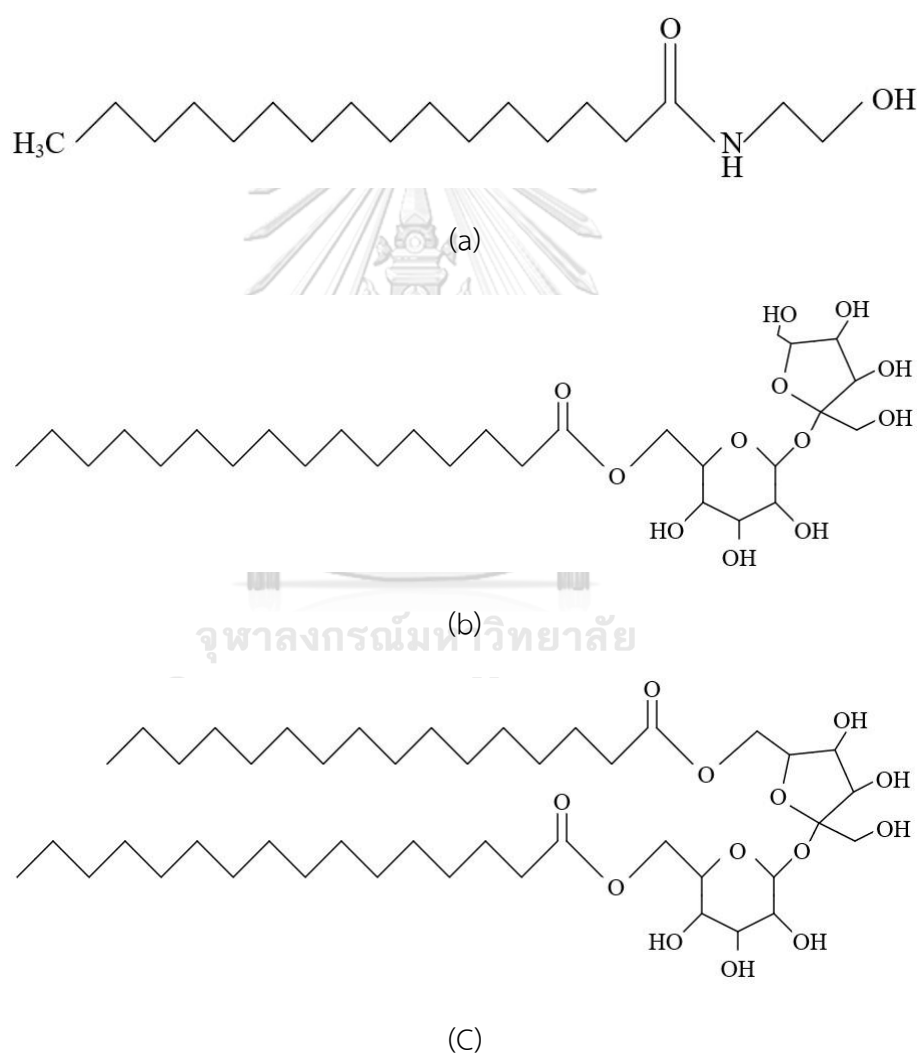
In this work, we compared the estimation results to the property parameters retrieved from databanks available in the Aspen Physical Property System. NIST-TRC Databank was used for 2-Acetamidoethanol and 1,3-Dipalmitin. Meanwhile, BIODIESEL databank was used for Monopalmitin. We compared the accuracy of each estimation method in terms of the absolute deviation (AD) and the absolute relative deviation (ARD) [36] as defined in equation (5) and (6). The estimation methods with the lowest AD and ARD values for each property would be used to estimate property parameters of palmitoylethanolamide and sucrose palmitate.

$$\text{Absolute deviation (AD)} = \left| \text{estimated value} - \text{experimental value} \right| \quad (5)$$

$$\text{Absolute relative deviation (ARD)} = \left| \frac{\text{estimated value} - \text{experimental value}}{\text{experimental value}} \right| \quad (6)$$

**Task 4A:** Property parameters estimation of palmitoylethanolamide and sucrose palmitate

We estimated the property parameters using the best estimation methods from task 3A by the procedure as for task 2A. The minimum required information such as molecular structure, molecular weight and normal boiling point are presented in Figure 13 and Table 12. Lastly, the estimated parameters were used for the simulation of palmitoylethanolamide and sucrose palmitate production processes.



**Figure 13** Molecular structures of palmitoylethanolamide (a), sucrose monopalmitate (b) and sucrose dipalmitate (c).



**Table 12** Properties of palmitoylethanolamide and sucrose palmitate [37].

Estimating compound	Formula	M.W.	NBP (°C)	Reference
(1) Palmitoylethanolamide	C <sub>15</sub> H <sub>37</sub> NO <sub>2</sub>	299.4919	461.5±28.0	ChemSpider
(2) Sucrose monopalmitate	C <sub>28</sub> H <sub>52</sub> O <sub>12</sub>	580.7053	744.9±60.0	ChemSpider
(3) Sucrose dipalmitate	C <sub>44</sub> H <sub>82</sub> O <sub>13</sub>	819.1273	863.2±65.0	ChemSpider

### 3.2. Conceptual process design

#### Task 1B: Data collection

The objective of task 1B was to define feed and product specifications such as purity, price and storage condition. Appendix B presents feed and product properties and specifications for the three production processes.

Moreover, reaction information was collected, such as the molar ratio of reactants, temperature, pressure, catalyst, solvent, reaction time, main reaction, side reaction, conversion and yield. The specifications of the reactor units were based on reaction information obtained from open literature, as presented in Table 13 – 15.

**Table 13** Reaction information for the palmitoylethanolamide production process.

Operating condition	Wang et al. [11]
Reaction	Amidation of methyl palmitate with monoethanolamine
Catalyst	3%wt sodium methoxide
Molar ratio of reactants	20: 1 of monoethanolamine to methyl palmitate
Temperature	60 °C
Pressure	Atmospheric pressure
Reaction time	1.5 h
Conversion	100% conversion of methyl palmitate
Reaction pathway	MP + MEA → PEA + MeOH

**Table 14** Reaction information for the sucrose palmitate production process.

Operating condition	Gutierrez et al. [12]
Reaction	Transesterification of methyl palmitate with sucrose
Catalyst	5%wt potassium carbonate
Surfactant	16.15%wt sucrose palmitate
Molar ratio of reactants	2.5: 1 of methyl palmitate to sucrose
Temperature	136 °C
Pressure	0.334 bar
Reaction time	3.92 h
Conversion	43.09% conversion of methyl palmitate
Yield	22.86%wt of sucrose palmitate (52.50% Mono-SE)
Reaction pathway	Sucrose + MP $\rightarrow$ Mono-SE + MeOH Mono-SE + MP $\rightarrow$ Di-SE + MeOH

**Table 15** Reaction information for the normal alkanes production process.

Operating condition	Yan et al. [13]
Reaction	Deoxygenation of methyl palmitate with hydrogen
Catalyst	3% Mo-Ni@PSi
Molar ratio of reactants	14: 1 of hydrogen to methyl palmitate [38]
Temperature	220 °C
Pressure	10 bar
Reaction time	2.5 h
Conversion	100% conversion of methyl palmitate
Yield	70.0%wt of pentadecane and 28.3% of hexadecane
Reaction pathway	MP + H <sub>2</sub> $\rightarrow$ Palmitic acid + CH <sub>4</sub> Palmitic acid + H <sub>2</sub> $\rightarrow$ Hexadecanal + H <sub>2</sub> O Hexadecanal $\rightarrow$ Pentadecane + CO Hexadecanal + H <sub>2</sub> $\rightarrow$ Hexadecanol Hexadecanol + H <sub>2</sub> $\rightarrow$ Hexadecane + H <sub>2</sub> O

**Task 2B:** Simple mass balance

The objective of task 2B was to perform an input-output structure and block flow diagram, which is composed of the reactor feed preparation system, reactor system, phase separation system and separation system. Besides, calculate a mass balance for all streams, including recycle streams, as shown in Appendix C.

**Task 3B:** Process flowsheet generation

The objective of task 3B was to define all unit operations in each system and their operating conditions such as temperature, pressure, reaction conversion and separation factor.

**Task 4B:** Process simulation

The objective of task 4B was to perform a simulation of the three production processes using Aspen Plus V11 software based on the information from the previous steps. The most appropriate property methods for each simulation were considered using the decision trees by Eric C. Carlson [39]. Lastly, we obtained the base case design with stream tables.

**Task 5B:** Equipment sizing and costing

The objective of task 5B was to perform equipment sizing and costing for the major equipment using Aspen Plus Process Economic Analyzer. First, we matched the equipment type with each unit operation in the flowsheet. After that, we clicked on “Evaluate Project” button to continue the sizing and costing calculations.

**Task 6B:** Economic analysis

The objective of task 6B was to evaluate economic profitability using Aspen Plus Process Economic Analyzer. In this work, we compared the three production processes in terms of discounted present value (DPV), discounted payback period (DPP) and discounted cash-flow rate of return (DCFROR). Moreover, we studied the sensitivity analysis by varying methyl palmitate purchasing cost, products selling prices and total

project cost. Table 16 and 17 provide the cost of utilities and the main parameters used for the economic analysis.

**Table 16** Cost of utilities [6].

Utility	Description	Cost (USD) for unit	Unit
Cooling tower water	inlet temperature = 35 °C outlet temperature = 50 °C	0.378	GJ
Refrigerated water	inlet temperature = 5 °C outlet temperature = 15 °C	4.77	GJ
Glycol solution	available at -13.7 °C	8.49	GJ
Low-pressure steam	5 barg, 160 °C	4.54	GJ
High-pressure steam	41 barg, 254 °C	5.66	GJ
Dowtherm	available at 400 °C	13.88	GJ
Electricity	-	0.0674	kWh
Air supply	3.3 barg (50 psig)	0.005	std m <sup>3</sup>
Process water	1/3 cost of potable water	0.177	tonne

**Table 17** Investment analysis parameters.

Parameter	Value
Project lifetime	20 years
Number of week per year	52 weeks
Tax rate	40%
Interest rate/Desired rate of return	20%
Working capital	5% of fixed capital investment
Operating charge	25% of operating labor costs
Plant overhead	50% of operating labor and maintenance costs
General and administrative costs	8% of subtotal operating costs

## CHAPTER 4

### RESULTS AND DISCUSSION

This chapter presents the results and interpretation of the results obtained from property estimation and conceptual process design of the three production processes. The contents are divided into six sections, as follows.

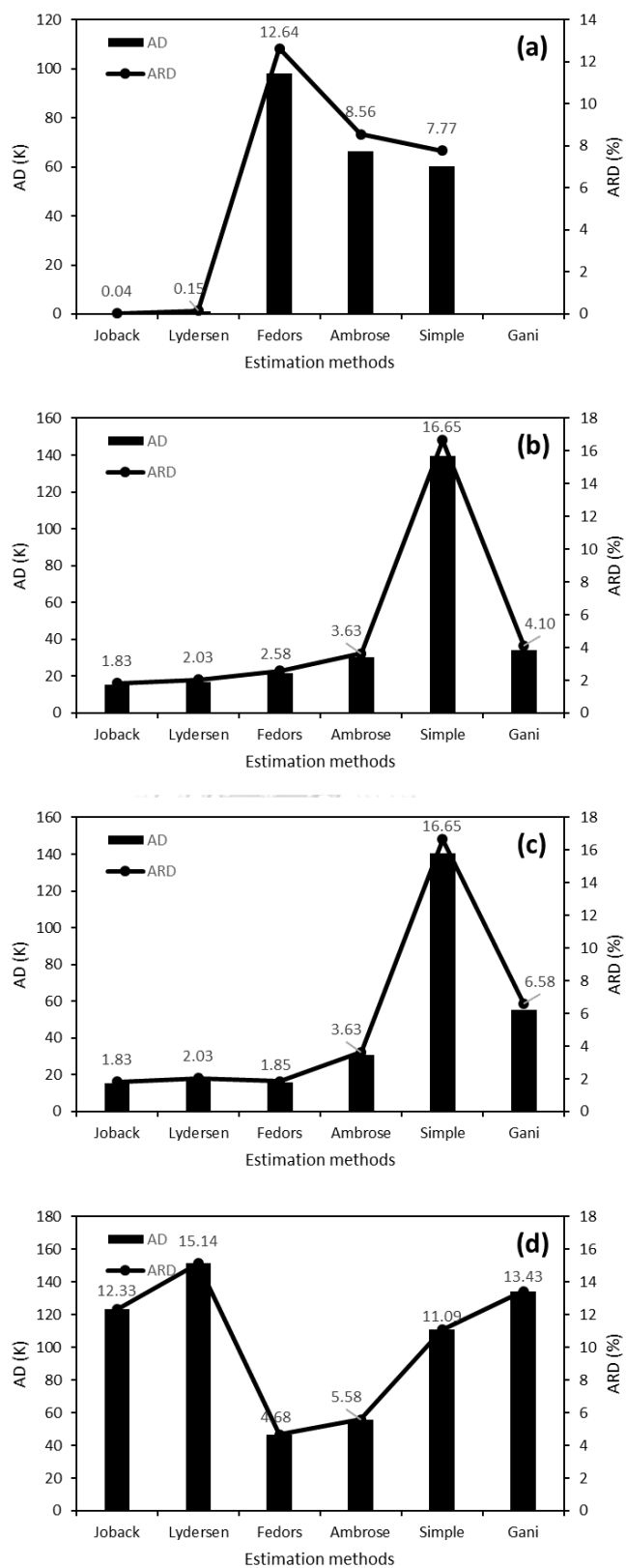
#### 4.1. Property estimation of the similar compounds

In this section, we summarized the comparison between the estimation results and the data retrieved from Aspen databanks. Figure 14 – 20 present in terms of the absolute deviation (AD) and the absolute relative deviation (ARD). Meanwhile, the property parameters obtained from estimation methods are presented in Appendix F.

##### 4.1.1. Critical temperature (TC)

From Figure 14 (a), the critical temperature of 2-Acetamidoethanol could not be estimated using GANI method because of missing group contribution values for some functional groups. In terms of deviations, Joback method provided less error than other methods for 2-Acetamidoethanol and Monopalmitin, as shown in Figure 14 (a), (b) and (c). Joback, Lydersen, Ambrose and Gani methods had similar accuracy (0.7 – 1.5%) [40]. All of the methods, except Gani method, used molecular structure and normal boiling point as input information. Whereas, Gani method used only molecular structure. The second-order groups account for the effect of neighboring atoms that make it has higher accuracy. However, Joback method was recommended for the broadest range of compounds except for silicon groups because it easiest to use [26].

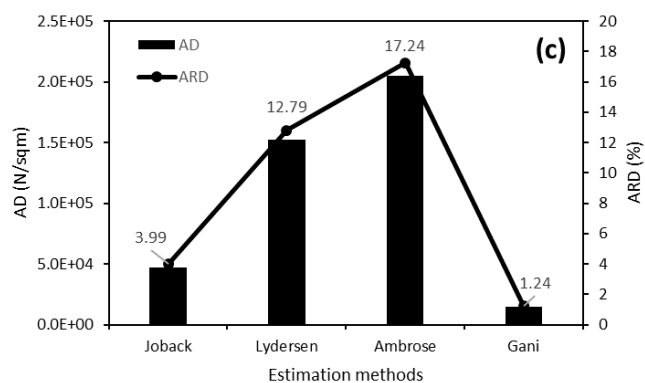
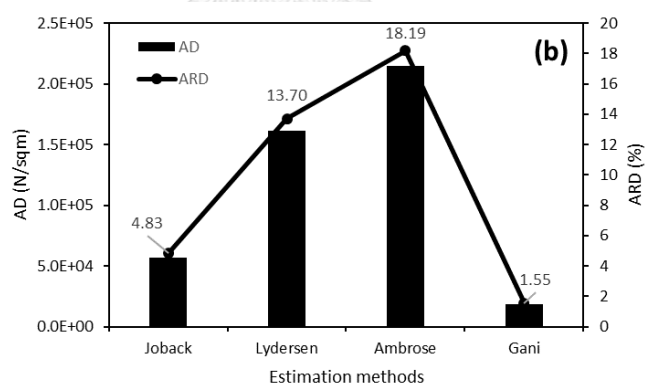
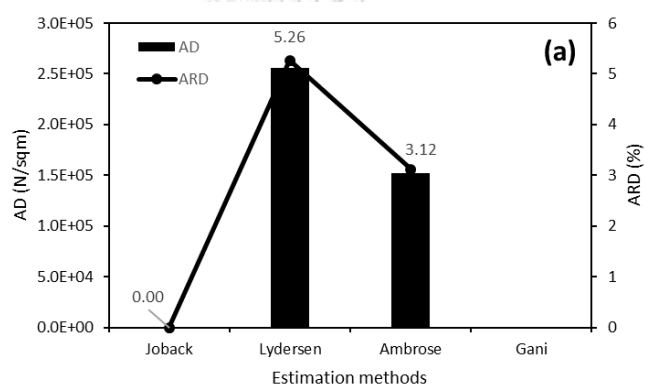
For 1,3-Dipalmitin compound, Fedors method showed the least deviation with 4.68% ARD, as shown in Figure 14 (d). This result is consistent with the work of Yener [41], who reported that Fedors and Ambrose methods provided the most accurate estimated results for long-chain lipids, especially for triglycerides.

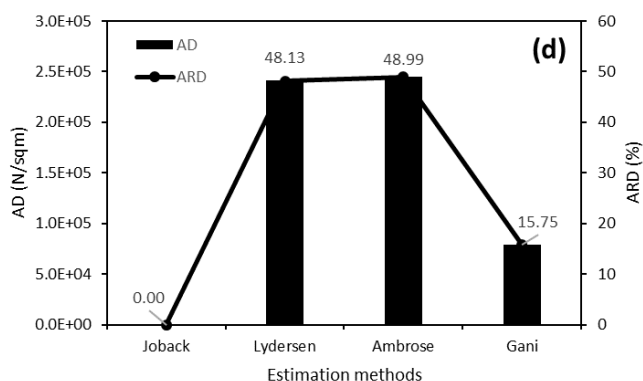


**Figure 14** Deviations of critical temperature estimation methods for 2-Acetamidoethanol (a), 1-Monopalmitin (b), 2-Monopalmitin (c) and 1,3-Dipalmitin (d).

#### 4.1.2. Critical pressure (PC)

Likewise, Gani method could not be used to predict the critical pressure of 2-Acetamidoethanol. As shown in Figure 15, Joback method gave the lowest deviations for 2-Acetamidoethanol and 1,3-Dipalmitin. Meanwhile, Gani method provided the best results for Monopalmitin. Tahami et al. [42] reported that Joback method and Gani methods presented the similar %AARD for nitrogen compounds (23.40%, 18.13%) and esters (5.46%, 5.11%). We thought that these two methods could be used to estimate the critical pressure because the deviations were not significant differences.





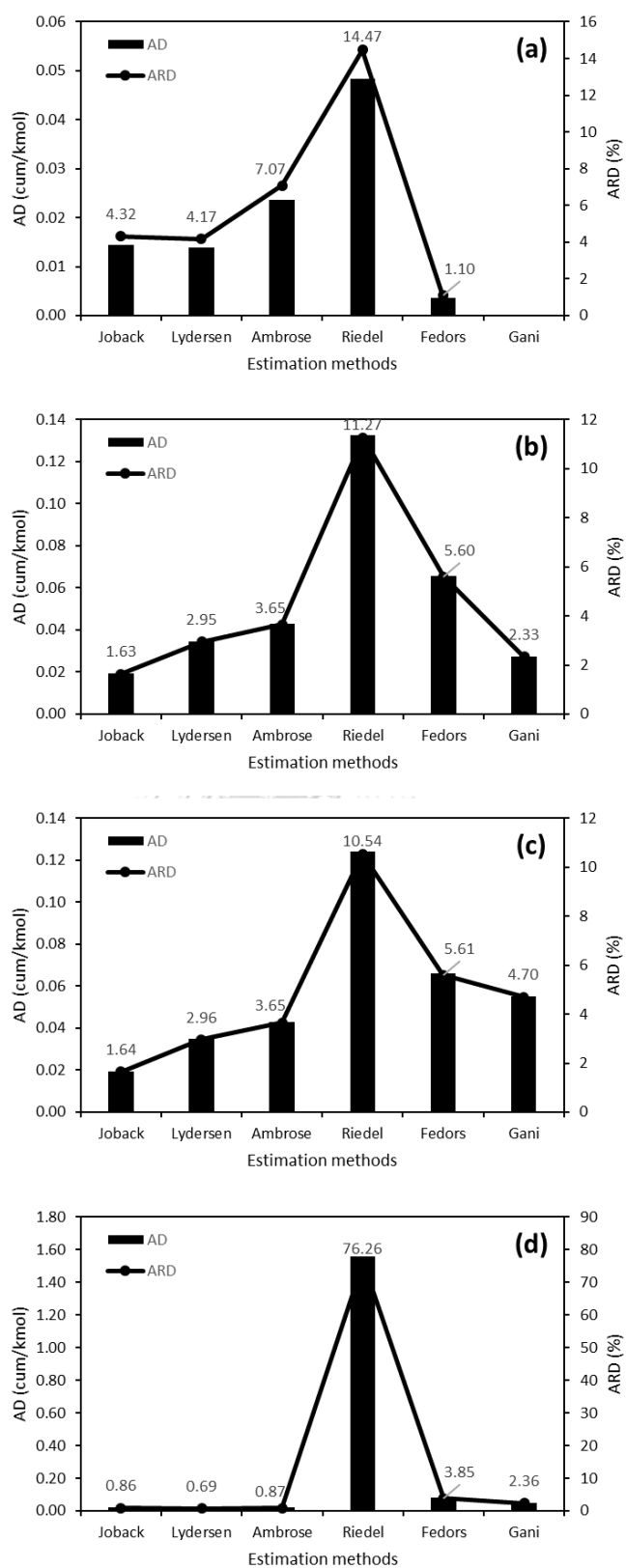
**Figure 15** Deviations of critical pressure estimation methods for 2-Acetamidoethanol (a), 1-Monopalmitin (b), 2-Monopalmitin (c) and 1,3-Dipalmitin (d).

#### 4.1.3. Critical volume (VC)

Riedel method required normal boiling point, critical temperature and critical pressure for critical volume estimation. We used the critical temperature estimated from Joback method for 2-Acetamidoethanol and Monopalmitin and Fedors method for 1,3-Dipalmitin. Meanwhile, we used critical pressure estimated from Joback method for 2-Acetamidoethanol and 1,3-Dipalmitin and Gani method for Monopalmitin. These selected methods were the methods giving the lowest deviations for each property. However, Riedel method gave the most considerable deviations for all compounds, as shown in Figure 16. This might happen because the Riedel method was recommended for hydrocarbon only [25].

As the same reason, Gani method also could not be used to estimate the critical volume of 2-Acetamidoethanol. The results showed that Fedors, Joback and Lydersen methods provided the lowest deviations for 2-Acetamidoethanol, Monopalmitin and 1,3-Dipalmitin, respectively. Sastri et al. [43] reported that these three methods gave a similar average absolute deviation (3.6 - 3.8%) for non-hydrocarbons. Whereas, Ambrose method provided less accuracy compared to Joback method.

