# Solvent Recovery and Recycle

John Gawalt
Jaired Re

Department of Chemical Engineering
Virginia Polytechnic Institute and State University

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## Acknowledgements

We are extremely grateful for the opportunity to revise our design report. The completion of our project would not have been possible without the continued support and guidance our professor, Dr. Bortner, and his teaching assistants. We would also like to thank Dr. Liu for his exceptional training in ASPEN Plus, and for providing us with relevant engineering heuristics necessary for a complete design.

Contents

Executive Summary

The object of this report is to propose a potential solvent recovery system for an existing siloxane polymerization unit. The polymerization unit has three waste streams, each of which is sequentially separated into the desired components: Acetonitrile, Toluene, and P-Xylene. Solvent grade Acetonitrile and Toluene are both expensive components and it would be in our best financial interest to maximize the amount of recycled solvent.

Our design incorporates two packed distillation towers along with a single stage flash drum to achieve mass purities of 99.83% Acetonitrile and 99.92% Toluene.

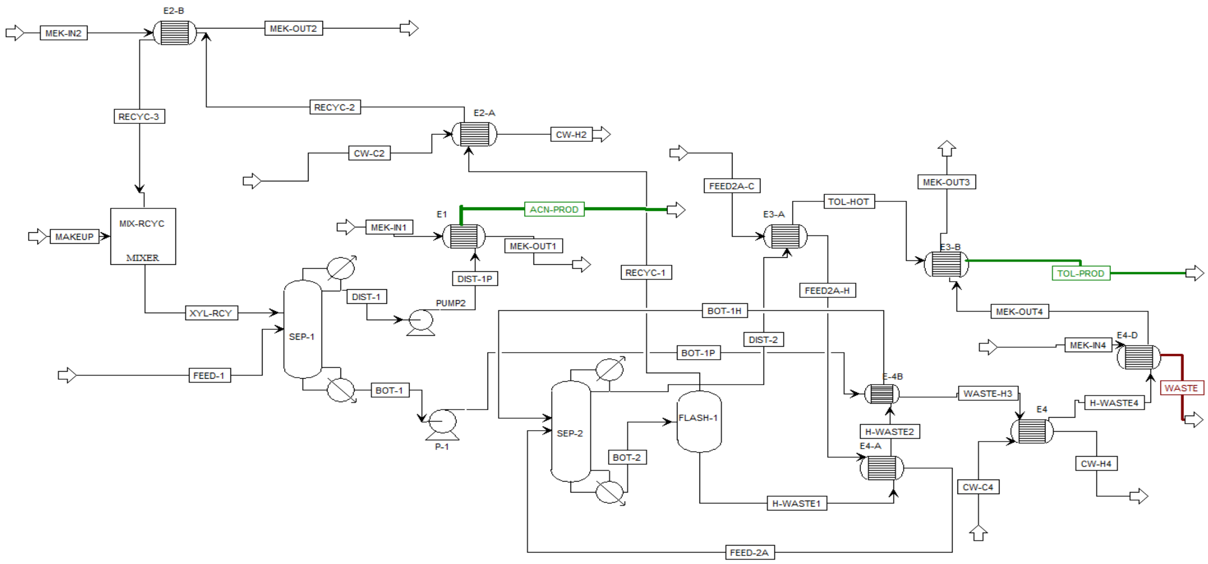


Figure I-1: Main process Flow Sheet

Figure I-1 displays all equipment used in our process with the exception of the backup pumps. All modeling calculations and sensitivity analyses are handled by ASPEN+. Our process description section goes into detail about each major unit and its associated auxiliary tasks such as pressure and temperature changes.

Our economic analysis for this process is conducted using a 20 year Sum of Years Digits depreciation scheme assuming a tax rate of 40%. For a total capital investment of $2.5 million our process earns an average of $3.7 million annually after taxes. This corresponds to a 144% rate of return on our investment. We also examine the effect of product sales price on our rate of return to predict the long term viability of our design.

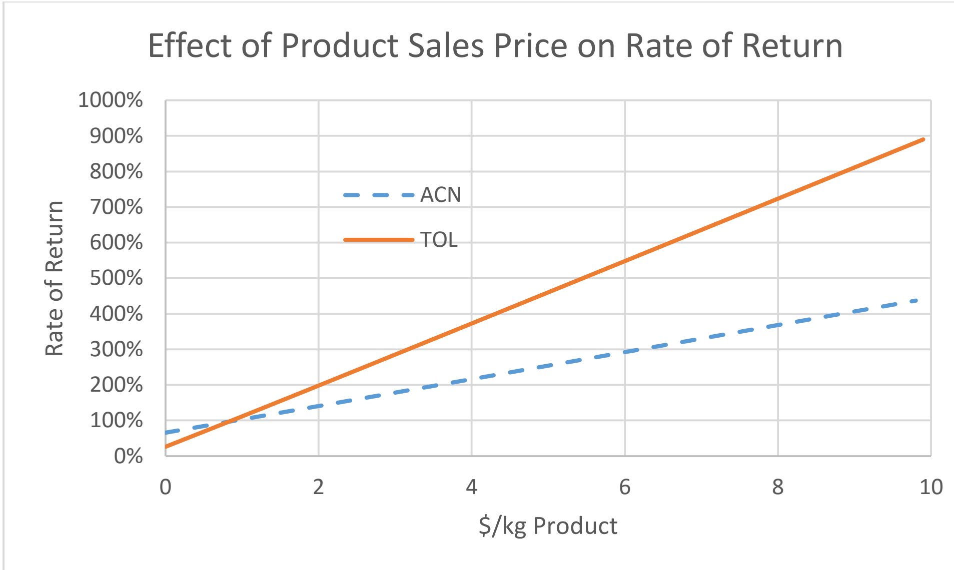


Figure I-1: This plot depicts the response of the rate of return when the product prices are subjected to change.

Figure I-1 Shows the behavior of our rate of return as a function of the product sales prices. From this plot it is clear that as long as the price for each component remains above $1/kg, our process will continuously add value to the company.

Our process is also designed with safety as the highest priority. HAZOP, FMEA, and Inherently safer design analyses found later in this report verify that our process is designed to minimize loss in terms of employee health and equipment safety.

We thank you for taking the time to consider our design solution. Please do not hesitate to contact us with any additional questions or concerns you may have.

# 1. Introduction

The formation of siloxane based polymers takes place in solution with strong solvents such as acetonitrile and toluene. When the polymerization is complete, the solvents must be separated once more before they can be reintroduced to the system. This is the basic idea behind our design: to minimize financial losses due to wasted solvent.

Acetonitrile is very prevalent in the chemical industry and is commonly used as a solvent for liquid-liquid or liquid-solid extraction. The major benefit of acetonitrile as a solvent is that it can dissolve both organic and inorganic materials. Similarly, toluene is commonly used in industry as an organic solvent, or gasoline additive. Our design is aimed at returning solvents to the polymerization unit to save on raw material cost for each of these solvents.

# 2. Process Description

*i. P&ID*

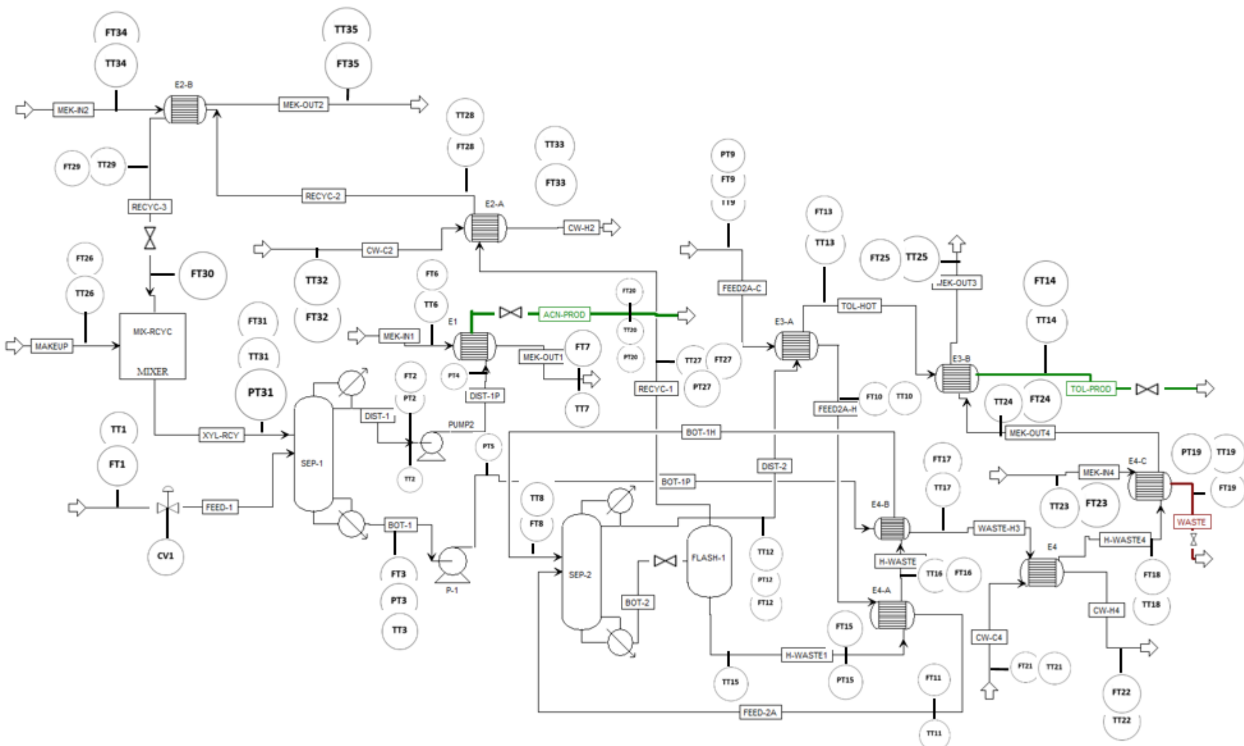

Figure 2-1: Process and Instrumentation Diagram for Solvent Recovery from a Siloxane Process.

P&IDs provide a basis in the developmental stage of system control schemes. This opens avenues to more in depth safety and operational investigations including FMEA and HAZOP. We converged on a system of sensors and controllers that will hold safe, steady state operation as long as possible. Streams around distillation columns should be equipped with temperature, flowrate, and pressure sensors. Streams entering and exiting heat exchangers should have temperature and flow sensors to ensure there is no cross flow, and sufficient heat is exchanged. Streams that enter or exit a pump must at least have a pressure sensor. Streams that exit into an open container that may contain chemicals above their flash point should have at least a temperature sensor and a control valve near the exit with an innate fail close setting. The recycle stream entering the heat exchanger must have a valve with an innate fail close setting. The stream exiting the mixer should have a temperature, pressure, and flow sensor to ensure the correct feed specifications are met. All additional sensors are added to facilitate quick, efficient troubleshooting when an issue arises.

*ii. Critical Streams*

Our process is designed with the intent of returning pure acetonitrile and toluene to the siloxane plant for reuse. The polymerization process produces three effluent flows named feeds A, B, and C. **Table 2-1** below shows the compositions and flowrates for each of these feed streams.

Table 2-1: Feed Stream Compositions

| Stream | Flow Rate $\left[\frac{kg}{hr}\right]$ | Composition (wt%) | | |
|---|---|---|---|---|
| | | Toluene | Acetonitrile | Siloxane |
| Feed A | 270 | 98.5 | 0 | 1.5 |
| Feed B | 60 | 96.5 | 2.0 | 1.5 |
| Feed C | 200 | 19.5 | 78.5 | 2.0 |

The main goal of this process is to return solvents of high enough purity to be reused in the initial polymerization plant. **Table 2-2** outlines the critical stream data for each effluent stream from our process.

Table 2-2: Critical Product Stream Data

| **Stream Name** | **Flow Rate** $\left[\frac{kg}{hr}\right]$ | **Temp** $[℃]$ | **Composition [wt. %]** | | | |
|---|---|---|---|---|---|---|
| | | | **Acetonitrile** | **Toluene** | **P-Xylene** | **Siloxane** |
| TOL Product | 362.8 | 4 | 0.073 | 99.92 | 0.003 | trace |
| ACN Product | 158.2 | 5 | 99.83 | 0.124 | 0.045 | trace |
| Waste | 36.6 | 27 | trace | 0.4 | 75.2 | 24.4 |
| Xylene Recycle | 85.0 | 27 | trace | 0.8 | 85.2 | 14 |

**Table 2-2** is a compilation of the results from our ASPEN Plus simulations, showing the outlet temperature of each stream before it enters storage as well as the composition of each stream. More extensive stream tables are located in **Appendix A.** The following subsection consists of an overview of each major separation unit used in our process.

*ii. Function of Major Equipment*

a. Acetonitrile Column

The first major unit in our process is a 25 stage packed vacuum distillation column measuring 0.76 m in diameter. A vacuum pump is attached to the total condenser in this tower to ensure the separation is run at 0.1 bar. This unit is charged with feeds B, C, and a P-Xylene stream and it tasked with separating acetonitrile from the remaining mixture. P-Xylene is used to keep siloxane in solution and facilitate the separation of acetonitrile. The distillate stream from this tower is the final acetonitrile product at 99.83 % purity. This stream is then cooled below to 5 ℃ and stored. The bottoms of this column is fed to the second distillation tower. Specific sizing and costing information is covered in the discussion as well as in the equipment summary.

b. Toluene Column

Toluene is separated at atmospheric pressure in a 24 stage packed column with a diameter of 0.6m. This column is charged with the bottoms flow out of column one as well as feed A on stages 15 and 8 respectively. This column produces a distillate stream composed of 99.92% toluene. Similar to the column before, the toluene product is cooled below it's to a temperature of $27\ ℃$ before being sent to storage. The bottom stream is comprised primarily of p-xylene and siloxane. This stream is fed to a flash drum to return xylene to the process.

c. Flash Drum

Our flash drum operates near the vaporization point of P-Xylene at a temperature of ##### ℃ and a vapor fraction of 0.72 entering the drum. Siloxane is an undesired waste product and must be make up no more than 25% of any stream to avoid solid formation within the system. We desire to recover as much of our separating agent as possible, therefore our flash drum is designed to dispose a waste stream containing 24.5% siloxane. We discuss the details of sizing and costing in Section 3.

# 3. Separation Tasks: Sizing and Costs

The separations are carried out in the order most fitting to that laid out by the separation heuristics. The goal of these separation processes is to yield the highest purity acetonitrile and toluene streams while minimizing both cost and waste. Acetonitrile has the lowest boiling point and is separated first, followed by toluene and finally p-xylene.

