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Chemical process plant design of a batch reactor for palm oil cracking

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Abstract

The concept of continuous process in producing oleochemicals from palm oil by using a batch reactor is discussed in this paper. It has been recognized that the batch stirred reactor is a primary mode used in the synthesis of oleochemicals. The design of a batch reactor is necessary for cracking of palm oil to produce oleochemicals. The proposed batch reactor is to crack 500Kg per day of palm oil aimed at producing Fatty acid ethyl ester (oleochemicals). This figure was chosen as the basis of the design. Also the energy and material balance of the batch process reactor plant was calculated. Finally the equipment design for the batch process reactor was carried out and the parameters obtained for its construction are: 4.76m^3 volume, 1.32m diameter, and 10hp electric motor for agitation.

Keywords: material balance, energy balance, palm oil cracking, oleochemicals, equipment design

1. Introduction

Oleochemicals are chemicals derived from oils and fats. They are analogous to petrochemicals which are chemicals derived from petroleum. Oleochemicals or derivatives based on C_{12}-C_{14} and C_{16}-C_{18} chain lengths have a variety of uses [1, 2]. The hydrolysis or alcoholysis of oils and fats formed the basis of the Oleochemicals industry. The five basic Oleochemicals are Fatty acids, Fatty Methyl esters and Ethyl esters, fatty alcohol, fatty nitrogen compounds and glycerol [2]. The process of derivation or obtaining these chemical intermediates from palm oil requires high temperature pyrolysis, alcoholysis, gasification or destructive distillation in the presence of a catalyst [3].

NOMENCLATURES

V_O	Volumetric flow rate, m^3/hr
X	Conversion
M_{AO}	Initial mass flow rate, kg/hr
ρ	Density, kg/m^3
K	Rate constant, g mol/min
T	Temperature, K
P	Power, kW
V	Reactor volume, m^3
H	Height, m
L	Baffle spacing, m
d_O	Baffle orifice diameter, m

2. Background to the study

The reactor is the starting point of the cracking process were the raw material which is the palm oil is introduced at an ambient temperature and is heated to a certain temperature made possible by the aid of a heat exchanger device embedded in the reactor [3]. Other key constituents are the Electric motor that houses the impeller (stirrer) for mixing of the raw material and also the baffle which act as a barrier to prevent vortex that results from centrifugal force during the working of the reactor. At the end of the cracking in the batch continuous stirrer reactor, the product can now be channeled to the fractionating column with will aid in its design. Material Balance is carried out which summarizes the sum of masses in the reactor in conformity with the law of conservation of matter. The Energy balance shows the heat effects of chemical reaction and physical transformation which occurs in the equipment. The equipment design shows the various design specifications and conditions for the design of the batch reactor in conformity with the standard design procedures and for the reactor to function effectively. The basic procedure that will lead to the yield of oleochemicals consists of pre-heating the palm oil (triglyceride) with the aid of a heat exchanger, and then passed to the pump, and from the pump it is charged into the reactor which operates at a chosen temperature of 374^{O}C and atmospheric pressure [1, 2, 3, 4].

3. Design Method for Batch Reactor

The geometric configuration is a proposed approach to design a batch reactor by maintaining dynamic stability using various constants, followed by the application of other empirical design correlations.

3.1 Equation of the reaction and mechanism

Equation for the reaction:

Triglycerides Heat ➔ Fatty Acids + Fatty acid Methyl Ester + Glycerol [4]. (1)

Triglycerides Heat ➔ Ethyl propanate + Stearic acid + Linoleic acid + Ketene (octadecatrien-1-ol) (2)

Mechanism

$CH_2\,OCOR^{I}$ CH_3

I I

$CHOCOCH_2R^{II} \rightarrow CH_2 + R^{I}COOH + R^{II}COOH + R^{III}CH{=}\,CHO$ (3)

I I

$CH_2\,OCOR^{III}$ $COOC_2H_5$

Triglyceride Ethyl Propanoate Stearic acid Linoleic acid Ketene (octadecatrien-1-ol) [5]