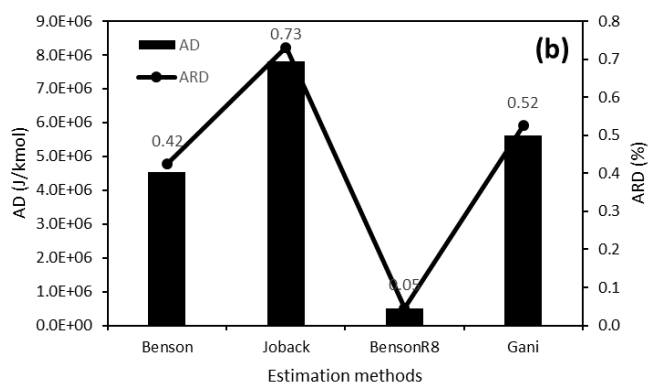
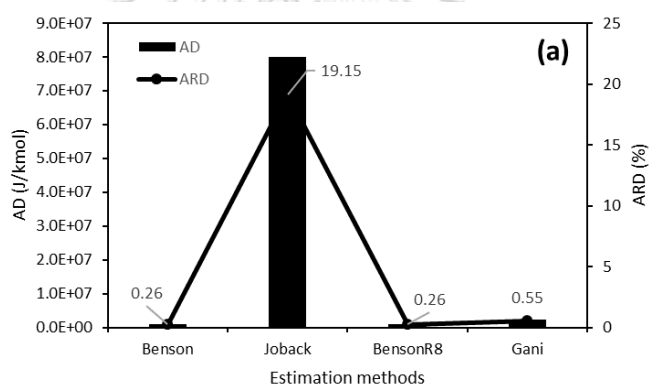


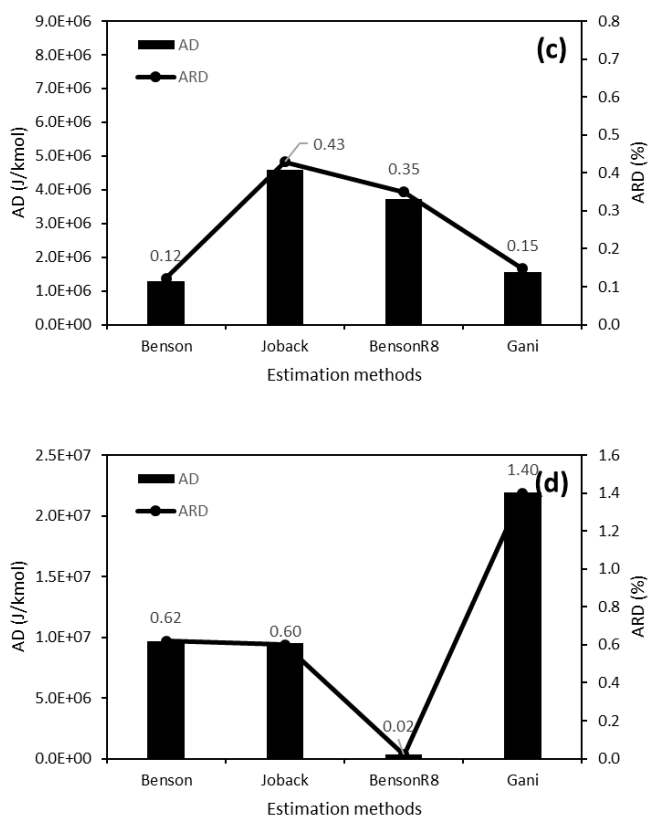


**Figure 16** Deviations of critical volume estimation methods for 2-Acetamidoethanol (a), 1-Monopalmitin (b), 2-Monopalmitin (c) and 1,3-Dipalmitin (d).

#### 4.1.4. Standard heat of formation (DHFORM)

As shown in Figure 17 (b) and (c), Benson and BensonR8 gave the lowest deviations for 1-Monopalmitin and 2-Monopalmitin. We would consider in term of the sum of squares of absolute deviation to compare these two methods. The result showed that BensonR8 provided the lower SSE, so we used this method for sucrose monopalmitate estimation. In Figure 17 (d), BensonR8 was the most accurate method for 1,3-Dipalmitin. For 2-Acetamidoethanol, the deviations from Benson and BensonR8 methods were equal. Therefore, we chose BensonR8 method like other compounds for further estimating. These estimation results were the same as described in [25], that Benson and BensonR8 methods gave higher accuracies than Joback and Gani methods.

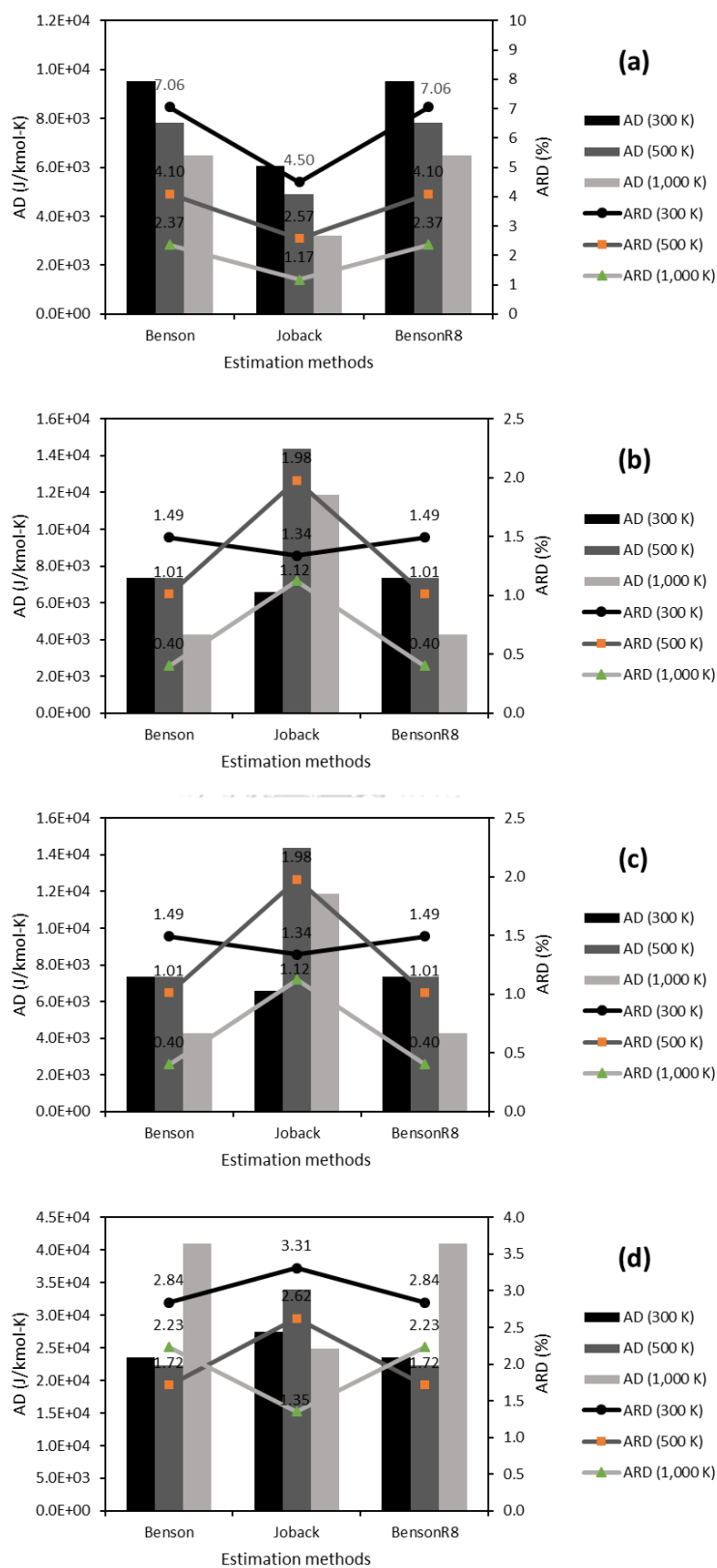




**Figure 17** Deviations of standard heat of formation estimation methods for 2-Acetamidoethanol (a), 1-Monopalmitin (b), 2-Monopalmitin (c) and 1,3-Dipalmitin (d).

#### 4.1.5. Ideal gas heat capacity (CPIG)

From Figure 18, the results of ideal gas heat capacity estimation are presented at various temperatures (300, 500 and 1,000 K). We would compare each method in term of the sum of squares of absolute deviation. The results showed that the Joback method gave the least SSE for 2-Acetamidoethanol and 1,3-Dipalmitin. On the contrary, Benson method provided the least SSE for Monopalmitin. However, these methods could be used to predict ideal gas heat capacity because they gave similar accurate results (1.1 – 1.4% ARD) [25].

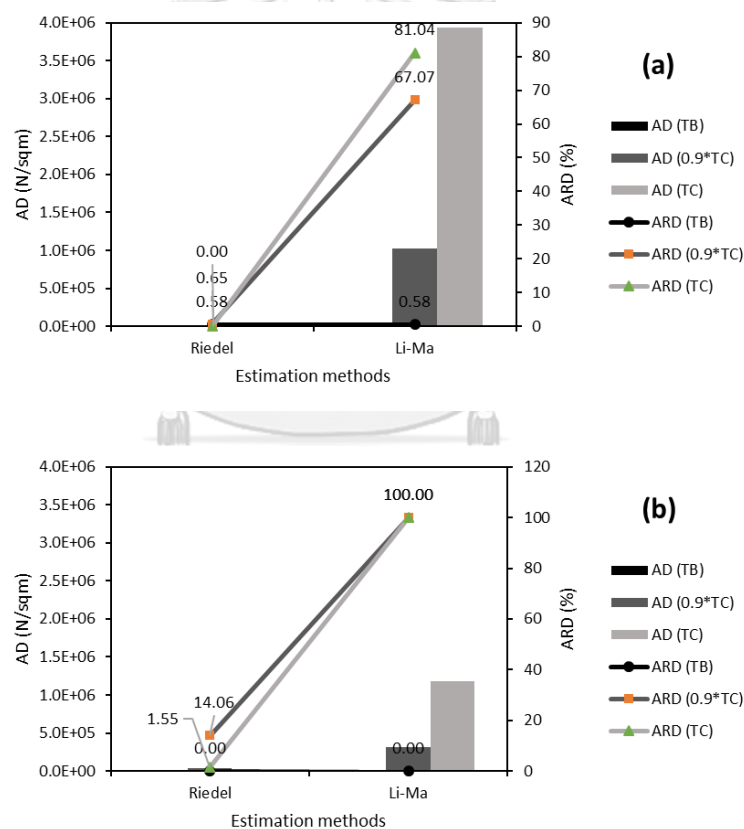


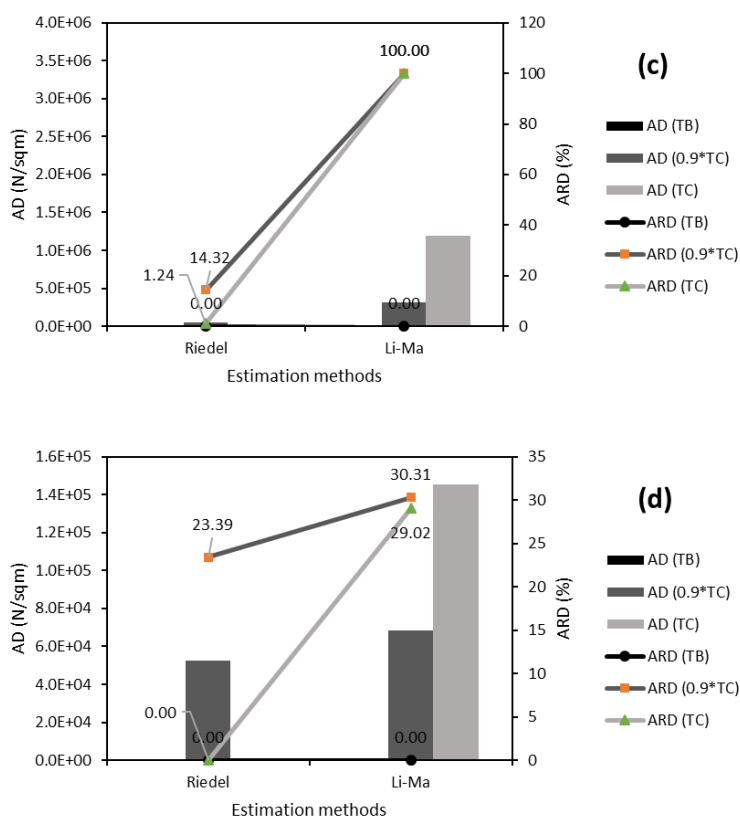
**Figure 18** Deviations of ideal gas heat capacity estimation methods for 2-Acetamidoethanol (a), 1-Monopalmitin (b), 2-Monopalmitin (c) and 1,3-Dipalmitin (d).

#### 4.1.6. Vapor pressure (PL)

Riedel method required normal boiling point, critical temperature and critical pressure for vapor pressure estimation. The values of these critical properties were obtained from the same methods as described in 4.1.3. From Figure 19, Riedel method provided lower deviations for all components at 0.9 of critical temperature and critical temperature.

These results were the same as in the work of Vlad et al [44]. They reported that Riedel method presented the more accurate vapor pressure than Li-Ma method for methyl oleate (Ester) when the normal boiling point was known.





**Figure 19** Deviations of vapor pressure estimation methods for 2-Acetamidoethanol (a), 1-Monopalmitin (b), 2-Monopalmitin (c) and 1,3-Dipalmitin (d).

#### 4.1.7. Enthalpy of vaporization (DHVL)

Enthalpy of vaporization can be calculated by definition, as presented in Table 9. The values of critical temperature and critical pressure were obtained from the same methods used in Riedel method as described in 4.1.3. For vapor pressure, we used the values estimated from the Riedel method for all compounds.

From Figure 20, The definition method gave the lowest deviations for all compounds. Whereas, Ducros method could not be used to estimate this property parameter for 2-Acetamidoethanol because of missing group contribution values for some functional groups.

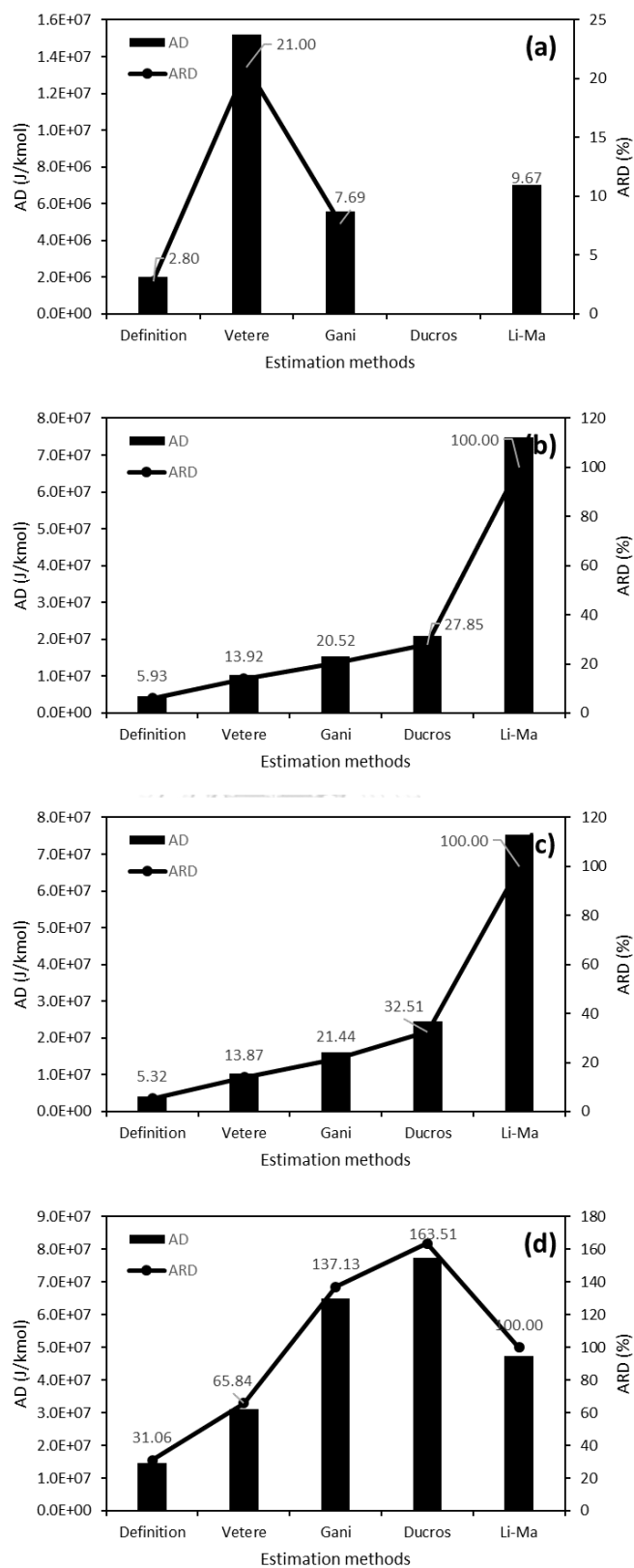


Figure 20 Deviations of enthalpy of vaporization (at TB) estimation methods for 2-Acetamidoethanol (a), 1-Monopalmitin (b), 2-Monopalmitin (c) and 1,3-Dipalmitin (d).

From the results, we would select the best estimation methods with the lowest AD and ARD values for estimating the properties of palmitoylethanolamide and sucrose palmitate. Table 18 summarizes the most appropriate method for each property and each compound.

**Table 18** The best methods for estimating the properties of palmitoylethanolamide and sucrose palmitate.

Property name	Parameter	PEA	MONO-SE	DI-SE
Critical temperature	TC	Joback	Joback	Fedors
Critical pressure	PC	Joback	Gani	Joback
Critical volume	VC	Fedors	Joback	Lydersen
Standard heat of formation	DHFORM	BensonR8	BensonR8	BensonR8
Ideal gas heat capacity	CPIG	Joback	Benson	Joback
Vapor pressure	PL	Riedel	Riedel	Riedel
Enthalpy of vaporization	DHVL	Definition	Definition	Definition

## 4.2. Property estimation of palmitoylethanolamide and sucrose palmitate

### 4.2.1. Palmitoylethanolamide

From Table 18, we used these property methods to estimate each property parameter. Table 19 and 20 present estimated pure component constants and temperature-dependent properties for palmitoylethanolamide.

**Table 19** Estimated pure component constants for palmitoylethanolamide.

Property name	Estimation method	Estimated value	Unit
Critical temperature	Joback	900	K
Critical pressure	Joback	1.296E+06	N/sqm
Critical volume	Fedors	1.076	cum/kmol
Standard heat of formation	Benson	-6.990E+08	J/kmol



**Table 20** Estimated temperature-dependent properties for palmitoylethanolamide.

Parameter	Ideal gas heat capacity	Vapor pressure	Enthalpy of vaporization
Estimation method	Joback	Riedel	Definition
$C_{1i}$	-2,034	147	7.943E+07
$C_{2i}$	1,796	-21,390	735
$C_{3i}$	-1.016	0	0.404
$C_{4i}$	2.143E-04	0	-0.948
$C_{5i}$	0	-16.1	735
$C_{6i}$	0	1.242E-18	-
$C_{7i}$	280	6	-
$C_{8i}$	1,100	735	-
$C_{9i}$	36,029	900	-
$C_{10i}$	83.2	-	-
$C_{11i}$	1.5	-	-
Temperature unit	K	K	K
Property unit	J/(kmol·K)	N/sqm	J/kmol

#### 4.2.2. Sucrose monopalmitate

From Table 18, we could not use GANI method to estimate the critical pressure of sucrose monopalmitate because of missing group contribution values for some functional groups. Thus, we replaced it with the Joback method, which had the second smallest AD and ARD values. Table 21 and 22 present estimated pure component constants and temperature-dependent properties for sucrose monopalmitate.

**Table 21** Estimated pure component constants for sucrose monopalmitate.

Property name	Estimation method	Estimated value	Unit
Critical temperature	Joback	2,014	K
Critical pressure	Joback	1.045E+06	N/sqm
Critical volume	Joback	1.688	cum/kmol
Standard heat of formation	BensonR8	-2.485E+09	J/kmol

**Table 22** Estimated temperature-dependent properties for sucrose monopalmitate.

Parameter	Ideal gas heat capacity	Vapor pressure	Enthalpy of vaporization
Estimation method	Benson	Riedel	Definition
$C_{1i}$	-86,421	-18.6	1.327E+07
$C_{2i}$	3,453	1,059	1,018
$C_{3i}$	-2.33	0	0.294
$C_{4i}$	5.931E-04	0	-2.642
$C_{5i}$	0	4.20	407
$C_{6i}$	0	-2.190E-22	-
$C_{7i}$	280	6	-
$C_{8i}$	1,100	1,018	-
$C_{9i}$	36,029	2,014	-
$C_{10i}$	144	-	-
$C_{11i}$	1.5	-	-
Temperature unit	K	K	K
Property unit	J/(kmol·K)	N/sqm	J/kmol

#### 4.2.3. Sucrose dipalmitate

Likewise, the property parameters of palmitoylethanolamide were predicted by the best estimation methods, as presented in Table 18. Table 23 and 24 present estimated pure component constants and temperature-dependent properties for sucrose dipalmitate.

**Table 23** Estimated pure component constants for sucrose dipalmitate.

Property name	Estimation method	Estimated value	Unit
Critical temperature	Joback	1,083	K
Critical pressure	Joback	4.496E+05	N/sqm
Critical volume	Joback	2.558	cum/kmol
Standard heat of formation	BensonR8	-2.982E+09	J/kmol

**Table 24** Estimated temperature-dependent properties for sucrose dipalmitate.

Parameter	Ideal gas heat capacity	Vapor pressure	Enthalpy of vaporization
Estimation method	Joback	Riedel	Definition
C <sub>1i</sub>	-28,909	-724	3.850E-07
C <sub>2i</sub>	4,569	1.1325E+05	758
C <sub>3i</sub>	-2.577	0	0.081
C <sub>4i</sub>	5.345E-04	0	2.096
C <sub>5i</sub>	0	91	303
C <sub>6i</sub>	0	-1.795E-18	-
C <sub>7i</sub>	280	6	-
C <sub>8i</sub>	1,100	758	-
C <sub>9i</sub>	36,029	1,083	-
C <sub>10i</sub>	219	-	-
C <sub>11i</sub>	1.5	-	-
Temperature unit	K	K	K
Property unit	J/(kmol·K)	N/sqm	J/kmol

#### 4.2.4. Solid-phase

Palmitoylethanolamide and sucrose palmitate remained in the solid phase at the end of processes. Thus, the simulations would require solid property parameters such as solid molar volume ( $V_S$ ), solid heat capacity (CPS) and solid standard enthalpy of formation (DHSFRM). Since Aspen Plus has no estimation method for solid molar volume, we would retrieve the data from the ChemSpider database, as shown in Table 25. For solid heat capacity and solid standard enthalpy of formation, only the Mostafa method is available for predicting these values. Table 26 and 27 present the solid properties estimated by Mostafa method.

**Table 25** Solid molar volume for palmitoylethanolamide and sucrose palmitate.

Compound	Solid molar volume	Unit	Reference
Palmitoylethanolamide	329.0	cc/mol	ChemSpider
Sucrose monopalmitate	456.3	cc/mol	ChemSpider
Sucrose dipalmitate	717.9	cc/mol	ChemSpider

**Table 26** Estimated solid heat capacity for palmitoylethanolamide and sucrose palmitate.

Parameter	PEA	MONO-SE	DI-SE
Estimation method	Mostafa	Mostafa	Mostafa
$C_{1i}$	4.082E+05	8.494E+05	1.167E+06
$C_{2i}$	1,061	1,459	2,324
$C_{3i}$	-0.057	-0.067	-0.113
$C_{4i}$	0	0	0
$C_{5i}$	-1.179E+10	-2.440E+10	-3.315E+10
$C_{6i}$	0	0	0
$C_{7i}$	280	280	280
$C_{8i}$	1,100	1,100	1,100
Temperature unit	K	K	K
Property unit	J/kmol	J/kmol	J/kmol

**Table 27** Estimated solid standard enthalpy of formation for palmitoylethanolamide and sucrose palmitate.

Compound	Estimation method	Estimated value	Unit
Palmitoylethanolamide	Mostafa	-5.437E+08	J/kmol
Sucrose monopalmitate	Mostafa	-4.060E+09	J/kmol
Sucrose dipalmitate	Mostafa	-4.149E+09	J/kmol

### 4.3. Conceptual process design

#### 4.3.1. Process description of palmitoylethanolamide production

Process flow diagram for the production of palmitoylethanolamide is shown in Figure 21. Fresh methyl palmitate (Stream 1) with a feed rate of 100,000 tonnes per year is mixed with fresh stream and recycle stream of monoethanolamine (Stream 2 and 4) in a liquid mixing tank (D-101). The temperature of the liquid mixture is adjusted to reaction temperature in a heat exchanger (E-101) before sent to the reactor (R-201). The operating conditions of the reactor are presented in Table 13. Next, the reactor effluent is sent to a vacuum distillation column (C-301) to remove the methanol by-product. The liquid bottom stream is mixed with the fresh water in a liquid mixing tank (D-401). The aqueous stream containing the desired product is cooled to a temperature of 6 °C through a heat exchanger (E-401) before sent to a crystallizer (CR-401). In the crystallizer, palmitoylethanolamide is converted from a liquid state to a solid-state. After that, the solid is isolated from the liquid by a filter (F-401). The liquid stream containing monoethanolamine and water is passed through a pump (P-401) and sent to a distillation column (D-401). The distillate product stream, which consists of water, is removed from the process. Meanwhile, monoethanolamine in the bottom stream is delivered to a pressure reducing valve (V-101) and recycled back to the mixing tank. Because some of the liquids remain in the solid stream, a dryer (DR-401) is used to evaporate these liquid compounds. Finally, we obtained 112,995 tonnes per year of 98%wt palmitoylethanolamide (Stream 21). Stream table of the process and summary of unit operating conditions are summarized in Appendix D.