## *i. ACN Column*

### a. Binary Analysis and Operating Pressure

Acetonitrile is the first component separated due its lower boiling point. This separation takes place in a staged packed distillation tower. The column pressure is determined by a binary analysis of acetonitrile and toluene. A higher level of separation is indicated by a greater distance between the equilibrium data and the y=x line.

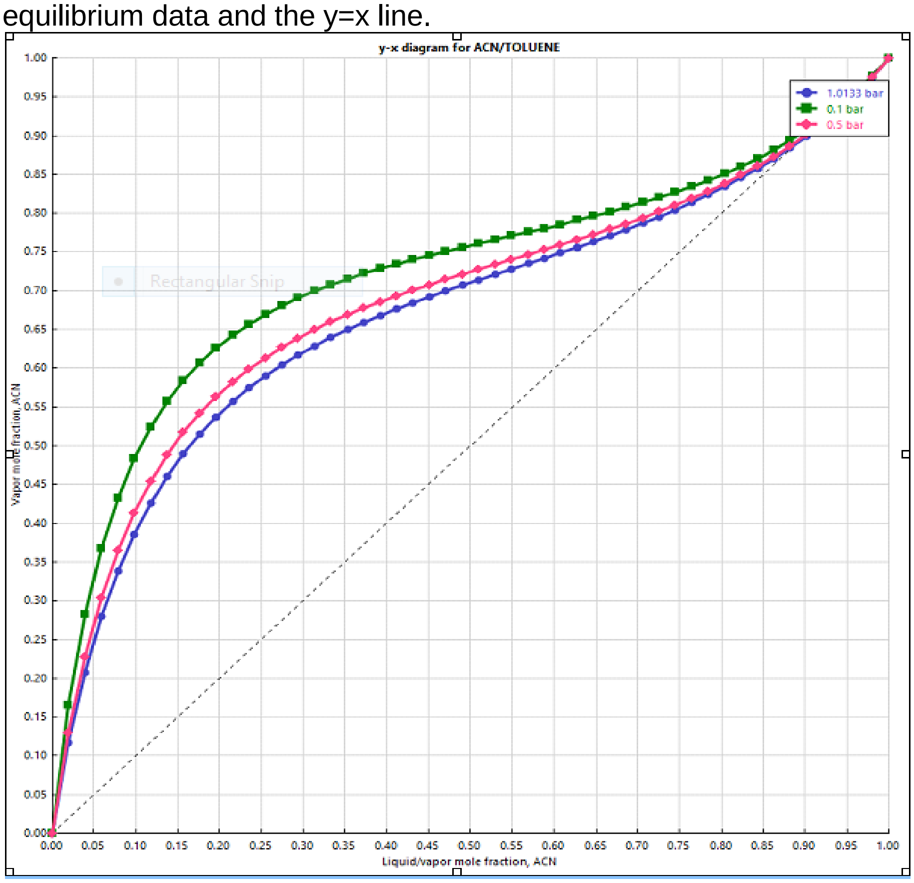


**Figure 3-1:** This represents the binary interaction between acetonitrile and toluene. The father the equilibrium line is from the y-x line, the greater the degree of separation.

The x-y diagram above shows that any pressure greater than 0.1 bar will prevent the purity of acetonitrile in the distillate stream from reaching its desired value of 99.82 %. This barrier is due to the azeotrope experienced by the mixture under those system conditions. The azeotrope composition is raised by adding P-Xylene. Xylene functions as a separating agent, increasing the relative volatility of acetonitrile while simultaneously entraining siloxane in the liquid phase. In order to achieve a vacuum of 0.1 bar, our design uses a liquid ring vacuum pump attached to the total condenser. Sizing information for the vacuum pump is located in Section 4.

b. Column Sizing and Pricing

Our ACN column is a packed column with 1.84m of Sulzer metal gauge packing, type CY with an equivalent of 25 ideal stages. We chose to use packed columns in our design because our columns are too narrow to accommodate stages. The feed is charged to the column on stage 22 with the xylene recycle stream entering on stage 8. The ideal operating temperature ranges from 52.8 C in the bottoms to 21.3 C in the distillate. Under these conditions, a purity of 99.83 % acetonitrile is recovered in the product stream.
A summary of the column one specifications is shown in **Table 3-1** below.

Table 3-1: Column 1 Specifications

| **Acetonitrile Column Specifications** | | |
|---|---|---|
| **Specifications** | Acetonitrile Tower | |
| **Bot. Temperature [°C]** | | 52.88 |
| **Top Temperature [°C]** | | 21.30 |
| **Pressure [bar]** | | 0.10 |
| **Diameter [m]** | | 0.77 |
| **Height [m]** | | 2.39 |
| **Pack Height [m]** | | 1.84 |
| **# of Trays** | | 23 |
| **Equivalent # Stages** | | 25 |
| **Feed-1** | Feed B + C | 22 |
| **Feed-2** | XyleneRcy | 8 |
| **Orientation** | Vertical | |
| **Structured Packing Type** | CY by Sulzer | |
| **HETP [m]** | 0.08 | |
| **Material** | STANDARD | |
| **Total Cost [$]** | | **$66,470** |
| **Distillate Stream Compositions** | **Species** | **wt. Frac** |
| | ACN | 0.9983 |
| | TOLUENE | 0.0012 |

| | | |
|---|---|---|
| | P-XYLENE | 0.0005 |
| | SILOXANE | ---trace-- |
| **Bottoms Stream Compositions** | **Species** | **wt. Frac** |
| | ACN | |
| | TOLUENE | 0.00121 |
| | P-XYLENE | 0.45646 |
| | SILOXANE | 0.07364 |

The table above lists operating conditions, and the sizing specifics of the distillation tower. The height of the column depended ultimately on the choice of packing material. We chose CY metal gauze packing because it offers a low overall height and is commonly used for vacuum operations. The HETP value of 0.08m is provided graphically by Sulzer; we chose the packing with the lowest possible HETP value that suits vacuum distillation. The height of packing is determined by the following equation:

$$H_{packing} = [\#\, Theoretical\ Stages] \cdot [HETP_{packing}] \qquad [3\text{-}1]$$

This equation gives us our pack height of 1.84 m. To calculate the column height we add an additional 15% of the pack height to the top and bottom of the column effectively increasing the pack height 30%. This additional height is to account for the space between the packing and the reboiler/condenser at the bottom/top of the column.

$$H_{Column} = 1.3 \cdot H_{packing} \qquad [3\text{-}2]$$

This give us our overall height of 2.39 m with a diameter of 0.77m as generated by ASPEN Plus.

The column is priced in EconExpert as a vertically oriented packed tower with the dimensions and operating conditions discussed above. For a packed height of 1.84 m and an operating pressure of 0.1 bar, the material and pressure factors are 4.0 and 1.7 respectively. This gives a base cost of $8,889 and a total cost, before delivery, of $60,420.

We will now consider the sizing and thermal duty of the condenser and reboiler.

c. Condenser and Reboiler Sizing

A 4.2 $m^2$ total condenser with a heat duty of -160 kW is used to condense the distillate which exits at a rate of 158.2 $\frac{kg}{hr}$ at 21.4 ℃. The specifications for the condenser and reboiler are shown below.

Table 3-2 ACN Tower Condenser and Reboiler

| ACN Column Total Condenser and Partial Reboiler Specifications |
|---|

| Specifications | R1 | | C1 | |
|---|---|---|---|---|
| Area $[m^2]$ | 3.9 | | 4.16 | |
| Duty [kW] | 185.1 | | -160.2 | |
| Type | kettle | | kettle | |
| | SEP-1 Bottoms | Low Pressure Steam | SEP-1 Distillate | MEK |
| Pressure in [kPa] | 10 | 172 | 10 | 100 |
| Pressure out [kPa] | 10 | 172 | 10 | 100 |
| Temperature in [°C] | 56 | 115.6 | 21.4 | -29 |
| Temperature Out [°C] | 51.6 | 115.6 | 21.4 | 11.3 4.0 |
| Vapor Fraction In | 0 | 1 | 1 | 0 |
| Vapor Fraction Out | 0.774 | 1 | 0 | 0 |
| Flow rate $\left[\frac{kg}{hr}\right]$ | 2160.5 | 1000 | 711.9 | 7190 |

To size the condensers we use Aspen Plus to generate condenser Hcurves. We use the Hcurves to determine the vapor fraction and temperature leaving the condenser as well as the heat duty required to make the change. We then specify a pseudo-stream as the vapor entering the condenser and connect that stream to a heat exchanger. Varying MEK as the cooling utility we set design specifications to the temperatures and vapor fractions found in the condenser Hcurves.

We use a similar method to size the reboilers. Reboiler Hcurves are generated using Aspen Plus to determine the temperature and vapor fraction leaving the reboiler as well as the heat duty required. A Pseudo-stream is created and used as the liquid entering the reboiler. This Pseudo-stream is fed into a heat exchanger. Using appropriate process steam as the heating utility set the design specifications in accordance with the values found by the reboiler Hcurves. For the Acetonitrile column we calculated a reboiler area of 3.8891 $m^2$ and a condenser area of 4.16 $m^2$.

### *ii. Toluene Tower*

#### a. Binary Analysis and Operating Pressure

The second separation in our process takes place between toluene and p-xylene. The operating pressure for the toluene tower is determined in the exact same fashion as for the acetonitrile tower. The results from the binary analysis are show below.

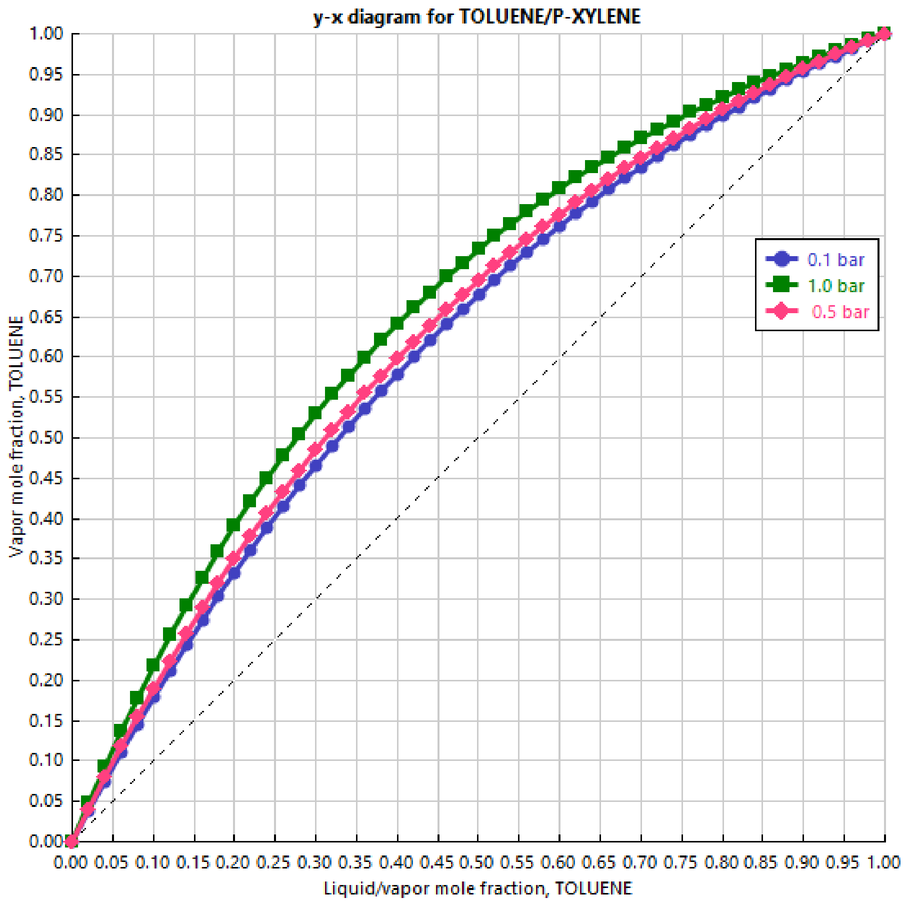


**Figure 3-2:** This represents the binary interaction between acetonitrile and toluene. The father the equilibrium line is from the y-x line, the greater the degree of separation.

b. Column Sizing and Pricing

This column produces 99.92 % toluene product at a rate of 362.8 $\frac{kg}{hr}$. Our Toluene tower is 0.447m in diameter and packed with 4.37m of FLEXIPAC metal packing material type 700Y with an HETP of 0.191m. This packing is equivalent to 24 theoretical stages in a traditional column. Our initial design used the same packing material in both columns but we did not account for the high temperature of column two which would not suit Sulzer type CY packing.

We determine the packed height and column height from equations [3-1] and [3-2] described in the ACN column sizing section. Our toluene column has a diameter of 0.62 m and a height of 4.56. Additional specifications including cost are shown in the table below.

Table 3-3: Toluene Column Summary

| Toluene Column Specifications | |
|---|---|
| **Specifications** | Toluene Tower |
| **Bot. Temperature [°C]** | 137.8 |
| **Top Temperature [°C]** | 109.9 |

| | | |
|---|---|---|
| **Pressure [bar]** | | 1.00 |
| **Diameter [m]** | | 0.617 |
| **Height [m]** | | 4.56 |
| **Pack Height [m]** | | 4.37 |
| **# of Trays** | | 21 |
| **Equivalent # Stages** | | 23 |
| **Feed 1 \| Stage** | Feed A | 8 |
| **Feed 2 \| Stage** | Bot-1 | 15 |
| **Orientation** | Vertical | |
| **Structured Packing Type** | 700Y | |
| **HETP [m]** | 0.191 | |
| **Material** | STANDARD | |
| **Total Cost [$]** | | $99,360 |
| **Distillate Stream Compositions** | **Species** | **wt. Frac** |
| | ACN | 0.00072 |
| | TOLUENE | 0.99925 |
| | P-XYLENE | 0.00003 |
| | SILOXANE | ---trace-- |
| **Bottoms Stream Compositions** | **Species** | **wt. Frac** |
| | ACN | ---trace-- |
| | TOLUENE | 0.00619 |
| | P-XYLENE | 0.82978 |
| | SILOXANE | 0.16403 |

Koch-Glitsch provides critical sizing information such as the HETP for each packing material. We chose to use 700Y FLEXIPAC because it is the most efficient packing material suited for all applications. The HETP value of 0.191m provided is based on a distillation at total reflux subjected to minor pressure/suction.

