Implementation of Mass Integration Design Concept for Material Preservation in Acrylonitrile Industry

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Abstract. The industrial production has suffered from huge amounts of waste discharges that contain valuable unreacted components as well as major contaminants that affect the environment. Just like heat integration, mass integration evolves around recycling the discharge streams back into the process to increase the overall plant performance and decrease the fresh feedstock resources used as well as extracting the valuable by-products whether in product streams or waste streams; thus, decreasing the overall cost and increasing the production value of outcomes. The study has tackled mass integration graphically on an existing production process, acrylonitrile, and evaluated the performance of mass-exchange networks. It also suggested improvements can be recommended in terms of composition driving forces inside mass exchangers. The mass network developed improved both the production yield and the product quality. In this research, the plant, located in Baroda complex, India, on a 500 m² area, has been studied for mass integration using mass separating agents. The mass separating agents used were water and benzene. A mass exchange network design has been conducted in the feasible design regions to achieve maximum mass recovery and mass targets of each mass exchanger. Three extra units were added for Acetonitrile removal, Hydrogen cyanide removal, and Acrylonitrile extraction.

Keywords: Acrylonitrile, Mass Exchange Network, Pinch Analysis, Mass Transfer

1. Introduction
Acrylonitrile (ACN) is one of the key monomers used in many production processes to produce day-to-day use products such as fibers, resins, intermediate chemical for certain products, synthetic rubber etc. It has been produced in many different methods. The “SOHIO Acrylonitrile Process” in the 1950’s by the Standard Oil Company, now part of British Petroleum has witnessed promising production route for acrylonitrile. The process was deemed a great success as for the first time it provides an economical one-step conversion from raw materials to products through gas phase ammonoxidation process over a catalyst [1].

Acrylonitrile is also used in fatty acid and vegetable oils extraction, unsaturated oil hydrocarbon extraction, plastic molding, removal of tars, phenols, and petroleum coloring substances, wool resin purification, steroid recrystallizing, DNA synthesis and sequence of peptides solvents, as reaction promotion medium, copper removal and refinement, chlorinated solvent stabilizer. It is also used in
chromatographic examination of high-pressure fluids, transition-metal component and catalyst component, production of perfumes and solvents [2].

Acrylonitrile can be produced either by the ammoxidation of propylene, heating of ethylene cyanohydrin in the presence of a dehydrating catalyst, by reacting acetylene and hydrogen cyanide in the presence of an aqueous solution of cuprous chloride catalyst or by the reaction of acetaldehyde-hydrogen cyanide reaction. Although a variety of chemical pathways have been shown and several techniques have been devised to acrylonitrile, the current paper focuses mainly on propylene ammoxidation. Standard Oil of Ohio (SOHIO) process fluid bed method is used in the vast majority of situations. This method is followed by approximately 90% of total acrylonitrile production plants. Reaction is too highly selective and fast for acrylonitrile production without the need for excessive recycling efforts [3].

\[2\text{CH}_2=\text{CH-CH}_3 + 2\text{NH}_3 + 3\text{O}_2 \rightarrow 2\text{CH}_2=\text{CH-C≡N} + 6\text{H}_2\text{O} \] (1)

In this paper, it is desired to implement the graphical mass integration method developed by Farrag et al. [4] on the SOHIO plant, as designed by Hansora in order to efficiently and economically separate acrylonitrile, and extract the useful side products as well as handle the toxic ones. Then the obtained results would be used to design mass exchanger units in order to be implemented in Hansora’s process for separation. The new renovated plant will be evaluated accordingly and compared to Hansora’s initially designed plant performance.

A strong motive for considering Mass Exchange network (MEN) was to deal with environmental concerns through using mass separating agents (MSAs) to remove the environment endangering species. It uses Pinch Analysis depending on the target and supply compositions of different streams. The streams are classified as lean or rich according to whether the composition of considered material in the stream is low or high, accordingly. Using these data, the cost of MSAs needed can be determined. Even though HI and MI is very similar, yet MI is far more complicated as it counts for more factors that affect the integration, such as the direct interactions between the streams in the mass exchangers and the MSA regeneration of considerations [5].