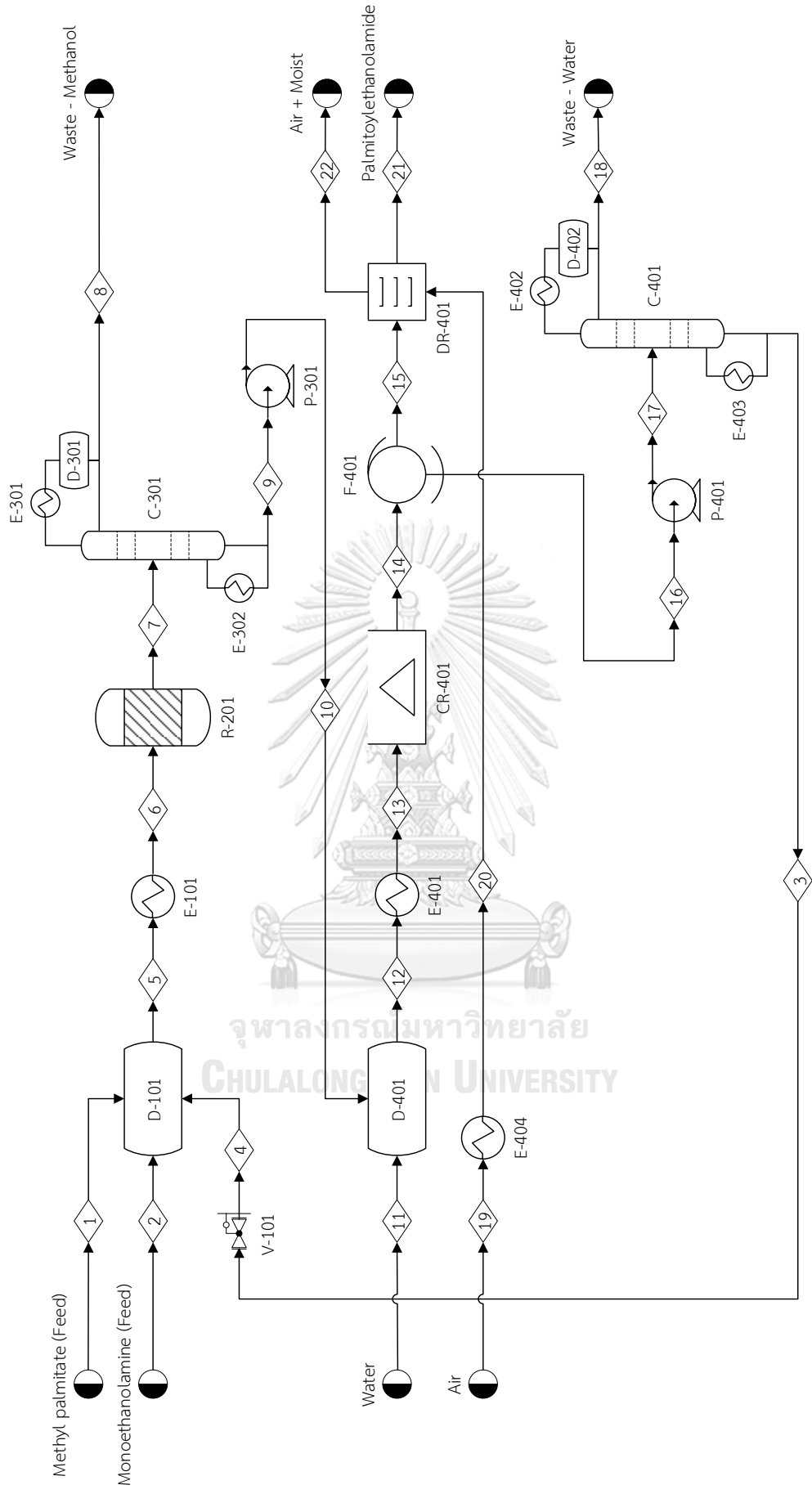


Figure 21 Process flow diagram for the production of palmitoylethanolamide.

#### 4.3.2. Process description of sucrose palmitate production

Process flow diagram for the production of sucrose palmitate is presented in Figure 22. 100,000 tonnes per year of methyl palmitate (Stream 1) are fed into a liquid mixing tank (D-101), which it is mixed with sucrose, sucrose palmitate (surfactant) and the recycled methyl palmitate (Stream 2, 3 and 5). This liquid mixture is sent to a pressure reducing valve (V-101) and a heat exchanger (E-101) to bring it to reaction pressure and temperature before entering a reactor (R-201). The operating conditions of the reactor are presented in Table 14. The outlet stream of the reactor is delivered to a flash drum (D-301) to remove methanol vapor. Then, the liquid effluent from D-301 is adjusted to room pressure and temperature by passing a pump (P-301) and a heat exchanger (E-301). For the product purification, this step is divided into 3 sub-steps. (1) Methyl palmitate separation: Ethyl acetate, which is used to extract the unreacted methyl palmitate, is mixed with the stream 13 in a mixing tank (D-401). After that, the solid and liquid are separated from each other by a filter (F-401). The liquid stream containing the unreacted methyl palmitate and ethyl acetate is sent to a distillation column (C-401). These two compounds are separated and then recycled to D-101 and D-403, respectively. Meanwhile, the solid stream is sent to the evaporator (EV-401) to vaporize the remaining ethyl acetate. The ethyl acetate vapor is condensed in a condenser (E-404) and then mixed with the ethyl acetate from C-401 in a mixing tank (D-402) before it recycles back to D-401. The solid is then cooled to the room temperature in a heat exchanger (E-405) and sent to the next sub-steps. (2) Sucrose separation: Water is added to dissolve the unreacted sucrose, and the additional sucrose is used to decrease the solubility of sucrose palmitate in water. Water, sucrose and the solid are mixed in a mixing tank (D-404). The aqueous solution is removed from the process by a filter (F-402). Next, the solid stream containing the desired product is delivered to (3) the drying process to remove the remaining water by a dryer (DR-401). Finally, we obtained 164,510 tonnes per year of 98%wt sucrose palmitate (Stream 34). These products consisted of sucrose monopalmitate and sucrose dipalmitate. Stream table of the process and summary of unit operating conditions are summarized in Appendix D.

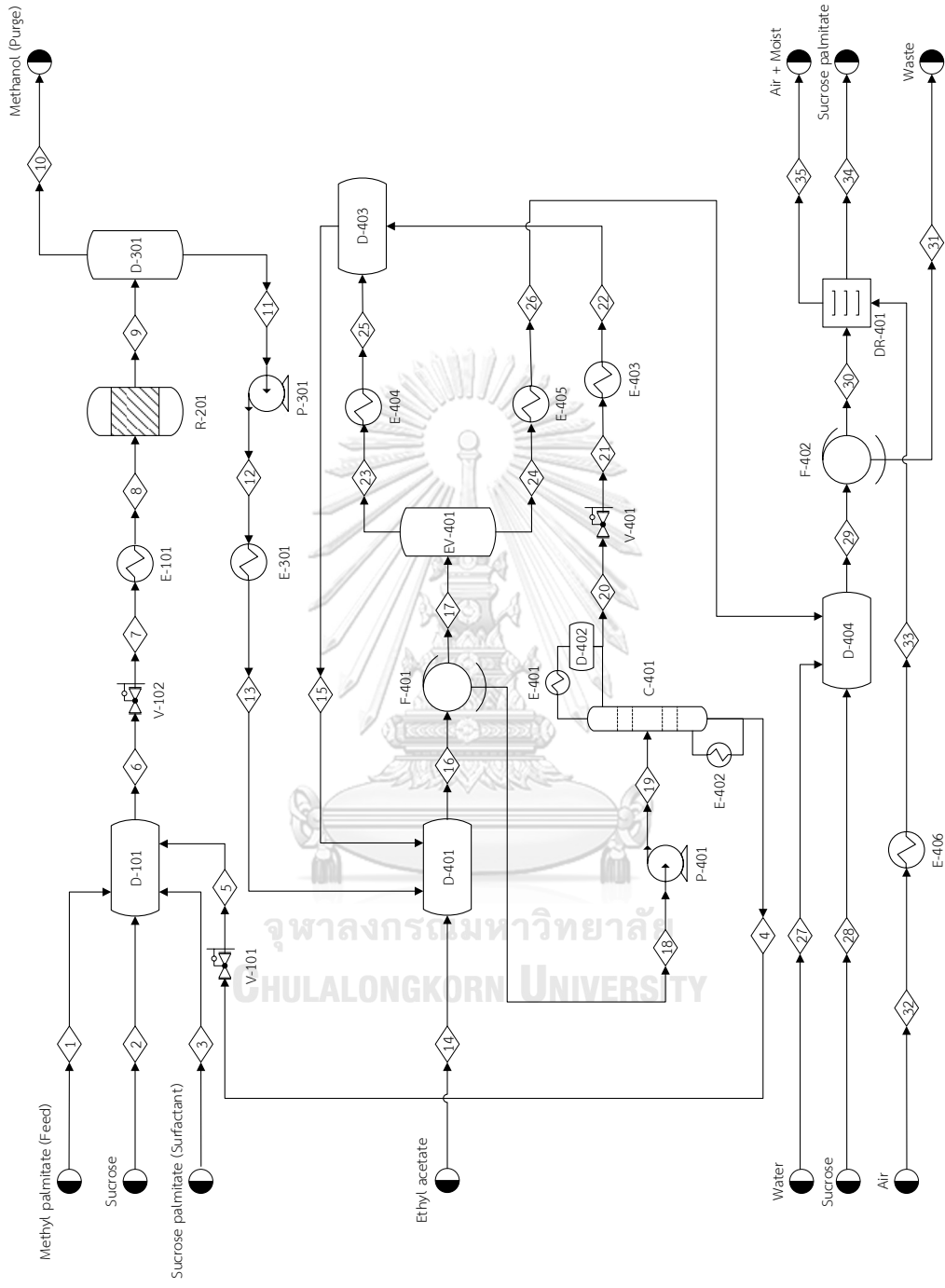


Figure 22 Process flow diagram for the production of sucrose palmitate.



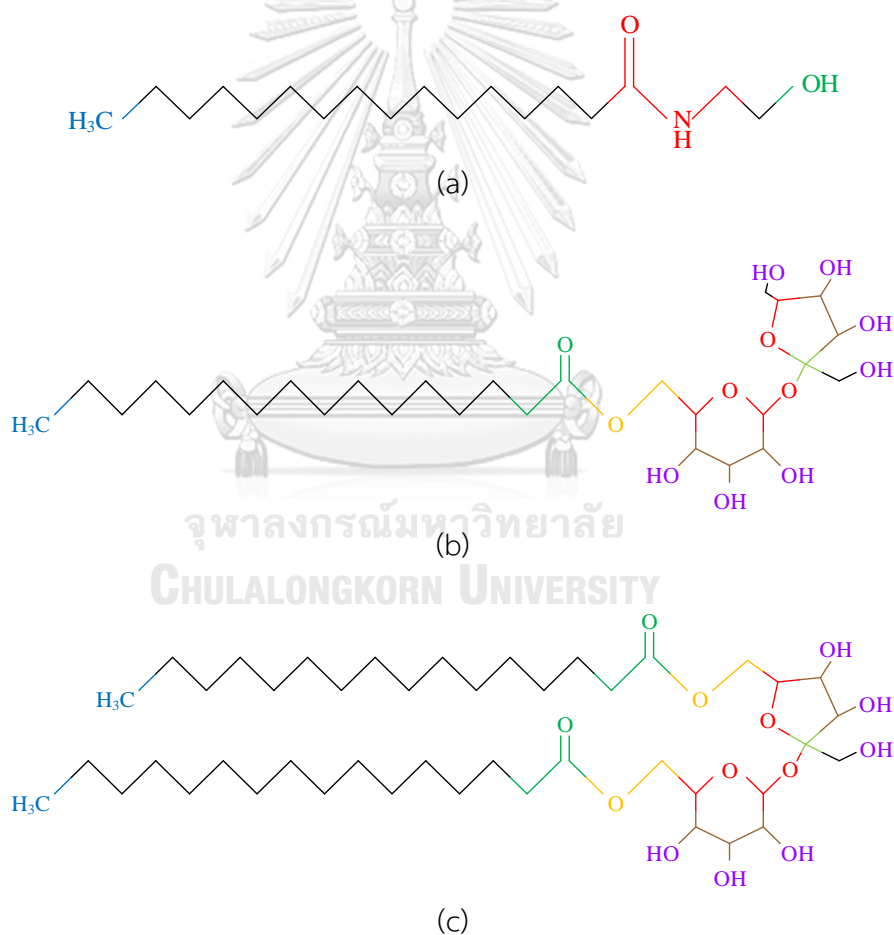
### 4.3.3. Process description of normal alkanes production

Figure 23 present the process flow diagram for the production of normal alkanes. Methyl palmitate with a feed rate of 100,000 tonnes/year (Stream 4) and recycled hexadecanol and palmitic acid (Stream 6) is fed to a liquid mixing tank (D-101). The liquid mixture is flowed through a pump (P-101) to increase the pressure as required in the reactor. Meanwhile, the hydrogen feed (Stream 1) is passed through a pressure reducing valve (V-101). The gas and liquid streams are mixed and then heated in a heat exchanger (E-101) before sent to the reactor (R-201). The operating conditions of the reactor are presented in Table 15. The reaction product stream is cooled in a heat exchanger (E-301) and then delivered to flash drum (D-301 and D-302) to separate the gas phase from the liquid phase. After that, the gaseous stream consisting mainly of the unreacted hydrogen is split into two streams: purge and recycle streams. The Purge stream is removed from the process to avoid an accumulation of by-products (CO and CH<sub>4</sub>), whereas the remaining stream is recycled back to the front end of this process. The two liquid streams from the flash drums are mixed in a mixing tank (D-303) and followed by a decanter (D-404) to remove water. The liquid mixture stream is then passed through a pressure reducing valve (V-401) and sent to a distillation column (C-401) equipped with a partial condenser. The vapor distillate stream, which consists of light gases (H<sub>2</sub>, CO and CH<sub>4</sub>), is removed from the process. The bottom product stream is delivered to the next distillation column (D-402). This column separates the desired products from hexadecanol and palmitic acid. These unreacted intermediates are recycled back to D-101 through a pressure reducing valve (V-102). The distillate product is delivered to a pump (P-401) and then sent to a final distillation column (C-403). Purified pentadecane and hexadecane streams are adjusted to the storage conditions via pressure-reducing valves (V-402 and V-403) and heat exchangers (E-407 and E-408). Finally, we obtained 55,448 and 24,612 tonnes per year of 99%wt pentadecane (Stream 31) and hexadecane (Stream 33), respectively. Stream table of the process and summary of unit operating conditions are summarized in Appendix D.



#### 4.3.4. Thermodynamics model selection

For the production of palmitoylethanolamide and sucrose palmitate, these processes contain some of the polar compounds, and no electrolytes are presented. According to the decision trees by Eric C. Carlson [39], activity coefficient models are preferred for these low-pressure systems. Since palmitoylethanolamide and sucrose palmitate are non-databank components, binary parameters are not available. Thus, we chose the UNIFAC method for these process simulations. The UNIFAC method uses the group contributions to predict the interaction parameters; hence we needed to add the group contributions of these products, as follows.



**Figure 24** The UNIFAC groups of palmitoylethanolamide (a), sucrose monopalmitate (b) and sucrose dipalmitate (c).

**Table 28** The UNIFAC groups of palmitoylethanolamide.

Group	Group number	Number of occurrences
CH2	1010	15
CH3	1015	1
OH (P)	1200	1
CONHCH2	3560	1

**Table 29** The UNIFAC groups of sucrose monopalmitate and sucrose dipalmitate.

Group	Group number	Number of occurrences	
		Sucrose monopalmitate	Sucrose dipalmitate
C	1000	1	1
CH	1005	5	5
CH2	1010	15	27
CH3	1015	1	2
OH (P)	1200	7	6
CH2CO	1400	1	2
CH-O	1605	3	3
CH2O	1610	1	2

For the production of normal alkanes, this simulation contains some of the polar compounds, and no electrolytes are presented. All components in this system are available in Aspen Plus, so they have the binary parameters in the databanks. According to the decision tree, we chose the PENG-ROB as the property method for the high-pressure ( $\geq 10$  bar) unit operations and the NRTL method for the remaining units. Moreover, Henry parameters are required because the supercritical gases ( $H_2$ ,  $CO$ , and  $CH_4$ ) are presented in this simulation.

#### 4.3.5. Value-added chemicals production yield

The feed rate of methyl palmitate was set equal to 100,000 tonnes per year for each process. Figure 25 presents the comparison of product yield from the three processes. The results showed that the sucrose palmitate production gave the highest product yield, followed by palmitoylethanolamide and normal alkanes, respectively. Considering the selling prices of products, even the price of sucrose palmitate was lower than palmitoylethanolamide and hexadecane, the total annual product sales of the sucrose palmitate production were still highest.

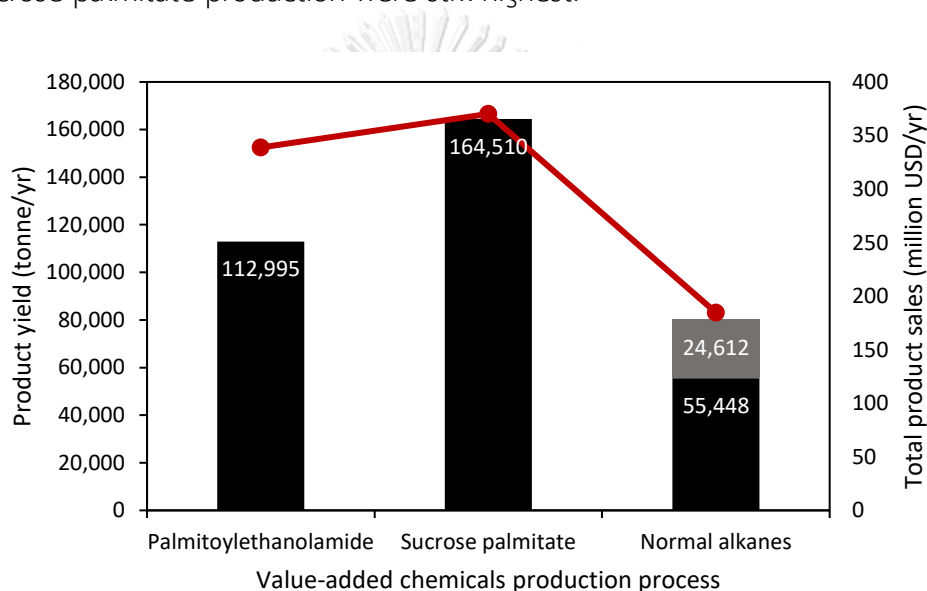


Figure 25 Product yield by 100,000 tonnes of methyl palmitate feedstock.

#### 4.4. Economic analysis

Table 30 summarized the sales and expenses for each process. Considering the total project cost, palmitoylethanolamide production is the most expensive process. This was caused by the high costs of crystallizer (CR-401), distillation column (C-401), and reboiler (E-403), as shown in Appendix E. These unit operations were larger than in other processes because of much higher inlet mass flow rates. Moreover, the total annual utilities cost of this process also higher than others. The cost of high-pressure steam influenced this cost because of the high energy consumption required in a reboiler (E-403). Even though palmitoylethanolamide's selling price was the highest,

this process had lower sales and higher expenses than the production of sucrose palmitate. This meant that the production of palmitoylethanolamide was not as economically attractive as sucrose palmitate production.

On the contrary, the production of normal alkanes was the cheapest process. This process had the lowest total equipment purchasing cost, although it had more equipment than other processes. The solvent did not present in this process that might cause smaller sizes of unit operations. Besides, this reduced the total annual raw material cost. Unfortunately, this alternative produced less amount of the primary product than other processes. The selling price of pentadecane was also the cheapest. When considering in terms of the annual profit, this process provided the lowest value.

For the production of sucrose palmitate, this alternative provided the most considerable sales with 370 million USD. In contrast, it had the second-largest total capital investment and total annual operating costs. Table 31 shows that sucrose palmitate production was the optimal alternative in terms of the highest discounted present value (DPV), lowest discounted payback period (DPP), and highest discounted cash-flow rate of return (DCFROR). The second and third attractive processes were the production of palmitoylethanolamide and normal alkanes, respectively.

Summary of sales and expenses for the three processes.

Item	Palmitoylethanolamide	Sucrose palmitate	Normal alkanes
<b>Gross profit margin (USD)</b>	170,000,000	220,000,000	41,000,000
<b>Total annual product sales (USD)</b>	339,000,000	370,000,000	185,000,000
Total equipment purchasing cost (USD)	7,820,000	3,680,000	3,340,000
Total equipment direct cost (USD)	15,500,000	10,200,000	7,070,000
Escalated project cost (USD)	37,200,000	28,000,000	21,500,000
Working capital (USD)	1,860,000	1,400,000	1,080,000
<b>Total capital investment, TCI (USD)</b>	<b>39,100,000</b>	<b>29,400,000</b>	<b>22,600,000</b>
Total annual raw material cost (USD)	172,000,000	186,000,000	144,000,000
Total annual operating labor cost (USD)	1,080,000	1,240,000	920,000
Total annual maintenance cost (USD)	479,000	239,000	321,000
Total annual utilities cost (USD)	46,700,000	21,800,000	4,630,000
Total annual operating charges (USD)	270,000	310,000	230,000
Total annual plant overhead (USD)	780,000	740,000	621,000
Total annual general and administrative costs (USD)	17,700,000	27,000,000	12,100,000
<b>Total annual operating costs (USD)</b>	<b>239,000,000</b>	<b>237,000,000</b>	<b>163,000,000</b>

**Table 30** Summary of the economic performances of the three processes.

Indicator	Palmitoylethanolamide	Sucrose palmitate	Normal alkanes
DPV (USD)	327,000,000	451,000,000	64,600,000
DPP (year)	3.10	2.97	7.15
DCFROR (%)	87.96	96.47	35.13

#### 4.5. Comparing the results with other literature

For the production of normal alkanes, we compared the economic analysis results with other literature. For example, we compared the total equipment direct cost with the work of Kantama et al. [45]. They studied the production of hydrogenated renewable diesel from palm fatty acid distillate (PFAD) with the feed rate of 17,250 tonnes/yr. The unit operation of their process also similar to our work. However, the feed rate was not equal to our work, so we should use the cost curve method, as presented in equation 7. The comparison of total equipment direct cost is shown in Table 32. We found that these values are similar.

$$\frac{\text{Cost A}}{\text{Cost B}} = \left( \frac{\text{Size A}}{\text{Size B}} \right)^{0.6} \quad (7)$$

**Table 31** The comparison of the total equipment direct cost.

	Our work	Kantama et al.
Total equipment direct cost (USD)	7,070,000	8,950,000



#### 4.6. Sensitivity analysis

In this work, a sensitivity analysis was conducted to study the effects of three variables such as methyl palmitate purchasing cost, products selling prices and total project cost. The results were compared in terms of DPV, DPP and DCFROR.

##### 4.6.1. Effect of variation of methyl palmitate purchasing cost

According to biodiesel prices reported by the Ministry of Energy of Thailand, the biodiesel price for the last 5 years was in the range of 19.32 to 42.10 bath/litre. This meant that it varied from -32% to 48% of the average price. Therefore, we studied the change of methyl palmitate purchasing cost between -50% to 50% of the original value (700 to 2,100 USD/tonne).

Figure 26 to 28 present the effect of methyl palmitate purchasing cost for the three production processes. The NPV value decreased by 46 – 51 million USD per 10% increased in methyl palmitate cost for palmitoylethanolamide and sucrose palmitate production processes. Meanwhile, the DPP values were less than 10 years, and the DCFROR values were more than 20% at the highest cost of methyl palmitate. This meant that these processes still kept profitable even if methyl palmitate purchasing cost would change from the original value.

For the production of normal alkanes, at methyl palmitate cost above 1,540 USD (10%), the NPV value would become negative. This process could not recover the total investment costs within 20 years. The results showed that this alternative was the most sensitive for the variation of the methyl palmitate purchasing cost.