The toluene column is priced using EconExpert and is classified as a vertically oriented process vessel with structured packing and an operating pressure of 1.0barg. EconExpert gives a base cost of $13,280. This cost is then multiplied by the pressure and material factors to give a final cost estimate of approximately $100,000.

### c. Condenser and Reboiler

In addition to the staged packing, the column is also equipped with a total condenser and a partial reboiler. The specifications for each are shown below.

Table 3-4: Toluene Column Condenser and Reboiler Summary

| Toluene Column Total Condenser and Partial Reboiler |
|---|

| Specifications | R2 | | C2 | |
|---|---|---|---|---|
| Area [m2] | 5.323 | | 2.79 | |
| Duty [kW] | 169.825 | | -165 | |
| Type | kettle | | kettle | |
| | SEP-2 Bottoms | High Pressure Steam | SEP-2 Distillate | Cooling Water |
| Pressure in [kPa] | 100 | 1033 | 100 | 100 |
| Pressure out [kPa] | 100 | 1033 | 100 | 100 |
| Temperature in [°C] | 137.7 | 181.4 | 109.81 | 35 |
| Temperature Out [°C] | 137.9 | 172.4 | 102 | 99.65 |
| Vapor Fraction In | 0 | 1 | 1 | 0 |
| Vapor Fraction Out | 0.783 | 1 | 0 | 0.074 |
| Flow rate [kg/hr] | 2339 | 13500 | 1632.6 | 2000 |

The sizing process for these reboilers and condensers is the same as the one taken for the ACN reboilers and condensers.

The bottoms stream from this column contains high grade p-xylene and therefore it is favorable to subject the stream to simple flash distillation and recycle the p-xylene back to the acetonitrile tower.

### *iii. Flash Drum*

The final separation is carried out in a flash drum immediately after the toluene separation column. The main function of this flash drum is to return xylene to the first column, and remove the siloxane waste from the original polymerization process.

The exiting stream compositions of the flash drum are highly sensitive to minor changes in flash temperature. We determine the optimum temperature of 138 C with a fraction vaporized of 0.7. Under these operating conditions, the flash drum returns xylene at 86 % purity. This recycle stream is mixed with pure xylene to maintain a constant feed of 100 $\frac{kg}{hr}$ to the acetonitrile column. The recycle stream has a flash point of 27.2 ℃ and must be cooled below this temperature before allowed to enter the mixer.

Table 3-5: Flash Drum Specifications

| Flash Separation of P-Xylene and Siloxane Operating Specifications | |
|---|---|
| Specifications | Flash Drum |
| **Temperature [°C]** | 138.00 |
| **Pressure [bar]** | 1.00 |
| **Diameter [m]** | 0.15 |
| **Height[m]** | 0.48 |
| **Volume [m$^3$]** | 0.01 |

| | | |
|---|---|---|
| **Heat Duty [kW]** | 7.77 | |
| **Material** | 316SS | |
| **Cost** | $14,581.00 | |
| | **Component** | **Weight Fraction** |
| **Vapor Stream Compositions (wt.frac.)** | Acetonitrile | -trace- |
| | Toluene | 0.0072 |
| | p-Xylene | 0.85 |
| | Water | 0 |
| | Siloxane | 0.14 |
| **Liquid Stream Compositions (wt. frac.)** | Acetonitrile | -trace- |
| | Toluene | 0.003 |
| | p-Xylene | 0.751 |
| | Water | 0 |
| | Siloxane | 0.245 |

# 4. Auxiliary Tasks: Sizing and Costing

In addition to the three main separation tasks several auxiliary units are incorporated in this process including:

i. Vacuum Pump
ii. Positive Displacement Pumps
iii. Reflux Drums
iv. Mixer – Motionless, Open Air
v. Heat Exchangers
vi. Storage Tanks
vii. Material of Construction Analysis

### *i. Vacuum Pump*

The separation carried out in the first column requires a sub-atmospheric pressure determined by our VLE binary analysis to be 0.1 bar. To pull the vacuum we chose to use a liquid ring pump because they are easy to maintain. Liquid ring pumps only have one moving part, leaving the majority of the mechanical duty to the fluid. To determine the power required to drive the pump we consult pump performance curves provided by Aerstin and Street (1978). The performance curve plots horse power and volume flow rate of the pump versus the suction head. Our design requires 0.9 bar of suction at a volume flow rate of 5.1 $\frac{L}{min}$ yielding a 20.4 kW power requirement. The equation below is used to calculate the purchase cost of the liquid-ring pump.

$$Installed\ Costs = \$28{,}000\left[\frac{HP}{10}\right]^{0.5} \cdot \left[\frac{1956}{745}\right] \quad [4\text{-}1]$$

In the above equation HP represents the power supplied to the fluid in horsepower. The second term in the equation is a corrective factor which adjusts the costs to the proper year. 1956 is the cost index for the current year, 745 was the cost index in 1981. These calculations yield a final estimated pump cost of $88,600. **Table 4-1** below displays the results of the pump sizing and costing analysis.

Table 4-1: Vacuum Pump Summary

| Vacuum Pump | |
|---|---|
| **Specification** | **Vacuum** |
| **Type** | Liquid Ring |
| **Power [kW]** | 20.4 |
| **Flowrate [l/min]** | 5.1 |
| **Pressure in [bar]** | 1.00 |
| **Pressure out [bar]** | 0.10 |
| **Cost [$]** | $88,574 |
| **Material** | Stainless Steel |

Table 4-1 is a summary of the sizing and costing analysis conducted for the vacuum pump. We double this cost in our economic analysis to purchase a backup pump that would allow for continuous production during primary pump maintenance or failure. Stainless Steel and bronze are the materials of choice for liquid-ring pumps as suggested by Aerstin and Street.

### *ii. Positive Displacement Pumps*

The distillate and bottoms streams of column one each require a pump to return the fluid to 1.0 bar of pressure before continuing in the process. Each pump is sized according to its suction pressure and power required. EconExpert gives material and pressure factors of 1.4 and 1.0 respectively, yielding a cost of $8,880 for each pump. It is not surprising that the cost for each pump is the same as they each operate under the same suction pressure with similar volume flow rates.

Table 4-2: Summary of Positive Displacement Pumps

| Pump Specification | | |
|---|---|---|
| **Specification** | **Pump 1** | **Pump 2** |
| **Type** | Positive Displacement | Positive Displacement |
| **Power [kW]** | 0.008 | 0.005 |
| **Flowrate [l/min]** | 0.257 | 0.2004 |
| **Differential Head [m]** | 11.10 | 11.64 |
| **Presure in [bar]** | 0.10 | 0.1 |
| **Pressure out [bar]** | 1.00 | 1.00 |
| **Cost [$]** | $8,880 | $8,880 |
| **Material** | Carbon Steel | Carbon Steel |

Table 4-2 summarizes the sizing and costing information for each rotary positive displacement pump in our process. As we did for the vacuum pump, we also include backups for each pump.

### *iii. Reflux Drums*

The reflux drums were sized with a holdup time of 8 minutes, at the end of which the reflux would be half full. These drums are considered to be horizontally aligned and are sized according to the volumetric flowrate from each column. Distillate 1 exits at 3.34 $\frac{L}{min}$ yielding a volume of 0.24$m^3$. In a similar fashion, the second reflux drum is found to have a volume of 7.73$m^3$. Each drum is sized with an optimal length to diameter ratio of 3.0. Using this ratio and the volume after 8 minutes, we are able to determine the dimensions of each drum.

Table 4-4: Summary of Reflux Drum Sizing

| Reflux Drum Sizing | | |
|---|---|---|
| Specification | Drum 1 | Drum 2 |
| Diameter [m] | 0.320 | 0.486 |
| Length[m] | 0.959 | 1.459 |
| Volume [m^3] | 0.2408 | 0.557 |
| Flow Rate [l/min] | 3.34 | 7.73 |

| | | |
|---|---|---|
| Holding Time [min] | 8 | 8 |
| Reflux Ratio | 3.5 | 3.5 |
| Liquid Space [%] | 50 | 50 |
| **Cost [$]** | $4,250 | $6,700 |
| **Material** | Carbon Steel | Carbon Steel |

Table 4-4 details each of the reflux drums including their cost. The pricing for these units was carried out in EconExpert. Each reflux drum has a material and pressure factor of 1.0 when carbon-steel is used yielding final costs of $4,250 and $6,700 for reflux drums one and two respectively.

*iii. Mixer*

The mixer in our process is designed to mix the recycled xylene with pure xylene to ensure column one receives a constant supply of separating agent. The ratio of makeup to recycled xylene is controlled in ASPEN Plus with an integrated FORTRAN algorithm. Our mixer of choice was an open top, unstirred mixer with a 70% liquid hold up time of 5 minutes. The mixed stream exits at a rate of 3.94 $\frac{L}{min}$ meaning the mixer must be able to hold 19.7L and remain 70% full. We assume a height to diameter ratio of 4 to calculate the dimensions of the mixer. These results are summarized in **Table 4-5** below.

Table 4-5: Unstirred Mixer Sizing

| Mixer 1 | | | |
|---|---|---|---|
| **Specification** | Unstirred, Motionless Mixer | | |
| **Hold Time [min]** | 5 | | |
| **Volume [m3]** | 0.0142 | | |
| **Diameter [m]** | 0.067 | | |
| | Makeup In | Recycle In | Recycle Out |
| **Pressure [bar]** | 1 | 0.98 | 1 |
| **Temperature [°C]** | 20 | 27 | 25.11 |
| **Mass Flow [$\frac{kg}{hr}$]** | 29.6 | 81.75 | 111.4 |
| **Cost [$]** | $1,780 | | |
| **Material** | Carbon Steel | | |

Table 4-5 includes the cost of the mixer at approximately $1,800 a total purchased cost of $1,190 and a bare module factor of 1.5.

*iv. Heat Exchanger Network*

Every exchange of heat that takes place in this process follows the guidelines of the table below. Acetonitrile and toluene have very low flash points and they must be cooled below these temperatures before being exposed to the atmosphere upon entering the storage vessel.

Table 4-6: Outlet Temperatures and Flash Points of Product Streams

| Product Flash Points | | | |
|---|---|---|---|
| **Product Stream** | **Inlet Temp [ ℃ ]** | **Outlet Temp [ ℃ ]** | **Flash Point [ ℃ ]** |
| ACN | 21.54 | 5 | 5.5 |
| TOL | 109.22 | 4 | 4.4 |
| Xylene Recycle | 137 | 27 | 27.2 |
| WASTE | 137 | 27 | 27.2 |

Our process uses counter-current shell and tube heat exchangers along with cooling water and MEK, an organic refrigerant. Neither the cooling water nor the MEK may raise more than 10 C above their supply temperatures of 35 ℃ and -29 C respectively. We set design specifications in ASPEN Plus to control the flowrate of each coolant stream, ensuring that no thermal crossovers took place.

Our initial process flowsheet included seven heat exchangers, incurred more utility cost because each exchanger had its own source of cooling utility. In our optimized design, we add two additional exchangers, one to heat each feed to the 2nd column, effectively reducing the reboiler duty. The waste stream is used to heat both the bottoms stream from the first column (bot-1 feed) as well as Feed 2A.

Table 4-7: Hot and Cold Stream Data for HEN Synthesis

| Stream Table for Heat Exchanger Network | | | | | | | |
|---|---|---|---|---|---|---|---|
| **Stream** | **ID** | **Supply T [C]** | **Target T [C]** | **m Flow $\left(\frac{kg}{hr}\right)$** | **Cp $\left(\frac{Kj}{kgK}\right)$** | **m Cp $\left(\frac{kJ}{hrK}\right)$** | **Q $\left(\frac{kJ}{hr}\right)$** |
| Dist-1 | SH 1 | 21.39 | 5 | 158.2 | 2.06 | 325.19 | 5329.90 |
| Dist-2 | SH 2 | 109.91 | 4 | 362.8 | 2.05 | 742.28 | 78614.62 |
| Recycle | SH 3 | 138 | 27 | 163.57 | 1.63 | 266.27 | 29556.08 |
| Waste | SH 4 | 138 | 27 | 248.95 | 1.71 | 424.54 | 47123.52 |
| | | | | | | | |
| Feed A | SC 1 | 20 | 100 | 270 | 1.658981 | 447.92 | -35833.99 |
| Bot-1 | SC 2 | 54 | 64 | 214.4 | 1.80 | 386.17 | -3861.67 |
| | | | | | | **Cooling Req.** | **120928.46** |

Table 4-7 shows the supply and target temperatures of each stream integrated in our heat exchanger network. Our integrated network reduces the cooling required in the system by using the Feed A and Bot-1 to remove 40MJ/hr from the hot streams. This value is determined by summing the total cooling provided by streams SC1 and SC2. It is impossible to cool SH1 with any process stream without violating minimum approach temperatures. A simplified version of our heat exchanger network is shown below in Figure 4-1.

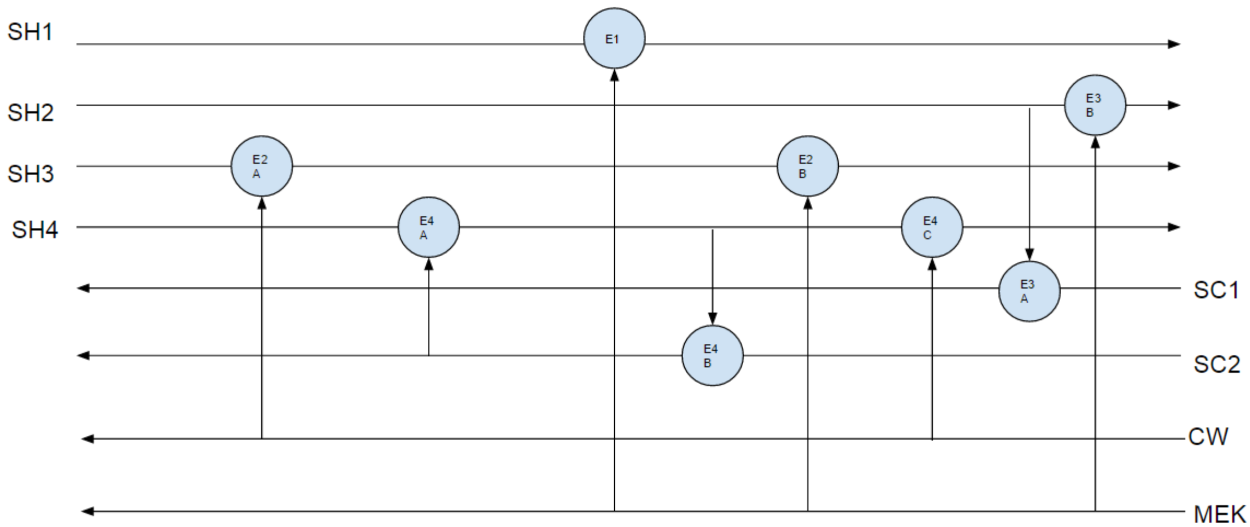


Figure 4-1: This figure depicts our simplified heat exchanger network. The inlet and outlet temperatures of each stream are displayed in Table 4-7. The cooling utilities, CW and MEK, are available at temperature rages of $[35\,℃\ to\ 45\,℃]$ and $[-29\,℃\ to -19\,℃]$ respectively.

