Technical Team

Nature of Invention: Process Flow Diagram , Mass Balance and Energy Balance

Applicant: QuantiVEX

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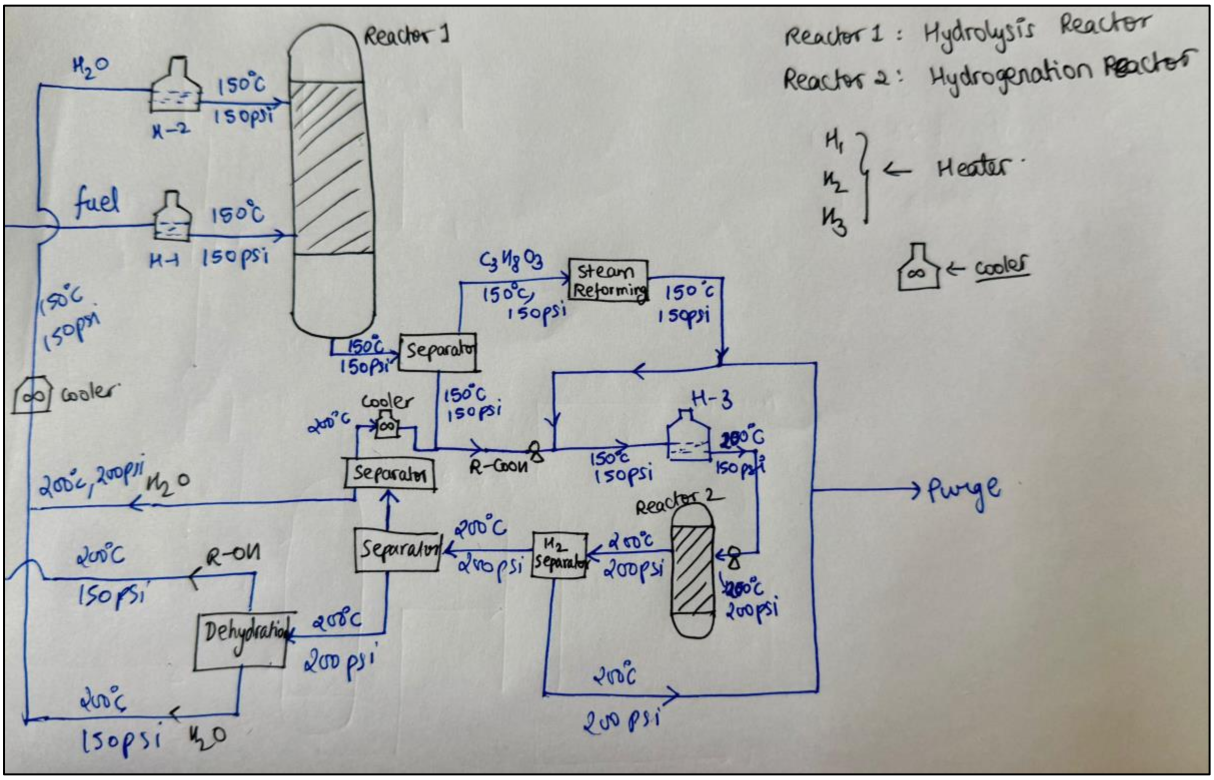
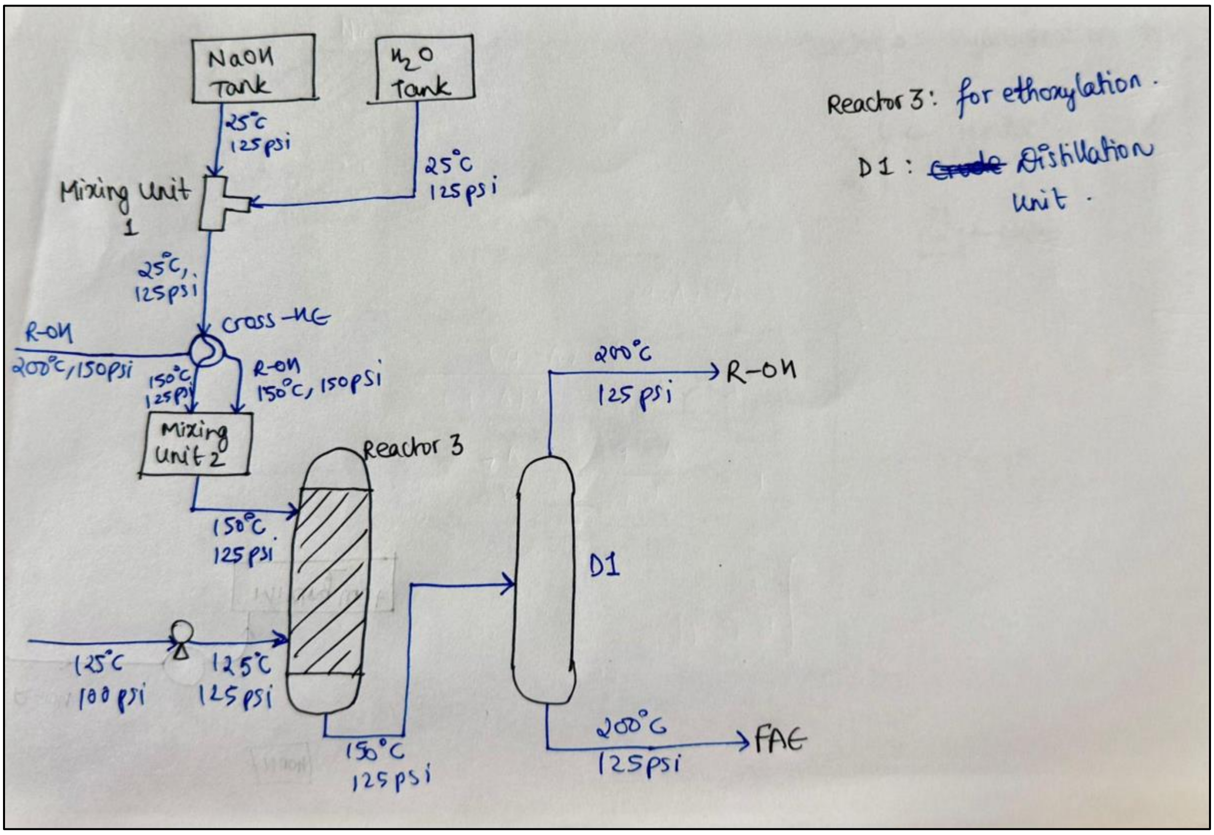
Chemical Formula: RO-(CH2CH2CO)nH

