CHE261A Patent Application

Applicant: SynergyX

Inventors: Diya Saraf, Sakshi Dargu, Aditya Gupta, Sanskaar Srivastava, Priyanshu Kamde

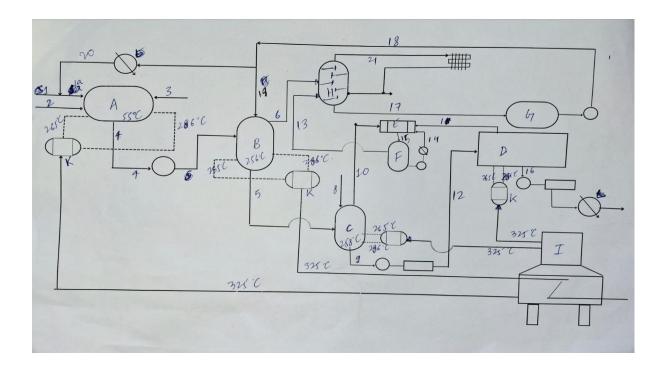
Chemical Formula: (C10H8O4)n

Chemical Name: Polyethylene terephthalate(PET)

Process Title: Production of PET from Pure Terephthalic Acid and Ethylene Glycol

Catalysts: Antimony TriAcetate

Process Description:
a. Process Flow Diagram:



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A-MIXING VESSEL
 B- ESTERIFIER
C- PRE-POLY CONDENSATION TANK
D- DISC RING REACTOR
E-SCRAPPER CONDENSER
F- CONDENSATE COLLECTOR
G- MOTHER VESSEL OF EG
M- DISTILLATION COLUMN
I - FURNACE
K- NEAT EXCUANGBERS
1. Fresh EG
                       17. Spent EG
2. Catalyst
                     18. Recovered EG
                       19. Recovered EG
3. PTA
4. Paste
                      20. Recycled EG
5. BMET
                       21. Water Vapors.
 6. Waste + Unseacted
         EG vaposs
7. Catalyst
8. Catalyst
9. Small chain PET
10. Eg vaposs
11- EG vaposs
12. small chain PET
13. Liquid EG
14. Cold EG
15. Condensed Eg
16. Long Chain PET
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b. Material Balance:

HODC-
$$\langle O \rangle$$
-COOH + HO(CH2)OH \longrightarrow HO-(OC- $\langle O \rangle$ -COO(CH2)O)H
(TPA) (EG) + 2NH2O (PET)
(MM=166.14) (MM=62.07) (H2O) (MM=192.2)
(MM=18)

- Basis = 100 tonnes PET/day = 4166.6 kg PET/hr = 100 $\times 10^3 \times 1 \text{ kg PET/hr} = 4166.6 \text{ kg PET/hr} = 21.68 \text{ kmol/hr} = 100 <math>\times 10^3 \times 1 \times 1 \text{ kmol PET/hr} = 21.68 \text{ kmol/hr} = 24 192.2$ For 90 % overall conversion,
- · EG required = 21.68 = 24.08 kmol/hr
- · TPA required = EG required = 24.08 kmol / hr

Balance across Mixer

- · Flowrate of Catalyst (Antimony TriAcetate) is taken to be 18 ppm
- · Also for the ratio, E|T=1.12
- Thus flowrate of MEG = (1.12)(24.08 kmo)/hr) = 26.97 kmol/hr
- · Fresh MEG = 24.08 kmol/hr
- MEG recycled = (26.97 24.08) kmol | hr
 = 2.89 kmol | hr
 = 2.89 x 62.07 kg | hr = 179.38 kg | hr
- · Flowrate of TPA = 24.08 kmol/hr

| | Input | Output |
|-------|-------|--------|
| TPA | 24.08 | |
| MEG | 26.97 | |
| Paste | | |
| Total | 51.05 | 51.05 |

```
Balance Across Esterifier:-
HOOC- (O) COOH + 2 HO (UN) OH -> HO (CH2) (UO) (O) COO- (U12) OH
               (MM=62.07) +2H2O (MM=254.24)
    (TPA)
                           (MM=18)
 (MM = 166.14)
· TPA reg for the above reaction is 24.08 kmol/hr
· Thus MEG reg = 2 (TPA reg) = 2(24.08) = 48.16 kmol/h
· MEG from paste of mixer = 26.97 kmol /hr
· Thus MEG obtained from recycle = (48-16-26-97)
  Due to 90 %. conversion,
 We have unreacted MEG as = (0.1)(48.16)
         = 4.816 kmol /hr
.: Reached MEG = (0.9) (48.16)
                        = 43.34 kmol hr
 We have unreacted TPA as = (0.1) (24.08)
                        = 2.408 kmol/hr
         :. Reacted TPA = (0,9) (24.08)
                        = 21.672 kmol | hr
 Also, BHET (bis (2-hydroxyethy) tereputhalate)
     produced in above reaction = no. of reacted
                                moler of TPA
                            = 21.672 kmol hr
  And Water produced = no. of reacted moles of MEG
                     = 43.34 kmol/hr
                       =780.12 Kg/M
```