After completing the HEN we verify our results by comparing the heat duties of the reboilers and condensers after heat integration. These results are outlined in table 4-8 below.

Table 4-8: Reboiler and Condenser Heat Duty Comparison

| Heat Integration Results | | | | |
|---|---|---|---|---|
| | Reboiler 1 | Reboiler 2 | Condenser 1 | Condenser 2 |
| Initial Heat Duty [kW] | 185.1 | 200.3 | -162.7 | -166.3 |
| Final Heat Duty [kW] | 185 | 169.8 | -160.2 | -165 |

The toluene column experienced the largest benefit from the heat integration process, reducing the heat duty approximately 40 kW. Specific information about each heat exchanger is located in Appendix C.

### *v. Storage Tanks*

The cost and size of a storage vessel is directly related to the inlet flowrate, and the desired fill time. Our tanks are designed to reach 50% of their maximum volume after 48 hours of continuous production. To calculate the required volume, we simply multiply the hourly inlet flowrate by 96 hrs to acquire the volume at max capacity.

Table 4-9: Storage Vessels

| Storage Vessel Sizing | | | | | | |
|---|---|---|---|---|---|---|
| **Storage Vessel** | **Inlet Flowrate** $[\frac{m^3}{day}]$ | **Volume [$m^3$ ]** | **Pressure [bar]** | **Material** | **Type** | **Cost** |
| **Acetonitrile Tank** | 4.70 | 18.80 | 1.0 | 316SS | Cone Roof | $13,880 |
| **Toluene Tank** | 9.84 | 39.36 | 1.0 | 316SS | Cone Roof | $19,600 |
| **Feed B+C Tank** | 1.11 | 29.42 | 1.0 | 316SS | Cone Roof | $17,000 |
| **Feed A Tank** | 7.36 | 32.80 | 1.0 | 316SS | Cone Roof | $18,000 |
| **Waste Tank** | 0.82 | 4.44 | 1.0 | 316SS | Cone Roof | $7,456 |
| **P-Xylene** | 8.20 | 3.28 | 1.0 | 316SS | Cone Roof | $6,620 |
| **Spill Containment** | Conditional | 59.04 | 1.0 | 316SS | Cone Roof | $23,970 |

The final item in Table 4-9 is the spill containment vessel which does not have a set inlet flowrate. This vessel is designed to contain 1.5 time the volume of the largest storage tank to ensure adequate chemical waste storage in the event of equipment failure. Spill containment is discussed in more detail in section 6.

# 5. Process Economics

### *i. Delivered Equipment Cos*

Each unit in our process is priced based on the EconExpert software package. We use a cost index of 556.7 in this program to ensure that the estimates we gather from EconExpert are appropriate for the current year. EconExpert supplies the total purchased cost as well as two dimensionless factors representing the material and conditions the unit is operating under. We calculate the true cost according to the equation below.

$$[True\ Cost] = [Base\ Purchased\ Cost] * [Material\ Factor] * [Pressure\ Factor] \quad [5\text{-}1]$$

It is typical for suppliers to provide 'free on board' service to load the equipment for you, excluding the delivery. Design heuristics suggest that the delivered equipment cost should be approximately 10 % greater than the true cost of the product. Table 5-1 below displays the total delivered equipment cost for our process.

Table 5-1: Total Delivered Equipment Cost

| Delivered Equipment Costs | | | | | |
|---|---|---|---|---|---|
| Mixer | $1,700 | 1.0 | 1.0 | $170 | $1,900 |
| ACN Tower | $8,900 | 4.0 | 1.7 | $6,052 | $66,600 |
| TOL Tower | $13,300 | 4.0 | 1.7 | $9,044 | $99,500 |
| Reb -1 | $10,800 | 1.0 | 1.0 | $1,080 | $11,900 |
| Cond - 1 | $4,700 | 1.0 | 1.0 | $470 | $5,200 |
| Reb - 2 | $10,800 | 1.0 | 1.0 | $1,080 | $11,900 |
| Cond -2 | $5,600 | 1.0 | 1.0 | $560 | $6,200 |
| Pump 1 | $2,200 | 1.4 | 1.0 | $308 | $3,400 |
| Pump 2 | $2,200 | 1.0 | 1.0 | $220 | $2,400 |
| Vacuum Pump | Costing Found in Table 4-1 | | | | $88,900 |
| Reflux Drum 1 | $3,600 | 1.0 | 1.0 | $360 | $4,000 |
| Reflux Drum 2 | $5,000 | 1.0 | 1.0 | $500 | $5,500 |
| Flash Drum | $14,600 | 1.0 | 1.0 | $1,460 | $16,100 |
| Heat Exchangers | $97,100 | 1.0 | 1.0 | $9,710 | $106,800 |
| Acetonitrile Tank | $13,900 | 1.0 | 1.0 | $1,390 | $15,300 |

| | | | | | |
|---|---|---|---|---|---|
| Toluene Tank | $19,600 | 1.0 | 1.0 | $1,960 | $21,600 |
| Feed B+C Tank | $17,100 | 1.0 | 1.0 | $1,710 | $18,800 |
| Feed A Tank | $18,000 | 1.0 | 1.0 | $1,800 | $19,800 |
| Waste Tank | $7,500 | 1.0 | 1.0 | $750 | $8,300 |
| P-Xylene | $6,600 | 1.0 | 1.0 | $660 | $7,300 |
| Spill Containment | $24,000 | 1.0 | 1.0 | $2,400 | $26,400 |
| Backup Pump 1 | $2,200 | 1.4 | 1.0 | $308 | $3,400 |
| Backup Pump 2 | $2,200 | 1.0 | 1.0 | $220 | $2,400 |
| Bkp Vc Pump | Costing Found in Table 4-1 | | | | $88,900 |
| | | | | **Total Cost** | **$532,500** |

In this table each heat exchanger is combined into a single cost as each exchanger costs exactly the same when sized in EconExpert. A simple summation gives our total delivered equipment cost (DEC). The DEC is an important value for the remaining economic analysis, it is used to determine the necessary investments in terms of fixed capital and operation costs.

### *I. Fixed Capital Investment*

To determine the fixed capital investment (FCI) for our process, we must calculate the direct, indirect, and contracting costs. Each cost in the subsequent table is based off of a percentage of the delivered equipment cost, and is subject to alteration by the engineer in charge of the process, within reason. Certain line items are excluded from our analysis because we are adding on to an existing plant. The land, service facilities, and buildings are already supplied by the company we are working for and therefore can be excluded from our total direct plant cost.

Table 5-2: Installation Costs

| **Install Costs** | | |
|---|---|---|
| **Direct Production Costs** | **[%] DEC** | Value |
| | | |
| Delivered Equipment Cost | 100 | $515,769 |
| Installation | 47 | $242,411 |
| Piping | 66 | $340,407 |
| Instrumentation and Controls | 15 | $77,365 |
| Electrical | 11 | $56,735 |
| Yard Improvements | 5 | $25,788 |
| | **Total Direct Plant Cost** | **$1,258,476** |
| | | |

| Indirect Costs | [%] DEC | Value |
|---|---|---|
| Engineering Supervision | 35 | $180,519 |
| Construction Expenses | 45 | $232,096 |
| | **Total Indirect** | **$412,615** |
| | | |
| **Other** | **[%] DEC** | Value |
| Contractor's Fee | 21 | $108,311 |
| Contingency | 42 | $216,623 |
| | **Total Other** | **$324,934** |

This table shows the cost of each service/improvement as compared to the DEC. We acquire the [%] DEC values from Peters and Timmerhaus (1981). Finally our FCI is calculated by adding up the Direct, Indirect, and Other costs to yield a value of $1,996,000.

Table 5-3: Summary of Key Investment Figures

| Capital Investment Summary | |
|---|---|
| DEC | $515,800 |
| FCI | $1,996,000 |
| WCI | $443,600 |
| TCI | $2,439,600 |

Table 5-3 summarizes the delivered equipment costs, fixed capital investment, working capital investment, and total capital investment.

*III. Labor*

Human labor is essential to the day-to-day operation of the plant, therefore we decided to hire several at an hourly rate of $25/hr for a total of 2000 hours/yr.

$$Labor\ Cost = \left[2000\frac{hrs}{worker\cdot year}\right] * [\#\ Workers] \cdot \left[\frac{\$}{hr}\right] \cdot [1.7] \qquad \text{[Eq 5-1]}$$

In addition to their $25/hr each worker will receive an additional 70% in benefits leaving us with a total labor cost of $680,000 annually.

*IV. Manufacturing Cost*

The manufacturing cost of this process takes into account periodic maintenance, required operating supplies, and laboratory charges. These are considered direct costs in the manufacturing process but in order to fully estimate the manufacturing cost, one must account for addition fixed costs, general expenses, and the plant overhead fees. The following table summarizes the cost of manufacturing on a yearly basis. All line items are from Peters and Timmerhaus (1991) for fluid processing plants.

Table 5-4: Calculation of Manufacturing Cost

| Manufacturing Cost | | | |
|---|---|---|---|
| **Direct Costs** | [%] | Percentage of | Value |
| Maintenance | 6 | FCI | $119,700 |
| Operating Supplies | 15 | FCI | $299,400 |
| Laboratory Charges | 15 | Operating Labor | $102,000 |
| **Fixed Charges** | | | |
| Local Taxes | 2.5 | FCI | $49,900 |
| Insurance | 0.7 | FCI | $13,900 |
| **Plant Overhead** | 55 | Labor, Supervision, Maintenance | $539,100 |
| **General Expenses** | | | |
| Administrative Costs | 15 | Labor, Supervision, Maintenance | $147,000 |
| Distribution and Selling | 15 | Manufacturing cost | $168,600 |

The manufacturing cost of a product plays into the operation cost of the plant and ultimately the rate of return.

*V. Rate of Return*

The rate of return is based on the after tax cash flow of the process. We determine this cash flow by following a 20 year SOYD depreciation scheme, assuming a salvage value of 0. This analysis also includes a 10% increase in operating cost during the first year to account for start-up and any additional costs it may bring with it. The results of this analysis are displayed below.

Table 5-5: Cash Flow Analysis

| 20 Year SOYD Cash Flow Analysis | | | | | | | |
|---|---|---|---|---|---|---|---|
| Year | Total Product Cost | Revenue From Sales | Before Tax Cash Flow | SOYD Depreciation Value | Taxable Income | Income Taxes | After Tax Cash Flow |
| 0 | -$2,518,700 | | | | | | -$2,518,700 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 1 | $3,935,900 | $9,679,800 | $5,743,900 | $203,897 | $5,540,003 | $2,216,001 | $3,527,900 |
| 2 | $3,578,100 | $9,679,800 | $6,101,700 | $193,702 | $5,907,998 | $2,363,199 | $3,738,500 |
| 3 | $3,578,100 | $9,679,800 | $6,101,700 | $183,507 | $5,918,193 | $2,367,277 | $3,734,400 |
| 4 | $3,578,100 | $9,679,800 | $6,101,700 | $173,312 | $5,928,388 | $2,371,355 | $3,730,300 |
| 5 | $3,578,100 | $9,679,800 | $6,101,700 | $163,117 | $5,938,583 | $2,375,433 | $3,726,300 |
| 6 | $3,578,100 | $9,679,800 | $6,101,700 | $152,923 | $5,948,777 | $2,379,511 | $3,722,200 |
| 7 | $3,578,100 | $9,679,800 | $6,101,700 | $142,728 | $5,958,972 | $2,383,589 | $3,718,100 |
| 8 | $3,578,100 | $9,679,800 | $6,101,700 | $132,533 | $5,969,167 | $2,387,667 | $3,714,000 |
| 9 | $3,578,100 | $9,679,800 | $6,101,700 | $122,338 | $5,979,362 | $2,391,745 | $3,710,000 |
| 10 | $3,578,100 | $9,679,800 | $6,101,700 | $112,143 | $5,989,557 | $2,395,823 | $3,705,900 |
| 11 | $3,578,100 | $9,679,800 | $6,101,700 | $101,948 | $5,999,752 | $2,399,901 | $3,701,800 |
| 12 | $3,578,100 | $9,679,800 | $6,101,700 | $91,754 | $6,009,946 | $2,403,979 | $3,697,700 |
| 13 | $3,578,100 | $9,679,800 | $6,101,700 | $81,559 | $6,020,141 | $2,408,057 | $3,693,600 |
| 14 | $3,578,100 | $9,679,800 | $6,101,700 | $71,364 | $6,030,336 | $2,412,134 | $3,689,600 |
| 15 | $3,578,100 | $9,679,800 | $6,101,700 | $61,169 | $6,040,531 | $2,416,212 | $3,685,500 |
| 16 | $3,578,100 | $9,679,800 | $6,101,700 | $50,974 | $6,050,726 | $2,420,290 | $3,681,400 |
| 17 | $3,578,100 | $9,679,800 | $6,101,700 | $40,779 | $6,060,921 | $2,424,368 | $3,677,300 |
| 18 | $3,578,100 | $9,679,800 | $6,101,700 | $30,585 | $6,071,115 | $2,428,446 | $3,673,300 |
| 19 | $3,578,100 | $9,679,800 | $6,101,700 | $20,390 | $6,081,310 | $2,432,524 | $3,669,200 |
| 20 | $3,578,100 | $10,137,700 | $6,559,600 | $10,195 | $6,549,405 | $2,619,762 | $3,939,800 |

The after tax cash flow, ATCF, is the most important column for calculating the rate of return on our initial investment. From this cash flow we calculate an annual rate of return of 144%. These values are based off of the 1981 cost index written by Peters and Timmerhaus. Based on this rate of return we can confidently recommend operating this solvent recovery system under the operating specifications displayed in the Equipment Summary.