Chemical Name: Fatty Alcohol Ethoxylates

Process Title: Production of Fatty Alcohol Ethoxylates from triglycerides (fuel)

(a) Process Diagram





NaOH Tank
H2O Tank
25°C 125psi
25°C 125psi
Mixing unit 1
25°C, 125psi
cross-HE
R-OH 200°C, 150psi
150°C 125psi
R-OH 150°C, 150psi
Mixing unit 2
Reactor 3
150°C 125psi
125°C 100psi
125°C 125psi
150°C 125psi
D1
200°C 125psi
R-OH
200°C 125psi
FAE
Reactor 3: for ethoxylation.
D1 : ~~Crude~~ Distillation unit.

1 Molecular Weights

Compound	Formula	Molecular Weight (kg/kmol)
Triglyceride	$(C_{17}H_{35}COO)_3C_3H_5$	891.48
Water	H_2O	18.02
Glycerol	$C_3H_8O_3$	92.09
Fatty Acid	$C_{17}H_{35}COOH$	284.47
Hydrogen	H_2	2.02
Fatty Alcohol	$C_{17}H_{35}CH_2OH$	270.49
Sodium Hydroxide	$NaOH$	40.00
Ethylene Oxide	C_2H_4O	44.05
Carbon Monoxide	CO	28.01
Carbon Dioxide	CO_2	44.01
Fatty Alcohol Ethoxylate	$C_{17}H_{35}CH_2(OCH_2CH_2)_5OH$	490.75

Table 1: Molecular Weights of Compounds Involved in the Process

2 Mass Balance

- We have chosen the alkyl group R to be $C_{17}H_{35}$.