| | Input: | Output | Stream |
|------------------|----------|---|---------------|
| recycled MEG | 21.19 | | |
| MEG in | 26.97 | Mar Wallan | 3 1- 14007 |
| TPA | 24.08 | DES STAME | /// |
| BUET | 11=14111 | 21.67 | |
| EG (un-reacted) | | 4.816 | dr 27 h |
| TPA (un-reacted) | 1 4 / | 2.408 | |
| Water | | 43.34 | |
| Total | 72.24 | 72.234 | |
| | | person de la constitución de la | 1111111111111 |

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Balance Across Extense PRE - Polycondinsation E Unit CJ
  Tank
n 40 (CM2) coo (O ) coo (CM2)204 -
        n nof c" (o) - courch; ) on + (n-1) nocu; chi
  n BHET - + n PET + (n-1) EG
1: 254.24 192.2 62.07
MM: 254.24
 mous of BMET available = Stream 5
           =21.679 kmolly
                     = 5511,62 kg lhe
 [conversion = 921.] [From RnD report]
  80, Reacted BMET = 92% X [21.678]
                 = 19.944 kmollhs
                 = 5070.56 kg/hl.
   A unreacted BMET: (available - reacted BMET)
            = (21.678 - 19.944) kmol/hr
                = 1.734 Kmol/hr
                  = 440.85 kg/hz
```

moles of PET produced = moles of BUET seached 30 PET preduced = 19,944 kmol /hs. = 3833.24 kg/hl. meles of MEG vapors = (anders of BMET reached = 18,944 Kmol/W = 1175.85 kg/hs i stream enput antport 5517.62 Kg/M BUETIN 400.19kg/W 400.19kg/W 5 un-reacted 440.85 kg/ly BUET 3833.24 Kg/M P 9 Loducel 1175.85 4/M 10 E9 vapors log brokents Balance across mother visul of SEG EGRin (uniton) Stream 7 = stream 18 EGRin EGRIN 18 EGRIN FGRIN 20 = Total EGR in mother ussel. : MEG recipled: 179.38 kg/hr = EGR in stleam 20 CFrom cockette barance & across mixel] MEG recycled in stream 19= 21,19 kmol the = 1315.26 kg/hl CFrom balance across esterifier] % Total MEG in Alcam 17= 1315.26 + 179.38 = 1494.64 kg/hs.

| | I enout the | (kg) | hr) Stream | |
|---|--|------------------|---------------|--------------------------|
| MEG | 1494.64 | - | 17 | - |
| EEG MEG | - | 1315.26 | 19 | |
| MEG | | 179.38 | | |
| Balar | nce acro | ss Distill | ation co | dunn |
| | Balance Across Distillation Column Curit HJ Mass input = mass centput | | | |
| =) 8 | =) stream 6+ stream 13 = stram21 + stream | | | |
| wa | ter vagado | s in z r | rates vap | iors out |
| = | H20 vap | ours in | steam ? | 4 = 40 in input stream 6 |
| 00 | water vapours in = water vapors out Hro vapours in stream 2 = 420 in input stream 6 stream 21 = 780.12 kg/h/ Errom barance across esterifier J | | | |
| AX | so) bach | and the court of | m- | |
| unseacted Eq in stream 6 + Eq recorded in stream 13 | | | | |
| = spent EG in stleam 17. | | | | |
| El secovered = (1494.64 - 298.93) kg/hs | | | | |
| | | 2 1195. | 71 kg/he | • |
| | | nput | output | Stleam |
| Equ | n-seacted): | 298.93/M | _ | 6 |
| wa | ites 7 | 80.12 kg/hg | _ | 6 |
| E9 81 | covered | 1195-71 kg/hl | - | 13 |
| spe | int Eg | - | 1494.64 kg/ | 42 17 |
| wa | vaposs. | _ | 180.12 kg/h | 21 |