Mass exchanger networks (MEN) work on matching the rich streams with lean streams and MSAs, accounting for their varying target and supply compositions, for the required load of mass exchange as per the targeted values using the equilibrium relations. Very often when using MSAs the flow of MSAs is determined according the requirements of the network to remove the predetermined mass load from the system [6].

Gadalla has developed the first of its kind graphical tool that can be used to assess existing as well as new network designs against the targets determined. The tool has PA principles integrated in a graphical tool that represents the compositions of lean streams versus it equivalent rich streams, as per equilibrium data, on the diagram. This is suggested to be used when revamping a plant with an already existing MEN to further improve the performances [7].

Using the composition driving forces, Farrag et al. developed another graphical tool to assess diminish losses, both environmental and economic. This method illustrates the lean streams compositions against the driving force for each individually considered exchanger, which is shown in forms of straight lines on the graphical tool. Since the costs are somewhat related to the driving forces as it affects the design considerations for the number of plates within the unit, the chosen method of assessing the performance was through the use of the composition driving force, within the mass exchange unit. The plot could be divided into different sections in order to determine the optimum section to place a mass exchanging unit and accordingly achieve the best possible solution. This method could also be used to assess existing plant in order to increase the resources sustainability and integration efficiency [8].

Farrag et al. further developed a graphical approach to evaluate the efficiencies of existing plants, and design new ones through using composition driving forces. This tool, using pinch concepts, plots the lean stream compositions, between the inlets and outlets, against the corresponding composition
driving force for each point in the mass exchanging unit. This method can also be used on new developing MEN or already existing ones to assess the performance. Moreover, it was uncovered that this method could be openly and efficiently used to evaluate linear systems with dilute streams. The decision of matches was taken as to pick the parameters that allow the most efficient target achievement such as low flows, highest driving forces and minimum costs [4].

In this project, the aim will be to implement the graphical mass integration method developed by Farrag et al. on the plant outlined in the previous section, as designed by Hansora in order to efficiently and economically separate ACN, and extract the useful side products as well as handle the toxic ones. Then the obtained results would be used to design mass exchanger units in order to be implemented in Hansora’s process for separation. The new renovated plant will be evaluated accordingly and compared to Hansora’s initially designed plant performance.

2. Synthesis of mass exchanger network

In the standard SOHIO process, air, ammonia, and propylene are introduced into a fluidized-bed catalytic (bismuth phosphomolybdate in silica) reactor operating at 0.3-2 bar pressure and 400-510°C. Ammonia and air are fed to the reactor in slight extra of stoichiometric proportions because extra ammonia drives the reaction closer to integration and air continually regenerates the catalyst. An important feature of the process is the high conversion of reactants on a once-through basis with only just a few seconds habitation time. The heat generated from the exothermic reaction is recovered via a waste-heat-recovery boiler. Figure 1 shows the standard SOHIO process.

Water acidified with sulphuric acid, which may retrieve by crystallization, removes unreacted ammonia, as aqueous ammonia sulphate. The product stream then flows through opposite current water absorber-stripper to reject inert gases and recover reaction products. The reaction products mixture of acrylonitrile, acetonitrile, and water and then is sent to a fractionator to remove hydrogen cyanide. The final two steps involve the drying of the acrylonitrile stream and the final distillation to route out heavy ends. The fiber-grade acrylonitrile obtained from the process is 99+% pure. Several fluid-bed catalysts have been used since the inception of the SOHIO ammoxidation process [9].

Hansora has used the developed process in order to construct a plant that processes 70,000 tons per year of acrylonitrile product on a basis of 24 hours per day, and 330 days per year. The reactor processes
ammonia, air and propylene yielding high conversion of propylene on a catalyst based on bismuth molybdenum. This in turn produces some side products such as toxic HCN, acetonitrile, acrylic acid, etc. [10].

2.1. Introduction
The idea and concept of the mass exchanger networks (MENs) was established by El-Halwagi (2017) [6]. The mass exchanger applies a direct interaction that occurs between two streams (rich stream and lean stream) to separate the components or species which are targeted to be removed from the rich streams. All strategies of the mass transfer which are adsorption, absorption, stripping, extraction, leaching, and ion exchange can be utilized in the mass exchange method. The leans streams (mass separating agents) could be found in the process itself or it could be achieved externally and thus they will be considered as external utilities, where these lean streams can be an adsorbent, a stripping agent, a solvent, an ion exchange resin. The rich streams are products streams or any type of wastes.