The success of our process is ultimately dependent on the market price of acetonitrile and toluene. We conduct a sensitivity analysis on the rate of return to examine its behavior as the market varies. The following plot displays the response of the rate of return when the product prices are changed.

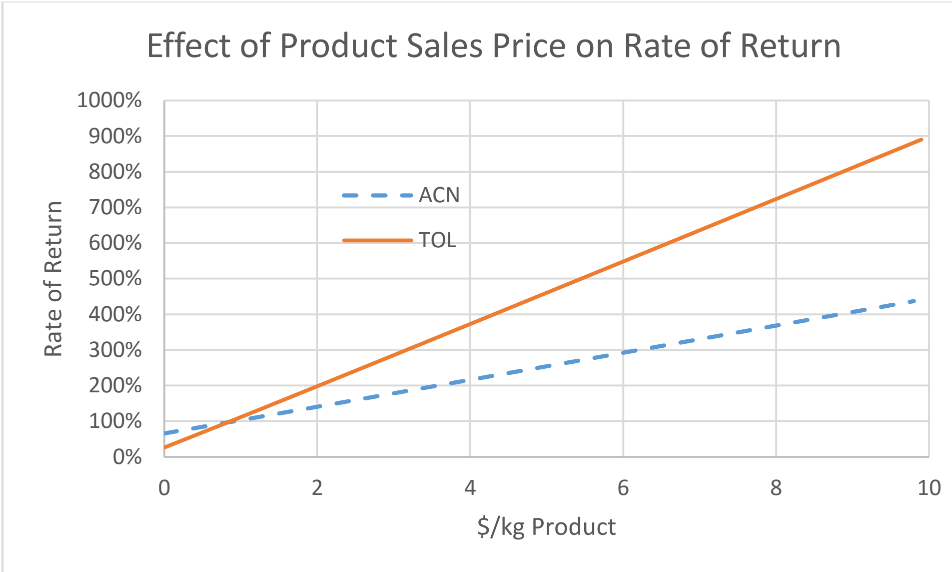


Figure 5-1: Sensitivity Analysis on the Rate of Return

According to figure 5-1, our profits are highly dependent on the price of toluene. This plot was generated using Excel and by varying each product price while holding the other constant at the value given in the design specifications.

# 6. Safety and quality control

The proposed recycle process involves a variety of hazardous materials and operating conditions that must be avoided through the design of a safe plant process. The first things to consider are the hazardous materials used in the process. Acetonitrile, Toluene, and Xylene have flash temperatures of 4.4, 5.5, and 27 $℃$ respectively. Unfortunately the mixer we use that contains mostly xylene is an open air mixer, and both the Acetonitrile and Toluene storage tanks are open to the atmosphere. We must cool these streams below their flash points before they can be stored or mixed. We consider all possibilities of failure along with the consequence of that failure. Failure Mode and Effects Analysis (FMEA) and Hazard Operability Analysis (HAZOP) are the preferred methods of risk assessment. FMEA is focused on how equipment failure affects the safety of the process and the economic impact. HAZOP is similar to FEMA, but focuses on safety in regards to personnel, the environment, and the safeguards that are necessary in order for the process to run smoothly. We increase the overall safety of the process by compiling widely accepted methods of systematic safety assessment: HAZOP, FMEA, and an inherently safer design checklist.

### *i. Spill Containment*

In the event of spillage, it is important to have a vessel large enough to contain the equivalent volume of the largest tank plus an additional 50% of that value. This ensures that even if our largest tank experiences failure, we will still be able to prevent the effluent fluids from exiting the plant. Our largest storage tank contains the toluene product and is 39 $m^3$ leading to a containment vessel with a volume of 59 $m^3$. In addition to containing the fluid in the drains, we must absorb the pooling liquids with a porous, inert material such as vermiculite. Above all else, we must be sure that all drainage is clear from all sources of ignition.

### *ii. Fire Prevention*

As mentioned previously Acetonitrile and toluene both have flash points below room temperature. Meaning a rupture in any of the networks containing Toluene or Acetonitrile could be a dangerous situation for surrounding personnel and equipment. The system of controllers explained in the P&ID diagram are the first line of defense, and should be designed to warn operators of data inconsistencies in the system. These inconsistencies could signify a leak or rupture in the system or possibly a hot flammable stream that is not cooled enough. In the case these controllers somehow fail additional passive and active prevention techniques will need to be installed. A passive solution could entail isolating the exits of the flammable streams in the design of the chemical plant from any spark sources. Conventional water spray systems will not extinguish flames made by a low flash point material. Acetonitrile can be extinguished using Bromochlorodifluoromethane (BCF). Acetonitrile can be extinguished by $CO_2$ portable extinguishers. The implementation of mobile foam monitors around the ACN and Toluene storage tanks as a last line of active fire protection.

*iii. Maximum Allowable operating Conditions*

The maximum allowable pressure and temperature of each unit are determined using heuristics as guidelines. The maximum allowable pressure is either 1.1 times the operating pressure, or 3.47 bar higher than the operating pressure, whichever gives a higher value. By these guidelines no vessel should exceed 4.5 bars of pressure at any point in our process.

Table 6-1: MAWP/MAWT Summary

| | Operating Pressure [bar] | MAWP [bar] | MAWT [C] |
|---|---|---|---|
| Mixer | 1 | 4.447 | 315.6 |
| ACN Tower | 0.1 | 3.547 | 315.6 |
| TOL Tower | 1 | 4.447 | 315.6 |
| Reb -1 | 0.1 | 3.547 | 315.6 |
| Cond - 1 | 0.1 | 3.547 | 315.6 |
| Reb - 2 | 1 | 4.447 | 315.6 |
| Cond -2 | 1 | 4.447 | 315.6 |
| Pump 1 | 0.1 | 3.547 | 315.6 |
| Pump 2 | 0.1 | 3.547 | 315.6 |
| Vacuum Pump | 0.1 | 3.547 | 315.6 |
| Reflux Drum 1 | 0.1 | 3.547 | 315.6 |
| Reflux Drum 2 | 1 | 4.447 | 315.6 |
| Flash Drum | 1 | 4.447 | 315.6 |
| Heat Exchangers | 1 | 4.447 | 315.6 |
| Acetonitrile Tank | 1 | 4.447 | 315.6 |
| Toluene Tank | 1 | 4.447 | 315.6 |
| Feed B+C Tank | 1 | 4.447 | 315.6 |
| Feed A Tank | 1 | 4.447 | 315.6 |
| Waste Tank | 1 | 4.447 | 315.6 |
| P-Xylene | 1 | 4.447 | 315.6 |
| Spill Containment | 1 | 4.447 | 315.6 |
| Backup Pump 1 | 0.1 | 3.547 | 315.6 |
| Backup Pump 2 | 0.1 | 3.547 | 315.6 |
| Bkp Vc Pump | 0.1 | 3.547 | 315.6 |

Table 6-1 above displays the maximum limits for each unit. The maximum temperature for each unit is the same because no unit exceed the limit of 315.6 C given by the design heuristic. The MAWP is very important to plant safety. The understanding of this limit helps reduce the chance of explosion due to overpressure.

### *iv. HAZOP*

List of chemicals involved in the proposed process are as follows:

- Acetonitrile (ACN)
- MethylEthylKetone (MEK)
- Siloxane
- Toluene
- Water
- P-Xylene

Potential Hazards:
Three of the main components that are being separated, Toluene, Acetonitrile, and p-Xylene, are exposed to temperatures above their flash points during the recycling process. Separation processes are also innately are run at high temperatures, relative to room temperature, to ensure sharp separations. Two of these components, Toluene and Acetonitrile have flash points of 5 and 4 °C respectively which are well below room temperature.
Analysis Boundaries:

1. Incidents that occur during the repair or maintenance process are not included.
2. Feeds enter the recycle process directly from the siloxane polymerization plant at a set steady flow rate that is closed from the atmosphere.
3. Cooling water and MEK flow rates are driven by gravity, and tuned using a control valve.
4. Stead-state operation
5. Equipment is well built and use as designed
6. Operators are properly trained
7. Procedures are clearly written
8. Maintenance and inspections are performed routinely

Analysis Results:
Strict enforcement of MSDS approved PPE, proper and relevant operator training as well as an emphasis on workplace safety. Any stream containing a material above its flash point must have temperature sensors as well as a pressure or a flow rate sensor to ensure there is no leak. Streams around heat exchangers should also be equipped with temperature and flow sensors to ensure there is no cross flow and the correct amount of heat is being exchanged. Extensive tables for the HAZOP analysis are located in Appendix –D

### *v. Personal Protective Equipment*

The safety data sheets described above outline the PPE requirements for all personnel who could potentially come in contact with hazardous materials. To ensure proper operator safety we require that gloves, insulated boots, full body suits, and safety glasses must be worn at all times. In the event that an operator must handle the materials directly, they are required to adorn addition protective equipment such as a self-contained respirator or breathing apparatus

Acetonitrile

Acetonitrile is highly flammable in its vapor state, and is flammable under room temperature at atmospheric pressure. Acetonitrile may also cause serious eye and skin irritation as well as toxic effects when inhaled or ingested. The use of personal protective equipment such as safety glasses, breathing apparatus, gloves, and lab coats should be required.

If personnel’s eyes come in contact, rinse out eye for at least 15 minutes. If personnel’s skin comes in contact with Acetonitrile wash the afflicted area with soap and water for at least 15 minutes. In the case of serious inhalation evacuate the afflicted personnel to a safe area with haste. Loosen any tight clothing collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, preform CPR (WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, In this case use a bag valve mask). In case of ingestion do not induce vomiting unless directed to do so by a medical professional. Never give anything by mouth to an unconscious person. Loosen any tight clothing and get medical attention if any symptoms appear.

The storage of acetonitrile must be in a tight ventilated container that is isolated from any heat or spark sources. In case of spill avoid contamination into the environment, and upgrade the level of personal protective equipment to a full body suit, self-contained breathing apparatus, vapor respirator, boots, and gloves. Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Toluene

Toluene is highly flammable as a vapor, hazardous to aquatic life, a skin irritant, can incur serious eye and organ damage, and may cause death if inhaled. Personal protective equipment such as a breathing apparatus, gloves, and eyewear should be required in operations involving toluene.
If skin comes in contact with toluene the MSDS procedure states to wash the affected area with soap and water for at least 20 minutes. If personnel’s eyes come in contact, rinse out eye for at least 15 minutes, and seek medical attention immediately. In the case of serious inhalation evacuate the afflicted personnel to a safe area with haste. Loosen any tight clothing collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, preform CPR (WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, In this case use a bag valve mask). In case of ingestion do not induce vomiting unless directed to do so by a medical professional. Never give anything by mouth to an unconscious person. Loosen any tight clothing and get medical attention if any symptoms appear.

Toluene needs to be stored in a sealed, well ventilated storage vessel that is isolated from any ignition sources. Drains and surface water must be protected from potential spills to avoid contamination. In case of spill avoid contamination into the environment, and upgrade the level of personal protective equipment to a full body suit, self-contained breathing apparatus, vapor respirator, boots, and gloves. Non sparking materials must be used in the cleanup of toluene. Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

P-Xylene

The MSDS lists p-xylene as a flammable liquid and vapor, hazardous to aquatic life, and harmful when in contact with skin and eyes, and has a toxicity when inhaled or ingested.
In case of contact with eyes flush with plenty of water for at least 15 minutes and seek medical attention if serious irritation persists. In the case of skin contact flush the afflicted area with an excess of water. Cover skin with an emollient, and remove any contaminated clothing and shoes. Thoroughly wash clothing and shoes before reuse. In the case of serious inhalation evacuate the afflicted personnel to a safe area with haste. Loosen any tight clothing collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, preform CPR (WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, In this case use a bag valve mask). In case of ingestion do not induce vomiting unless directed to do so by a medical professional. Never give anything by mouth to an unconscious person. Loosen any tight clothing and get medical attention if any symptoms appear.

P-Xylene should be stored in a sealed, well ventilated storage vessel that is isolated from any ignition sources. Drains and surface water must be protected from potential spills to avoid contamination. In case of spill avoid contamination into the environment, and upgrade the level of personal protective equipment to a full body suit, self-contained breathing apparatus, vapor respirator, boots, and gloves. Non sparking materials must be used in the cleanup of p-xylene. Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location

## 7. Conclusion

The recovery of solvents, toluene and acetonitrile, from a polymerization plant is best carried out using two distillation towers and one flash drum. Our process utilizes the packed columns to separate out the solvents independently while the flash drum separates the waste from recycled separating agent. The results from or HAZOP and FMEA analyses allow us to confidently present a safe design for the solvent recovery. Not only is our process efficient, it also generates a large savings value.

Our process generates a 144% rate of return on a total investment of $2.52 million with an annual after tax cash flow of approximately $3.7 million. Sensitivity analysis on the rate of return determined that our process will remain profitable as long as the pure component prices remain above $1 per kilogram. If further adjustments were to be made to our design, we would recommend integration of the column one feed into our heat exchanger network.

Thank you for the opportunity to work on this design project, feel free to contact us with any question or concerns you may have.