```
Balance Across Disc Ring Reactor
                      (unit D)
 cerrenced Reaction Yield & = 96%.
       [Flow RnD Repost]
stocker of en
unseacted BUET in stream 9= unreacted BUET
                           in stream 12
   BUETIN
 A stream 12 = 440, 85 kg lhs.
 BUET that will react = 0.96 × 440.85
                  =423. 20 kg /he =1. 6646 kmd/he
 BHET unreacted = 440.85-423.21
                  = 17.64 kg/hs.
                  = 0.069 kmol/hg
 PET formed = 300 kg the mous of BNET reacted
            = 1.6646 kmol 1 hg
             = # 319,94 kg/hs
 * small chain PET input = 3833, 24 kg lhs
                               [Stream 97
                                = Stlem 12
   EG vapots = 41,27 kg/hs
                                   = 19.944kmol)
               = 0.665 kmol/hr.
               [= fundes of BUET - 1)]
  Long chain PET = PET formed +
                   small chain PET input
              = 4153, 18 kg lhs
            2 21.608 knowl / hs
```

Input = contput PET in + BUET wasercled = solids + Eq vaposs thong chain 440.85 + 3833.24 = solids + 41.27 + 21.608 4153.18 solids = 49.6 4 kg/hr Input (19ths output 19ths) Streams PET input 3833.24 311 ET unseacted 940.85 #7.64 12 dy 16 solids 79.64 11 EG vapors - 41.27 11 Long Chain 4153.18 16 Balance Across Scrapper Condenser y Distillate Total input of EG = Stream 10 + stream !! = 1217.12 kg/hs. Let showering cold Eq = X kg/h/. Condensed EG = Y kg/hs uncondensed vapors out = 7 kg/hs By wass balance, input = output 1083.028 + X= 4+ Z -- O 4= X+ 1076.48 -- @ A Z = 21. 065 kg/hg

| 801 | | | tion col | |
|-----------|---------|------------------------|----------|---------|
| | | -X = 797 | | |
| | | = Y = 199 | | |
| _scrap | per con | denser kg/m) output | alhs) | |
| | Input | 19 m outpu | St. | leans |
| 9 vapors | 41.27 | - | 10 | |
| vapors | 1175.88 | - | 10 | |
| Showered | | - | 14 | |
| mdensote | - | 1993.48 | 15 | |
| ondensed | _ | 21.065 | | |
| Cone | densale | Collector | | |
| | 1 | 1 | D 1+ | |
| | | put | output | Streams |
| iondenso | tity 19 | 93.48 | - | 15 |
| cold Eg | | - 7 | 197.394 | 14 |
| Liquid EC | j l | - # | 195071 | 13 |

c. Energy Balance:

Balance Across Mixer

$$T = 328 \text{ K}$$
 $P = 1 \text{ atm}$
 $(CP)_{PPA} = 2.82 \times 10^{5} \frac{kT}{kmol.K}$
 $(CP)_{PPA} = 2.69 \times 10^{5} \frac{kT}{kmol.K}$
 $(CP)_{PP$

```
For EG vapor (unreacted),
     Q= (4.816 kmo) (130 kmol K) (256) K
     + (4.816 \frac{\text{kmol}}{\text{hr}}) (6.56 \times 10^{4} \frac{\text{kJ}}{\text{kmol}})
0 = (1.6 + 3.16) \times 10^{5} \text{ kJ/hr} = 4.76 \text{ kJ/hr}
For TPA (unreacted)
    Q = (2.408 kmol) (350 KJ ) (256K)
     Q= 2.16 ×103 ×J/hr
For Water vapor,
      Q= mGAT+ mix
     a = (43.34 × (256 k)) (35.7 k) (256 k)
     \dot{Q} = (3.96 \times 10^{5} + 17.6 \times 10^{5}) (4.07 \times 10^{6} \frac{kJ}{km-1})
     Q = 2.16 \times 10^6 \text{ kJ/hr}
150 \quad \text{Total Qout} = 5.09 \times 10^6 \text{ kJ/hr}
  Also.
  Heat of reaction:
  TPA -8.16×165 KJ/kmol BHET -10.94×105 KJ/kmol
MEG -3.85×105 KJ/kmol Water -2.42×105 KJ/kmol
   Total Hr = - 9.16 ×106 rt | Kmol hr
    Q'in + Hr 1 - Dow = Qnet
        Q_{\text{net}} = (0.947 - 4.16 - 5.09) \times 10^6 \text{ kJ/hr}