Where

$R^{I} = (CH_2)_{16}\,CH_3,$

$R^{II} = (CH_2)_6\,CH = CH\,(CH_2)_7\,CH_3$

$R^{III} = (CH_2)_7\,CH = CH - CH_2\text{-}CH = (CH_2)_4\,CH_3$

Assumptions

1. 95% of FAEE produced at reactor is recovered as distillate.
2. For practical purpose, steady state condition is assumed
3. Batch operation
4. A day is assumed to be 8 hours
5. 85% conversion

Basis: 1 day operation

Plant capacity = 500kg/day

3.2 Calculation parameters used

Physical/Chemical Properties of Equation of Reaction [6]

Density

- Triglyceride- $0.928 g/cm^3$
- Ethyl propanoate- $0.8844 g/cm^3$
- Stearic Acid- $0.847 g/cm^3$ at 70^oC, $1.017 g/cm^3$ at 17^oC
- Ketene (octadecatrien-1-ol):$1.08 g/cm^3$
- Linoleic Acid- $0.90 g/cm^3$

Vapour Pressure

- Triglyceride- Between 25-760mmHg
- Ethyl propanoate- 35.90mmHg, 5.32kpa/27^oC, 44mmHg at 27.2^oC
- Stearic Acid- 10mmHg at 21^oC, 1mmHg at 344.7^oF, 5mmHg at 408.2^oF
- Ketene (Octadecatrien-1-ol): Greater than 1atm, $1.4*10^3$kPa at 25^oC
- Linoleic Acid- 3.5mmHg at 25^oC, 1.0mmHg at 180^oC, 1.0mmHg at 176.5^oF

Viscosity

- Triglyceride- 15.9cSt at 40^oC
- Also Palm Oil (Triglyceride):
- Kinematic Viscosity is $39.6 mm^2/s$ at 38^oC,
- Density is $0.9180 g/cm^3$
- Therefore Viscosity = Kinematic Visco. * Density = 39.6 * 0.9180 = 36.3528
- At room temp. Viscosity is 8.46Pa.s
- Ethyl propanoate- 0.426cP at 25^oC
- Stearic Acid- 176.50cP (160^oC), 9.04cP (75^oC), 7.79mPa.s (80^oC), 6.29mPa.s (90^oC)
- Linoleic Acid- 29.0cP(25^oC), 17.7cP(38^oC), 13.1cP(50^oC), 9.41cP(60^oC), 3.41cP(110^oC)

Rate Constant Values

K values of the cracking of palm oil in autoclave Batch reactor

Temperature	Rate constant
623	0.0053gmol/min
648	0.0021gmol/min
673	0.0060gmol/min

4. Results and Discussion

4.1 Material balance over the Reactor

Plant capacity = 500kg/day

$$\text{Capacity} = \frac{500}{8} = 62.5\text{kg/hr}$$

Considering 20% Safety factor

$$\text{Plant through put} = \frac{20}{100} \text{ x } 62.5 = 75\text{kg/hr}$$

Note: This safety factor takes care of material loss due to over pressure and other losses

From assumption, 95% of FAEE expected to be produced at reactor is recovered as distillate

$$\text{FAEE is } S_2 = \frac{75}{95} \text{ x} \frac{100}{1} = 78.95\text{kg/hr}$$

$$\text{Kmol of FAEE produced from reactor} = \frac{\text{mass}}{\text{molar mass}} = \frac{78.95}{102.13} = 0.733$$

Kmol of FAEE produced= 0.773kmol/hr

$$\text{Conversion} = \frac{\text{kmoles of palm oil consumed}}{\text{kmoles of palm oil fed}} \text{ x } \frac{100}{1} \qquad (4)$$

Similarly,

$$\text{Reactor Yield} = \frac{\text{kmoles of FAEE produced}}{\text{kmoles of palm oil fed}} \text{ x } \frac{100}{1} \qquad (5)$$