# Appendix A: Stream Tables

*i. Table A-1 – Stream Table Part 1*

| | ACN-PROD | BOT-1 | BOT-1H | BOT-1P | BOT-2 | CW-C2 | CW-C4 | CW-H2 |
|---|---|---|---|---|---|---|---|---|
| **From** | | P-1 | 2-Sep | E-4B | FLASH-1 | E2-A | E4 | |
| **To** | E1 | 1-Sep | E-4B | P-1 | 2-Sep | | | E2-A |
| **Substream: MIXED** | | | | | | | | |
| **Mass Flow kg/hr** | | | | | | | | |
| **ACN** | 157.9412 | 0.2587969 | 0.2587969 | 0.2587969 | 1.62E-11 | 0 | | |
| **TOLUENE** | 0.1883581 | 97.32374 | 97.32374 | 97.32374 | 0.744797 | 0 | | |
| **P-XYLENE** | 0.0704428 | 99.92956 | 99.92956 | 99.92956 | 99.91296 | 0 | 0 | 0 |
| **WATER** | 0 | 0 | 0 | 0 | 0 | 940.7379 | 0 | 0 |
| **MEK** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **SILOXANE** | 3.22E-22 | 15.70086 | 15.70086 | 15.70086 | 19.75072 | 0 | 42.05953 | 940.7379 |
| **Mass Frac** | | | | | | | 0 | 0 |
| **ACN** | 0.9983641 | 1.21E-03 | 1.21E-03 | 1.21E-03 | 1.34E-13 | 0 | 0 | 0 |
| **TOLUENE** | 1.19E-03 | 0.4564626 | 0.4564626 | 0.4564626 | 6.19E-03 | 0 | | |
| **P-XYLENE** | 4.45E-04 | 0.4686843 | 0.4686843 | 0.4686843 | 0.829784 | 0 | 0 | 0 |
| **WATER** | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 |
| **MEK** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **SILOXANE** | 2.03E-24 | 0.0736393 | 0.0736393 | 0.0736393 | 0.164031 | 0 | 1 | 1 |
| **Total Flow kg/hr** | 158.2 | 213.213 | 213.213 | 213.213 | 120.4085 | 940.7379 | 0 | 0 |
| **Vapor Frac** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Liquid Frac** | 1 | 1 | 1 | 1 | 1 | 1 | 42.05953 | 940.7379 |
| **Solid Frac** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Temperature C** | 5 | 53.87832 | 63.90875 | 53.90486 | 138.2141 | 35 | 1 | 1 |
| **Pressure bar** | 1 | 0.1 | 1 | 1 | 1 | 1 | 0 | 0 |
| **Enthalpy Btu/lb** | 311.0895 | -53.86925 | -45.97711 | -53.81416 | -112.976 | -6802.71 | 35 | 45.00039 |

*ii. Table A-2 – Stream Table Part 2*

| | CW-H4 | DIST-1 | DIST-1P | DIST-2 | FEED-1 | FEED-2A | FEED2A-C | FEED2A-H | WASTE-H3 |
|---|---|---|---|---|---|---|---|---|---|
| **From** | | PUMP2 | E1 | E3-A | 1-Sep | 2-Sep | E3-A | E4-A | E4 |
| **To** | E4 | 1-Sep | PUMP2 | 2-Sep | | E4-A | | E3-A | E-4B |
| **Substream: MIXED** | | | | | | | | | |
| **Mass Flow kg/hr** | | | | | | | | | |
| **ACN** | | | | | | | | | |
| **TOLUENE** | | | | | | | | | |
| **P-XYLENE** | 0 | 157.9412 | 157.9412 | 0.261136 | 158.2 | 0 | 0 | 0 | 7.77E-13 |
| **WATER** | 0 | 0.188358 | 0.188358 | 362.5272 | 96.9 | 265.95 | 265.95 | 265.95 | 0.132707 |
| **MEK** | 0 | 0.070443 | 0.070443 | 0.0117 | 0 | 0 | 0 | 0 | 29.53713 |
| **SILOXANE** | 42.05953 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Mass Frac** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **ACN** | 0 | 3.22E-22 | 3.22E-22 | 2.29E-06 | 4.9 | 4.05 | 4.05 | 4.05 | 8.949852 |
| **TOLUENE** | | | | | | | | | |
| **P-XYLENE** | 0 | 0.998364 | 0.998364 | 7.20E-04 | 0.608462 | 0 | 0 | 0 | 2.01E-14 |
| **WATER** | 0 | 1.19E-03 | 1.19E-03 | 0.999248 | 0.372692 | 0.985 | 0.985 | 0.985 | 3.44E-03 |
| **MEK** | 0 | 4.45E-04 | 4.45E-04 | 3.22E-05 | 0 | 0 | 0 | 0 | 0.764821 |
| **SILOXANE** | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Total Flow kg/hr** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Vapor Frac** | 0 | 2.03E-24 | 2.03E-24 | 6.31E-09 | 0.018846 | 0.015 | 0.015 | 0.015 | 0.231743 |
| **Liquid Frac** | 42.05953 | 158.2 | 158.2 | 362.8 | 260 | 270 | 270 | 270 | 38.61969 |
| **Solid Frac** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Temperature C** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| **Pressure bar** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Enthalpy Btu/lb** | 44.99976 | 21.39113 | 21.54418 | 109.8909 | 20 | 100 | 20 | 97.96897 | 70.64693 |
| **Entropy Btu/lb-R** | 1 | 0.1 | 1 | 1 | 1 | 1 | 1 | 1 | 0.955735 |
| **Average MW** | -6784.8 | 325.2858 | 325.4519 | 125.445 | 207.1597 | 104.378 | 41.38287 | 102.6347 | -214.947 |

*iii. Table A-3 – Stream Table Part 3*

| | H-WASTE1 | H-WASTE2 | H-WASTE4 | MAKEUP | MEK-IN1 | MEK-IN2 | MEK-IN4 | MEK-OUT1 | XYL-RCY |
|---|---|---|---|---|---|---|---|---|---|
| **From** | E4-A | E-4B | E4-D | Mixer | E1 | E2-B | E4-D | | 1-Sep |
| **To** | FLASH-1 | E4-A | E4 | | | | | E1 | MIX-RCYC |
| **Substream: MIXED** | | | | | | | | | |
| **Mass Flow kg/hr** | | | | | | | | | |
| **ACN** | | | | | | | | | |
| **TOLUENE** | | | | | | | | | |
| **P-XYLENE** | 7.77E-13 | 7.77E-13 | 7.77E-13 | 0 | 0 | 0 | 0 | 0 | 1.54E-11 |
| **WATER** | 0.132707 | 0.132707 | 0.132707 | 0 | 0 | 0 | 0 | 0 | 0.61209 |
| **MEK** | 29.53713 | 29.53713 | 29.53713 | 29.62417 | 0 | 0 | 0 | 0 | 100 |
| **SILOXANE** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Mass Frac** | 0 | 0 | 0 | 0 | 280 | 330 | 1689.806 | 280 | 0 |
| **ACN** | 8.949852 | 8.949852 | 8.949852 | 0 | 0 | 0 | 0 | 0 | 10.80086 |
| **TOLUENE** | | | | | | | | | |
| **P-XYLENE** | 2.01E-14 | 2.01E-14 | 2.01E-14 | 0 | 0 | 0 | 0 | 0 | 1.38E-13 |
| **WATER** | 3.44E-03 | 3.44E-03 | 3.44E-03 | 0 | 0 | 0 | 0 | 0 | 5.49E-03 |
| **MEK** | 0.764821 | 0.764821 | 0.764821 | 1 | 0 | 0 | 0 | 0 | 0.897562 |
| **SILOXANE** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Total Flow kg/hr** | 0 | 0 | 0 | 0 | 1 | 1 | 1 | 1 | 0 |
| **Vapor Frac** | 0.231743 | 0.231743 | 0.231743 | 0 | 0 | 0 | 0 | 0 | 0.096944 |
| **Liquid Frac** | 38.61969 | 38.61969 | 38.61969 | 29.62417 | 280 | 330 | 1689.806 | 280 | 111.413 |
| **Solid Frac** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Temperature C** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| **Pressure bar** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Enthalpy Btu/lb** | 137 | 123.0842 | 45 | 20 | -29 | -29 | -29 | -19.2409 | 25.11668 |
| **Entropy Btu/lb-R** | 0.955735 | 0.955735 | 0.955735 | 1 | 1 | 1 | 1 | 1 | 1 |
| **Average MW** | -159.492 | -171.68 | -234.447 | -102.209 | -1677.49 | -1677.49 | -1677.49 | -1669.38 | -160.735 |

*iv. Table A-4 – Stream Table Part 4*

| | MEK-OUT2 | MEK-OUT3 | MEK-OUT4 | RECYC-1 | RECYC-2 | RECYC-3 | TOL-HOT | TOL-PROD |
|---|---|---|---|---|---|---|---|---|
| **From** | | | E3-B | E2-A | E2-B | Mixer | E3-B | |
| **To** | E2-B | E3-B | E4-D | FLASH-1 | E2-A | E2-B | E3-A | E3-B |
| **Substream: MIXED** | | | | | | | | |
| **Mass Flow kg/hr** | | | | | | | | |
| **ACN** | | | | | | | | |
| **TOLUENE** | | | | | | | | |
| **P-XYLENE** | 0 | 0 | 0 | 1.54E-11 | 1.54E-11 | 1.54E-11 | 0.26113 | 0.26113 |
| **WATER** | 0 | 0 | 0 | 0.61209 | 0.61209 | 0.61209 | 362.527 | 362.527 |
| **MEK** | 0 | 0 | 0 | 70.37583 | 70.37583 | 70.37583 | 0.0117 | 0.0117 |
| **SILOXANE** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Mass Frac** | 330 | 1689.806 | 1689.806 | 0 | 0 | 0 | 0 | 0 |
| **ACN** | 0 | 0 | 0 | 10.80086 | 10.80086 | 10.80086 | 2.29E-06 | 2.29E-06 |
| **TOLUENE** | | | | | | | | |
| **P-XYLENE** | 0 | 0 | 0 | 1.88E-13 | 1.88E-13 | 1.88E-13 | 7.20E-04 | 7.20E-04 |
| **WATER** | 0 | 0 | 0 | 7.48E-03 | 7.48E-03 | 7.48E-03 | 0.999248 | 0.999248 |
| **MEK** | 0 | 0 | 0 | 0.860458 | 0.860458 | 0.860458 | 3.22E-05 | 3.22E-05 |
| **SILOXANE** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Total Flow kg/hr** | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 0 |
| **Vapor Frac** | 0 | 0 | 0 | 0.132058 | 0.132058 | 0.132058 | 6.31E-09 | 6.31E-09 |
| **Liquid Frac** | 330 | 1689.806 | 1689.806 | 81.78879 | 81.78879 | 81.78879 | 362.8 | 362.8 |
| **Solid Frac** | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |
| **Temperature C** | 1 | 1 | 1 | 0 | 1 | 1 | 1 | 1 |
| **Pressure bar** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Enthalpy Btu/lb** | -25.0352 | -18.993 | -28.6394 | 137 | 45 | 27 | 55 | 4 |
| **Entropy Btu/lb-R** | 1 | 1 | 1 | 0.955735 | 0.955735 | 0.955735 | 1 | 1 |
| **Average MW** | -1674.21 | -1669.17 | -1677.19 | 37.27103 | -168.686 | -181.933 | 79.86073 | 42.48466 |

<u>Appendix B: Main Process Flowsheet</u>

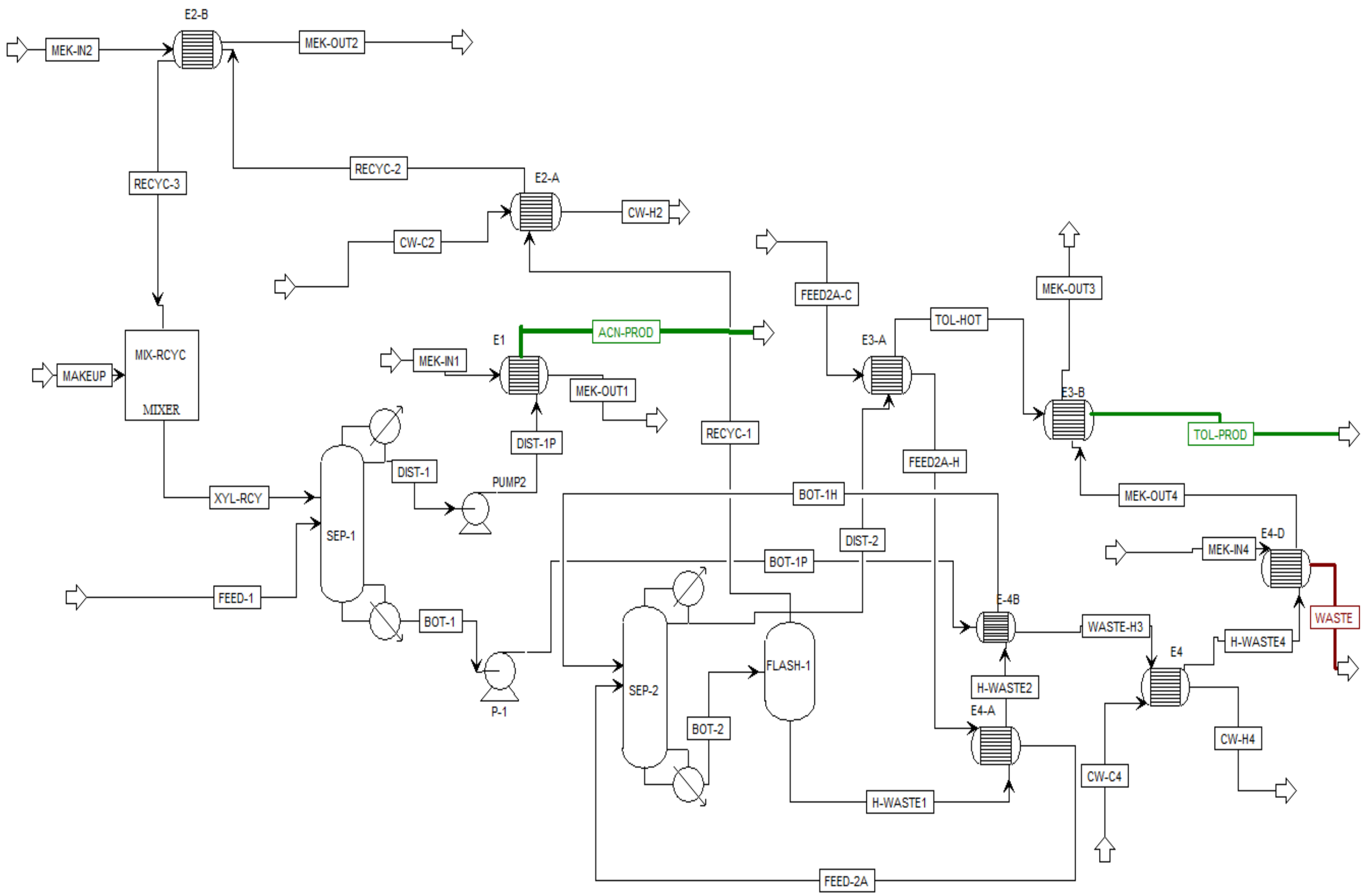


Figure B-1: Main process flow sheet as generated by ASPEN Plus V8.8

Appendix C: Equipment Summary

*I. Distillation Column Summary*

Table C-1: RADFRAC Column Design Summary

| RADFRAC Specifications | | | | |
|---|---|---|---|---|
| **Specifications** | Acetonitrile Tower | | Toluene Tower | |
| **Bot. Temperature [°C]** | 52.88 | | 137.8 | |
| **Top Temperature [°C]** | 21.30 | | 109.9 | |
| **Pressure [bar]** | 0.10 | | 1 | |
| **Diameter [m]** | 0.77 | | 0.617 | |
| **Height [m]** | 2.39 | | 4.56 | |
| **Pack Height [m]** | 1.84 | | 4.37 | |
| **# of Trays** | 23 | | 21 | |
| **# Stages** | | 23 | 23 | |
| **Feed-1** | 22 | | Feed A | 8 |
| **Feed-2** | XYLRCY | 8 | Bot-1 | 15 |
| **Orientation** | Vertical | | Vertical | |
| **Structured Packing Type** | CY by Sulzer | | 700Y FlexiPac | |
| **HETP [m]** | 0.08 | | 0.191 | |
| **Material** | STANDARD | | STANDARD | |
| **Total Cost [$]** | $66,467 | | $99,357 | |
| **Distillate Stream Compositions** | **Species** | **wt. Frac** | **Species** | **wt. Frac** |
| | ACN | 0.99836 | ACN | 0.00072 |
| | TOLUENE | 0.00119 | TOLUENE | 0.99925 |
| | P-XYLENE | 0.00045 | P-XYLENE | 0.00003 |
| | SILOXANE | ---trace--- | SILOXANE | ---trace-- |
| **Bottoms Stream Compositions** | **Species** | **wt. Frac** | **Species** | **wt. Frac** |
| | ACN | | ACN | ---trace-- |
| | TOLUENE | 0.00121 | TOLUENE | 0.00619 |
| | P-XYLENE | 0.45646 | P-XYLENE | 0.82978 |
| | SILOXANE | 0.07364 | SILOXANE | 0.16403 |