Q_{\text{net}} = -8.3 \times 10^6 \text{ kJ/hr}
```

```
For EG vapors, 1

\lambda = 6.56 \times 10^4 \text{ kJ [kmo]}
     Q=mGAT+ml
    0 = (18,944 kmol) (131 KT) (272 K) +
                 (18.944 Kmol) (6.56 × 104 KJ)
    \hat{Q} = (6.75 + 12.4) \times 10^5 \text{ kJ/hr}

\hat{Q} = 19.2 \text{ kJ/hr} = 1.92 \times 10^6 \text{ kJ/hr}
  Total Qow = 3.05 x 107 kJ/hr
   Also, Heat of Reaction
    BHET -10.94 \times 10^5 ESTERNOT Hr = -248.36 \times 10^5
PET -19.74 \times 10^5 ESTERNOT FSTERNOT hr
    MEG - 3.85 X105 KJ (KMI)
· Flow Rate of Dow Therm required for this heat
      T = 284^{\circ}C = 557 + \Delta T = (557 - 545) K

Cp = 842.61 \ \text{KJ} | \text{kmol, k} = 12 \text{ k}
     Onet = Oin - Oout + Hr
   = (0.246 - 3.05 - 2.48) \times 10^{7} \text{ kJ/hr}
= -5.29 \text{ kJ/hr}
(M)_{dowtherm} = 0 = 5.29 \times 10^{7} \text{ kJ/hr}
(M)_{dowtherm} = 5229.56 \text{ kmol/hr}
(M)_{dowtherm} = 5229.56 \text{ kmol/hr}
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```
Balance Across DRR
   T= 548 K
   P=1.5-1.2 mbar
  [nput] => @ T=545K DT = 272K
 For BHET unreacted, Q= mCp DT
       Q= (1-734 kmol) (405 kmol K) (272 K)
       Q = 1.91 X105 11/hr
 For PET, Q= (19.944 kmol) (5190 kJ) (272K)
          a = 2.82 x107 kJ/hr
  Total Oin= 2.83 X107 KJ/hr
 ONDW => @ T= 548K DT= 275 K
 For BHET unreacted, \dot{Q} = (0.0643 \frac{\text{kmol}}{\text{hr}}) (405 \frac{\text{kJ}}{\text{kmol}}) (275)
 For Long Chain PET, Q= (21.61 kmol) (5160 KJ) (275 K)
                   0 = 3.07 XID7
 For EG vapors, A = 6.56×109 Let | Kmo)
  Q= mCpAT+mA
  \hat{Q} = (0.665 \frac{\text{kinol}}{\text{hr}})(132 \frac{\text{KJ}}{\text{mod h}})(275 \text{ k}) +
   \hat{Q} = 6.78 \times 10^4 \text{ kJ} / \text{hr}
(0.665 \frac{\text{kmol.k}}{\text{hr}}) (6.56 \times 10^4 \frac{\text{kJ}}{\text{kmol}})
Total Oom = 3.07 ×107 kJ/hr
  Qnet = Qin - Qow = (2.83-3.07) X107 KJ
Qnet = 2.39 X106 KJ hr
```

```
Flow Rate of Dow Therm required for this heat,
        T = 286 °C = 559 k

C_9 = 842.61 \frac{kJ}{kmol.k}

\Delta T = (559 - 548)k

\Delta T = 11 k
      \frac{(m)_{dowtherm}}{(m)_{dowtherm}} = \frac{0}{Cp \Delta T} = \frac{2.39 \times 10^6 \text{ kJ/hr}}{(842.61 \text{ kJ})(11 \text{ k})} 
 \frac{(m)_{dowtherm}}{(m)_{dowtherm}} = \frac{258.17 \text{ kmol}}{hr} 
 Balance Across Distillation Column
      P= 260 mbar
Input |
For EG vapor unreacted, \dot{Q} = (4.82 \frac{\text{kmol}}{\text{Nr}})(130 \frac{\text{kJ}}{\text{kmol K}})(256\text{K})

(1 = 6.56 \times 10^4 \frac{\text{ks}}{\text{kmol}}) + (4.82 \frac{\text{kmol}}{\text{Nr}})(6.56 \times 16^4 \frac{\text{kJ}}{\text{kmol}})