2.2. Composition driving force graphical design
The transfer of the targeted components needed to be removed from the rich streams and sending them to the lean streams, are ruled by the composition driving force, moreover, to achieve the theoretical plates number and the composition driving force. The total cost estimation is related to the composition driving force. For sizing the equipment’s of mass exchanger, the graphical approach of the composition driving force is considered.

A straight line that has a slope which is linked with the rich and lean streams mass flows, refer to the unit of mass exchanging. The length of this straight line is proportional to the transferred mass capacity that occurred inside the exchanger unit. The mass exchangers are analyzed and located according to the pinch analysis rules. [4, 8].

2.3. Mass integration analysis and network design
The compositions of the rich stream and the lean stream are shown in figure 2. The lines of the lean streams are constructed as vertical straight lines which begins from the \((\text{x}_{\text{eqv}})\) point that rely on the \(\text{x}\)-axis. The lines of the rich streams are straight lines that intercepts at the points \((\text{y})\) where they are constructed by an inclination of 45° and they carry slopes equal to \((-1)\) as shown in figure 2. The construction of the rich stream-lines begins from the \(\text{y}\)-axis where the \(\Delta \text{C} = \text{y}\) that corresponds to \(\text{x}_{\text{eqv}} = 0\) on the \(\text{x}\)-axis, and the end of the rich stream-lines lies on the \(\text{x}\)-axis on the points which is \(\text{y} = \text{x}_{\text{eqv}}\) and \(\Delta \text{C} = 0\). The composition of the lean pinch is constructed parallel to the lean streams and the same for the composition of the rich pinch where it is constructed parallel to the parallel to the rich streams.

![Figure 2. Streams representation for network design.](image-url)
The mass networks are described in the (CDF) graphical representation by means of three dimensions. Across the inlet or exit of the exchanger the composition driving force is displayed by the first coordinate, the second coordinate indicates the equivalent compositions of the lean streams, and the third one shows the compositions of the rich streams that passes through the exchanger [4, 8].

2.4. Process description and rigorous modelling

The process described by Hansora is for the purpose of increasing an industrial capacity of an Indian acrylonitrile plant by the ammoxidation of propylene mechanism. The initial process achieves the product separation through the consecutive distillation units in order to obtain the required product specifications as well as remove the contaminants in the product mixture [10].

In order to achieve the required processes efficiently, the efficient use of streams within the system to remove the components desired, in the main aim of reducing the process use of external resources. The limit is achieved within the materialistic and utilities use; in other words, this limits the reagents as well as heating system uses.

The project is going to do so by first removing the key contaminants from the product stream which is rich in some components that must be removed; acetonitrile and hydrogen cyanide. Acetonitrile is easily removed by the use of water, which demonstrates highly miscible characteristics [11]. Also as water demonstrates limited solubility of acrylonitrile, this shows that the water may be used as a solvent [12].

The simulation, illustrated in figure 3, was done in order to extract the main data to be used in mass exchanger network design.

![Acrylonitrile plant simulation.](image)

2.5. Network Design Calculations

It is assumed in the separation system that $\varepsilon=0.001$, and that the product stream is at 1 atm and 40°C. The product (Rich) stream is separated into three different streams using three phase separators. The gas stream ($G_1$) flows at 896.4 kg/h, the liquid stream ($G_2$) flows at 5243 kg/h, while the aqueous stream ($G_3$) flows at 35540 kg/h. The key contaminants will be removed using separating agent to reduce the duty of the used separators.

2.6. Choice of Separating agents

The plant provides a stream of waste water that has been used to remove unreacted ammonia with sulphuric acid dissolved within the mixture. Due to the miscibility of acetonitrile and HCN in water, the stream will be used to target these key concentration components in the streams. Looking at the
mass separation coefficient dependent on which the separation quality is determined, it was chosen to carry out the processes at 40°C and 1 atm for water as a separating agent.