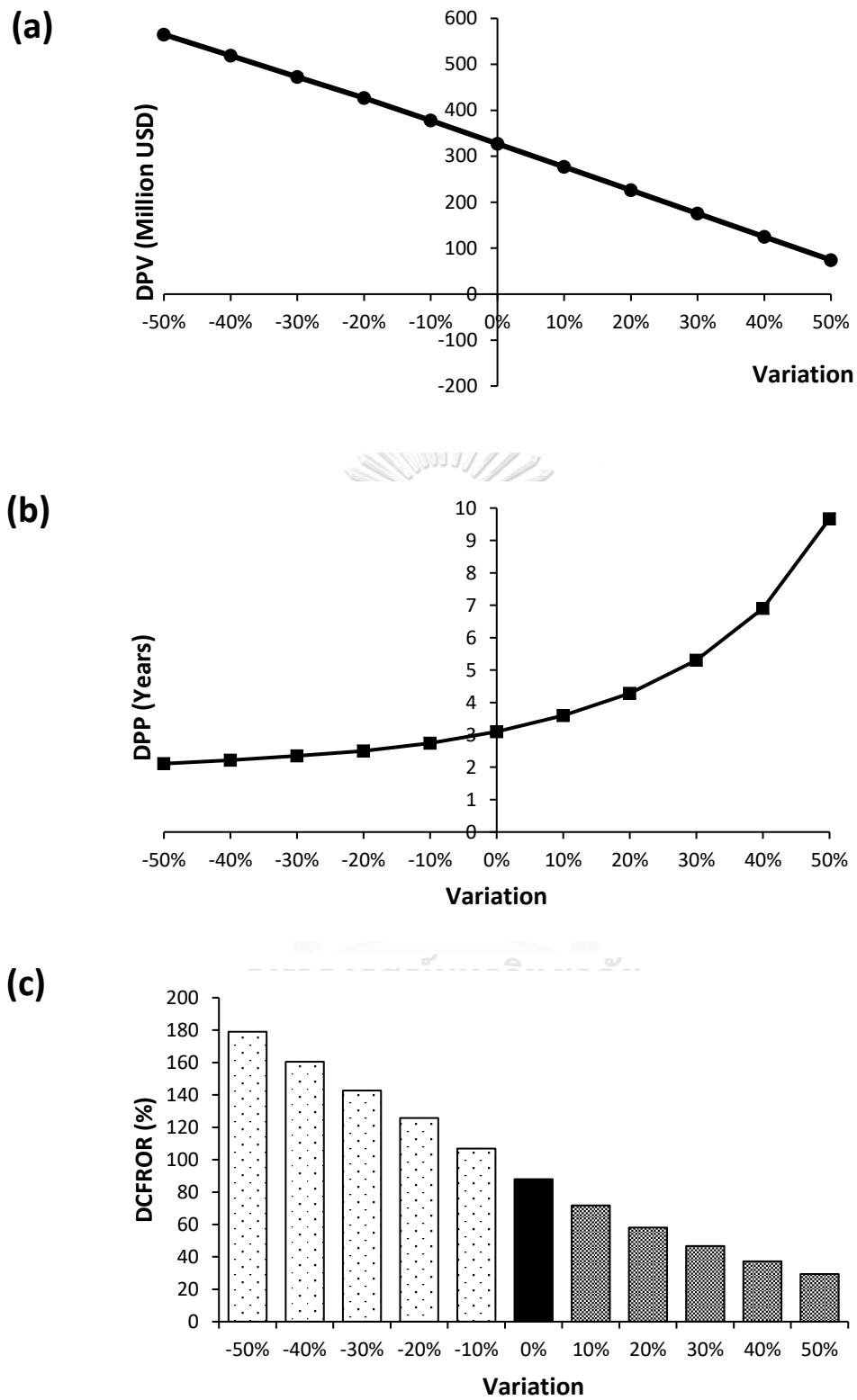


Figure 26 The effect of methyl palmitate purchasing cost on DPV (a), DPP (b) and DCFROR (c) for palmitoylethanolamide production.

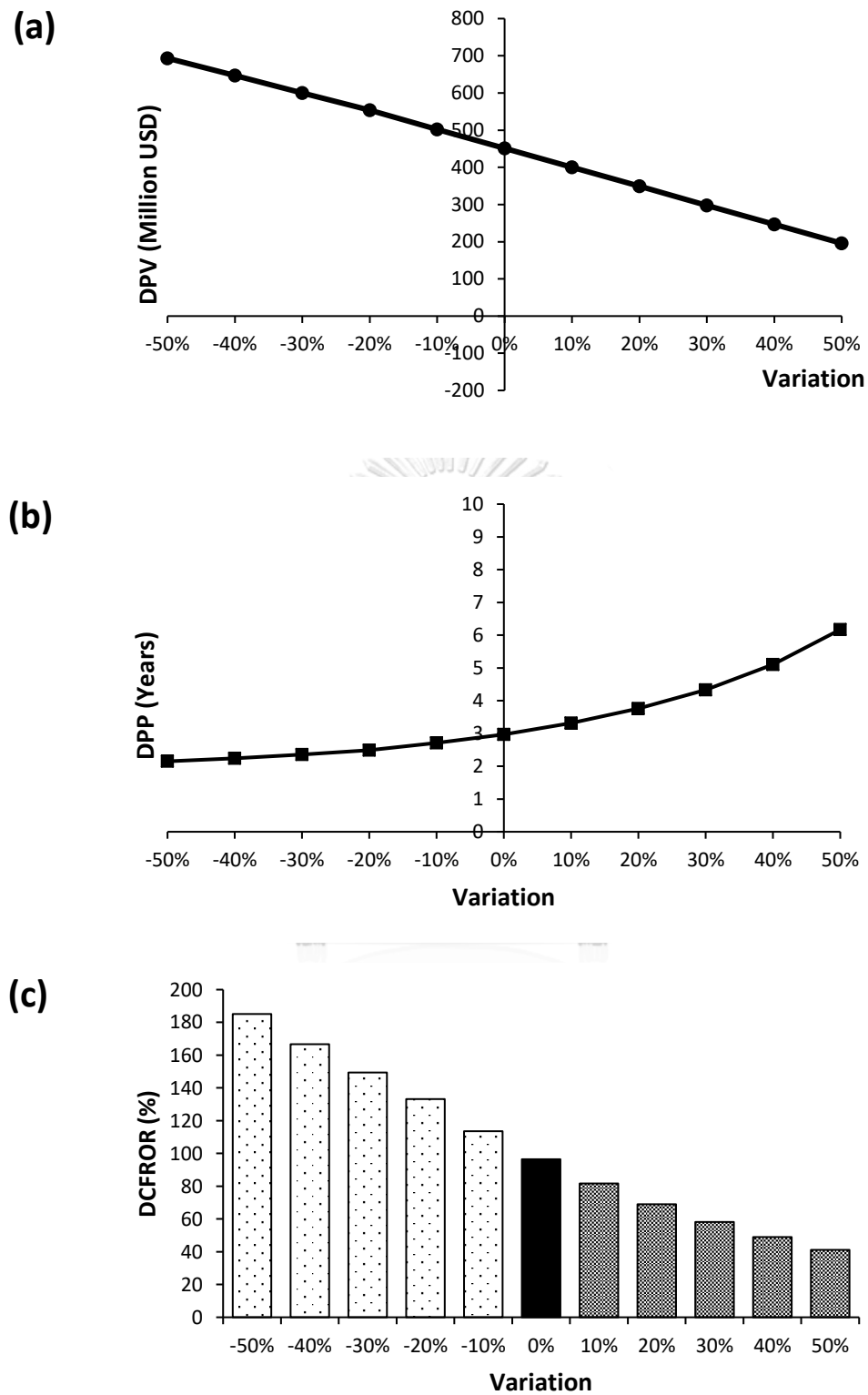


Figure 27 The effect of methyl palmitate purchasing cost on DPV (a), DPP (b) and DCFROR (c) for sucrose palmitate production.

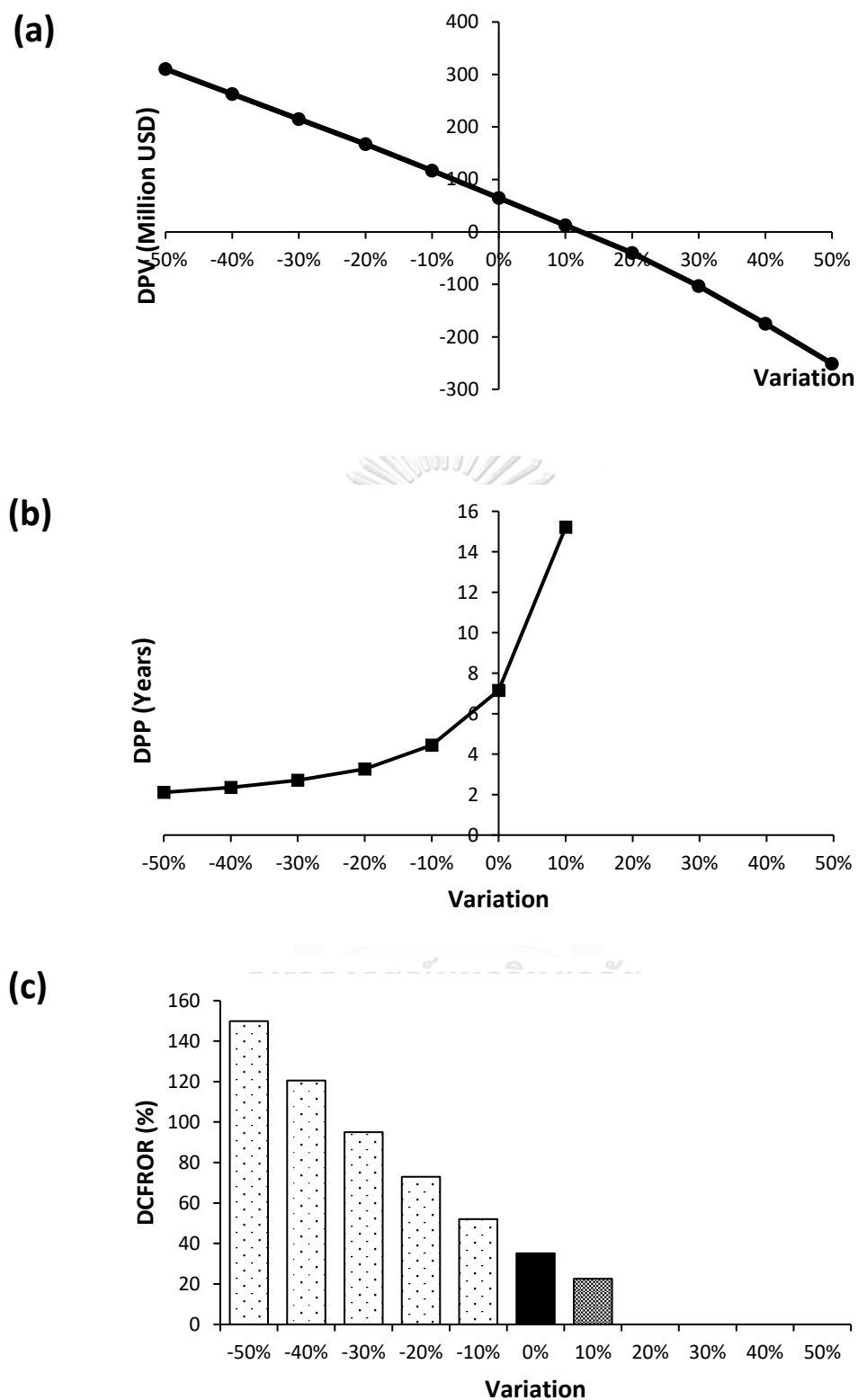
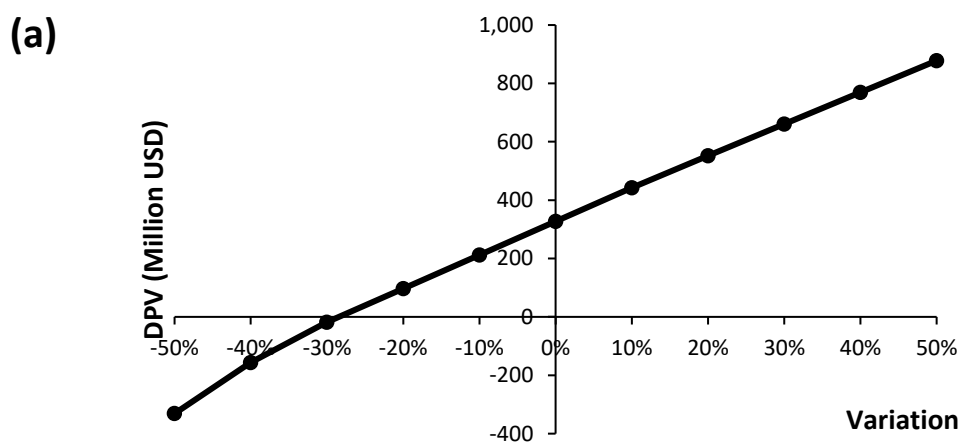


Figure 28 The effect of methyl palmitate purchasing cost on DPV (a), DPP (b) and DCFROR (c) for normal alkanes production.

#### 4.6.2. Effect of variation of product selling prices

Likewise, we studied the change of product selling price between -50% to 50% of the original value. Figure 29 shows the effect of the palmitoylethanolamide selling price between 1,500 and 4,500 USD/tonne. When the product selling price was less than or equal to 2,100 USD/tonne (-30%), this process would provide negative NPV, and the DPP value was beyond the project lifetime. As shown in Figure 30 to 31, the prices of products changed from 1,125 to 3,375 USD/tonne for sucrose palmitate, 1,000 to 3,000 USD/tonne for pentadecane and 1,500 to 4,500 USD/tonne for hexadecane. The sucrose palmitate selling prices were required more than 1,350 USD/tonne (-40%) to make this alternative feasible. Meanwhile, normal alkanes production required product selling prices of pentadecane and hexadecane greater than or equal to 1,800 and 2,700 USD/tonne (-10%). The results showed that sucrose palmitate production could be profitable at the lowest of product selling price among other processes.



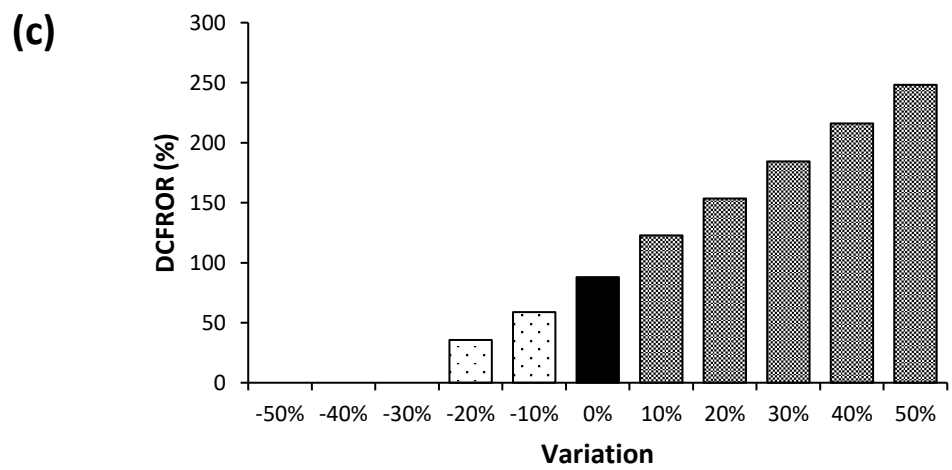
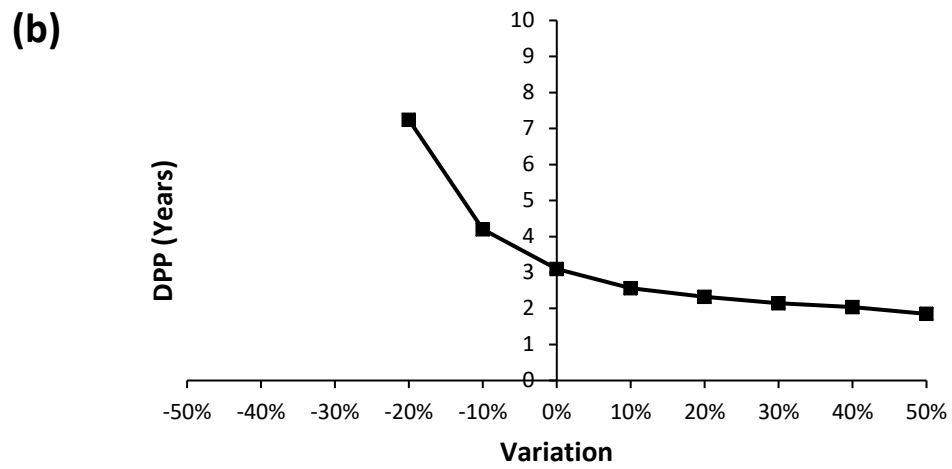
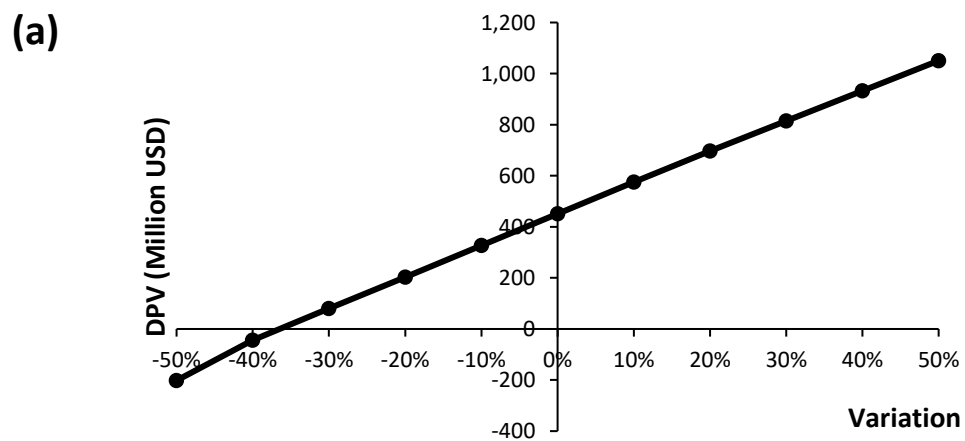


Figure 29 The effect of palmitoylethanolamide selling price on DPV (a), DPP (b) and DCFROR (c) for palmitoylethanolamide production.



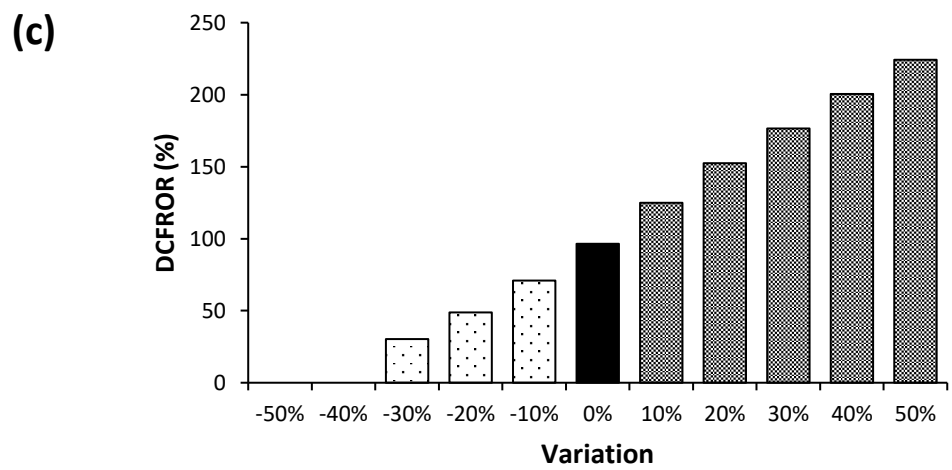
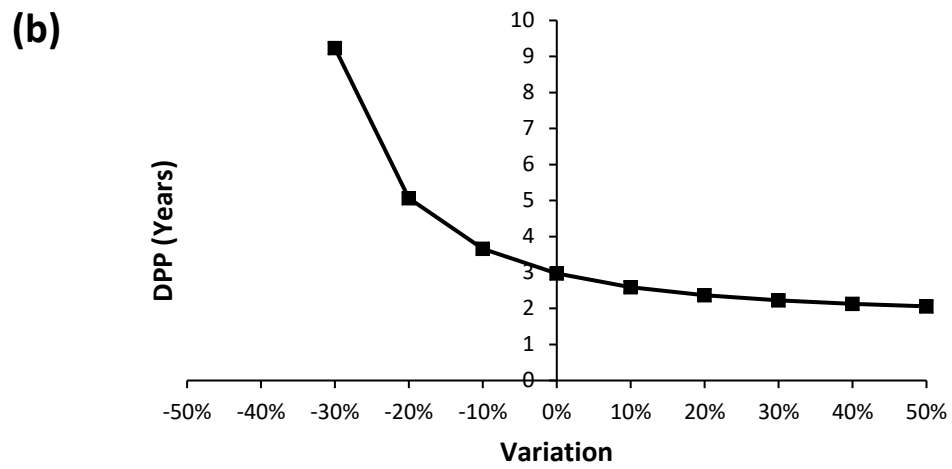
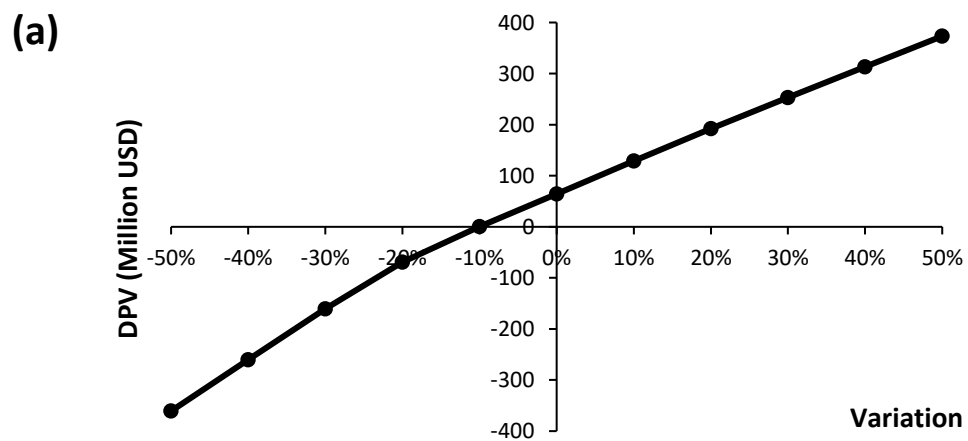
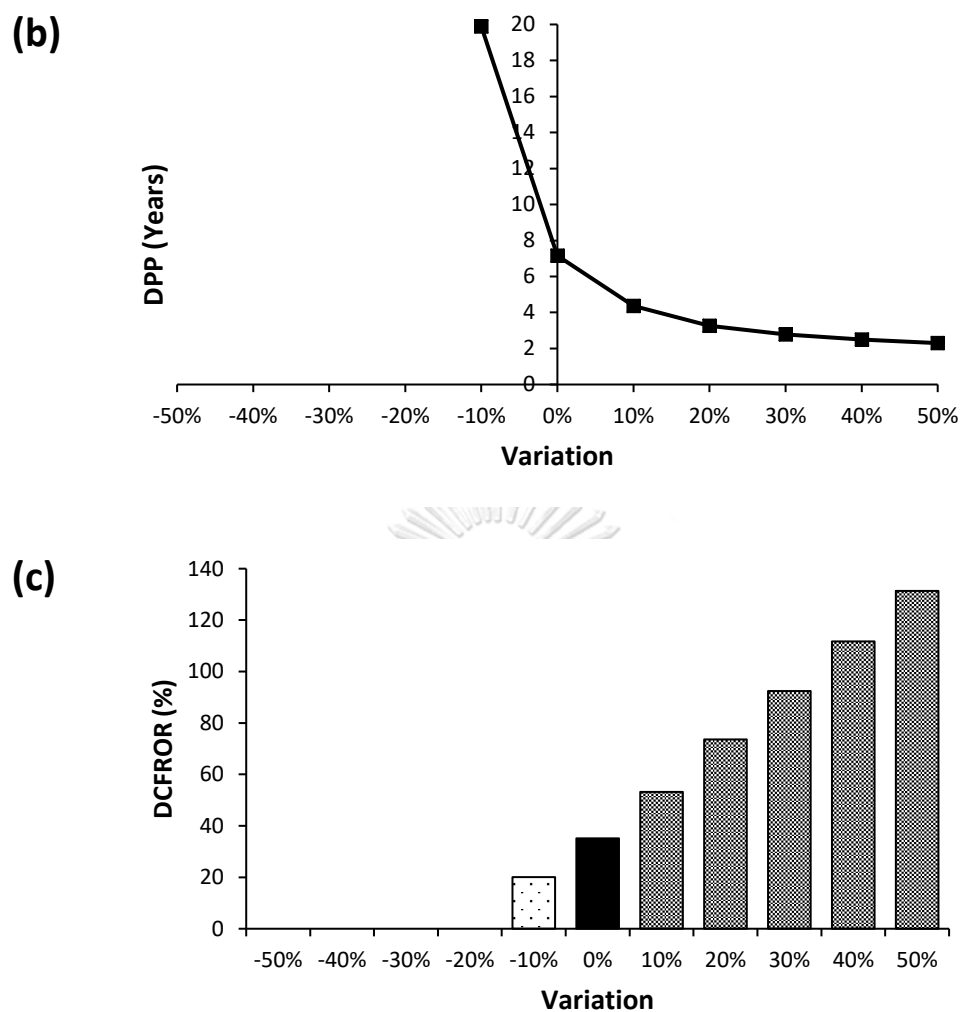


Figure 30 The effect of sucrose palmitate selling price on DPV (a), DPP (b) and DCFROR (c) for sucrose palmitate production.