\dot{Q} = (1.6 + 3.16) \times 10^5 \frac{\text{kJ}}{\text{kmol}}
                                            Q= 4.76 ×105 kJ/hr
 For Water vapors, A = 4.07 XID4 KJ/kmo)
Q= mCp DT+ind
   Q= (43.34 kmol) (35.7 kt ) (256 k)
           + (43.34) (4.07 ×104 +7/kmol)
   \hat{Q} = (3.96 + 17.6) \times 10^5 \text{ kJ/hr}

\hat{G} = 2.16 \times 10^6 \text{ kJ/hr}
Fir EG lig recovery, G=mcp DT, DT=80K
   Q = (19.27 kmol) (183 KJ ) (80K)
   $ = 2.82 X105 KJ/hr
Qin (total) = 2.92 x 106 kg/hr
```

```
] Output |
  For EGlig, A = 6.56 X104 KJ/kmol, DT=100 K
    Q = mcp AT + mx
    Q = (24.08 kmol) (160 KT) (100 K)
      + (24.08 kmol) (6.56 X104 kJ)
     0 = 3.85 kJ | hr
   For Condensed water, DT=40K
        à= (43.34 kmol) (65 ks) (40 K)
          Q = 1.13 KJ | hr
     total Qout = (1.13 +3.85) 105 KJ/hr
            · Qout = 4.98x10 kJ/hr
    \dot{Q}_{net} (Net Heat) = \dot{Q}_{in} - \dot{Q}_{out}

\dot{Q}_{net} = (2.92 \times 10^6 - 4.98 \times 10^5) \text{ kg/hr}

\dot{Q}_{net} = 2.42 \times 10^6 \text{ kg/hr}
 Balance Across Scrapper Condenser
  [Input]
   For EG vapors, \lambda = 6.56 \times 10^4 \text{ kJ/kmo}, \Delta T = 295 \text{ KG}
    Q = mcp AT + mid
    Q = (0.665 kmol) (132 kJ ) (275 K)
    \hat{\Phi} = \frac{(0.665 \text{ kmol})(6.56 \times 16^4 \text{ kJ/kmol})}{(2.42+4.36)(0^4 \text{ kJ/hr})} = 6.78 \times 16^4 \text{ kJ/hr}
```

Also for EG vapors,

$$\dot{Q} = (18.95 \frac{\text{kmol}}{\text{hr}})(132 \frac{\text{kJ}}{\text{kmol}})(275 \text{ K})$$
 $+ (18.95 \frac{\text{kmol}}{\text{hr}})(6.56 \times 10^4 \frac{\text{kJ}}{\text{kmol}})$
 $\dot{Q} = (6.88 + 12.4) \times 10^5 \text{ kJ/hr}$

For EG showered, $\dot{Q} = \dot{m} C_{p} \Delta T$
 $\dot{Q} = (12.85 \frac{\text{kmol}}{\text{hr}})(154 \frac{\text{kJ}}{\text{kmol}})(40 \text{ K})$
 $\dot{Q} = 7.9 \times 10^4 \text{ kJ/hr}$

Total $\dot{Q}_{1n} = (1.93 + 0.079 + 0.068) \times 10^6 \text{ kJ/hr}$
 $\dot{Q}_{1n} = 2.07 \times 10^6 \text{ kJ/hr}$

Output \Rightarrow

For Condensed EG, $\dot{Q} = \dot{m} C_{p} \Delta T$, $\Delta t = 80 \text{ K}$
 $\dot{Q} = (32.12 \frac{\text{kmol}}{\text{hr}})(157 \frac{\text{kJ}}{\text{kmol}})(80 \text{ K})$
 $\dot{Q} = 4.03 \times 10^5 \text{ kJ/hr}$

Total $\dot{Q}_{000} = 4.03 \times 10^5 \text{ kJ/hr}$

Net Heat, $\dot{Q}_{1n} = (2.07 - 0.403) \times 10^6 \text{ kJ/hr}$
 $\dot{Q}_{1n} = (2.07 - 0.403) \times 10^6 \text{ kJ/hr}$

Contributions of each Author:

- a. Process Flow Diagram: Diya Saraf, Sanskaar Srivastava
- b. Material Balance: Sakshi Dargu ,Aditya Gupta, Priyanshu Kamde
- Energy Balance: Sakshi Dargu, Diya Saraf

| Sign the pdf and upload. | | |
|--------------------------|---------|-----------|
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