Although HCN is toxic and would contaminate water, water has been chosen as a separating agent to remove the component from the mixture in order to allow for better extraction of the desired product from all other by-products and unreacted materials. Also due to the miscibility of acrylonitrile in benzene, this is the separating agent decided to be used for the extraction of acrylonitrile from the streams for which key contaminants have been removed before the process of acrylonitrile extraction.

3. Results for the integrated process

3.1. Acetonitrile removal

3.1.1. Pinch determination

The mass exchange from the rich stream to the lean stream is determined across the different ranges of the mass fraction of the acetonitrile content. This depends on the total flow rate of the rich streams for each range. The mass exchanged from each of the streams is calculated for each range using the following equation.

\[ \Delta M_i = \Delta y_i \times G_i \]  

(2)

For the range \( y = 0.0005 \) to 0.0040

\[ \Delta M_{y=0.0005 \text{ to } 0.0040} = (0.0040 - 0.0005) \times 5243 = 18.3505 \text{ kg/h} \]

For the range \( y = 0.0040 \) to 0.0048

\[ \Delta M_{y=0.0040 \text{ to } 0.0048} = (0.0048 - 0.0040) \times (896.4 + 5243) = 4.9115 \text{ kg/h} \]

For the range \( y = 0.0048 \) to 0.0191

\[ \Delta M_{y=0.0048 \text{ to } 0.0191} = (0.0191 - 0.0048) \times 5243 = 74.9749 \text{ kg/h} \]

The pinch plot will be plotted using the data found in table 1.

| \( y \) (wt/wt) | \( \Delta M \) (kg/h) |
|---------------|------------------|
| 0             | 0                |
| 0.0005        | 0                |
| 0.004         | 18.3505          |
| 0.0048        | 23.2620          |
| 0.0191        | 98.2369          |

Table 1. Pinch stream plot data.

For \( T = 40^\circ C \) and pressure = 1 atm, \( m = 0.07715 \)
\[ y = m (x + \epsilon) + b \]  

(3)

\( b \) is neglected as it only affects the position not the behavior of mass transfer in the network.
\[ x_{eq} = y - m \epsilon \]  

(4)

Table 2 shows the lean stream compositions on different scales.

| Point  | Mass fraction of acrylonitrile in lean stream, \( x \) (wt/wt) | Corresponding mass fraction in rich stream, \( y \) (wt/wt) | \( x_{eq} \) (wt/wt) |
|--------|-------------------------------------------------------------|----------------------------------------------------------|-------------------|
| Supply | 0.0007                                                      | 1.3116x10^{-6}                                           | 5.4005x10^{-5}    |
According to figure 4, the pinch points upon which the network is classified were determined to illustrate the acrylonitrile pinch diagram.

![Acrylonitrile pinch diagram](image)

**Figure 4.** Acrylonitrile pinch diagram.

The point of intersection which also the pinch point is at \( y = 0.0005 \) and \( \Delta M = 0 \text{ kg/h} \), on the equivalent scale this represents an acetonitrile composition of \( x = 0.005 \) and a composition of \( x_{eq} = 0.0004285 \).

### 3.1.2 Streams compositions

The acetonitrile is present in significant concentrations in order to affect the quality of extraction of acrylonitrile using benzene, it is also very highly soluble. The acrylonitrile composition \( (y_{in}) \) is 0.0048, 0.0191 and 0.0054 in \((G_1), (G_2)\) and \((G_3)\), respectively.

Acetonitrile is infinitely soluble in water. The outlet mass fraction will be limited to 0.3 in order to dodge the azeotrope effect during extraction of acetonitrile. The target mass fraction of acrylonitrile \( (y_{out}) \) is 0.004 and 0.0005 in \((G_1)\) and \((G_2)\), respectively. The concentrations of acetonitrile are going to be reduced in the rich streams using the process lean stream.

### 3.1.3 Mass exchanger network design

The acetonitrile mass exchanger network includes two streams, gas phase stream \((G_1)\) and liquid phase stream \((G_2)\). The gas phase \((G_1)\) has a supply composition of \( y_{in} = 0.0048 \) and the liquid phase \((G_2)\) has a supply composition of \( y_{in} = 0.0191 \). The gas phase \((G_1)\) has a targeted composition of \( y_{out} = 0.004 \) and the liquid phase \((G_2)\) has a targeted composition of \( y_{out} = 0.0005 \). This is presented as follows on the mass exchanger network in figure 5. The lean stream is represented by two vertical lines at the equivalent \( x \) mass fraction.
Figure 5. Acetonitrile mass exchanger network before applying mass exchangers.