SC = stoichiometric factor = ratio of stoichiometric moles of product to reactant = 1

Stoichiometric Equation of the Reaction

Triglycerides => Ethyl propanoate (FAEE) + Stearic acid + Linoleic acid + ketenes (6)

$$0.95 = \frac{0.773}{\text{Kmole of palm oil converted}} \text{ x } \frac{1}{1}$$

$$\text{Kmoles of palm oil converted} = \frac{0.773}{0.95} = 0.814\text{kmol/hr}$$

$$\text{Triglyceride fed} = \frac{0.814}{0.85} = 0.958 \text{ kmoles}$$

Kmoles of Stearic acid produced= 0.773,

Kmoles of Linoleic acid produced = 0.773

Kmoles of ketene produced= 0.773,

Kmoles of triglyceride unconverted = 0.958 - 0.814 = 0.114

Mass of triglyceride fed to the reactor

Kmoles fed = 0.958, Molar mass = 846.26

Mass of Triglyceride fed = 0.958 x 846.26 = 810.72kg/hr

Mass of triglyceride unconverted = (0.958-0.814) x 846.26 = 121.86kg/hr

Calculation of Mass of Ketene (Octadecatrien-1-ol) Produced

From the stoichiometric equation, 1 kmole of ketene is produced along with 1 kmole of FAEE, 1 kmole of Stearic acid and 1 kmole of Linoleic acid.

Hence, total kmoles of ketene produced = 0.773

Molar mass of ketene = 223.42kg/kmol, Mass of ketene = 0.773 x 223.42= 172.72kg/hr

Calculation of Mass of Stearic Acid Produced

From stoichiometric equation, 1 kmole of stearic acid was produced.

Hence total kmol of stearic acid produced = 0.773

Molar mass of stearic acid = 284.48kg/kmol, Mass of Stearic acid = 0.773 x 284.48 = 219.9kg/hr

Calculation of Mass of Linoleic Acid Produced

From the stoichiometric equation, 1 kmole of Linoleic acid produced.

Hence total kmoles of linoleic acid produced = 0.773

Molar mass = 280.45kg/kmol., Mass of Linoleic acid = 280.45 x 0.773 = 216.79kg/hr

Material Balance Summary

Compd mass composition (%) (kg/hr) compd Mass composition (%) (kg/hr)

Inlet Stream

Triglyceride (Mass: 810.72kg/hr, Composition: 100%)

Outlet Streams

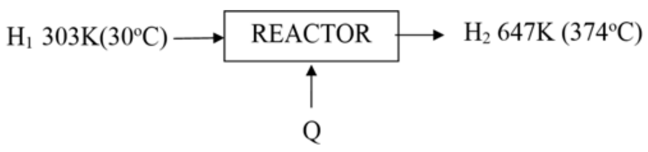
Compound	**Mass (kg/hr)**	**Composition (%)**
Ethyl Propanoate (FAEE)	78.95	9.74
Stearic acid	219.9	27.14
Linoleic acid	216.79	26.76
Ketenes	172.7	21.32
Triglyceride Unconverted	121.86	15.04
Total	810.2	

Table 1: Summary of material balance at reactor

	Reactor		**Quantity**	
Stream	**Component**	**Mol.wt Kg/kmol**	**Kmole /hr**	**Kg/ hr**
S_1 (Input)	Triglyceride	846.26	0.958	810.72
		ΣS_1		810.72
S_2 (Output)	FAEE (Ethyl propanoate)	102.13	0.773	78.95
	Stearic acid	284.48	0.773	219.9
	Linoleic acid	280.45	0.733	216.79
	Ketenes	223.42	0.773	172.7
	Triglyceride Unconverted	846.26	0.144	121.86
		ΣS_2		810.2