Step 1: Hydrolysis of Triglycerides

Key Assumption: 95% conversion of triglycerides

$$C_3H_5(OOCR)_3 + 3\,H_2O \longrightarrow C_3H_8O_3 + 3\,RCOOH \tag{1}$$

Input:

- Triglycerides: x kmol/hr
- Water: Excess (from recycle streams + fresh feed as needed)

Output (95% conversion):

- Fatty acids: $3x \times 0.95 = 2.85x$ kmol/hr
- Glycerol: $x \times 0.95 = 0.95x$ kmol/hr
- Unreacted triglycerides: $x - 0.95x = 0.05x$ kmol/hr (Recycled)

Recycle:

- Unreacted triglycerides are recycled back to the hydrolysis step.
- Excess water from downstream processes is recycled to minimize fresh water usage.

Step 2: Steam Reforming of Glycerol

Key Assumption: Complete combustion of glycerol occurs

$$C_3H_8O_3 + 3\,H_2O \longrightarrow 3\,CO_2 + 7\,H_2 \tag{2}$$

Input:

- Glycerol: $0.95x$ kmol/hr
- Water: Excess (recycled + fresh as needed)

Output:

- Hydrogen: $7x$ kmol/hr
- Carbon dioxide: $2.85x$ kmol/hr

Recycle:

- Unreacted hydrogen from hydrogenation is recycled here.
- Excess water is reused to minimize fresh water input.

Step 3: Hydrogenation of Fatty Acids

Key Assumption: 95% conversion of fatty acids

$$RCOOH + 2\,H_2 \longrightarrow RCH_2OH + H_2O \tag{3}$$

Input:

- Fatty acids: $2.85x$ kmol/hr
- Hydrogen: $2 \times 2.85x \times 0.95 = 5.42x$ kmol/hr

Output:

- Fatty alcohol: $2.71x$ kmol/hr
- Water: $2.71x$ kmol/hr
- Unreacted fatty acids: $0.14x$ kmol/hr (Recycled)
- Unreacted hydrogen: $1.58x$ kmol/hr (Recycled)

Recycle:

- Unreacted fatty acid is recycled.
- Unreacted hydrogen is recycled to hydrogenation or steam reforming.

Step 4: Alkoxide Formation

$$RCH_2OH + NaOH \longrightarrow RCH_2O^-Na^+ + H_2O \tag{4}$$

Input:

- Fatty alcohol: $2.71x$ kmol/hr
- NaOH: $2.71x$ kmol/hr

Output:

- Alkoxide: $2.71x$ kmol/hr
- Water: $2.71x$ kmol/hr

Recycle:

- Excess water is recycled.
- Some NaOH is recovered and reused in neutralization.

Step 5: Ethoxylation (FAE Formation)

$$RCH_2O^-Na^+ + 5\,C_2H_4O + H_2O \longrightarrow RCH_2(OCH_2CH_2)_5OH + NaOH \tag{5}$$

Input:

- Alkoxide: $2.71x$ kmol/hr
- Ethylene oxide: $13.55x$ kmol/hr
- Water: $2.71x$ kmol/hr

Output:

- Fatty Alcohol Ethoxylates (FAE): $2.71x$ kmol/hr
- NaOH: $2.71x$ kmol/hr

Recycle:

- Excess water is recycled.
- Unreacted ethylene oxide is separated and reused.
- Excess NaOH is reused in neutralization.

Determining the value of x

- Our given basis ($\dot{m}_{FAE}$) is 1000 kg/day of neutralized FAE
- $\dot{m}_{FAE} = 1000 \text{ kg/day} = \frac{1000 \text{ kg}}{24 \text{ hr}} = 41.67 \text{ kg/hr}$
- Hence its molar flow rate $\dot{n}_{FAE} = \frac{\dot{m}_{FAE}}{M_{FAE}} = \frac{41.67 \text{ kg/hr}}{476.72 \text{ kg/kmol}} = 0.0874 \text{ kmol/hr}$
- Since we got the final molar flow rate of FAE = $2.71x$ kmol/hr, we can equate it with the above obtained molar flow rate of FAE to solve for x.
- $2.71x = 0.0874 \implies \boxed{x = 0.032}$

3 Mass Balance Tables

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Triglycerides	28.53	1.43
Water	1.728	0.086
Fatty Acid	-	25.94
Glycerol	-	2.80
Total	**30.26**	**30.26**