Acetonitrile mass exchanger network above allows for two mass exchangers one for each of the rich streams \( G_1 = 896.4 \text{ kg/h} \) and \( G_2 = 5243 \text{ kg/h} \).

\[
L' = \frac{L}{m} = \frac{900.7}{0.07715} = 11674.65 \text{ kg/h}
\]  

(5)

Using the following equation to get the slope of each exchanger line in the network

\[
S = \frac{L'}{G} - 1
\]  

(6)

For \( G_1 \):

\[
S_{G1} = \frac{11674.65}{896.4} - 1 = 12.0394
\]

For \( G_2 \):

\[
S_{G2} = \frac{11674.65}{5243} - 1 = 1.2267
\]

Using \( S_{G1} = 12.0394 \), starting at the intersection of the pinch line with the line representing the outlet stream \( \Delta C = 0.004 - x_{eq} \) The exchanger line stops at \( \Delta C = 0.0043 \) and \( x_{eq} = 0.00048 \). For the second stream, using \( S_{G2} = 1.2267 \), starting at the intersection of the pinch line with the line representing the outlet stream \( \Delta C = 0.0005 - x_{eq} \) The exchanger line stops at \( \Delta C = 0.0103 \) and \( x_{eq} = 0.0087760 \). Figure 6 illustrates the acetonitrile mass exchanger network with mass exchangers.
Using the equation derived for the number of theoretical plates in terms of the slope, the mass exchanger can be designed

\[
NTP = \frac{\ln \left( \frac{1}{S+1} \frac{S\Delta y}{\Delta C_{\text{lean}} + m\Delta C_{\text{rich}}} + S+1 \right)}{\ln(S+1)}
\]

For Gas Stream the NTP is 1.006, with 60% plate efficiency, thus the actual number of plates is almost 2.

From Hysys, the gas stream is evaluated to have a volumetric flow rate of 2 m$^3$/h and a lean stream flow rate of 0.7379 m$^3$/h, based on which, the unit will be designed. The velocity is taken as 1.2 m/s in a vessel with diameter 1 m. For a residence time of 20 min, height will be 2.16 m.

For Liquid Stream: NTP is 8, with 60% plate efficiency, thus the actual number of plates is almost 14.

From Hysys, the gas stream is evaluated to have a volumetric flow rate of 6.4257 m$^3$/h and a lean stream flow rate of 0.7379 m$^3$/h, based on which, the unit will be designed. The velocity is taken as 1.2 m/s in a vessel with diameter 1 m. For a residence time of 20 min, height will be 10 m.

3.2. Hydrogen cyanide removal

A process for the removal of hydrogen cyanide from gas streams which comprises contacting the gas stream in the presence of water in an amount at least sufficient to hydrolyze the contained hydrogen cyanide with a catalyst consisting of at least one alkali metal hydroxide deposited on a support selected from the group consisting of alumina, silica, alumina silica and the zeolites in which the alkali metal hydroxide deposited on the support as alkali metal is present in an amount of from about 0.1 to about 10 percent in on the total weight of the alkali metal and the support at a temperature from about 200°F to about 800°F for a time sufficient to hydrolyze a substantial quantity of the hydrogen cyanide present in the gas stream to ammonia.

3.2.1. Pinch determination

The mass exchange from the rich stream to the lean stream is determined across the different ranges of the mass fraction of the hydrogen cyanide content. This depends on the total flow rate of the rich streams for each range. The mass exchanged from each of the streams is calculated for each range using equation (1).

For the range $y = 0.01$ to $0.02$

\[
\Delta M_{y=0.01~\text{to}~0.02} = (0.02 - 0.01) \times 5243 = 52.43 \text{ kg/h}
\]
For the range \( y = 0.02 \) to 0.0417
\[
\Delta M_{y=0.0040 \text{ to } 0.0048} = (0.0417 - 0.02) \times (896.4 + 5243) = 133.225 \text{ kg/h}
\]

For the range \( y = 0.0417 \) to 0.0787
\[
\Delta M_{y=0.0048 \text{ to } 0.0191} = (0.0787 - 0.0417) \times 5243 = 193.991 \text{ kg/h}
\]

The pinch plot will be plotted using the data found in table 3.