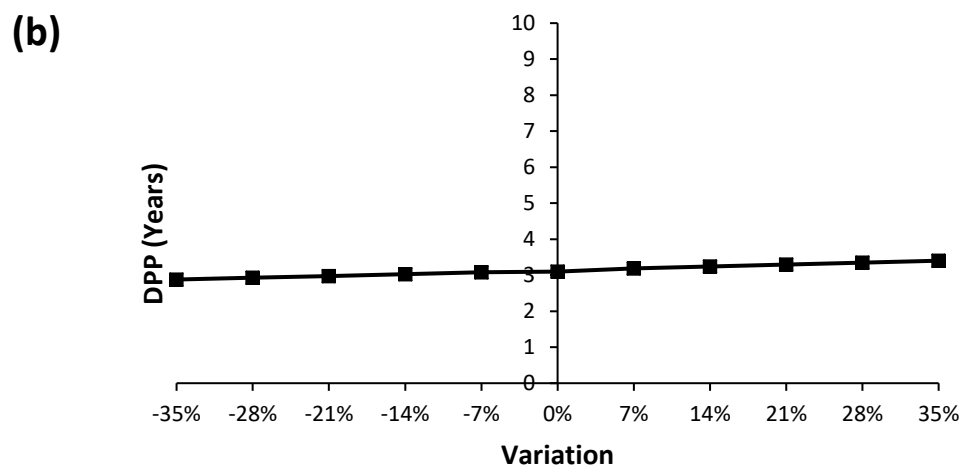
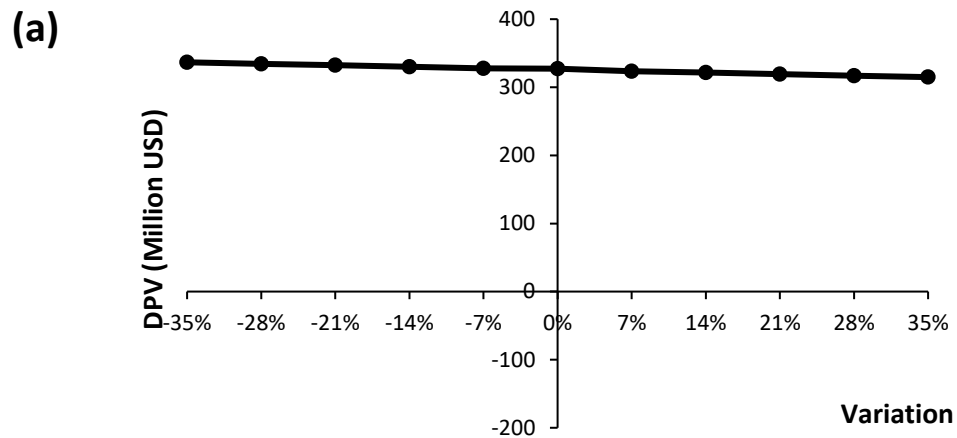
**Figure 31** The effect of pentadecane and hexadecane selling prices on DPV (a), DPP (b) and DCFROR (c) for normal alkanes production.

#### 4.6.3. Effect of variation of fixed capital investment (FCI)

According to the cost estimation method, it has an error of  $\pm 35\%$ . Therefore, we studied the change of fixed capital investment between  $-35\%$  to  $35\%$  of the original value. Figure 32 to 34 presents the effect of fixed capital investment on the economic indicators for the palmitoylethanolamide, sucrose palmitate and normal alkanes production processes. The NPV values decreased by 1 – 4, 2, and 1 million USD per 10% increased in fixed capital investment for the three processes. Whereas, the DPP values increased by 0.02 – 0.09, 0.03, and 0.14 - 0.15 years. The DCFROR value



decreased by 1 - 5%, 1 - 3%, and 0.4 - 0.8%, respectively. However, these processes still kept profitable. We could see that the change in fixed capital investment between -35% and 35% had less impact than the cost of raw material and products for all processes.



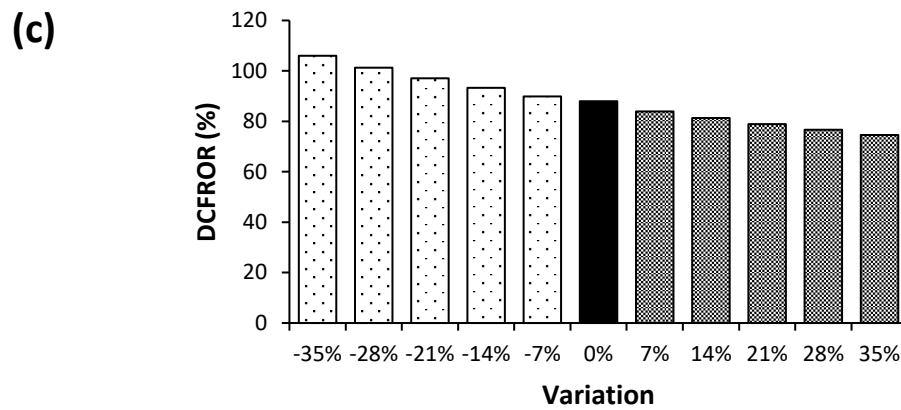
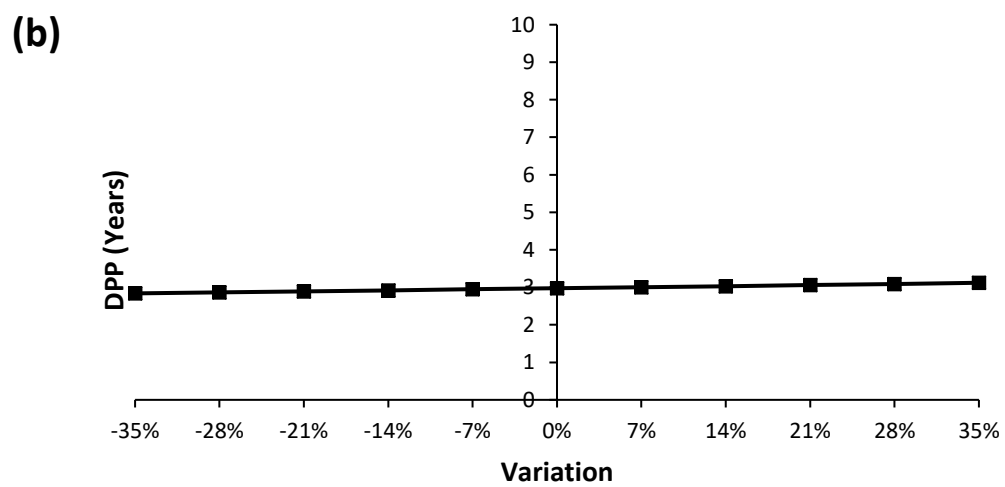
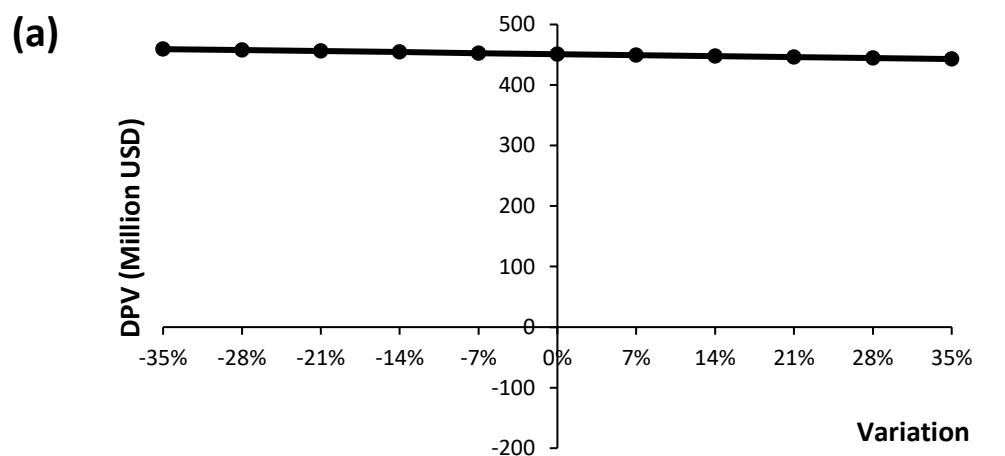


Figure 32 The effect of total capital investment on DPV (a), DPP (b) and DCFROR (c) for palmitoylethanolamide production.



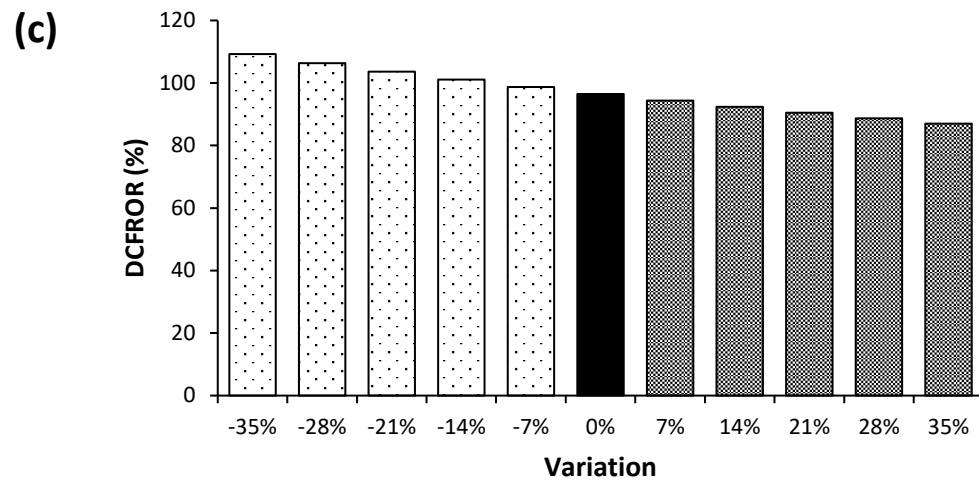
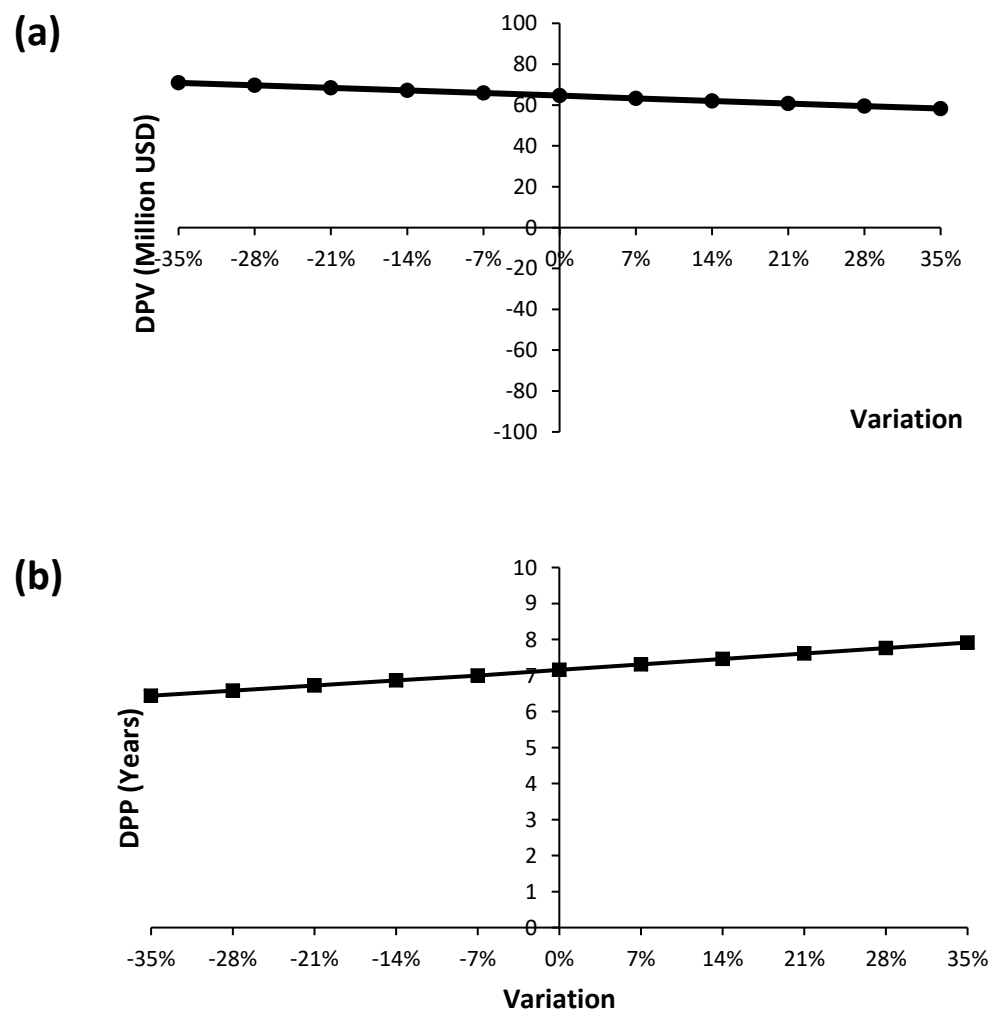
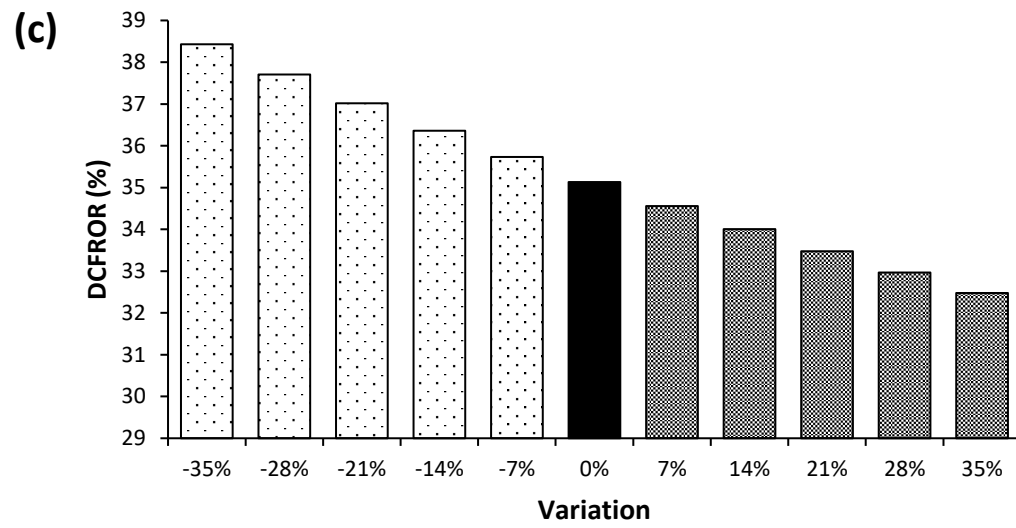


Figure 33 The effect of total capital investment on DPV (a), DPP (b) and DCFROR (c) for sucrose palmitate production.





**Figure 34** The effect of total capital investment on DPV (a), DPP (b) and DCFROR (c) for normal alkanes production



## CHAPTER 5

### CONCLUSION

#### 5.1. Conclusion

In this work, we presented an alternative for using methyl palmitate as a raw material to produce the value-added chemicals instead of selling as a biofuel. These chemicals were palmitoylethanolamide, sucrose palmitate and normal alkanes. Firstly, we estimated property parameters of palmitoylethanolamide and sucrose palmitate, which were not available in Aspen Plus V11. We chose the most accurate Aspen Plus's built-in estimation methods based on the results of property estimation of structurally similar compounds to our chemicals. They were 2-Acetamidoethanol, 1-Monopalmitin, 2-Monopalmitin and 1,3-Dipalmitin, which had experimental properties. The expected estimation results of palmitoylethanolamide and sucrose palmitate were further used in the process simulation step. Next, the three production processes were simulated using Aspen Plus V11. We specified the methyl palmitate feed rate of 100,000 tonnes/year for all processes. The simulation results reported that the production rates were 112,995 tonnes/year, 164,510 tonnes/year and 80,060 tonnes/year for the production of palmitoylethanolamide, sucrose palmitate and normal alkanes, respectively. Finally, we performed an economic analysis of each process using Aspen Process Economic Analyzer. The results presented that the production of sucrose palmitate was the best alternative with the higher NPV, higher DCFROR and lower DPV values. Besides, this process was the least sensitive alternative to the changes in methyl palmitate cost and product selling price.

#### 5.2. Recommendation

- 5.2.1. The more structurally similar compounds can provide more accuracy of the estimation property parameters.
- 5.2.2. Vary the operating conditions of solid handling equipment to find the optimal conditions for each process.
- 5.2.3. Compare the three production processes in terms of energy consumption and carbon dioxide emissions.

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## APPENDIX A

### GROSS PROFIT MARGIN ANALYSIS

#### Assumption

- The amount of methyl palmitate (feedstock) is 1 tonne.
- Process conversion (x) = 1
- No capital costs, utility costs, and operating costs have been considered.
- By-products are classified as non-valuable products.

Gross profit margin is obtained by subtracting the raw materials costs from revenue products [6]. Table 33 presents raw materials costs and products selling prices. The gross profit margin for each alternative process is given in Table 34.

**Table 32** Raw materials costs and products selling prices

Chemicals	CAS No.	Prices (USD/tonne)	Reference
Ascorbic acid	50-81-7	4,800	[46]
Ascorbyl palmitate	137-66-6	5,000	[47]
Butanol	71-36-3	781	[46]
Butyl palmitate	111-06-8	1,000	[48]
Cetyl alcohol	36653-82-4	1,200	[47]
Cetyl palmitate	540-10-3	1,000	[48]
Ethanol	64-175-5	1,028	[46]
Ethyl palmitate	628-97-7	1,000	[47]
Hexadecane	544-76-3	3,000	[47]
Hydrogen	1333-74-0	2,000	[49]
Isopropanol	67-63-0	1,208	[46]
Isopropyl palmitate	142-91-6	1,500	[47]
Methanol	67-56-1	287	[46]
Methyl palmitate	112-39-0	1,400	[47]
Monoethanolamine	141-43-5	1,000	[47]
Palmitic acid	57-10-3	1,200	[47]

**Table 33** Raw materials costs and products selling prices (cont.)

Chemicals	CAS No.	Prices (USD/tonne)	Reference
Palmitoylethanolamide	544-31-0	3,000	[47]
Pentadecane	629-62-9	2,000	[47]
Retinol	68-26-8	1,990	[47]
Retinyl palmitate	79-81-2	2,550	[47]
Sucrose	57-50-1	370	[9]
Sucrose palmitate	26446-38-8	2,250	[9]

**Example** Gross profit margin for ascorbyl palmitate production process

Reaction	Methyl palmitate + Ascorbic acid $\rightarrow$ Ascorbyl palmitate + Methanol			
MW	270.45	176.12	414.53	32.04
Mole stoi	1	1	1	1
Mass stoi	270.45	176.12	414.53	32.04
Feed (tonne)	1	$= \frac{1}{270.45} \times 176.12$ = 0.651	$= \frac{1}{270.45} \times 414.53$ = 1.533	$= \frac{1}{270.45} \times 32.04$ = 0.118

$$\text{Gross profit margin} = (1.533 \text{ tonne})(5,000 \text{ USD/tonne}) - (1 \text{ tonne})(1,400 \text{ USD/tonne}) - (0.651 \text{ tonne})(4,800 \text{ USD/tonne})$$

$$\text{Gross profit margin} = 3,138 \text{ USD}$$

Table 33 Gross profit margin analysis results.

Chemical product	Reaction	Margin (USD)
(1) Ascorbyl palmitate	Methyl palmitate + Ascorbic acid $\rightarrow$ Ascorbyl palmitate + Methanol	+ 3,138
(2) Sucrose palmitate	Methyl palmitate + Sucrose $\rightarrow$ Sucrose palmitate + Methanol	+ 2,963
(3) Palmitoylethanolamide	Methyl palmitate + Monoethanolamine $\rightarrow$ Palmitoylethanolamine + Methanol	+ 1,696
(4) Retinyl palmitate	Methyl palmitate + Retinol $\rightarrow$ Retinyl palmitate	+ 1,441
(5) Hexadecane	Methyl palmitate + Hydrogen $\rightarrow$ Palmitic acid + Methane Palmitic acid + Hydrogen $\rightarrow$ Hexadecanal + Water Hexadecanal + Hydrogen $\rightarrow$ Cetyl alcohol Cetyl alcohol + Hydrogen $\rightarrow$ Hexadecane + Water	+ 1,052
(6) Pentadecane	Methyl palmitate + Hydrogen $\rightarrow$ Palmitic acid + Methane Palmitic acid + Hydrogen $\rightarrow$ Hexadecanal + Water Hexadecanal $\rightarrow$ Pentadecane + carbon monoxide	+ 141
(7) Isopropyl palmitate	Methyl palmitate + Isopropanol $\rightarrow$ Isopropyl palmitate + Methanol	- 13
(8) Palmitic acid	Methyl palmitate + Hydrogen $\rightarrow$ Palmitic acid + Methane	- 227
(9) Cetyl alcohol	Same as Equation (1) – (3) of Hexadecane	- 369
(10) Ethyl palmitate	Methyl palmitate + Ethanol $\rightarrow$ Ethyl palmitate + Methanol	- 523
(11) Cetyl palmitate	Methyl palmitate + Cetyl alcohol $\rightarrow$ Cetyl palmitate + Methanol	- 1,264
(12) Butyl palmitate	Methyl palmitate + 1-Butanol $\rightarrow$ Butyl palmitate + Methanol	- 1,614

**APPENDIX B**  
**FEED AND PRODUCT SPECIFICATIONS**

**Table 34** Properties and specification of methyl palmitate

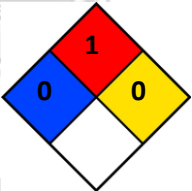
Property	Methyl palmitate
<b>Physical and chemical properties</b>	
Chemical formula	$C_{17}H_{34}O_2$
Molecular weight	270.456
Appearance	Light yellow clear liquid
Odor	Wax-like
Melting point	29.9 °C
Boiling point	324.55 °C
Vapor pressure	1.49E-04 Torr at 25 °C
Density	0.852 g/cm <sup>3</sup>
Solubility	Insoluble in water
<b>Storage</b>	35 °C, 1 atm
<b>Cost</b>	1,400 USD/tonne
<b>NFPA Classification</b>	<div style="display: flex; align-items: center;">  <div style="margin-left: 10px;"> <p>Health: 0</p> <p>Flammability: 1</p> <p>Instability: 0</p> <p>Specific hazard: N/A</p> </div> </div>

Table 35 Feed and product specification for the production of palmitoylethanolamide.

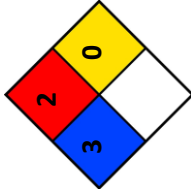
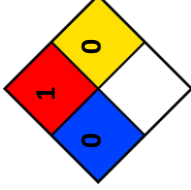
Property	Monoethanolamine	Palmitoylethanolamide
<b>Physical and chemical properties</b>		
Chemical formula	$C_2H_7NO$	$C_{18}H_{37}NO_2$
Molecular weight	61.084	299.4919
Appearance	Colorless liquid	White/off-white solid (Fine powder)
Odor	Ammonia-like	Odorless
Melting point	10.5 °C	98.5 °C
Boiling point	170 °C	461.5±28.0 °C
Vapor pressure	0.458 Torr at 25 °C	1.87E-10 Torr at 25 °C
Density	1.018 g/cm <sup>3</sup>	0.910±0.06 g/cm <sup>3</sup>
Solubility	Soluble in water	Poorly soluble in water
<b>Storage</b>	20 °C, 1 atm	- 20 °C, 1 atm
<b>Cost</b>	1,000 USD/tonne	3,000 USD/tonne
<b>NFPA Classification</b>		
	 <p>Health: 3 Flammability: 2 Instability: 0 Specific hazard: N/A</p>	 <p>Health: 0 Flammability: 1 Instability: 0 Specific hazard: N/A</p>



Table 36 Feed and product specification for the production of sucrose palmitate.