Input, ΣS_1 = 810.72 kg/hr, Output, ΣS_2 = 810. 2 kg/hr

4.2 Energy Balance over the Reactor



$H_1 + Q = H_2$

Assumptions

1. Steady State Operation
2. Datum Temperature

- Hence, the input to the reactor
- Triglyceride = 810.72kg
- H_1=MCpT_1,=810.72x2425.78x303=595888.39KJ/hr=595.888MJ/hr
- Effluents, from the reactor
- Ethyl propanoate = 78.95kg/hr, Stearic acid = 219.9kg/hr, Linoleic acid = 216.79 kg/hr
- Ketene = 172.7kg/hr, Triglyceride uncovered = 121.86 kg/hr

:. $Q = H_{out} - H_{in}$

Heat output, $H_{out} = \Sigma mc_pT$

= (mc_pT) + (mc_pT) + (mc_pT) + (mc_pT) + (mc_pT) +

Ethyl propanoate, stearic acid, Linoleic acid, Ketene, Unconverted Triglyceride

a. Head output for Ethyl propanoate = mc_pT = 78.95 x 1.920 x 647 = 98074.848 = 98.074KJ/hr

b. Heat output for Stearic acid = mc_pT = 219.9 x 2359.42 x 647 = 335687.183KJ/hr

c. Heat output for Linoleic acid = mc_pT = 216.79 x 2884.27 x 647 = 404556.738KJ/hr

d. Heat output for Ketene = mc_pT, H_{out} = 172.7 x 3.568 x 647 = 398.677KJ/hr
e. Heat output for unconverted Triglyceride = mc_pT = 121.86 x 2425.78 x 647 = 191256.791KJ/hr

Total Heat output = 931.997MJ/hr
$Q = H_2 – H_1$ = 931.997 - 595.888 = <u>336.109</u> MJ/hr
Heat added to the reaction for cracking of the palm oil
= 336.109MJ/hr = 336109KJ/hr

$$\text{Power} = \frac{336109 \times 10^3}{60 \times 60} = 93363.6\text{W}$$
$$= 93.3636 \text{ KW}$$

4.3 Energy Balance Summary

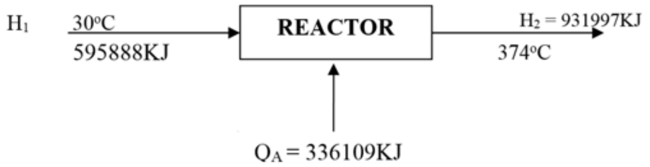


Table 2: Summary of energy balance

Input	Output
H_1: 595888	H_2: 931997
Q: 336109	-
931997	931997

4.4 Equipment design calculations for the reactor

A) Detailed Design of the Batch Reactor

Since the process is batch operation, batch stirred reactor is used. The volume for batch reactor is given as [7]

$$\frac{dN}{dt} = -r_A V \qquad (7)$$

After simplication of the above

$$V = \frac{V_o}{K} \ln \frac{1}{1-x} \qquad (8)$$

Where
V_o = volumetric flow rate, K = rate constant
V = volume of the liquid, X = conversion

Mass flow rate = Density x volumetric flow rate
Initial mass flow rate, M_{AO}= 810.72kg/hr
Density of triglyceride = 928kg/m^3

$$M_{AO} = \frac{\rho V_o}{V_o} = \frac{M_{AO}}{\rho} = \frac{810.72}{928} = 0.8736\text{m}^3/\text{hr}$$

Using K-values of the cracking of palm oil in autoclave batch reactor
K_{647} = 0.0060 gmol/min
K_{647} = 0.464hr^{-1}

$$V = \frac{0.8736}{0.464} \ln \frac{1}{1-0.85} = \frac{0.873 \times 1.897}{0.464} = 3.57\text{m}^3$$

Volume of liquid content, V_C= 3.57m^3
From Perry 5th Edition [8]
For safety
Void space, V_V = 25% of total volume
$V_T = V_c + V_v$
$V_v = 0.25V_T$
$V_T = V_C + 0.25 V_T$
$V_C = V_T - 0.25 V_T = V_T (1- 0.25)$

$$V_T = \frac{V_C}{0.75} = \frac{3.57}{0.75} = 4.76\text{m}^3$$

Total volume of the reactor, V_T = <u>4.76m^3</u>

$$V = \frac{\pi D^2 h}{4} \qquad (9)$$

h = 3.48m
Total height of the reactor, h= 3.48m
Since viscosity of the reactant is low, meaning turbulence will be needed, therefore, baffle is incorporated to avoid vortex and create turbulent mixing.