**Table 3.** Hydrogen Cyanide pinch streams plot data.

| \( y \) (wt/wt) | \( \Delta M \) (kg/h) |
|-----------------|---------------------|
| 0               | 0                   |
| 0.01            | 0                   |
| 0.02            | 52.43               |
| 0.0417          | 185.655             |
| 0.0787          | 379.646             |

For \( T = 40^\circ C \) and pressure = 1 atm, \( m = 0.07715 \)
\[
y = m (x + \varepsilon) + b
\]

\( b \) is neglected as it only affects the position not the behavior of mass transfer in thenetwork.
\[
x_{eq} = y - m\varepsilon
\]

Table 4 shows the lean stream composition on different scales.

**Table 4.** Lean stream compositions on different scales.

| Point   | Mass fraction of HCN in lean stream, \( x \) (wt/wt) | Corresponding mass fraction in rich stream, \( y \) (wt/wt) | \( x_{eq} \) (wt/wt) |
|---------|--------------------------------------------------|----------------------------------------------------------|--------------------|
| Supply  | 0.0007                                           | 7.5023x10^{-5}                                           | 3.0892x10^{-5}     |
| Target  | 0.01                                             | 4.8544x10^{-4}                                           | 1.31x10^{-6}       |

The range at which the lean stream will fall on the pinch diagram does not intersect with the rich composite curve thus, the pinch point cannot be determined. Also, since the rich streams have equivalent compositions higher than that the water stream has, mass transfer is impractical. Thus, an external lean stream, or an external mass separating agent will be used.

The water supply will be assumed at a negligible concentration of hydrogen cyanide of \( x_{in} = 0.001 \) which is equivalent to \( x_{eq} = 0.0004 \). The target composition would be limited to \( x_{out} = 0.025 \) which is equivalent to \( x_{eq} = 0.0114 \).

3.2.2. Streams compositions

The hydrogen cyanide is also present in considerable concentrations that would affect the quality of extraction of acrylonitrile from the mixture. The hydrogen cyanide has the following compositions in the three streams as listed below in table 5.
Table 5. Hydrogen Cyanide mass fractions.

| Stream            | Symbol | Flow rate (kg/h) | Mass fraction of HCN, y_in |
|-------------------|--------|------------------|---------------------------|
| Gas steam         | G₁     | 896.4            | 0.0787                    |
| Liquid stream     | G₂     | 5243             | 0.0471                    |
| Aqueous stream    | G₃     | 35540            | 0.0201                    |

Hydrogen cyanide is soluble in water. The outlet mass fraction will be reduced in order to allow for the better extraction of acrylonitrile from the product streams. Water used to remove the hydrogen cyanide must be treated later on as hydrogen cyanide is toxic, so it should not be thrown out directly. Table 6 illustrates the supply and target mass fraction of Hydrogen Cyanide.

Table 6. Supply and target mass fraction of hydrogen cyanide.

| Stream            | Symbol | Supply mass fraction of HCN, y_in | Target mass fraction of HCN, y_out |
|-------------------|--------|----------------------------------|-----------------------------------|
| Gas steam         | G₁     | 0.0787                           | 0.01                              |
| Liquid stream     | G₂     | 0.0471                           | 0.02                              |

The concentrations of hydrogen cyanide are targeted to be removed from the rich streams (0.004 and 0.0005 in Gas and Liquid streams respectively) using the process lean stream.

The hydrogen cyanide mass exchanger network includes two streams, gas phase stream (G₁) and liquid phase stream (G₂). The gas phase (G₁) has a supply composition of y_in = 0.0787 and the liquid phase (G₂) has a supply composition of y_in = 0.0471. The gas phase (G₁) has a targeted composition of y_out = 0.01 and the liquid phase (G₂) has a targeted composition of y_out = 0.02. This is presented as follows on the mass exchanger network in figure 7.