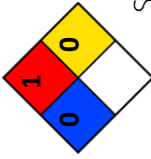
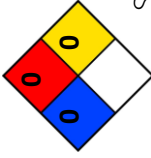
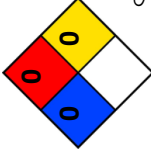
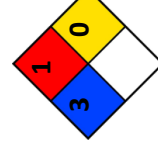
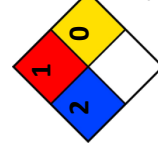
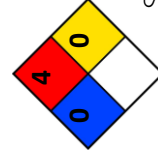
Property	Sucrose	Sucrose monopalmitate	Sucrose dipalmitate
<b>Physical and chemical properties</b>			
Chemical formula	$C_{12}H_{22}O_{11}$	$C_{28}H_{52}O_{12}$	$C_{44}H_{82}O_{13}$
Molecular weight	342.3	580.7053	819.1141
Appearance	White solid	White/off-white solid	White/off-white solid
Odor	Odorless	Odorless	Odorless
Melting point	186 °C	45 - 65 °C	45 - 65 °C
Boiling point	477.85 °C	744.9±60.0 °C	863.2±65.0 °C
Vapor pressure	1.79E-22 Torr at 25 °C	0.0±5.6 mmHg at 25 °C	0.0±0.6 mmHg at 25 °C
Density	1.5805 g/cm	1.3±0.1 g/cm <sup>3</sup>	1.1±0.1 g/cm <sup>3</sup>
Solubility	Soluble in water	Partly soluble	Partly soluble
<b>Storage</b>	23 °C, 1 atm	35 °C, 1 atm	35 °C, 1 atm
<b>Cost</b>	370 USD/tonne	2,250 USD/tonne	2,250 USD/tonne
<b>NFPA Classification</b>	 Health: 0 Flammability: 1 Instability: 0 Specific hazard: N/A	 Health: 0 Flammability: 0 Instability: 0 Specific hazard: N/A	 Health: 0 Flammability: 0 Instability: 0 Specific hazard: N/A

Table 37 Feed and product specification for the production of normal alkanes.

Property	Hydrogen	Pentadecane	Hexadecane
<b>Physical and chemical properties</b>			
Chemical formula	H <sub>2</sub>	C <sub>15</sub> H <sub>32</sub>	C <sub>16</sub> H <sub>34</sub>
Molecular weight	2.016	212.419	226.446
Appearance	Colorless gas	Colorless liquid	Colorless liquid
Odor	Odorless	Mild waxy	Odorless
Melting point	- 259.2 °C	9.92 °C	18.16 °C
Boiling point	- 252.76 °C	270.69 °C	286.86 °C
Vapor pressure	-	0.0112 Torr at 25 °C	4.52E-03 Torr at 25 °C
Density	0.089 g/cm <sup>3</sup>	0.7687 g/cm <sup>3</sup>	0.7734 g/cm <sup>3</sup>
Solubility	Poorly soluble in water	Insoluble in water	Insoluble in water
<b>Storage</b>	35 °C, 2000 psia	35 °C, 1 atm	35 °C, 1 atm
<b>Cost</b>	2,000 USD/tonne	2,000 USD/tonne	3,000 USD/tonne
<b>NFPA Classification</b>	Health: 0 Flammability: 4 Instability: 0 Specific hazard: N/A	Health: 2 Flammability: 1 Instability: 0 Specific hazard: N/A	Health: 3 Flammability: 1 Instability: 0 Specific hazard: N/A



## APPENDIX C

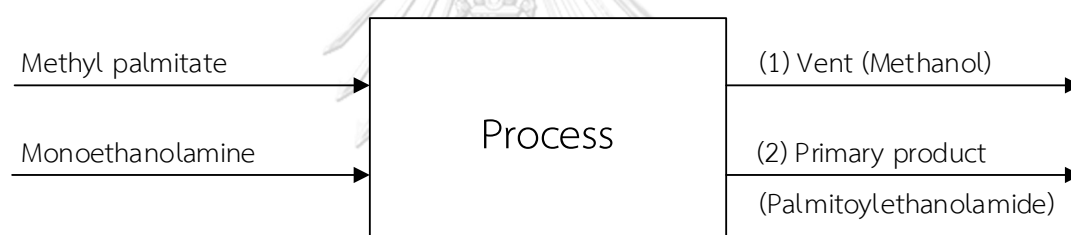
### SIMPLE MASS BALANCE

#### C.1. Palmitoylethanolamide production

**Table 38** Input-output structure of palmitoylethanolamide production.

Component	Classification	Destination code	NBP (°C)	
Methanol	Gas Byproduct	Vent	64.7	(1)
Monoethanolamine	Liquid Reactant	Recycle	170.0	
Methyl palmitate	Liquid Reactant	-	324.6	
Palmitoylethanolamide	Solid Product	Primary product	461.5	(2)

\* Methyl palmitate is completely consumed.



**Figure 35** Input-output structure of palmitoylethanolamide production.

#### Design basis

- Methyl palmitate feed rate of 100,000 tonnes/year
- Reaction conversion:  $x = 1$  (Reaction pathway as in Table 13)
- Process conversion:  $x = 1$
- No excess of the reactant at process inlet
- Calculation basis 12,500 kg/h of methyl palmitate (S1)

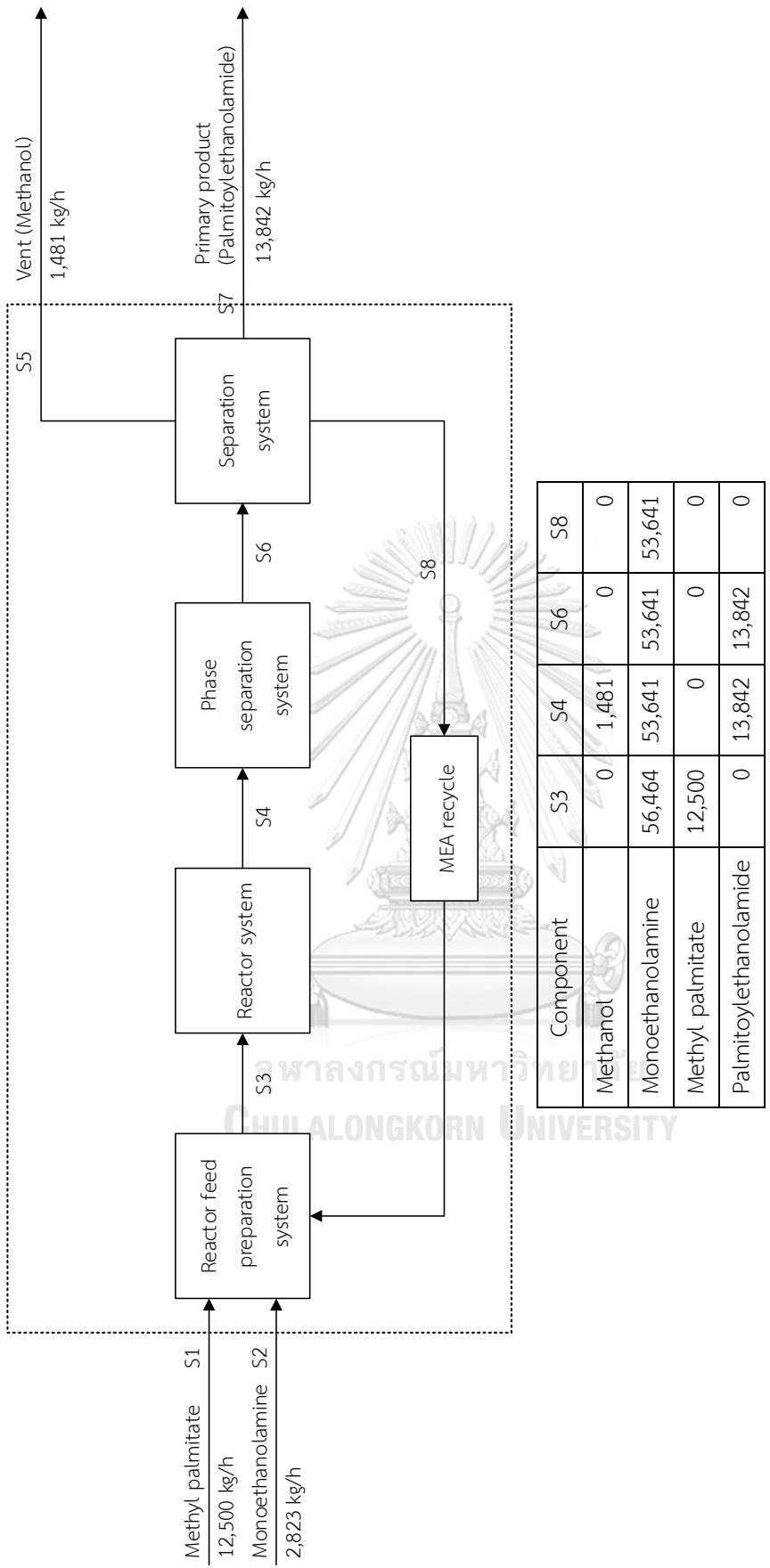
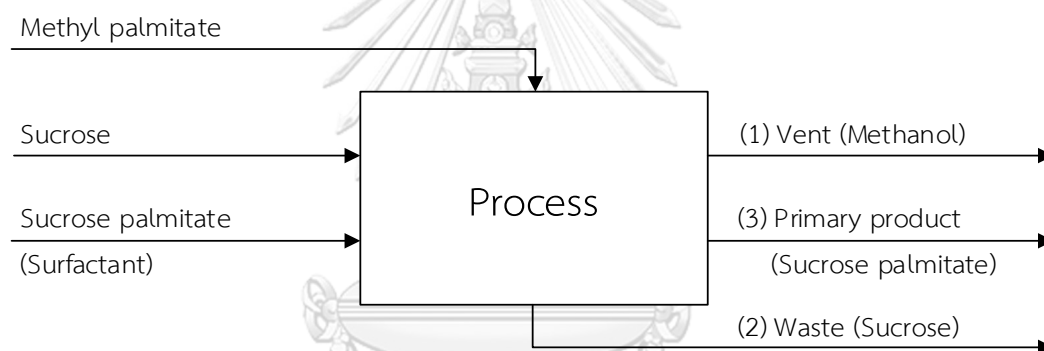


Figure 36 Material balance for palmitoylethanolamide production.

## C.2. Sucrose palmitate production

**Table 39** Input-output structure of sucrose palmitate production.

Component	Classification	Destination code	NBP (°C)	
Methanol	Gas Byproduct	Vent	64.7	(1)
Methyl palmitate	Liquid Reactant	Recycle	324.6	
Sucrose	Solid Reactant	Waste	477.9	(2)
Sucrose monopalmitate	Solid Product/ Surfactant	Primary product	744.9	
Sucrose dipalmitate	Solid Product/ Surfactant	Primary product	863.2	(3)



**Figure 37** Input-output structure of sucrose palmitate production.

### Design basis

- Methyl palmitate feed rate of 100,000 tonnes/year
- Reaction conversion:  $x_1 = 0.3098$ ,  $x_2 = 0.1755$   
(Reaction pathway as in Table 14)
- Process conversion:  $x_1 = 1$
- No excess of the reactant at process inlet
- Calculation basis 12,500 kg/h of methyl palmitate (S1)

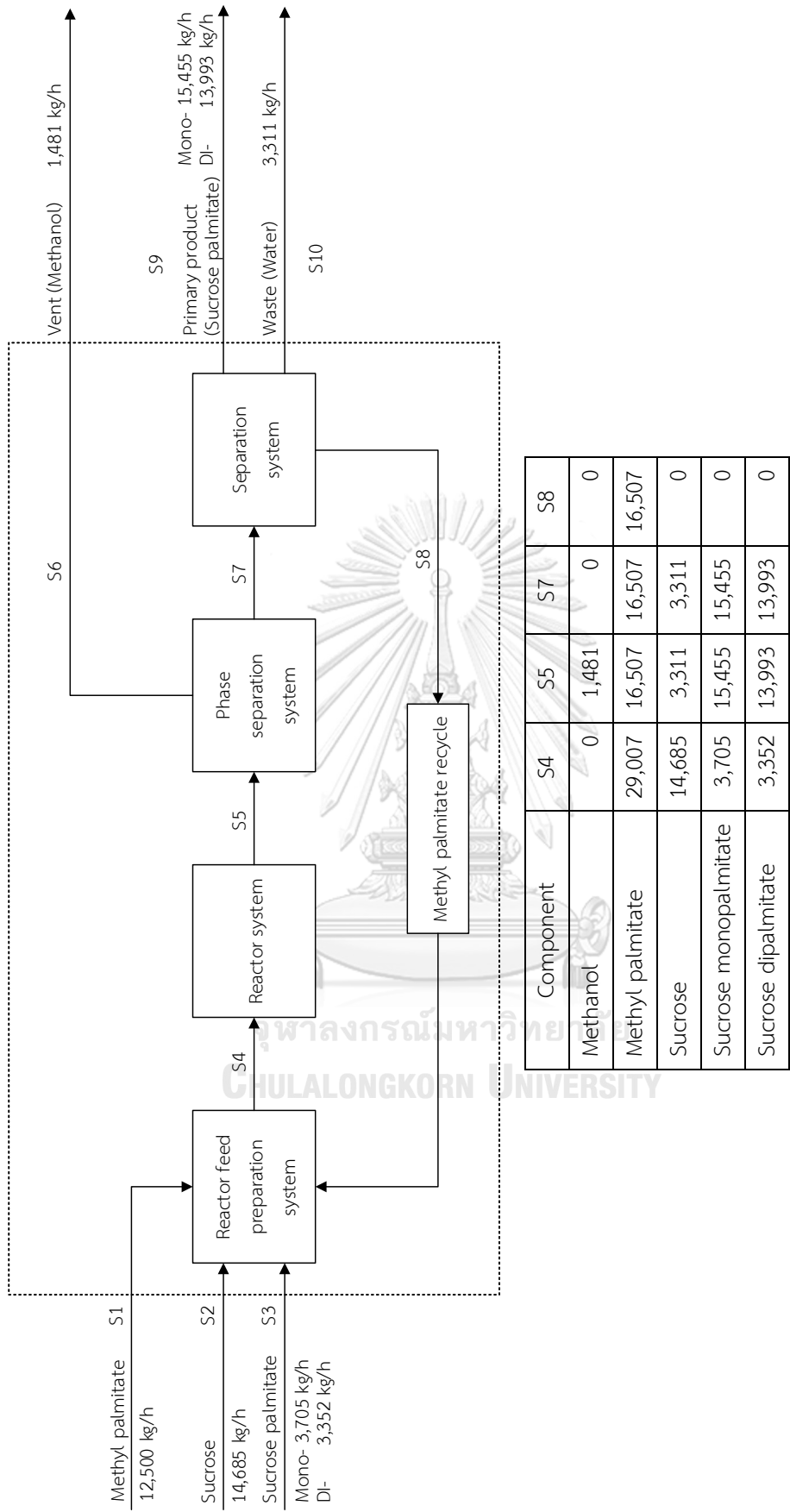


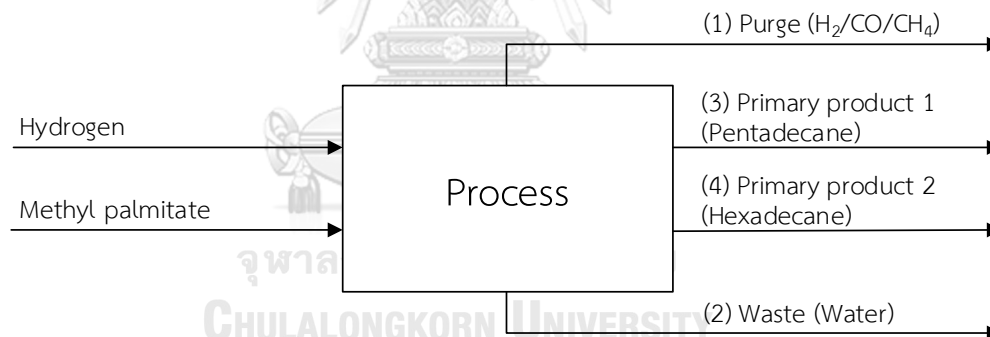
Figure 38 Material balance for sucrose palmitate production.

### C.3. Normal alkanes production

**Table 40** Input-output structure of normal alkanes production.

Component	Classification	Destination code	NBP (°C)
Hydrogen	Gas Reactant	Recycle and purge	-252.8
Carbon monoxide	Gas Byproduct	Recycle and purge	-191.5 (1)
Methane	Gas Byproduct	Recycle and purge	-161.5
Water	Liquid Byproduct	Waste	100.0 (2)
Pentadecane	Liquid Product	Primary product 1	270.7 (3)
Hexadecane	Liquid Product	Primary product 2	286.9 (4)
Hexadecanal	Liquid Reactant	-	320.6
Methyl palmitate	Liquid Reactant	-	324.6
Hexadecanol	Liquid Reactant	Recycle	324.9
Palmitic acid	Liquid Reactant	Recycle	350.0

\* Hexadecanal and methyl palmitate are completely consumed.



**Figure 39** Input-output structure of normal alkanes production.

#### Design basis

- Methyl palmitate feed rate of 100,000 tonnes/year
- Reaction conversion:  $x_1 = 1$ ,  $x_2 = 0.9915$ ,  $x_3 = 0.706$ ,  $X_4 = 0.294$ ,  $X_5 = 0.9708$   
(Reaction pathway as in Table 15)
- Process conversion:  $x_1 = 1$
- 10% excess hydrogen at process inlet
- Calculation basis 12,500 kg/h of methyl palmitate (S1)

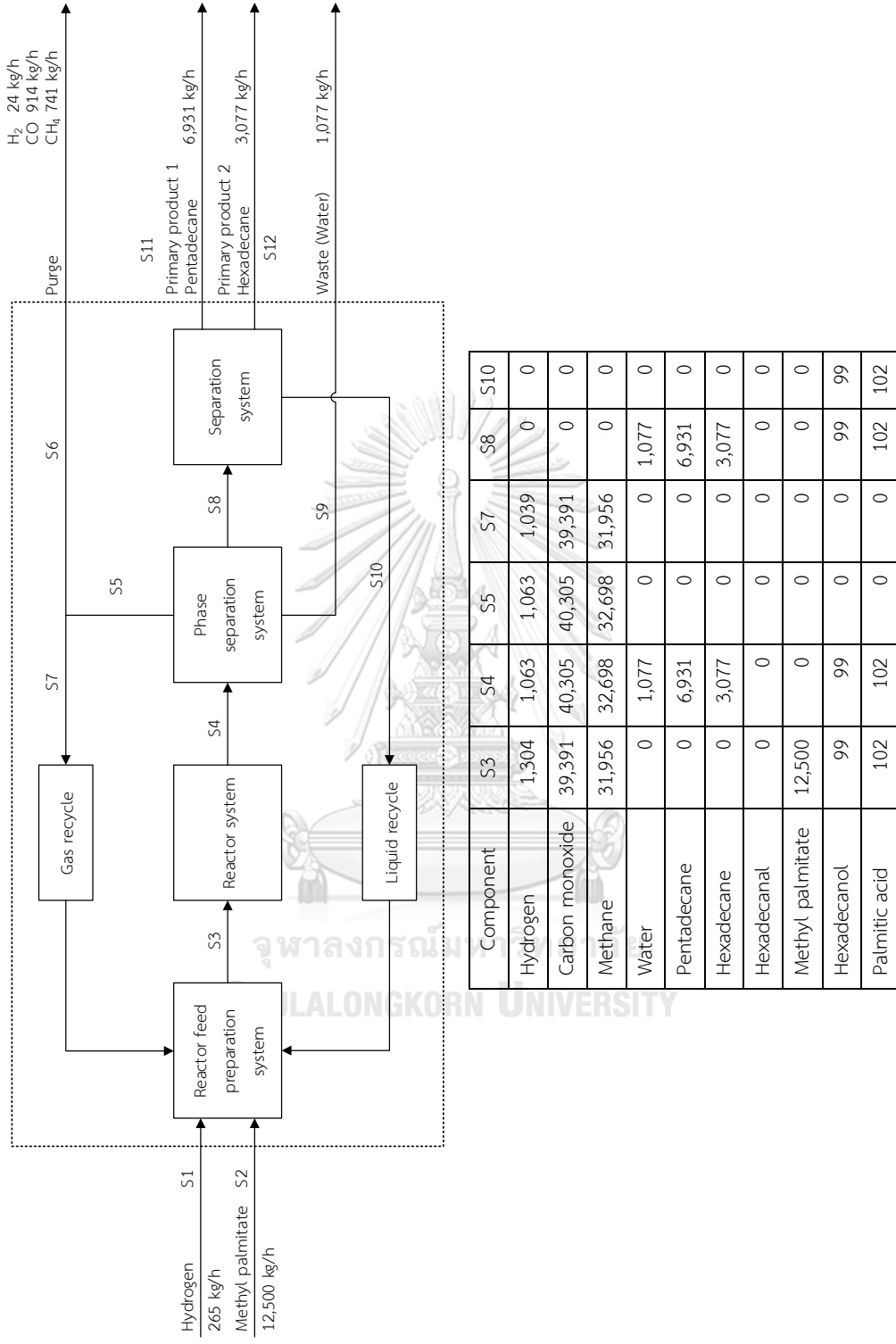


Figure 40 Material balance for normal alkanes production.



**APPENDIX D**  
**STREAM TABLE AND EQUIPMENT SUMMARY**

**D.1. Palmitoylethanolamide production**

**Table 41** Stream table for the production of palmitoylethanolamide.

<b>Stream number</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>
Temperature (°C)	35.0	20.0	192.4	169.5	162.8	60.0
Pressure (bar)	1.01	1.01	2.00	1.01	1.01	1.01
Vapor mole fraction	0.0	0.0	0.0	0.10	0.0	0.0
Total flow (kg/h)	12,500	3,954	52,533	52,533	68,987	68,987
Total flow (kmol/h)	46.22	64.74	860.89	860.89	971.84	971.84
<b>Component flowrates (kmol/h)</b>						
Methanol	0.0	0.0	0.0	0.0	0.0	0.0
Water	0.0	0.0	1.26	1.26	1.26	1.26
Monoethanolamine	0.0	64.74	859.63	859.63	924.37	924.37
Methyl palmitate	46.22	0.0	0.0	0.0	46.22	46.22
Palmitoylethanolamide	0.0	0.0	0.0	0.0	0.0	0.0
Air	0.0	0.0	0.0	0.0	0.0	0.0
<b>Stream number</b>	<b>7</b>	<b>8</b>	<b>9</b>	<b>10</b>	<b>11</b>	<b>12</b>
Temperature (°C)	60.0	23.2	140.1	140.2	35.0	56.8
Pressure (bar)	1.01	0.15	0.35	1.01	1.01	1.01
Vapor mole fraction	0.0	0.0	0.0	0.0	0.0	0.0
Total flow (kg/h)	68,987	1,507	67,480	67,480	231,172	298,652
Total flow (kmol/h)	971.84	47.47	924.38	924.38	12,832	13,756
<b>Component flowrates (kmol/h)</b>						
Methanol	46.22	46.17	0.0	0.0	0.0	0.0
Water	1.26	1.21	0.05	0.05	12,832	12,832
Monoethanolamine	878.15	0.09	878.06	878.06	0.0	878.06
Methyl palmitate	0.0	0.0	0.0	0.0	0.0	0.0
Palmitoylethanolamide	46.22	0.0	46.22	46.22	0.0	46.22
Air	0.0	0.0	0.0	0.0	0.0	0.0

**Table 42** Stream table for the production of palmitoylethanolamide (cont.).

Stream number	13	14	15	16	17	18
Temperature (°C)	6.0	6.0	6.0	6.0	6.0	111.4
Pressure (bar)	1.01	1.01	1.01	1.01	2.00	1.50
Vapor mole fraction	0.0	0.0	0.0	0.00	0.0	0.0
Total flow (kg/h)	298,652	298,652	19,794	278,858	278,858	226,326
Total flow (kmol/h)	13,756	13,756	332.74	13,424	13,424	12,563
<b>Component flowrates (kmol/h)</b>						
Methanol	0.05	0.05	0.0	0.05	0.05	0.05
Water	12,832	12,832	268.17	12,564	12,564	12,563
Monoethanolamine	878.06	878.06	18.35	859.71	859.71	0.09
Methyl palmitate	0.0	0.0	0.0	0.0	0.0	0.0
Palmitoylethanolamide	46.22	46.22	46.22	0.0	0.0	0.0
Air	0.0	0.0	0.0	0.0	0.0	0.0
Stream number	19	20	21	22		
Temperature (°C)	35.0	300.0	125.0	125.0		
Pressure (bar)	1.01	1.01	1.01	1.01		
Vapor mole fraction	1.0	1.0	0.0	1.00		
Total flow (kg/h)	100,164	100,164	14,124	105,834		
Total flow (kmol/h)	3,460	3,460	50.84	3,742		
<b>Component flowrates (kmol/h)</b>						
Methanol	0.0	0.0	0.0	0.0		
Water	0.0	0.0	0.00	268.17		
Monoethanolamine	0.0	0.0	4.62	13.73		
Methyl palmitate	0.0	0.0	0.0	0.0		
Palmitoylethanolamide	0.0	0.0	46.22	0.0		
Air	3,460	3,460	0.0	3,460		

Table 42 Operating conditions of unit operations for palmitoylethanolamide production.