*II. Reflux Drum Summary*

Table C-2: Reflux Drums

| Reflux Drum Sizing | | |
|---|---|---|
| Specification | Drum 1 | Drum 2 |
| Diameter [m] | 0.320 | 0.486 |
| Length[m] | 0.959 | 1.459 |
| Volume [m^3] | 0.2408 | 0.557 |
| Flow Rate [l/min] | 3.34 | 7.73 |
| Holding Time [min] | 8 | 8 |
| Reflux Ratio | 3.5 | 3.5 |
| Liquid Space [%] | 50 | 50 |
| **Cost [$]** | $4,251.00 | $6,992.00 |
| **Material** | Carbon Steel | Carbon Steel |

*III. Pump Summary*

Table C-3: Pumps

| **Pump Operation and Cost** | | | |
|---|---|---|---|
| **Specification** | **Pump 1** | **Pump 2** | **Vacuum** |
| **Type** | Rotary | Rotary | Liquid Ring |
| **Power [kW]** | 0.008 | 0.005 | 20.4 |
| **Flowrate [l/min]** | 0.257 | 0.2004 | 0.306 |
| **Differential Head [m]** | 11.10 | 11.64 | ----------- |
| **Pressure in [bar]** | 0.10 | 0.1 | 1.00 |
| **Pressure out [bar]** | 1.00 | 1.00 | 0.10 |
| **Cost [$]** | $8,880 | $8,880 | $33,883 |
| **Material** | Carbon Steel | Carbon Steel | Stainless Steel |

## IV. Flash Drum Summary

Table C-4: Flash Drum Specifications

| Drum Separator Summary | | |
|---|---|---|
| **Specifications** | **Flash Drum** | |
| **Temperature [°C]** | 138.00 | |
| **Pressure [bar]** | 1.00 | |
| **Diameter [m]** | 0.15 | |
| **Height[m]** | 0.48 | |
| **Volume [m^3]** | 0.01 | |
| **Heat Duty [kW]** | 7.77 | |
| **Type** | Vertical | |
| **Material** | 316SS | |
| **Cost** | $14,581 | |
| | **Component** | **Wt. Fraction** |
| **Vapor Stream Compositions** | Acetonitrile | -trace- |
| | Toluene | 0.007 |
| | p-Xylene | 0.861 |
| | Water | 0 |
| | Siloxane | 0.131 |
| **Liquid Stream Compositions** | Acetonitrile | -trace- |
| | Toluene | 0.003 |
| | p-Xylene | 0.765 |
| | Water | 0 |
| | Siloxane | 0.245 |

## V. Storage Vessels

Table C-5: Storage Tank Sizing

| Storage Vessel Sizing | | | | | |
|---|---|---|---|---|---|
| **Storage Vessel** | **Volume [m$^3$]** | **Pressure [bar]** | **Material** | **Type** | **Cost** |
| **Acetonitrile Tank** | 18.80 | 1.0 | 316SS | Cone Roof | $13,880 |
| **Toluene Tank** | 39.36 | 1.0 | 316SS | Cone Roof | $19,630 |
| **Feed B+C Tank** | 29.42 | 1.0 | 316SS | Cone Roof | $17,090 |
| **Feed A Tank** | 32.80 | 1.0 | 316SS | Cone Roof | $18,000 |

| | | | | | |
|---|---|---|---|---|---|
| **Waste Tank** | 4.44 | 1.0 | 316SS | Cone Roof | $7,456 |
| **P-Xylene** | 3.28 | 1.0 | 316SS | Cone Roof | $6,623 |
| **Spill Containment** | 59.04 | 1.0 | 316SS | Cone Roof | $23,972 |

*VI. Heat Exchanger Summary Part 1: E1 - E3,B*

Table C-6: Summary of the first 5 heat exchangers in our process

| Heat Exchanger Summary | | | | | |
|---|---|---|---|---|---|
| **Block ID** | E1 | E2-A | E2-B | E3-A | E3-B |
| **Specification** | | | | | |
| **Heat duty [kW]** | 1.459 | 10.88 | 0.7 | 10.684 | 8.76 |
| **Actual exchanger area [sqm]** | 0.046 | 0.207 | 0.013 | 0.575 | 0.204 |
| **Minimum temperature approach [°C]** | 10.0 | 10.0 | 10.0 | 10.0 | 10.0 |
| **Type** | S&T | S&T | S&T | S&T | S&T |
| **Flow Pattern** | C-C | C-C | C-C | C-C | C-C |
| **Hot Stream ID** | ACN | XYL-RCY | XYL-RCY | TOL | TOL |
| **Cooling Stream** | MEK | CW | MEK | FEED-2A | MEK |
| **Inlet hot stream temperature [°C]** | 21.54 | 137.00 | 45.00 | 109.22 | 55.00 |
| **Inlet hot stream pressure [bar]** | 1.00 | 0.96 | 0.96 | 1.00 | 1.00 |
| **Outlet hot stream temperature [°C]** | 5.00 | 45.00 | 27.00 | 55.00 | 4.00 |
| **Outlet hot stream pressure [bar]** | 1.00 | 0.96 | 0.96 | 1.00 | 1.00 |
| **Inlet cold stream temperature [°C]** | -29.00 | 35.00 | -29.00 | 20.00 | -28.64 |
| **Inlet cold stream pressure [bar]** | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| **Outlet cold stream temperature [°C]** | -19.25 | 45.00 | -25.04 | 97.06 | -18.99 |
| **Outlet cold stream pressure [bar]** | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| **Cost** | $10,793 | $10,793 | $10,793 | $10,793 | $10,793 |

*VII: Heat Exchanger Summary: E4,A-D*

Table C-7: Summary of the final 4 heat exchangers

| *Heat Exchanger Summary* | | | | |
|---|---|---|---|---|
| ***Block ID*** | *E4-A* | *E4-B* | *E4-C* | *E4-D* |
| ***Specification*** | | | | |
| ***Heat duty [kW]*** | *.4857* | *.304* | *8.76* | *.3251* |
| ***Actual exchanger area [sqm]*** | *0.029* | *0.019* | *0.049* | *0.006* |
| ***Minimum temperature approach [°C]*** | *10.0* | *10.0* | *10.0* | *10.0* |
| ***Type*** | S&T | S&T | S&T | S&T |

| | | | | |
|---|---|---|---|---|
| ***Flow Pattern*** | C-C | C-C | C-C | C-C |
| ***Hot Stream ID*** | *WASTE* | *WASTE* | *WASTE* | *WASTE* |
| ***Cooling Stream*** | *FEED-2A* | *BOT-1* | *CW* | *MEK* |
| ***Inlet hot stream temperature [°C]*** | *63.18* | *137.00* | *116.76* | *45.00* |
| ***Inlet hot stream pressure [bar]*** | *0.96* | *0.96* | *0.96* | *0.96* |
| ***Outlet hot stream temperature [°C]*** | *45.00* | *116.76* | *63.18* | *27.00* |
| ***Outlet hot stream pressure [bar]*** | *0.96* | *0.96* | *0.96* | *0.96* |
| ***Inlet cold stream temperature [°C]*** | *35.00* | *97.06* | *52.91* | *-29.00* |
| ***Inlet cold stream pressure [bar]*** | *1.00* | *1.00* | *1.00* | *1.00* |
| ***Outlet cold stream temperature [°C]*** | *45.00* | *100.00* | *62.91* | *-28.64* |
| ***Outlet cold stream pressure [bar]*** | *1.00* | *1.00* | *1.00* | *1.00* |
| ***Cost*** | *$10,790* | *$10,790* | *$10,790* | *$10,790* |

*VIII: Mixer Summary*

Table C-8: Mixer Sizing

| Mixer 1 | | | |
|---|---|---|---|
| **Specification** | Unstirred, Motionless Mixer | | |
| **Hold Time [min]** | 5 | | |
| **Volume [m3]** | 0.0142 | | |
| **Diameter [m]** | 0.0399 | | |
| | Makeup In | Recycle In | Recycle Out |
| **Pressure [bar]** | 1 | 0.98 | 1 |
| **Temperature [°C]** | 20 | 27 | 25.11 |
| **Mass Flow [kg/hr]** | 29.6 | 81.75 | 111.4 |
| **Cost [$]** | $1,785.00 | | |
| **Material** | Carbon Steel | | |

*IX: Condenser and Reboiler Summary*

Table C-9: Condenser and Reboilers

| Condenser and Reboiler Summary |
|---|

| Specifications | R1 | | R2 | | C1 | | C2 | |
|---|---|---|---|---|---|---|---|---|
| Area [$m^2$] | 3.8891 | | 5.323 | | 4.16 | | 2.79 | |
| Duty [kW] | 185.05 | | 169.8 | | -160.2 | | -165 | |
| Type | kettle | | kettle | | kettle | | kettle | |
| | SEP-1 Bottoms | Low Pressure Steam | SEP-2 Bottoms | High Pressure Steam | SEP-1 Distillate | MEK | SEP-2 Distillate | Cooling Water |
| Pressure in [bar] | 0.10 | 1.72 | 1.00 | 10.33 | 0.10 | 1.00 | 1.00 | 1.00 |
| Pressure out [bar]] | 0.10 | 1.72 | 1.00 | 10.33 | 0.10 | 1.00 | 1.00 | 100 |
| Temperature in [°C] | 56 | 115.6 | 137.7 | 181.4 | 21.4 | -29 | 109.81 | 35 |
| Temperature Out [°C] | 51.6952 | 115.56 | 137.9 | 172.4 | 21.39 | 11.34 | 102 | 99.65 |
| Vapor Fraction In | 0 | 1 | 0 | 1 | 1 | 0 | 1 | 0 |
| Vapor Fraction Out | 0.774 | 1 | 0.783 | 1 | 0 | 0 | 0 | 0.074 |
| Flow rate [kg/hr] | 2160.5 | 1000 | 2339 | 13500 | 711.9 | 71 90 | 1632.6 | 14350 |

*X: Summary of Delivered Equipment Costs*

Table C-10: Equipment Cost Summary

| Delivered Equipment Costs | | | | | |
|---|---|---|---|---|---|
| | **Base Cost** | **Material Factor** | **Pressure Factor** | **Delivery Fee** | **True Cost** |
| Mixer | $1,732 | 1.0 | 1.0 | $173 | $1,905 |
| ACN Tower | $8,886 | 4.0 | 1.7 | $6,042 | $66,467 |
| TOL Tower | $13,283 | 4.0 | 1.7 | $9,032 | $99,357 |
| Reb -1 | $10,793 | 1.0 | 1.0 | $1,079 | $11,872 |
| Cond - 1 | $4,658 | 1.0 | 1.0 | $466 | $5,124 |
| Reb - 2 | $10,793 | 1.0 | 1.0 | $1,079 | $11,872 |
| Cond -2 | $5,551 | 1.0 | 1.0 | $555 | $6,106 |
| Pump 1 | $2,222 | 1.4 | 1.0 | $311 | $3,422 |
| Pump 2 | $2,222 | 1.0 | 1.0 | $222 | $2,444 |
| Vacuum Pump | $16,212 | 1.9 | 1.0 | $3,080 | $33,883 |
| Reflux Drum 1 | $3,581 | 1.0 | 1.0 | $358 | $3,939 |
| Reflux Drum 2 | $4,971 | 1.0 | 1.0 | $497 | $5,468 |
| Flash Drum | $14,581 | 1.0 | 1.0 | $1,458 | $16,039 |
| Heat Exchangers | $97,137 | 1.0 | 1.0 | $9,714 | $106,851 |
| Acetonitrile Tank | $13,880 | 1.0 | 1.0 | $1,388 | $15,268 |
| Toluene Tank | $19,631 | 1.0 | 1.0 | $1,963 | $21,594 |
| Feed B+C Tank | $17,093 | 1.0 | 1.0 | $1,709 | $18,802 |
| Feed A Tank | $17,999 | 1.0 | 1.0 | $1,800 | $19,799 |
| Waste Tank | $7,456 | 1.0 | 1.0 | $746 | $8,202 |
| P-Xylene | $6,623 | 1.0 | 1.0 | $662 | $7,285 |
| Spill Containment | $23,972 | 1.0 | 1.0 | $2,397 | $26,369 |
| Backup Pump 1 | $2,222 | 1.4 | 1.0 | $311 | $3,422 |
| Backup Pump 2 | $2,222 | 1.0 | 1.0 | $222 | $2,444 |
| Bkp Vc Pump | $16,212 | 1.9 | 1.0 | $3,080 | $33,883 |
| | | | | **Total Cost** | **$531,819** |