![Figure 7. Streams representation for the removal of hydrogen cyanide mass exchanger network.](image)

3.2.3. Mass exchanger network design

Since no pinch conditions can be determined due to the unknown flowrate of external mass separating agent, the mass exchangers will be placed on the network as to remove all the required contaminant, by
using the constraints set on the concentration of the streams flowing into and out of the mass exchanger. Hydrogen cyanide mass exchanger network is developed for two mass exchangers one for each of the rich streams $G_1 = 896.4$ kg/h and $G_2 = 5243$ kg/h.

Using the following equation to get the slope of each exchanger line in the network:

$$ S = \frac{\Delta y}{\Delta x_{eq}} - 1 $$

For $G_1$: $S_{G1} = \frac{0.0687}{0.011} - 1 = 6.2455$

For $G_2$: $S_{G2} = \frac{0.0217}{0.011} - 1 = 0.9727$

Matching the two points through which the mass exchange happens for each stream the following network is obtained as a result. Figure 8 illustrates the hydrogen cyanide mass exchanger network.

![Figure 8. Hydrogen cyanide mass exchanger network.](image)

For gas stream: NTP is 1.3, with 60% plate efficiency, thus the actual number of plates is almost 3.

From Hysys, the gas stream is evaluated to have a volumetric flow rate of $2 \text{ m}^3/\text{h}$ and an external lean stream can be calculated to be $808.3735$ kg/h or $0.9308 \text{ m}^3/\text{h}$ (assuming benzene density of 868.5). The velocity is taken as 1.2 m/s in a vessel with diameter 1 m. For a residence time of 20 min, height will be 2.24 m. For liquid stream: NTP is 3, with 60% plate efficiency, thus the actual number of plates is almost 6.

From Hysys, the gas stream is evaluated to have a volumetric flow rate of $6.4257 \text{ m}^3/\text{h}$ and an external lean stream can be calculated to be $34737.15$ kg/h or $39.9967 \text{ m}^3/\text{h}$ (assuming benzene density of 868.5). The velocity is taken as 1.2 m/s in a vessel with diameter 1 m. For a residence time of 20 min, height will be 11.75 m. For aqueous Stream: NTP is 1.12, with 60% plate efficiency, thus the actual number of plates is almost 2.

From Hysys, the gas stream is evaluated to have a volumetric flow rate of $37.0089 \text{ m}^3/\text{h}$ and an external lean stream can be calculated to be $32049.972$ kg/h or $36.9027 \text{ m}^3/\text{h}$ (assuming benzene density of 868.5). The velocity is taken as 1.2 m/s in a vessel with diameter 1 m. For a residence time of 20 min, height will be 8 m.
3.3. Acrylonitrile extraction

3.3.1. Pinch determination

The mass exchange from the rich stream to the lean stream is determined across the different ranges of the mass fraction of the acrylonitrile content. This depends on the total flow rate of the rich streams for each range. The mass exchanged from each of the streams is calculated for each range using equation (1).

For the range $y = 0.0005$ to $0.0048$

$$\Delta M_{y=0.0005 \text{ to } 0.0048} = (0.0048 - 0.0005) \times (5243 + 896.4) = 26.39942 \text{ kg/h}$$

For the range $y = 0.0048$ to $0.077$

$$\Delta M_{y=0.0048 \text{ to } 0.077} = (0.077 - 0.0048) \times 5243 = 378.544 \text{ kg/h}$$

For the range $y = 0.077$ to $0.1209$

$$\Delta M_{y=0.077 \text{ to } 0.1209} = (0.1209 - 0.077) \times (5243 + 35540) = 1790.3737 \text{ kg/h}$$

For the range $y = 0.1209$ to $0.8285$

$$\Delta M_{y=0.1209 \text{ to } 0.8285} = (0.8285 - 0.1209) \times 5243 = 3709.9468 \text{ kg/h}$$

For $T = 30^\circ C$ and pressure = 1 atm, $m = 0.9018$

$$y = m(x + \varepsilon) + b$$

$b$ is neglected as it only affects the position not the behavior of mass transfer in the network.

$$x_{eq} = y - m\varepsilon$$

Table 7 shows the lean stream compositions on different scales.