Unit	Equipment type	Model	Operating condition	Note
<b>(1) Reactor feed preparation system</b>				
V-101	Pressure reducing valve	Valve	Outlet pressure = 1.01325 bar	
D-101	Liquid mixing tank	Mixer	Pressure drop = 0	
E-101	Floating head heat exchanger	Heater	Outlet temperature = 60 °C Pressure drop = 0	- $T_{\text{outlet}}$ = Reaction temperature based on the work of Wang et al. [11]
<b>(2) Reactor system</b>				
R-201	Fixed bed reactor	RStoic	Isothermal operation Temperature = 60 °C Pressure drop = 0	- Adiabatic temperature rise was more than 15% of $T_{\text{inlet}}$ . - Reactions based on the work of Wang et al. [11] MP + MEA $\rightarrow$ PEA + MeOH ; $X_{\text{MP}} = 1$
<b>(3) Phase separation system</b>				
C-301	Distillation column (Total condenser)	RadFrac	No. of stages = 8, Feed stage = 4 Condenser pressure = 0.15 bar Reboiler pressure = 0.35 bar Distillate rate = 47.47 kmol/h Molar reflux ratio = 3.27 Discharge pressure = 1.01325 bar	- The number of stages and feed location were obtained from DSTWU model. - The optimum distillate rate and molar reflux ratio were obtained from the design spec.
P-301	Centrifugal pump	Pump		
<b>(4) Separation system</b>				
D-401	Liquid mixing tank	Mixer	Pressure drop = 0	

Table 43 Operating conditions of unit operations for palmitoylethanolamide production (cont.).

Unit	Equipment type	Model	Operating condition	Note
<b>(4) Separation system (cont.)</b>				
E-401	Fixed tube sheet heat exchanger	Heater	Outlet temperature = 6 °C Pressure drop = 0	- $T_{\text{outlet}}$ based on the work of Wang et al. [11]
CR-401	Oslo growth type crystallizer	Crystallizer	Temperature = 6 °C Pressure drop = 0 Physical reaction: PEA $\rightarrow$ PEA (S) Solubility of PEA in water = 4.01 mg/l at 20 °C Model = Solids separator Fraction of solids to solid outlet = 1 Liquid load of solid outlet = 0.43 Pressure drop = 0 Duty = 0	- Temperature based on the work of Wang et al. [11]
F-401	Rotary drum filter	Filter		- Assumption: Percent solid recovery = 100% - Moisture in filter cake for rotary drum filter was obtained from the work of Parekh [50].
P-401	Centrifugal pump	Pump	Discharge pressure = 2 bar	
C-401	Distillation column (Total condenser)	RadFrac	No. of stages = 13, Feed stage = 8 Condenser pressure = 1.5 bar Reboiler pressure = 2.0 bar Distillate rate = 12,563 kmol/h Molar reflux ratio = 0.323	- The number of stages and feed location were obtained from DSTWU model. - The optimum distillate rate and molar reflux ratio were obtained from the design spec.

**Table 43** Operating conditions of unit operations for palmitoylethanolamide production (cont.).

Unit	Equipment type	Model	Operating condition	Note
<b>(4) Separation system (cont.)</b>				
E-404	Floating head heat exchanger	Heater	Outlet temperature = 300 °C Pressure drop = 0	- The inlet air temperature to the rotary dryer was obtained from the Handbook of industrial drying [51].
DR-401	Direct rotary dryer	Dryer	Operation mode = Continuous Dryer type = Shortcut Pressure drop = 0 Heat Duty = 0 Exit stream moisture contents: MEA = 0.02 (wet basis) Inlet air flow rate = 100,164 kg/h	- We specified the outlet air temperature = 125 °C [52] and then used the design spec to find the optimum inlet air flow rate.

## D.2. Sucrose palmitate production

**Table 43** Stream table for the production of sucrose palmitate.

Stream number	1	2	3	4	5	6
Temperature (°C)	35.0	23.0	35.0	355.7	323.8	153.8
Pressure (bar)	1.01	1.01	1.01	2.00	1.01	1.01
Vapor mole fraction	0.0	0.0	0.0	0.0	0.47	0.0
Total flow (kg/h)	12,500	13,122	7,057	13,438	13,438	46,118
Total flow (kmol/h)	46.22	38.34	10.47	49.83	49.83	144.85
<b>Component flowrates (kmol/h)</b>						
Methanol	0.0	0.0	0.0	0.0	0.0	0.0
Ethyl acetate	0.0	0.0	0.0	0.20	0.20	0.20
Water	0.0	0.0	0.0	0.0	0.0	0.0
Methyl palmitate	46.22	0.0	0.0	49.62	49.62	95.84
Sucrose	0.0	38.34	0.0	0.0	0.0	38.34
Sucrose monopalmitate	0.0	0.0	6.38	0.0	0.0	6.38
Sucrose dipalmitate	0.0	0.0	4.09	0.0	0.0	4.09
Stream number	7	8	9	10	11	12
Temperature (°C)	153.8	136.0	136.0	136.0	136.0	136.0
Pressure (bar)	0.33	0.33	0.33	0.33	0.33	1.01
Vapor mole fraction	0.0	0.0	0.28	1.00	0.0	0.0
Total flow (kg/h)	46,118	46,118	46,118	1,352	44,766	44,766
Total flow (kmol/h)	144.85	144.85	144.85	40.73	104.12	104.12
<b>Component flowrates (kmol/h)</b>						
Methanol	0.0	0.0	41.30	40.39	0.91	0.91
Ethyl acetate	0.20	0.20	0.20	0.18	0.02	0.02
Water	0.0	0.0	0.0	0.0	0.0	0.0
Methyl palmitate	95.84	95.84	54.54	0.15	54.39	54.39
Sucrose	38.34	38.34	8.64	0.0	8.64	8.64
Sucrose monopalmitate	6.38	6.38	24.46	0.0	24.46	24.46
Sucrose dipalmitate	4.09	4.09	15.70	0.0	15.70	15.70



**Table 44** Stream table for the production of sucrose palmitate (cont.).

Stream number	25	26	27	28	29	30
Temperature (°C)	35.0	35.0	35.0	23.0	35.2	35.2
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01
Vapor mole fraction	0.0	0.0	0.0	0.0	0.0	0.0
Total flow (kg/h)	17,682	31,454	71,019	1,896	104,370	28,613
Total flow (kmol/h)	200.51	55.16	3,942	5.54	4,003	119.42
<b>Component flowrates (kmol/h)</b>						
Methanol	0.17	0.0	0.0	0.0	0.0	0.0
Ethyl acetate	200.19	1.58	0.0	0.0	1.59	0.03
Water	0.0	0.0	3,942	0.0	3,942	78.84
Methyl palmitate	0.14	4.76	0.0	0.0	4.77	0.10
Sucrose	0.0	8.64	0.0	0.0	0.0	0.0
Sucrose monopalmitate	0.0	24.46	0.0	0.0	24.46	24.46
Sucrose dipalmitate	0.0	15.70	0.0	0.0	15.70	15.70
Stream number	31	32	33	34	35	
Temperature (°C)	35.2	35.0	300.0	125.0	125.0	
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	
Vapor mole fraction	0.0	1.00	1.00	0.0	1.00	
Total flow (kg/h)	75,757	43,013	43,013	27,621	44,005	
Total flow (kmol/h)	3,883	1,486	1,486	64.46	1,541	
<b>Component flowrates (kmol/h)</b>						
Methanol	0.0	0.0	0.0	0.0	0.0	
Ethyl acetate	1.56	0.0	0.0	0.0	0.03	
Water	3,863	0.0	0.0	23.92	54.93	
Methyl palmitate	4.67	0.0	0.0	0.10	0.0	
Sucrose	0.0	0.0	0.0	0.28	0.0	
Sucrose monopalmitate	0.0	0.0	0.0	24.46	0.0	
Sucrose dipalmitate	0.0	0.0	0.0	15.70	0.0	
Air	0.0	1,486	1,486	0.0	1,486	



Table 44 Operating conditions of unit operations for sucrose palmitate production.

Unit	Equipment type	Model	Operating condition	Note
<b>(1) Reactor feed preparation system</b>				
V-101	Pressure reducing valve	Valve	Outlet pressure = 1.01325 bar Pressure drop = 0	
D-101	Liquid mixing tank	Mixer		
V-102	Pressure reducing valve	Valve	Outlet pressure = 0.334 bar	- $P_{\text{outlet}}$ = Reaction pressure based on the work of Gutierrez et al. [12]
E-101	Double pipe heat exchanger	Heater	Outlet temperature = 136 °C Pressure drop = 0	- $T_{\text{outlet}}$ = Reaction temperature based on the work of Gutierrez et al. [12]
<b>(2) Reactor system</b>				
R-201	Fixed bed reactor	RStoic	Isothermal operation Temperature = 136 °C Pressure drop = 0	- Adiabatic temperature rise was more than 15% of $T_{\text{inlet}}$ . - Reactions based on the work of Gutierrez et al. [12] ( $X_{\text{MP1}} = 0.3098$ , $X_{\text{MP2}} = 0.1755$ ) SC + MP $\rightarrow$ MONO-SE + MeOH MONO-SE + MP $\rightarrow$ DI-SE + MeOH
<b>(3) Phase separation system</b>				
D-301	Flash drum	Flash2	Pressure drop = 0 Duty = 0	
P-301	Centrifugal pump	Pump	Discharge pressure = 1.01325 bar	
E-301	Floating head heat exchanger	Heater	Outlet temperature = 35 °C Pressure drop = 0	

Table 45 Operating conditions of unit operations for sucrose palmitate production (cont.).

Unit	Equipment type	Model	Operating condition	Note
<b>(4) Separation system</b>				
D-401	Liquid mixing tank	Mixer	Pressure drop = 0	
F-401	Rotary drum filter	Filter	Model = Solids separator Fraction of solids to solid outlet = 1 Fraction of liquid to liquid outlet = 0.91 Pressure drop = 0 Duty = 0	- Assumption: Percent solid recovery = 100% - Yield of methyl palmitate extraction = 91% [9]
P-401	Centrifugal pump	Pump	Discharge pressure = 2 bar	
C-401	Distillation column (Total condenser)	RadFrac	No. of stages = 5, Feed stage = 3 Condenser pressure = 1.5 bar Reboiler pressure = 2.0 bar Distillate rate = 2,042 kmol/h Molar reflux ratio = 1 Outlet pressure = 1.01325 bar	- The number of stages, feed location, and molar reflux ratio were obtained from the DSTWU model. - The optimum distillate rate was obtained from the design spec.
V-401	Pressure reducing valve	Valve	Outlet pressure = 1.01325 bar	
E-403	Fixed tube sheet heat exchanger	Heater	Outlet temperature = 35 °C Pressure drop = 0	
EV-401	Forced circulation evaporator	Flash2	Temperature = 130 °C Pressure drop = 0	- The optimum temperature was obtained from sensitivity analysis: $T \geq 130 \text{ °C} \rightarrow$ ETA removal > 99%

Table 45 Operating conditions of unit operations for sucrose palmitate production (cont.).

Unit	Equipment type	Model	Operating condition	Note
<b>(4) Separation system (cont.)</b>				
E-404	Floating head heat exchanger	Heater	Outlet temperature = 35 °C Pressure drop = 0	
D-403	Liquid mixing tank	Mixer	Pressure drop = 0	
E-405	Floating head heat exchanger	Heater	Outlet temperature = 35 °C Pressure drop = 0	
D-404	Liquid mixing tank	Mixer	Pressure drop = 0	
F-402	Rotary drum filter	Filter	Model = Solids separator Fraction of solids to solid outlet = 1 Fraction of liquid to liquid outlet = 0.98 Pressure drop = 0 Duty = 0	- Assumption: Percent solid recovery = 100% - Yield of sucrose extraction = 98% [9]
E-406	Floating head heat exchanger	Heater	Outlet temperature = 300 °C Pressure drop = 0	- The inlet air temperature to the rotary dryer was obtained from the Handbook of industrial drying [51].
DR-401	Direct rotary dryer	Dryer	Operation mode = Continuous Dryer type = Shortcut Pressure drop = 0, Heat Duty = 0 Exit stream moisture contents: Water = 0.0156 (wet basis) Inlet air flow rate = 43,013 kg/h	- We specified the outlet air temperature = 125 °C [52] and then used the design spec to find the optimum inlet air flow rate.

### D.3. Normal alkanes production

Table 45 Stream table for the production of normal alkanes.

Stream number	1	2	3	4	5	6	7	8	9
Temperature (°C)	35.0	38.3	20.0	35.0	371.9	334.7	42.3	42.8	20.4
Pressure (bar)	137.90	10.00	10.00	1.01	2.00	1.01	1.01	10.00	10.00
Vapor mole fraction	1.00	1.00	1.00	0.0	0.0	0.52	0.0	0.0	1.00
Total flow (kg/h)	265	265	72,485	12,500	201	201	12,701	12,701	72,750
Total flow (kmol/h)	131.46	131.46	3,918.93	46.22	0.81	0.81	47.02	47.02	4,050.39
<b>Component flowrates (kmol/h)</b>									
Hydrogen	131.46	131.46	515.15	0.0	0.0	0.0	0.0	0.0	646.61
Carbon monoxide	0.0	0.0	1,405.81	0.0	0.0	0.0	0.0	0.0	1,405.81
Methane	0.0	0.0	1,989.82	0.0	0.0	0.0	0.0	0.0	1,989.82
Water	0.0	0.0	8.15	0.0	0.0	0.0	0.0	0.0	8.15
Pentadecane	0.0	0.0	0.003	0.0	0.0	0.0	0.0	0.0	0.003
Hexadecane	0.0	0.0	0.0	0.0	0.001	0.001	0.001	0.001	0.0
Hexadecanal	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Methyl palmitate	0.0	0.0	0.0	46.22	0.0	0.0	46.22	46.22	0.0
Hexadecanol	0.0	0.0	0.0	0.0	0.41	0.41	0.41	0.41	0.0
Palmitic acid	0.0	0.0	0.0	0.0	0.40	0.40	0.40	0.40	0.0

Table 46 Stream table for the production of normal alkanes (cont.).

Stream number	10	11	12	13	14	15	16	17	18
Temperature (°C)	24.0	220.0	220.0	60.0	60.0	60.0	20.0	20.0	20.0
Pressure (bar)	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00
Vapor mole fraction	0.99	1.00	1.00	0.99	1.00	0.0	0.99	1.00	0.0
Total flow (kg/h)	85,451	85,451	85,451	85,451	75,204	10,248	75,204	74,138	1,066
Total flow (kmol/h)	4,097.41	4,097.41	4,116.45	4,116.45	4,066.36	50.09	4,066.36	4,008.13	58.23
<b>Component flowrates (kmol/h)</b>									
Hydrogen	646.61	646.61	527.00	527.00	526.94	0.06	526.94	526.94	0.0
Carbon monoxide	1,405.81	1,405.81	1,438.44	1,438.44	1,438.07	0.37	1,438.07	1,438.07	0.001
Methane	1,989.82	1,989.82	2,036.04	2,036.04	2,034.79	1.25	2,034.79	2,034.79	0.003
Water	8.15	8.15	67.95	67.95	66.47	1.48	66.47	8.33	58.14
Pentadecane	0.003	0.003	32.63	32.63	0.08	32.56	0.076	0.003	0.073
Hexadecane	0.002	0.002	13.59	13.59	0.0	13.58	0.014	0.0	0.014
Hexadecanal	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Methyl palmitate	46.22	46.22	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hexadecanol	0.41	0.41	0.41	0.41	0.0	0.41	0.0	0.0	0.0
Palmitic acid	0.40	0.40	0.40	0.40	0.0	0.40	0.0	0.0	0.0

Table 46 Stream table for the production of normal alkanes (cont.).

Stream number	19	20	21	22	23	24	25	26	27
Temperature (°C)	20.0	53.0	53.0	53.0	53.2	91.5	308.3	293.2	293.2
Pressure (bar)	10.00	10.00	10.00	10.00	2.00	1.50	2.00	1.50	2.00
Vapor mole fraction	1.00	0.0	0.0	0.0	0.027	1.00	0.0	0.0	0.0
Total flow (kg/h)	1,676	11,314	10,266	1,048	10,266	57	10,208	10,007	10,007
Total flow (kmol/h)	90.58	108.32	50.13	58.19	50.13	3.11	47.02	46.22	46.22
<b>Component flowrates (kmol/h)</b>									
Hydrogen	11.91	0.055	0.055	0.0	0.0554	0.0554	0.0	0.0	0.0
Carbon monoxide	32.50	0.37	0.37	0.0	0.37	0.37	0.0	0.0	0.0
Methane	45.99	1.25	1.25	0.001	1.25	1.25	0.0	0.0	0.0
Water	0.19	59.62	1.43	58.19	1.43	1.43	0.001	0.001	0.001
Pentadecane	0.0	32.63	32.63	0.0	32.63	0.003	32.63	32.63	32.63
Hexadecane	0.0	13.59	13.59	0.0	13.59	0.001	13.59	13.59	13.59
Hexadecanal	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Methyl palmitate	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hexadecanol	0.0	0.41	0.41	0.0	0.41	0.0	0.41	0.0	0.0
Palmitic acid	0.0	0.40	0.40	0.0	0.40	0.0	0.40	0.0	0.0

Table 46 Stream table for the production of normal alkanes (cont.).

Stream number	28	29	30	31	32	33
Temperature (°C)	288.8	320.4	270.5	6.0	6.0	6.0
Pressure (bar)	1.50	2.00	1.01	1.01	1.01	1.01
Vapor mole fraction	0.0	0.0	0.26	0.0	0.0	0.0
Total flow (kg/h)	6,931	3,076	6,931	298,652	298,652	19,794
Total flow (kmol/h)	32.63	13.59	32.63	13,756	13,756	332.74
<b>Component flowrates (kmol/h)</b>						
Hydrogen	0.0	0.0	0.0	0.0	0.0	0.0
Carbon monoxide	0.0	0.0	0.0	0.0	0.0	0.0
Methane	0.0	0.0	0.0	0.0	0.0	0.0
Water	0.001	0.0	0.001	0.001	0.0	0.0
Pentadecane	32.63	0.001	32.63	32.63	0.001	0.001
Hexadecane	0.003	13.58	0.003	0.003	13.58	13.58
Hexadecanal	0.0	0.0	0.0	0.0	0.0	0.0
Methyl palmitate	0.0	0.0	0.0	0.0	0.0	0.0
Hexadecanol	0.0	0.0	0.0	0.0	0.0	0.0
Palmitic acid	0.0	0.0	0.0	0.0	0.0	0.0

**Table 46** Operating conditions of unit operations for normal alkanes production.

Unit	Equipment type	Model	Operating condition	Note
<b>(1) Reactor feed preparation system</b>				
V-101	Pressure reducing valve	Valve	Outlet pressure = 10 bar	
V-102	Pressure reducing valve	Valve	Outlet pressure = 1.01325 bar	
D-101	Liquid mixing tank	Mixer	Pressure drop = 0	
P-101	Centrifugal pump	Pump	Discharge pressure = 10 bar	- $P_{\text{outlet}}$ = Reaction pressure based on the work of Yan et al. [13]
E-101	U-tube heat exchanger	Heater	Outlet temperature = 220 °C Pressure drop = 0	- $T_{\text{outlet}}$ = Reaction temperature based on the work of Yan et al. [13]
<b>(2) Reactor system</b>				
R-201	Trickle bed reactor	RStoic	Isothermal operation Temperature = 220 °C Pressure drop = 0	- Adiabatic temperature rise was more than 15% of $T_{\text{inlet}}$ . - Reactions based on the work of Yan et al. [13] $\text{MP} + \text{H}_2 \rightarrow \text{PA} + \text{MeOH}; X_{\text{MP}}=1$ $\text{PA} + \text{H}_2 \rightarrow \text{Hexadecanal} + \text{Water}; X_{\text{PA}}=0.9915$ $\text{Hexadecanal} \rightarrow \text{N-PEN} + \text{CO}; X_{\text{NAL}}=0.706$ $\text{Hexadecanal} + \text{H}_2 \rightarrow \text{Hexadecanol}; X_{\text{NAL}}=1$ $\text{Hexadecanol} + \text{H}_2 \rightarrow \text{N-HEX} + \text{Water}; X_{\text{NOL}}=0.9708$



Table 47 Operating conditions of unit operations for normal alkanes production (cont.).

Unit	Equipment type	Model	Operating condition	Note
<b>(3) Phase separation system</b>				
E-301	Floating head heat exchanger	Heater	Outlet temperature = 60 °C Pressure drop = 0	- The optimum temperature was obtained from sensitivity analysis.
D-301	Flash drum	Flash2	Pressure drop = 0 Duty = 0	
E-302	Fixed tube sheet heat exchanger	Heater	Outlet temperature = 20 °C Pressure drop = 0	- The optimum temperature was obtained from sensitivity analysis.
D-302	Flash drum	Flash2	Pressure drop = 0 Duty = 0	
D-303	Liquid mixing tank	Mixer	Pressure drop = 0	
D-304	Decanter	Decanter	Pressure drop = 0 Duty = 0 Key component = Water	
<b>(4) Separation system</b>				
V-401	Pressure reducing valve	Valve	Outlet pressure = 2 bar	
C-401	Distillation column (Partial condenser)	RadFrac	No. of stages = 6 Feed stage = 3 Condenser pressure = 1.5 bar Reboiler pressure = 2.0 bar Distillate rate = 3.11 kmol/h Molar reflux ratio = 0.2	- The number of stages and feed location were obtained from the DSTWU model. - The optimum distillate rate and molar reflux ratio were obtained from the design spec.

Table 47 Operating conditions of unit operations for normal alkanes production (cont.).

