### **DETAILED MATERIAL BALANCE**

Basis: 200 TPD of Acrylic Acid.

( Plant works continuously for 24 hours a day )

$$CH_2$$
= $CHCH_3 + O_2 \rightarrow CH_2 = CHCHO + H_2O$   
acrolein

$$CH_2$$
= $CHCHO + \frac{1}{2}O_2 \rightarrow CH_2$ = $CHCOOH$  acrylic acid

# **Compound** Molecular weight

Propylene	42
Acrylic acid(AA)	72
Acetic acid	60
Acrolein	56
Oxygen	16
Carbon dioxide	44

# Propylene required to produce 200 TPD of AA

1 kmol of 
$$C_3H_6 \rightarrow 1$$
 kmol of AA  
42 kg/hr of  $C_3H_6 \rightarrow 72$  kg/hr of AA

$$C_3H_6$$
 required to produce 200 TPD of AA  
= 200 x (42/72) = 116.67 TPD of  $C_3H_6$ 

At a yield of 78%

kmol of 
$$C_3H_6$$
 required = 116.67 / 0.78 = 149.57 TPD = 148.38 kmol/hr

## Oxygen required:

1 kmol of 
$$C_3H_6$$
 requires  $\rightarrow$  3/2 kmol of  $O_2$   
Hence  $O_2$  required = 3/2 x 148.38 kmol/ hr  
= 222.57 kmol/ hr

#### REACTOR I

## Oxidation of Propylene to Acrolein .

(From Literature)

$$CH_2$$
= $CHCH_3 + O_2 \rightarrow CH_2 = CHCHO + H_2O$   
acrolein

Catalyst composition: Ni. Fe. Zn. Bi. or Zn + Co (Fe promotion)

Contact time = 3.6 sec

Average temperature = 355° C

Feed Composition:  $C_3H_6$ : Air: Steam:: 1:7.75:3.75

Overall conversion of  $C_3H_6 = 100\%$ 

Conversion to acrolein = 70% Conversion to AA = 11%

> $C_3H_6$  fed = 148.38 kmol/hr Steam fed = 556.42 kmol/hr

Air fed =  $148.38 \times 7.75 = 1149.94 \text{ kmol/hr}$ 

 $O_2$  entering = 241.48 kmol/hr

 $N_2$  in =  $N_2$  out = 908.45 kmol/ hr

 $O_2$  used in the reactor = 148.38 kmol/hr

 $O_2$  left unreacted = 93.1 kmol/hr

Acrolein produced =  $148.38 \times 0.7 = 103.866 \text{ kmol/hr}$ 

AA produced = 148.0.11 = 16.32 kmol/hr

Steam produced = 103.866 kmol/hr

Side products produced ( $CO_2$  + Acetic acid)= $48.38 \times 0.19 = 28.192$ 

(in equal quantities) kmol/hr

Total steam leaving the reactor = 660.286 kmol/hr

#### **REACTOR II**

# Oxidation of Acrolein to Acrylic acid

(From literature)

$$CH_2$$
= $CHCHO + \frac{1}{2}O_2 \rightarrow CH_2$ = $CHCOOH$  acrylic acid

Catalyst composition: Mo<sub>12</sub> V<sub>1.9</sub> Al <sub>1.0</sub> Cu<sub>2.2</sub> (support - Al sponge)

Contact time: 1 - 3 sec

Average temperature - 300°C

Acrolein conversion - 100%

Yield of AA - 97.5%

### Feed:

 $O_2 = 93.1 \text{ kmol/hr}$ 

 $N_2 = 908.45 \text{ kmol/hr}$ 

Steam = 660.286 kmol/hr

Acrolein = 103.866 kmol/hr

Acylic acid = 16.32 kmol/hr

Acetic acid = 14.096 kmol/hr

 $CO_2 = 14.096 \text{ kmol/hr}$ 

AA formed in reactor II = 101.26 kmol/hr

By products formed = 2.5966 kmol/hr

 $O_2$  reacted = 51.352 kmol/hr

 $O_2$  unreacted = 41.167 kmol/hr

 $N_2$  in =  $N_2$  out = 908.45 kmol/hr

```
Total AA formed in 2 reactors = 101.26 + 16.32 = 117.58 kmol/hr
Total Acetic acid produced = 15.3942 kmol/hr
Total CO<sub>2</sub> produced = 15.3942kmol/hr
```

#### ABSORBER:

Feed entering at the bottom of the absorber.

```
Acrylic acid = 117.58 \text{ kmol/hr}

Acetic acid = 15.38 \text{ kmol/hr}

CO_2 = 15.38 \text{ kmol/hr}

O_2 = 41.167 \text{kmol/hr}

N_2 = 908.47 \text{ kmol/hr}

Steam = 660.286 \text{ kmol/hr}
```

#### From literature:

Acrylic acid and acetic acid is absorbed using water as solvent. Gases  $CO_2$ ,  $O_2$ ,  $N_2$  and small amount of steam leave the absorber at the top.