| Point   | Mass fraction of HCN in lean stream, $x$ (wt/wt) | Corresponding mass fraction in rich stream, $y$ (wt/wt) | $x_{eq}$ (wt/wt) |
|---------|-----------------------------------------------|--------------------------------------------------------|-----------------|
| Supply  | 0.0000                                        | 0.0009                                                 | 0               |
| Target  | 0.1250                                        | 0.1136                                                 | 0.1127          |

3.3.2. Mass exchanger network

The acrylonitrile mass exchanger network is to include three streams, gas phase stream ($G_1$), liquid phase stream ($G_2$) and aqueous phase stream ($G_3$). The gas phase ($G_1$) has a supply composition of $y_{in} = 0.0048$, the liquid phase ($G_2$) has a supply composition of $y_{in} = 0.8285$ and the aqueous phase ($G_3$) has a supply composition of $y_{in} = 0.1209$. The gas phase ($G_1$) has a targeted composition of $y_{out} = 0.0005$ and the liquid phase ($G_2$) has a targeted composition of $y_{out} = 0.0005$ and the aqueous phase ($G_3$) has a supply composition of $y_{in} = 0.0770$.

Acrylonitrile mass exchanger network above allows for three mass exchangers one for each of the rich streams $G_1 = 896.4 \text{ kg/h}, G_2 = 5243 \text{ kg/h}$ and $G_3 = 35540 \text{ kg/h}$.

Using the following equation to get the slope of each exchanger line in the network:

$$S = \frac{\Delta y}{\Delta x_{eq}} - 1$$

After calculating the slope of each exchanger line, figure 9 is developed to represent the acrylonitrile mass exchanger network after implementing mass integration.
3.3.3. Mass exchanger design
For gas stream: NTP is 1.12, with 60% plate efficiency, thus the actual number of plates is almost 2.

From Hysys, the gas stream is evaluated to have a volumetric flow rate of 2 m$^3$/h and an external lean stream can be calculated to be 808.3735 kg/h or 0.9308 m$^3$/h (assuming benzene density of 868.5). The velocity is taken as 1.2 m/s in a vessel with diameter 1 m. For a residence time of 20 min, height will be 2.24 m. For liquid stream: NTP is 3, with 60% plate efficiency, thus the actual number of plates is almost 6.

For liquid stream: NTP is 3, with 60% plate efficiency, thus the actual number of plates is almost 6.

From Hysys, the gas stream is evaluated to have a volumetric flow rate of 6.4257 m$^3$/h and an external lean stream can be calculated to be 34737.15 kg/h or 39.9967 m$^3$/h. The vessel with diameter 1.5 m, for a residence time of 20 min, height will be 11.75 m.

For Aqueous stream: NTP is 1.12, with 60% plate efficiency, thus the actual number of plates is almost 2.

From Hysys, the gas stream is evaluated to have a volumetric flow rate of 37.0089 m$^3$/h and an external lean stream can be calculated to be 32049.972 kg/h or 36.9027 m$^3$/h. The vessel with diameter 1.5 m, for a residence time of 20 min, height will be 8 m.

4. Conclusion
This study addressed the implementation of mass exchange design concept for the acrylonitrile production plant based in India located on a 500 m$^2$ land. The mass exchanger networks were designed using graphical design approach. The product stream was split into three different streams; gas, liquid, and aqueous phase streams. Two mass separating agents were utilized, which were benzene and water. The mass separating agents were used to remove the contaminants attached with the main production stream. These contaminants were mainly acetonitrile and hydrogen cyanide. The acetonitrile was in the gas stream, liquid stream, and aqueous stream. The concentrations of acetonitrile and hydrogen cyanide was reduced in the rich stream (main product stream) using the process mass separating agents (water and benzene). For the acetonitrile removal, the mass load integrated was 0.72 kg/h and 97.52 kg/h for gas and liquid streams, respectively. For its removal no surplus loads of external mass separating agents were needed, the process lean stream was sufficient. For the hydrogen cyanide removal, the mass load integrated was 61.58 kg/h and 113.77 kg/h for gas and liquid streams, respectively. For its removal surplus loads of external mass separating agents were added for more efficient mass separation. Finally, the extraction of acrylonitrile took place over three cascaded units where the maximum mass transfer loads reached were 3.85 kg/h, 434.12 kg/h and 156 kg/h.
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