Unit	Equipment type	Model	Operating condition	Note
<b>(4) Separation system (cont.)</b>				
C-402	Distillation column (Total condenser)	RadFrac	No. of stages = 48 Feed stage = 27 Condenser pressure = 1.5 bar Reboiler pressure = 2.0 bar Distillate rate = 46.22 kmol/h Molar reflux ratio = 0.99	- The number of stages and feed location were obtained from the DSTWU model. - The optimum distillate rate and molar reflux ratio were obtained from the design spec.
P-401	Centrifugal pump	Pump	Discharge pressure = 2 bar	
C-403	Distillation column (Total condenser)	RadFrac	No. of stages = 99 Feed stage = 55 Condenser pressure = 1.5 bar Reboiler pressure = 2.0 bar Distillate rate = 32.63 kmol/h Molar reflux ratio = 4.84	- The number of stages and feed location were obtained from the DSTWU model. - The optimum distillate rate and molar reflux ratio were obtained from the design spec.
V-402	Pressure reducing valve	Valve	Outlet pressure = 1.01325 bar	
V-403	Pressure reducing valve	Valve	Outlet pressure = 1.01325 bar	
E-407	Floating head heat exchanger	Heater	Outlet temperature = 35 °C Pressure drop = 0	
E-408	Double pipe heat exchanger	Heater	Outlet temperature = 35 °C Pressure drop = 0	

**APPENDIX E**  
**TOTAL PROJECT COST OF PLANT**

**E.1. Palmitoylethanolamide production**

**Table 47** Total project cost of palmitoylethanolamide production (USD).

Items	Labor cost	Material cost	Total cost	Percentages
Equipment	198,000	8,060,000	8,260,000	47.1% of TDC
Piping	1,440,000	3,570,000	5,010,000	28.6% of TDC
Civil	341,000	419,000	760,000	4.3% of TDC
Steel	28,300	167,000	195,000	1.1% of TDC
Instruments	183,000	1,100,000	1,280,000	7.2% of TDC
Electrical	148,000	1,010,000	1,160,000	6.6% of TDC
Insulation	362,000	376,000	738,000	4.2% of TDC
Paint	82,200	33,700	116,000	0.7% of TDC
<b>Total Direct Field Cost</b>	<b>2,790,000 (TDL)</b>	<b>14,700,000 (TDM)</b>	<b>17,500,000 (TDC)</b>	<b>100.0% of TDC</b>
<b>Indirect Field Cost</b>			<b>3,380,000</b>	<b>121.3% of TDL</b>
<b>Total Field Cost</b>			<b>20,900,000</b>	<b>67.1% of TIC</b>
Freight			147,000	1.0% of TDM
Taxes and Permits			884,000	5.0% of TDC
Engineering and HO			2,660,000	8.5% of TIC
Other Project Costs			1,820,000	5.8% of TIC
Contingency			4,750,000	15.3% of TIC
<b>Total Non-Field Cost</b>			<b>10,300,000</b>	<b>32.9% of TIC</b>
<b>Total Project Cost</b>			<b>31,200,000 (TIC)</b>	<b>177.9% of TDC</b>
<b>Adjusted Total Project Cost</b>			<b>35,500,000</b>	
<b>Escalated Total Project Cost</b>			<b>37,200,000</b>	

**Table 48** Equipment cost of palmitoylethanolamide production (USD).

Unit	Equipment type	Total Direct cost	Equipment cost
<b>(1) Reactor feed preparation system</b>			
D-101	Liquid mixing tank	250,000	129,000
E-101	Floating head heat exchanger	175,000	51,400
<b>(2) Reactor system</b>			
R-201	Fixed bed reactor	317,000	155,000
<b>(3) Phase separation system</b>			
C-301	Distillation column	510,000	185,000
E-301	Condenser (fixed tube sheet)	126,000	31,900
E-302	Reboiler (U-tube)	221,000	97,500
D-301	Reflux drum	82,500	12,700
P-301	Centrifugal pump	52,400	7,700
<b>(4) Separation system</b>			
D-401	Liquid mixing tank	389,000	228,000
E-401	Fixed tube sheet heat exchanger	613,000	351,000
CR-401	Oslo growth type crystallizer	1,950,000	1,500,000
F-401	Rotary drum filter	342,000	242,000
P-401	Centrifugal pump	76,000	13,600
C-401	Distillation column	5,710,000	2,330,000
E-402	Condenser (fixed tube sheet)	539,000	309,000
E-403	Reboiler (U-tube)	3,620,000	1,990,000
D-402	Reflux drum	210,000	43,500
E-404	Floating head heat exchanger	267,000	96,400
DR-401	Direct rotary dryer	66,800	41,600

## E.2. Sucrose palmitate production

**Table 49** Total project cost of sucrose palmitate production (USD).

Items	Labor cost	Material cost	Total cost	Percentages
Equipment	67,200	3,790,000	3,860,000	47.1% of TDC
Piping	1,510,000	2,820,000	4,330,000	28.6% of TDC
Civil	198,000	247,000	444,000	4.3% of TDC
Steel	27,400	160,000	187,000	1.1% of TDC
Instruments	196,000	1,250,000	1,450,000	7.3% of TDC
Electrical	150,000	992,000	1,140,000	6.6% of TDC
Insulation	225,000	284,000	509,000	4.2% of TDC
Paint	107,000	36,200	144,000	0.7% of TDC
<b>Total Direct Field Cost</b>	<b>2,480,000 (TDL)</b>	<b>9,580,000 (TDM)</b>	<b>12,100,000 (TDC)</b>	<b>100.0% of TDC</b>
<b>Indirect Field Cost</b>			<b>2,990,000</b>	<b>120.9% of TDL</b>
<b>Total Field Cost</b>			<b>15,100,000</b>	<b>64.3% of TIC</b>
Freight			95,800	1.0% of TDM
Taxes and Permits			575,000	4.8% of TDC
Engineering and HO			2,660,000	11.4% of TIC
Other Project Costs			1,450,000	6.2% of TIC
Contingency			3,570,000	15.3% of TIC
<b>Total Non-Field Cost</b>			<b>8,350,000</b>	<b>35.7% of TIC</b>
<b>Total Project Cost</b>			<b>23,400,000 (TIC)</b>	<b>194.1% of TDC</b>
<b>Adjusted Total Project Cost</b>			<b>26,600,000</b>	
<b>Escalated Total Project Cost</b>			<b>28,000,000</b>	

**Table 50** Equipment cost of sucrose palmitate production (USD).

Unit	Equipment type	Total Direct cost	Equipment cost
<b>(1) Reactor feed preparation system</b>			
D-101	Liquid mixing tank	260,000	86,700
E-101	Double pipe heat exchanger	77,200	12,300
<b>(2) Reactor system</b>			
R-201	Fixed bed reactor	266,000	107,000
<b>(3) Phase separation system</b>			
D-301	Flash drum	145,000	25,000
P-301	Centrifugal pump	50,700	6,000
E-301	Floating head heat exchanger	105,000	22,000
<b>(4) Separation system</b>			
D-401	Liquid mixing tank	357,000	204,000
F-401	Rotary drum filter	955,000	658,000
P-401	Centrifugal pump	78,700	14,000
C-401	Distillation column	4,250,000	707,000
E-401	Condenser (fixed tube sheet)	329,000	151,000
E-402	Reboiler (floating head)	777,000	453,000
D-402	Reflux drum	232,000	48,900
E-403	Fixed tube sheet heat exchanger	136,000	37,100
EV-401	Forced circulation evaporator	661,000	362,000
E-404	Floating head heat exchanger	87,500	16,700
D-403	Liquid mixing tank	336,000	200,000
E-405	Floating head heat exchanger	87,800	17,000
D-404	Liquid mixing tank	246,000	128,000
F-402	Rotary drum filter	477,000	329,000
E-406	Floating head heat exchanger	198,000	56,000
DR-401	Direct rotary dryer	66,800	41,600

## E.3. Normal alkanes production

**Table 51** Total project cost of normal alkanes production (USD).

Items	Labor cost	Material cost	Total cost	Percentages
Equipment	175,000	3,440,000	3,610,000	40.8% of TDC
Piping	518,000	986,000	1,500,000	17.0% of TDC
Civil	124,000	202,000	325,000	3.7% of TDC
Steel	36,300	199,000	235,000	2.7% of TDC
Instruments	226,000	1,230,000	1,460,000	16.5% of TDC
Electrical	132,000	943,000	1,080,000	12.1% of TDC
Insulation	256,000	304,000	560,000	6.3% of TDC
Paint	60,000	25,700	85,700	1.0% of TDC
<b>Total Direct Field Cost</b>	<b>1,530,000</b> (TDL)	<b>7,330,000</b> (TDM)	<b>8,860,000</b> (TDC)	<b>100.0% of TDC</b>
<b>Indirect Field Cost</b>			<b>2,060,000</b>	<b>135.0% of TDL</b>
<b>Total Field Cost</b>			<b>10,900,000</b>	<b>60.6% of TIC</b>
Freight			73,300	1.0% of TDM
Taxes and Permits			440,000	5.0% of TDC
Engineering and HO			2,740,000	15.2% of TIC
Other Project Costs			1,090,000	6.1% of TIC
Contingency			2,750,000	15.3% of TIC
<b>Total Non-Field Cost</b>			<b>7,100,000</b>	<b>39.4% of TIC</b>
<b>Total Project Cost</b>			<b>18,000,000</b> (TIC)	<b>203.4% of TDC</b>
<b>Adjusted Total Project Cost</b>			<b>20,500,000</b>	
<b>Escalated Total Project Cost</b>			<b>21,500,000</b>	

**Table 52** Equipment cost of normal alkanes production (USD).

Unit	Equipment type	Total Direct cost	Equipment cost
<b>(1) Reactor feed preparation system</b>			
D-101	Liquid mixing tank	245,000	74,700
P-101	Centrifugal pump	50,200	17,400
E-101	U-tube heat exchanger	101,000	20,400
<b>(2) Reactor system</b>			
R-201	Trickle bed reactor	238,000	71,000
<b>(3) Phase separation system</b>			
E-301	Floating head heat exchanger	132,000	30,300
D-301	Flash drum	141,000	32,900
E-302	Fixed tube sheet heat exchanger	99,700	21,900
D-302	Flash drum	137,000	32,900
D-303	Liquid mixing tank	185,000	75,200
D-304	Decanter	93,300	15,800
<b>(4) Separation system</b>			
C-401	Distillation column	332,000	90,400
E-401	Condenser (double pipe)	45,700	2,600
E-402	Reboiler (floating head)	153,000	36,500
D-401	Reflux drum	100,000	15,000
C-402	Distillation column	897,000	403,000
E-403	Condenser (double pipe)	81,300	11,900
E-404	Reboiler (fixed tube sheet)	153,000	37,500
D-402	Reflux drum	134,000	17,000
P-401	Centrifugal pump	38,000	4,500
C-403	Distillation column	3,130,000	2,220,000
E-405	Condenser (floating head)	76,600	13,200
E-406	Reboiler (fixed tube sheet)	186,000	45,800
D-403	Reflux drum	161,000	23,400
E-407	Floating head heat exchanger	84,600	13,200
E-408	Double pipe heat exchanger	85,400	15,000



## APPENDIX F

### PROPERTY PARAMETERS OF SIMILAR COMPOUNDS

Appendix F shows the comparison of each property parameter obtained from Aspen's databanks and estimation methods. As shown in the tables below, (a), (b), (c) and (d) are 2-Acetamidoethanol, 1-Monopalmitin, 2-Monopalmitin and 1,3-Dipalmitin, respectively.

**Table 53** Comparison of critical temperature obtained from databanks and estimation.

Method	(a)	(b)	(c)	(d)
Databank	776.0	837.0	843.0	1,000.0
Joback	776.3	852.4	858.5	1,123.3
Lydersen	774.9	854.0	860.1	1,151.4
Fedors	677.9	858.6	858.6	953.2
Ambrose	824.4	867.4	873.6	944.2
Simple	836.3	976.4	983.4	1,110.9
GANI	-	802.7	787.6	856.7

\* The unit of critical temperature is Kelvin (K).

**Table 54** Comparison of critical pressure obtained from databanks and estimation.

Method	(a)	(b)	(c)	(d)
Databank	4.863E+06	1.179E+06	1.188E+06	5.009E+05
Joback	4.863E+06	1.235E+06	1.235E+06	5.009E+05
Lydersen	4.607E+06	1.340E+06	1.340E+06	7.420E+05
Ambrose	5.015E+06	1.393E+06	1.393E+06	7.463E+05
Gani	-	1.160E+06	1.173E+06	5.789E+05

\* The unit of critical pressure is N/sqm.

**Table 55** Comparison of critical volume obtained from databanks and estimation.

Method	(a)	(b)	(c)	(d)
Databank	0.334	1.177	1.177	2.043
Joback	0.320	1.158	1.158	2.061
Lydersen	0.320	1.142	1.142	2.029
Ambrose	0.310	1.134	1.134	2.025
Riedel	0.286	1.309	1.301	3.601
Fedors	0.338	1.111	1.111	1.964
Gani	-	1.149	1.122	1.995

\* The unit of critical volume is cum/kmol.

**Table 56** Comparison of critical compressibility factor obtained from databanks and estimation.

Method	(a)	(b)	(c)	(d)
Databank	0.252	0.199	0.199	N/A
Definition	0.241	0.190	0.190	0.128

\* Critical compressibility factor has no unit.

**Table 57** Comparison of standard heat of formation obtained from databanks and estimation.

Method	(a)	(b)	(c)	(d)
Databank	-4.171E+08	-1.070E+09	-1.067E+09	-1.567E+09
Benson	-4.182E+08	-1.066E+09	-1.066E+09	-1.558E+09
Joback	-3.372E+08	-1.063E+09	-1.063E+09	-1.558E+09
BensonR8	-4.182E+08	-1.071E+09	-1.071E+09	-1.568E+09
Gani	-4.194E+08	-1.076E+09	-1.069E+09	-1.545E+09

\* The unit of standard heat of formation is J/kmol.

**Table 58** Coefficients for ideal gas heat capacity equation for 2-Acetamidoethanol.

Parameter	Databank	Benson	Joback	BensonR8
Equation	NIST Aly-Lee	Ideal gas heat capacity polynomial		
C <sub>1i</sub>	86,771	2,675	10,682	2,675
C <sub>2i</sub>	141,461	492	466	492
C <sub>3i</sub>	570	-0.295	-0.254	-0.295
C <sub>4i</sub>	152,880	6.789E-05	4.766E-05	6.789E-05
C <sub>5i</sub>	1,579	0	0	0
C <sub>6i</sub>	0	0	0	0
C <sub>7i</sub>	8.31	280	280	280
C <sub>8i</sub>	200	1,100	1,100	1,100
C <sub>9i</sub>	1,000	36,029	36,029	36,029
C <sub>10i</sub>	-	18	18	18
C <sub>11i</sub>	-	1.5	1.5	1.5

**Table 59** Coefficients for ideal gas heat capacity equation for 1,3-Dipalmitin.

Parameter	Databank	Benson	Joback	BensonR8
Equation	NIST Aly-Lee	Ideal gas heat capacity polynomial		
C <sub>1i</sub>	629,795	-18,485	25,500	-18,485
C <sub>2i</sub>	1.493E+06	3,428	3,259	3,428
C <sub>3i</sub>	809	-1.85	-1.72	-1.85
C <sub>4i</sub>	6.145E+05	3.125E-04	3.00E-04	3.125E-04
C <sub>5i</sub>	-1.064E+04	0	0	0
C <sub>6i</sub>	0	0	0	0
C <sub>7i</sub>	8.31	280	280	280
C <sub>8i</sub>	200	1,100	1,100	1,100
C <sub>9i</sub>	1,000	36,029	36,029	36,029
C <sub>10i</sub>	-	164	165	164
C <sub>11i</sub>	-	1.5	1.5	1.5

**Table 60** Coefficients for ideal gas heat capacity equation for 1,3-Dipalmitin.

Parameter	Databank	Benson	Joback	BensonR8
Equation	NIST Aly-Lee	Ideal gas heat capacity polynomial		
$C_{1i}$	629,795	-18,485	25,500	-18,485
$C_{2i}$	1.493E+06	3,428	3,259	3,428
$C_{3i}$	809	-1.85	-1.72	-1.85
$C_{4i}$	6.145E+05	3.125E-04	3.00E-04	3.125E-04
$C_{5i}$	-1.064E+04	0	0	0
$C_{6i}$	0	0	0	0
$C_{7i}$	8.31	280	280	280
$C_{8i}$	200	1,100	1,100	1,100
$C_{9i}$	1,000	36,029	36,029	36,029
$C_{10i}$	-	164	165	164
$C_{11i}$	-	1.5	1.5	1.5

\* The unit of ideal gas heat capacity is J/(kmol·K).

The unit of temperature is Kelvin (K).

**Table 61** Comparison of ideal gas heat capacity of 2- Acetamidoethanol obtained from databanks and estimation.

Method	CPIG at 300 K	CPIG at 500 K	CPIG at 1,000 K
Databank	1.350E+05	1.910E+05	2.735E+05
Benson	1.255E+05	1.832E+05	2.670E+05
Joback	1.289E+05	1.861E+05	2.703E+05
BensonR8	1.255E+05	1.832E+05	2.670E+05

\* The unit of ideal gas heat capacity is J/(kmol·K).

**Table 62** Comparison of ideal gas heat capacity of Monopalmitin (b,c) obtained from databanks and estimation.

Method	CPIG at 300 K	CPIG at 500 K	CPIG at 1,000 K
Databank	4.915E+05	7.256E+05	1.057E+06
Benson	4.842E+05	7.182E+05	1.053E+06
Joback	4.850E+05	7.112E+05	1.046E+06
BensonR8	4.842E+05	7.182E+05	1.053E+06

\* The unit of ideal gas heat capacity is J/(kmol·K).

**Table 63** Comparison of ideal gas heat capacity of 1,3-Dipalmitin obtained from databanks and estimation.

Method	CPIG at 300 K	CPIG at 500 K	CPIG at 1,000 K
Databank	8.287E+05	1.295E+06	1.836E+06
Benson	8.522E+05	1.273E+06	1.877E+06
Joback	8.561E+05	1.261E+06	1.860E+06
BensonR8	8.522E+05	1.273E+06	1.877E+06

\* The unit of ideal gas heat capacity is J/(kmol·K).

**Table 64** Coefficients for vapor pressure equation for 2-Acetamidoethanol.

Parameter	Databank	Riedel	Li-Ma
Equation	NIST Wagner 25	Extended Antoine	
C <sub>1i</sub>	-11.7	128	70.0
C <sub>2i</sub>	4.87	-16,395	-9,070
C <sub>3i</sub>	-10.38	0	0
C <sub>4i</sub>	-5.29	0	0
C <sub>5i</sub>	15.4	-13.9	-6.71
C <sub>6i</sub>	776	2.681E-18	2.125E-19
C <sub>7i</sub>	240	6	6
C <sub>8i</sub>	776	569	569
C <sub>9i</sub>	-	776	776

**Table 65** Coefficients for vapor pressure equation for 1-Monopalmitin.

Parameter	Databank	Riedel	Li-Ma
Equation	NIST Wagner 25	Extended Antoine	
C <sub>1i</sub>	-13.8	134	-2.423E+05
C <sub>2i</sub>	6.98	-18,708	1.921E+07
C <sub>3i</sub>	-15.2	0	0
C <sub>4i</sub>	-5.26	0	0
C <sub>5i</sub>	14.0	-14.6	32,946
C <sub>6i</sub>	837	1.590E-18	-8.129E-15
C <sub>7i</sub>	350	6	6
C <sub>8i</sub>	837	694	694
C <sub>9i</sub>	-	852	852

**Table 66** Coefficients for vapor pressure equation for 2-Monopalmitin.

Parameter	Databank	Riedel	Li-Ma
Equation	NIST Wagner 25	Extended Antoine	
C <sub>1i</sub>	-13.8	135	-2.425E+05
C <sub>2i</sub>	7.04	-18,969	1.934E+07
C <sub>3i</sub>	-15.3	0	0
C <sub>4i</sub>	-5.25	0	0
C <sub>5i</sub>	14.0	-14.7	32,946
C <sub>6i</sub>	843	1.534E-18	-7.789E-15
C <sub>7i</sub>	298	6	6
C <sub>8i</sub>	843	699	699
C <sub>9i</sub>	-	858	858

**Table 67** Coefficients for vapor pressure equation for 1,3-Dipalmitin.

Parameter	Databank	Riedel	Li-Ma
Equation	NIST Wagner 25	Extended Antoine	
C <sub>1i</sub>	-7.73	112	72.4
C <sub>2i</sub>	1.94	-17,700	-13,015
C <sub>3i</sub>	-2.88	0	0
C <sub>4i</sub>	-3.20	0	0
C <sub>5i</sub>	13.1	-11.8	-6.71
C <sub>6i</sub>	727	6.875E-19	2.434E-20
C <sub>7i</sub>	71	6	6
C <sub>8i</sub>	727	817	817
C <sub>9i</sub>	-	953	953

\* The unit of vapor pressure is N/sqm.

The unit of temperature is Kelvin (K).

**Table 68** Comparison of vapor pressure of 2- Acetamidoethanol obtained from databanks and estimation.

Method	PL at TB	PL at 0.9*TC	PL at TC
Databank	1.019E+05	1.516E+06	4.863E+06
Riedel	1.013E+05	1.526E+06	4.863E+06
Li-Ma	1.013E+05	4.993E+05	9.219E+05

\* The unit of vapor pressure is N/sqm.

**Table 69** Comparison of vapor pressure of 1-Monopalmitin obtained from databanks and estimation.

Method	PL at TB	PL at 0.9*TC	PL at TC
Databank	1.013E+05	3.098E+05	1.179E+06
Riedel	1.013E+05	3.534E+05	1.160E+06
Li-Ma	1.013E+05	5.218E-33	1.805E-35

\* The unit of vapor pressure is N/sqm.

**Table 70** Comparison of vapor pressure of 2-Monopalmitin obtained from databanks and estimation.

Method	PL at TB	PL at 0.9*TC	PL at TC
Databank	1.013E+05	3.109E+05	1.188E+06
Riedel	1.013E+05	3.555E+05	1.173E+06
Li-Ma	1.013E+05	5.218E-33	1.805E-35

\* The unit of vapor pressure is N/sqm.

**Table 71** Comparison of vapor pressure of 1,3-Dipalmitin obtained from databanks and estimation.

Method	PL at TB	PL at 0.9*TC	PL at TC
Databank	1.013E+05	2.250E+05	5.009E+05
Riedel	1.013E+05	1.724E+05	5.009E+05
Li-Ma	1.013E+05	1.568E+05	3.556E+05

\* The unit of vapor pressure is N/sqm.

**Table 72** Coefficients for enthalpy of vaporization equation for 2-Acetamidoethanol.

Parameter	Databank	Definition	Vetere	Gani	Li-Ma
Equation	NIST TDE Watson		Watson		
C <sub>1i</sub>	19.1	7.041E+07	5.723E+07	9.191E+07	6.544E+07
C <sub>2i</sub>	1.71	569	569	298	569
C <sub>3i</sub>	-1.54	0.402	0.380	0.380	0.460
C <sub>4i</sub>	0.292	-0.580	0	0	0
C <sub>5i</sub>	776	569	569	298	785
C <sub>6i</sub>	4	-	-	-	-
C <sub>7i</sub>	245	-	-	-	-
C <sub>8i</sub>	776	-	-	-	-



**Table 73** Coefficients for enthalpy of vaporization equation for 1-Monopalmitin.

Parameter	Databank	Definition	Vetere	Gani	Ducros	Li-Ma
Equation	NIST TDE Watson			Watson		
C <sub>1i</sub>	19.3	7.036E+07	6.439E+07	1.452E+08	1.541E+08	4.330E+07
C <sub>2i</sub>	1.66	694	694	298	298	694
C <sub>3i</sub>	-1.46	0.409	0.380	0.380	0.380	0.327
C <sub>4i</sub>	0.351	-0.869	0	0	0	0
C <sub>5i</sub>	837	278	278	119	119	278
C <sub>6i</sub>	4	-	-	-	-	-
C <sub>7i</sub>	350	-	-	-	-	-
C <sub>8i</sub>	837	-	-	-	-	-

**Table 74** Coefficients for enthalpy of vaporization equation for 2-Monopalmitin.

Parameter	Databank	Definition	Vetere	Gani	Ducros	Li-Ma
Equation	NIST TDE Watson			Watson		
C <sub>1i</sub>	19.3	7.128E+07	6.485E+07	1.475E+08	1.610E+08	4.363E+07
C <sub>2i</sub>	1.48	699	699	298	298	699
C <sub>3i</sub>	-1.18	0.409	0.380	0.380	0.380	0.327
C <sub>4i</sub>	0.244	-0.875	0	0	0	0
C <sub>5i</sub>	843	280	280	119	119	280
C <sub>6i</sub>	4	-	-	-	-	-
C <sub>7i</sub>	300	-	-	-	-	-
C <sub>8i</sub>	814	-	-	-	-	-

**Table 75** Coefficients for enthalpy of vaporization equation for 1,3-Dipalmitin.

Parameter	Databank	Definition	Vetere	Gani	Ducros	Li-Ma
Equation	NIST TDE Watson			Watson		
C <sub>1i</sub>	19.0	6.194E+07	7.838E+07	2.034E+08	2.261E+08	3.980E+07
C <sub>2i</sub>	3.21	817	817	298	298	817
C <sub>3i</sub>	-5.12	0.428	0.380	0.380	0.380	0.327
C <sub>4i</sub>	2.59	-0.900	0	0	0	0
C <sub>5i</sub>	1,000	327	327	119	119	327
C <sub>6i</sub>	4	-	-	-	-	-
C <sub>7i</sub>	345	-	-	-	-	-
C <sub>8i</sub>	1,000	-	-	-	-	-

\* The unit of vapor pressure is J/kmol.

The unit of temperature is Kelvin (K).

**Table 76** Comparison of enthalpy of vaporization at TB obtained from databanks and estimation.

Method	(a)	(b)	(c)	(d)
Databank	7.244E+07	7.479E+07	7.529E+07	4.726E+07
Definition	7.041E+07	7.036E+07	7.128E+07	6.194E+07
Vetere	5.723E+07	6.439E+07	6.485E+07	7.838E+07
Gani	6.687E+07	9.014E+07	9.143E+07	1.121E+08
Ducros	-	9.563E+07	9.977E+07	1.245E+08
Li-Ma	6.544E+07	0	0	0

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