Table 2: Mass Flow Summary of Compounds in Hydrolysis of Triglycerides

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Glycerol	2.80	-
Water	1.64	-
Hydrogen	-	0.43
Carbon Dioxide	-	4.01
Total	**4.44**	**4.44**

Table 3: Mass Flow Summary of Compounds in Steam Reforming of Glycerol

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Fatty acids	25.94	1.27
Hydrogen	0.35	0.10
Fatty alcohol	-	23.46
Water	-	1.56
Total	**26.3**	**26.4**

Table 4: Mass Flow Summary of Compounds in Hydrogenation of Fatty Acids

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Fatty alcohol	23.46	-
Sodium Hydroxide	3.47	-
Alkoxide	-	25.37
Water	-	1.56
Total	**26.93**	**26.93**

Table 5: Mass Flow Summary of Compounds in Alkoxide Formation

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Alkoxide	25.37	-
Ethylene Oxide	19.10	-
Water	1.56	-
Fatty Alcohol Ethoxylates	-	42.56
Sodium Hydroxide	-	3.47
Total	**46.03**	**46.03**

Table 6: Mass Flow Summary of Compounds in Ethoxylation

4 Energy Balance

4.1 Specific Heat Capacities

Substance	Specific Heat Capacity (C_p) [kJ/kg·K]
Triglyceride	2.0
Water	4.18
Hydrogen gas (H_2)	14.3
$C_{17}H_{35}COOH$	1.9
Glycerol	2.4
$C_{17}H_{35}CH_2OH$	2.2
Ethylene Oxide	1.18
Fatty Acid Ethoxylate (FAE)	2.5
NaOH (aq·)	3.7

Table 7: Specific Heat Capacity of Various Substances

4.2 Energy Balance Calculations

4.2.1 Preheating the Feed

Temperature change:

$$\Delta T = 150 - 25 = 125°C$$

Heat required:

$$\dot{Q}_{in} = \dot{m}C_p\Delta T \quad \text{(kJ/hour)}$$

For individual components:

$$\dot{Q}_{TG} = \dot{m}_{TG}C_{p,TG}\Delta T \implies 28.53 \times 2 \times 125 = 7132.5 \text{ kJ/hr}$$

$$\dot{Q}_{H_2O} = \dot{m}_{H_2O}C_{p,\mathrm{H_2O}}\Delta T \implies 1.728 \times 4.18 \times 125 = 902.88 \text{ kJ/hr}$$

$$\dot{Q}_{pre-heat} = \dot{Q}_{TG} + \dot{Q}_{\mathrm{H_2O}} = 8035.38 \text{ kJ/hr}$$

4.2.2 Hydrolysis Reactor

Reaction enthalpy:

$$\Delta H_r = -1213 \text{ kJ/kmol}$$

Total heat released:

$$\dot{Q}_{out} = -1213 \times \dot{n} \quad \text{(kJ/hour)}$$

$$\dot{Q}_{hydr,out} = -1213 \times 0.95 \times 0.032 = -36.87 \text{ kJ/hr}$$

4.2.3 Steam Reforming Reactor

Reaction enthalpy:

$$\Delta H_r = 742.5 \text{ kJ/kmol}$$

Total heat input:

$$\dot{Q}_{in} = 742.5 \times \dot{n} \quad \text{(kJ/hour)}$$

$$\dot{Q}_{SR,in} = 742.5 \times 0.95 \times 0.032 = 22.57 \text{ kJ/hr}$$

4.2.4 Heating Fatty Acid and Hydrogen to 200°C

$$\dot{Q}_{in,total} = \dot{m}_{H_2} C_{p,\mathrm{H}_2}(200 - 150) + \dot{m}_{FA} C_{p,FA}(200 - 150) \quad \text{(kJ/hour)}$$
$$\implies \dot{Q}_{in,total} = 0.35 \times 14.3 \times 50 + 25.94 \times 1.9 \times 50 = 2714.55 \text{ kJ/hr}$$

4.2.5 Hydrogenation of Fatty Acid

Reaction enthalpy:
$$\Delta H_r = 180.32 \text{ kJ/kmol}$$
Total heat input:
$$\dot{Q}_{in} = 180.32 \times \dot{n} \quad \text{(kJ/hour)}$$
$$\implies \dot{Q}_{in} = 180.32 \times 2.71 \times 0.032 = 15.64 \text{ kJ/hr}$$