$$\text{Baffle width, } w = d/8 = 0.66 = \frac{0.083\text{m}}{8}$$
$$\text{Off set of baffle above liquid top} = \frac{w}{6} = \frac{0.083}{6} = 0.0138\text{m}$$
$$\text{Off set of baffle bottom} = \frac{d}{2} = \frac{0.66}{2} = 0.33\text{m}$$
$$\text{Height of baffle} = H + \frac{w}{6} - \frac{d}{2} = 2.64 + 0.0138 - 0.33 = 2.32\text{m}$$

The volume of liquid content required for the batch stirred reaction = 3.57m^3

$$\text{Volume of a content using cylindrical tanks} = \frac{\pi D^2 H}{4}$$

From Perry 5th Edition [8]: H/D = 2 to 3
-: choosing 2
H = 2D

$$\text{Volume} = \frac{\pi D^2 \times 2D}{4} \qquad (10)$$

D = <u>1.32m</u>

Diameter of the batch stirred reactor = 1.32m
Height of liquid, H = 2D = 2.64m

Also from Perry 5th Edition [8]
For a radial impeller (impeller to be used for the stirring)
$0.3 \leq (d/D) \leq 0.5$ (ratio of impeller diameter to column diameter) Assuming 0.5
d/D = 0.5
d = 0.5D
d = 0.5 x 1.32 = 0.66m

The diameter of the radial impeller for the Batch stirred tanks, d = 0.66m

Power Requirement

Mean efficiency will depend on the following:

i) The width and span of the propeller

ii) Its speed of rotation

Conversely, the values of these quantities will determine the power demand

If the span of the propeller 2r and the speed 1000rpm

The power consumption of the mixer

$$P = k\mu^3 D^5 \quad (11)$$

Where

k = 1. 711 $lb_f\ s^2/ft^4$ or 874.2 Ns^2/M^4 for low viscous liquid

Viscosity of oil, $\mu = 36.35\ mNs/m^2$

$\mu = 350rpm = 5.83rps$

For the pilot unit, taking the impeller diameter as ΔT/3 [9].

In the turbulent regime, at high values of Re, p is independent of Re

$$\frac{P}{\rho\mu^3 D^5} = f\frac{(\rho\mu D^2)}{U}, \frac{(\mu^2 D)}{g}, \frac{\Delta T}{\Delta} \quad (12)$$

$$Re = \rho\mu D^2/U = \frac{0.44^2 \times 928 \times 5.83}{36.35 \times 10^3} = 28814.9 = 28815$$

$$P = K^1N^3D^5 = 874.2 + (5.83)^3 + (0.528)^5$$

P= 7108.63 (10hp)

Power requirement of the impeller = **7.108 kW (10hp)**

Equipment Design summary

Summary of reactor design

Volume of reactor:	$4.76m^3$
Diameter of reactor:	1.32m
Volume of liquid content:	$3.57m^3$
Height of liquid level:	2.64m
Impeller type:	Orientation
Impeller diameter:	0.66m
Power requirement of impeller:	(7.108 kW) 10hp
Height of the baffle:	2.32m

5. Conclusion

The design for a batch reactor follows an appropriate methodology based on the standard shell and tube heat exchanger. Other criteria employed to take into account are the effect of baffles and the rate of reaction. The study shows the importance of a batch stirred reactor in cracking of palm oil which buttresses the point that complete conversion of triglyceride to oleo chemicals can be achieved at long residence time with relatively compact batch stirred reactor. The parameters for fabrication of the reactor are as follows: $4.76m^3$ volume, 1.32m diameter, and 10hp electric motor for agitation.

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