## Assumptions:

90% of the steam entering gets condensed.

#### Solvent:

Water entering at the top = 488.6 kmol/hr

Off gases leaving at the top:

```
CO_2 = 15.38 \text{ kmol/hr}

N_2 = 908.4 \text{ kmol/hr}

O_2 = 41.167 \text{ kmol/hr}

AA = 1.1758 \text{ kmol/hr}

Acetic acid = 0.1539kmol/hr
```

Product liquid leaving at the bottom of the absorber to recovery section:

```
Acrylic acid = 116.404 kmol/hr
Acetic acid = 15.236 kmol/hr
water = 1082.85 kmol/hr
```

Mol fraction of AA in the product stream = 0.0958 = 9.58%Weight fraction of AA in the product stream = 0.2911 = 29.11%

#### **SOLVENT EXTRACTION COLUMN:**

Feed from the bottom of the absorber:

Acrylic acid = 116.404 kmol/hr Acetic acid = 15.236 kmol/hr water = 1082.85 kmol/hr

Solvent with high solubility for acrylic acid and acetic acid, and low solubility with water is used to extract AA acid from absorber stream.

Assumption: Solvent required for 99 .5% extraction of AA is 500 kmol/hr.

Recycled stream from solvent recovery column and waste tower.

Acrylic acid = 0.53 kmol/hr Acetic acid = 0.08 kmol/hr Water = 129.94 kmol/hr

Total Acrylic acid in = 116.934 kmol/hr Total Acetic acid in = 15.316 kmol/hr Total water in = 1212.79 kmol/hr

Extract phase contains (to solvent recovery plant):

Acrylic acid =  $0.995 \times 116.404 = 115.83 \text{ kmol/hr}$ . Acetic acid = 15.16 kmol/hr

Water = 21.657 kmol/hrSolvent = 488.5 kmol/hr

Raffinate phase contains ( to waste tower):

Acrylic acid = 1.104 kmol/hr Acetic acid = 0.156 kmol/hr Water = 1191.13 kmol/hr Solvent = 11.5 kmol/ hr

#### **SOLVENT RECOVERY COLUMN:**

Assumption: Complete recovery of solvent occurs.

Bottom product contains only acetic acid and acrylic acid.

Feed: Extract phase from the liquid-liquid extractor:

Acrylic acid = 115.83 kmol/hr. Acetic acid = 15.16 kmol/hr Water = 21.657 kmol/hr

```
Solvent = 488.5 \text{ kmol/hr}
```

Upstream contains (recycled to extraction column):

```
Solvent = 488.5 kmol/hr
Acrylic acid = 0.53 kmol/hr
Acetic acid = 0.08 kmol/hr
Water = 21.657 kmol/hr
```

Column bottoms contain ( to acid tower ):

```
Acrylic acid = 115.3 kmol/hr
Acetic acid = 15.08 kmol/hr
```

#### WASTE TOWER

Assumption: Bottom product contains water and all acrylic acid, acetic acid entering the column.

Feed: Raffinate phase from the liquid-liquid extractor.

```
Acrylic acid = 1.104 kmol/hr

Acetic acid = 0.156 kmol/hr

Water = 1191.13 kmol/hr

Solvent = 11.5 kmol/ hr
```

Column bottom stream ( to waste water treatment plant)

```
Water = 1082 .845 kmol/hr
Acetic acid = 0.156 kmol/hr
Acrylic acid = 1.104 kmol/hr
```

Column overhead stream (recycled to extraction column)

```
Solvent = 11.5 kmol/hr
Water = 108.2 kmol/hr
```

**ACID TOWER** ( Designed as a major equipment )

Assumption: Top product is 95 wt. % acetic acid Bottom product is 99.5 wt.% acrylic acid.

Feed:

Acrylic acid = 115.3 kmol/hr Acetic acid = 15.08 kmol/hr

# Top product

Acetic acid = 14.883 kmol/hr Acrylic acid = 0.14 kmol/hr

Acetic acid produced = 21.67 TPD at 95 % purity

# Bottom product

Acrylic acid = 115.16 kmol/hr Acetic acid = 0.197 kmol/hr

Acrylic acid produced = 200 TPD at 99.5% purity