4.2.6 Mixing Unit

Reaction enthalpy:
$$\Delta H_r = -117 \text{ kJ/kmol}$$
Total heat:
$$\dot{Q}_{total} = \dot{Q}_{cooling}(\mathrm{RCH_2OH}) + \dot{Q}_{heating}(NaOH) + \Delta H_r \times \dot{n} \quad \text{(kJ/hour)}$$
$$\implies \dot{m}_1 C_p(200 - 150) + \dot{m}_2 C_p(150 - 25) + \Delta H_r \times \dot{n}$$
$$\implies 23.46{\times}2.2{\times}(150{-}200){+}3.47{\times}3.7{\times}(150{-}25){+}({-}117){\times}2.71{\times}0.032 = -985.87 \text{ kJ/hr}$$

4.2.7 Preheating Ethylene Oxide

Temperature change:
$$\Delta T = 150 - 25 = 125°C$$
Heat required:
$$\dot{Q}_{in} = \dot{m} C_p \Delta T \quad \text{(kJ/hour)}$$
$$\implies \dot{Q}_{in} = 19.1 \times 1.18 \times 125 = 2817.25 \text{ kJ/hr}$$

4.2.8 Ethoxylation Reactor

Reaction enthalpy:
$$\Delta H_r = -231 \text{ kJ/kmol}$$
Total heat released:
$$\dot{Q}_{out} = \Delta H_r \times \dot{n} \quad \text{(kJ/hour)}$$
$$\implies \dot{Q}_{out} = (-231) \times 2.71 \times 0.032 = -19.16 \text{ kJ/hour}$$

4.3 Total Heat Given or Consumed

The total energy input/output in the process is calculated as:
$$\dot{Q}_{net} = \sum \dot{Q}_{in} - \sum \dot{Q}_{out} \quad \text{(kJ/hour)}$$
$$\implies \dot{Q}_{net} = 13605.39 - 1041.90 = 12563.49 \text{ kJ/hr}$$

Capital cost (only for the reactor):

Equipment	Design Capacity (L)	No. of units	Cost/unit ($ for year 2014)	Total Cost ($ for year 2014)
REACTOR 1 (Jacketed reactor, agitated, Carbon steel, pressure of 150 psi)	2000	1	39,500	39,500
REACTOR 2 (Jacketed, agitated, carbon steel, pressure of 300 psi)	1000	1	37,100	37,100
REACTOR 3 (Jacketed, agitated, carbon steel, pressure of 150 psi)	1000	1	25,600	25,600

References: Provide reference for a research paper or an actual patent.

1. http://www.matche.com/equipcost/Reactor.html
2. https://patents.google.com/patent/US4218386A/en#:~:text=A%20process%20for%20hydrolyzing%20triglyceride,to%20produce%20carboxylic%20acids%20corresponding
3. https://patents.google.com/patent/US1839974A/en
4. https://patents.google.com/patent/EP0310194A1/en
5. https://docs.google.com/document/d/1oPy2cF__JycGj6WjQylfV7wy3jah52hNr2eDtSsBZRo/edit?usp=sharing

List the contributions of each author:

- **Process flow diagram:** Sarthak Singh
- **Material Balance:** Bipin Kumar Jaiswal, Nonit Gupta, Peeyush Sahu
- **Energy Balance:** Bipin Kumar Jaiswal, Nonit Gupta, Peeyush Sahu
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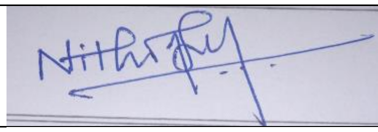
CEO Name	230709	
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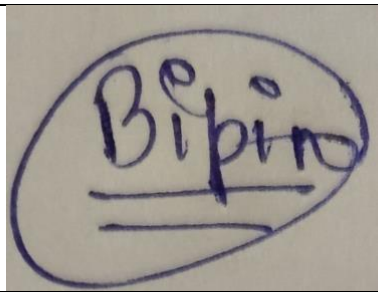
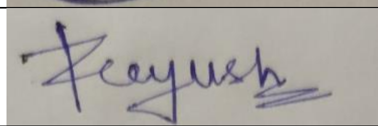
Bipin Kumar Jaiswal)	230300	
Peeyush Sahu	230750	
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