*Delivery Costs assumed to be ~10% of base cost

Appendix D: FMEA Summary

*i. FMEA Definitions*

*The subsequent pages outline the results of our Failure Mode and Effects Analysis. The tables below define the rank ordered severity, occurrence, and detection parameters.*

| **SEVERITY** | | |
|---|---|---|
| **Rank** | **Effect rate** | **Criteria** |
| **10** | Hazardous- without warning | Very high severity ranking when a potential failure mode affects personal safety, safe item operation and/or involves non-compliance with government regulation without warning |
| **9** | Hazardous- with warning | Very high severity ranking when a potential failure mode affects safe item operation and/or involves non-compliance with government regulation with warning |
| **8** | Very High | Item inoperable, with loss of primary function. |
| **7** | High | Item operable, but at reduced level of performance. Customer dissatisfied. |
| **6** | Moderate | Item operable, but Comfort/ Convenience item(s) inoperable. Customer experiences discomfort. |
| **5** | Low | Item operable, but Comfort/ convenience item(s) operable at reduced level of performance. Customer experiences some dissatisfaction. |
| **4** | Very low | Fit & finish/Squeak & Rattle item does not conform. Defect noticed by average customers. |
| **3** | Minor | Fit & finish/Squeak & Rattle item does not conform. Defect noticed by most customers. |
| **2** | Very minor | Fit & finish/Squeak & Rattle item does not conform. Defect noticed by discriminating customers. |
| **1** | None | No effect. |

| **OCCURRENCE** |
|---|

| Rank | CPK | Failure Rate | Criteria |
|---|---|---|---|
| **10** | ≤ 0.33 | < 1 in 2 | **Very High:** |
| **9** | ≥ 0.33 | 1 in 3 | Failure almost inevitable |
| **8** | ≥ 0.51 | 1 in 8 | **High:** |
| **7** | ≥ 0.67 | 1 in 20 | Repeated failures |
| **6** | ≥ 0.83 | 1 in 80 | **Moderate:** |
| **5** | ≥ 1.00 | 1 in 400 | Occasional failures |
| **4** | ≥ 1.17 | 1 in 2000 | |
| **3** | ≥ 1.33 | 1 in 15 000 | **Low:** |
| **2** | ≥ 1.50 | 1 in 150 000 | Relatively few failures |
| **1** | ≥ 1.67 | ≤ 1 in 1 500 000 | **Remote:** Failure is unlikely |

| DETECTION | | |
|---|---|---|
| **Rank** | **Detection rate** | **Criteria** |
| 10 | Absolute uncertainty | Design Control will not and/or cannot detect a potential cause/ mechanism and subsequent failure mode; or there is no Design Control. |
| 9 | Very remote | Very Remote chance the Design Control will detect a potential cause/mechanism and subsequent failure mode. |
| 8 | Remote | Remote chance the Design Control will detect a potential cause/ mechanism and subsequent failure mode. |
| 7 | Very low | Very Low chance the Design Control will detect a potential cause/ mechanism and subsequent failure mode. |
| 6 | Low | Low chance the Design Control will detect a potential cause/mechanism and subsequent failure mode. |
| 5 | Moderate | Moderate chance the Design Control will detect a potential cause/mechanism and subsequent failure mode. |
| 4 | Moderately high | Moderately High chance the Design Control will detect a potential cause/mechanism and subsequent failure mode. |
| 3 | High | High chance the Design Control will detect a potential cause/mechanism and subsequent failure mode. |
| 2 | Very high | Very High chance the Design Control will detect a potential cause/mechanism and subsequent failure mode. |
| 1 | Almost certain | Design Controls will almost certainly detect a potential cause/mechanism and subsequent failure mode. |

*ii. FMEA Tables*

Table D.1: FMEA of RADFRAC Column and Pump

| **Subsystem No.** | **FUNCTION** | **POTENTIAL FAILURE MODE** | **POTENTIAL CAUSES** | **POTENTIAL EFFECTS** | **DETECTION METHOD** | **SEV** | **OCC** | **DET** | **RPN** | **Recommended Action(s)** | **Responsibility Completion date** | **SEV** | **OCC** | **DET** | **RPN** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| RADFrac Column | **Separator** | Stage Drying up | Too much heat/Low liquid flow rate | Separation will be off specification. Most material in distillate | bottoms flow rate sensor and feed flow rate sensor | 8 | 1 | 1 | 8 | | | | | | 0 |
| | | Foaming | Vapor Flow rate to large | Hinder vapor flow rate, and will possibly lead to flooding | Distillate flow rate sensor and feed flow rate sensor | 5 | 2 | 1 | 10 | | | | | | 0 |
| | | Stage Flooding | Too little heat/Low vapor Flow rate | Separation is off specification. Most material in bottoms | Distillate flow rate sensor and feed flow rate sensor | 8 | 1 | 1 | 8 | | | | | | 0 |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pump | **Vacuum** | Jam closed | Solid particulate blocking pump | No flow/reduced flow out of pump. Incorrect operating pressure | Flow rate sensor at pump exit to detect decrease in flow rate | 10 | 1 | 1 | 10 | | | | | | 0 |
| | **Compressor** | Motor Fails while running | Mechanical malfunction | Separation is off specification, and production will be stopped | Flow rate sensor at pump exit | 8 | 7.5 | 1 | 60 | | | | | | 0 |
| | | Electrical contacts fail to start | Equipment Malfunction | Separation is off specification | Flow rate sensor at pump exit | 8 | 2 | 1 | 16 | | | | | | 0 |

Table D.2: FMEA of Flash Drum, Shell and Tube Heat Exchanger, and Piping

| Subsystem No. | FUNCTION | POTENTIAL FAILURE MODE | POTENTIAL CAUSES | POTENTIAL EFFECTS | DETECTION METHOD | SEV | OCC | DET | RPN | Recommended Action(s) | Responsibility Completion date | SEV | OCC | DET | RPN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Flash Drum | Single stage separation | Flooding | Inlet temperature too low/pressure to high, or flow rate is too large | Reverse Flow | flow rate sensor on inlet stream | 8 | 1 | 1 | 8 | | | | | | 0 |
| | | drying up | Inlet Temperature too high/pressure too low, or flow rate is too low | No liquid flow. Which would result in incorrect recycle concentrations | flow rate sensor on liquid exit stream | 8 | 1 | 1 | 8 | | | | | | 0 |
| Shell and Tube Heat Exchanger | Cooling | Outlet temperature too high | incorrect flow rates/fouling | Material may be above flash point | Temperature sensor on hot stream exit | 10 | 1 | 1 | 10 | yearly maintenance to reduce risk of fouling | | | | | 0 |
| | | Tube failure | Leak/Rupture | Contamination of streams | Temperature sensors on inlet | 8 | 8 | 3 | 192 | flow sensor on inlet and exit stream | | 8 | 8 | 1 | 64 |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | **and exit streams** | | | | | | | | | | |
| **Piping** | **Piping Joint** | **leak** | **wear and tear** | **possible health effects and the small possibility that a material will be released from a stream with low pressure and high temperature that will be well above the flash point and i** | **Operator awareness** | **10** | **1** | **6** | **60** | | | | | | |

Table D.3: FMEA for Mixer, Processing and Intermediate Units, Operator, and Control System/Process Automation

| Subsystem No. | FUNCTION | POTENTIAL FAILURE MODE | POTENTIAL CAUSES | POTENTIAL EFFECTS | DETECTION METHOD | SEV | OCC | DET | RPN | Recommended Action(s) | Responsibility Completion date | SEV | OCC | DET | RPN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Mixer** | **Containment** | **Overflow** | **Inlet flow rate too large, or exit flow rate is too low** | **could lead to spills, and potential health effects to anyone in proximity with the mixer** | **Liquid level sensor** | **9** | **1** | **1** | **9** | **Include a spill/overflow tank with a fail open switch** | | | | | **0** |
| **Processing and Intermediate Units** | **Power** | **Power failure for more than 20 minutes** | **Blackout, Electrical issues, etc** | **Plant inoperable** | **Operator awareness** | **8** | **10** | **1** | **80** | | | | | | **0** |
| **Operator** | **Unit Operation and Maintenance** | **Procedural Violation** | **Human error** | **Serious injury** | **Operator awareness** | **10** | **1** | **1** | **10** | | | | | | **0** |
| **Control System and Process Automation** | **Thermocouple** | **Equipment malfunction** | **wear and tear** | **Incorrect input into controll loop, which could result in the** | **automated comparison with thermocouples downstream and comparis** | **10** | **8** | **2** | **160** | **include thermocouples inside vessels that are hazardous as well** | | **8** | **6** | **2** | **96** |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | **system being off specific ation** | **on to literature values** | | | | | **at at the inlet/exit** | | | | | |
| | **Generic Control Loop** | **Compu ter error** | **Power surge** | **System off spec possibl e safety hazards** | **Thermoc ouples at points of potential hazards** | **10** | **6** | **1** | **60** | | | | | | **0** |

Table D.4: FMEA for Control Systems and Process Automation Continued

| Subsystem No. | FUNCTION | POTENTIAL FAILURE MODE | POTENTIAL CAUSES | POTENTIAL EFFECTS | DETECTION METHOD | SEV | OCC | DET | RPN | Recommended Action(s) | Responsibility Completion date | SEV | OCC | DET | RPN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Control System and Process Automation | Differential Pressure Sensor | Malfunctioning part | wear and tear | Separation will be off specification | Check during startup. If no change in Pressure there's a problem | 8 | 10 | 1 | 80 | | | | | | 0 |
| | Differential Pressure Transducer (Level Sensor) | Malfunctioning. Incorrect level recorded | Blocked entrance/exit of sensor. Electrical issues. Incorrect connection etc.. | Overflow | Incrementally drain storage tanks to determine flow rate, pressure, then ultimately Height of fluid. Could be Automated | 4 | 10 | 2 | 80 | | | | | | 0 |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **Control Valve** | **fail open/close** | **Computer/ logic controller malfunction.** | **Separation off specification. Loss of material** | **Flow rate sensor at inlet and exit of valve to ensure the valve position corresponds to measured values** | **8** | **6** | **1** | **48** | | | | | | **0** |

Appendix E: HAZOP Summary

*i. Determination of risk hierarchy*

| **Qualitative Method** | **Risk Matrix Example** | | | | **Quantitative Method** |
|---|---|---|---|---|---|
| Frequency Categories | Death, Equipment or Facility Loss (Hazard Severity 1) | Severe Injury, Major Facility Damage (Hazard Severity 2) | Injury, Illness, Minor Equipment or Facility Damage (Hazard Severity 3) | Minor Injury or Minor Equipment Damage (Hazard Severity 4) | Probability of Incident per hour or per operation |
| A Frequent | Risk Level I | Risk Level I | Risk Level I | Risk Level III | Greater than 1E-3 /hr or /op |
| B Probable | Risk Level I | Risk Level I | Risk Level II | Risk Level III | Greater than 1E-4 or equal to 1E-3/hr or /op |
| C Occasional | Risk Level I | Risk Level II | Risk Level II | Risk Level IV | Greater than 1E-5 or equal to 1E-4 /hr or /op |
| D Remote | Risk Level II | Risk Level II | Risk Level IV | Risk Level IV | Greater than 1E-6 or equal to 1E-5 /hr or /op |
| E Improbable | Risk Level IV | Risk Level IV | Risk Level IV | Risk Level IV | Less than or equal to 1E-6 /hr or /op |

Figure E-1: Risk Matrix Used in HAZOP Analysis

Table E-1: Potential Hazards

| Potential Hazards, Consequences, and Prevention Techniques | | | |
|---|---|---|---|
| Potential Hazard | Consequence | Prevention Tactic | Action Taken |
| Components exposed to temperatures above flash temperature | Serious Injury or possibly death. Possible damage to surrounding equipment | Implement a Control loop equipped with thermocouples at cooler exits and at the entrances to the mixer and storage tanks. | Include an intrinsic fire alarm system. |
| Operator skin contact or inhalation of hazardous components | Health issues of worker and possible liability. | Minimize open containers, and conduct routine equipment checks for leaks, ruptures, etc. | Require personnel to wear light PPE inside the plant. Isolate the mixer and storage tanks to minimize contact, and post pertinent MSDS around equipment. |
| Low and high pressure steam | Can cause serious injury | Include caution signs and railing around equipment using steam. Practice good | Require PPE around plant |
| Operator in contact with MEK | Will cause injury if in contact with skin | In the design of the plant limit piping exposure of MEK | Include MSDS, caution signs, and conduct routine maintenance on pipes and storage containers that include MEK. |
| Toluene, ACN, and Xylene vapor release | All three components have environmental impacts and are volatile liquids at room temperature | Components are cooled to avoid flash. This also decreases volatility | Emphasis on daily safety checks, and in leak prevention specifically |

*ii. Key Tables*

| Name | Guide word | Parameter | Potential Hazard | Effect | Safeguard | Consequence | Frequency | Risk | Actions/Comments |
|---|---|---|---|---|---|---|---|---|---|
| Feed-1 | Low | Flow | No immediate hazard | Products off specification. Incorrect temperatures and pressures will result through the system due to Heat exchanger/pump sizing | Flow sensor at entrance to column | 3 | 1 | IV | Don’t need the flow sensor, however it will be useful for detecting if the feed is off specification |
| | High | Flow | none | Separation off specification. High distillate flow in first column. | Differential pressure sensor at entrance to column 1 with control valve | 3 | 1 | IV | |
| | No | Flow | none | No product being made | Differential pressure sensor at entrance to column 1 | 2 | 2 | IV | Not hazardous, but costly and will halt production for a variety of time, depending how automated the system is. |
| | Reverse | Flow | Could result in | Recycle process does not yield product, and can | Differential pressure sensor to | 3 | 1 | IV | Would imply a serious issue at the end of the siloxane |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | equipment failure. | disrupt the siloxane polymerization process | determine the direction of flow. | | | | polymerization process, or a buildup of pressure in the column over time. |
| | High | Temperature | none | larger column1 feed temperature | Thermocouple on feed | 1.5 | 2 | IV | One heat exchangers would not function properly |
| | Low | Temperature | none | Separation will be off specification | Thermocouple along the feed | 1 | 2 | IV | Thermocouple not required |
| | High | Pressure | none | Separation will be off specification | Pressure sensor in feed | 2 | 2 | IV | |
| | Low | Pressure | none | Better separation, Higher operating cost | Pressure sensor in feed | 2 | 1 | IV | |

| Name | Guide Word | Parameter | Potential Hazard | Effect | Safeguard | Consequence | Frequency | Risk | Actions/Comments |
|---|---|---|---|---|---|---|---|---|---|
| Distkkkkkkkkkkkkkkkkkkkkkkk-1 | Low | Flow | none | More cooling utility used than needed | Flow sensor at the exit of the reflux drum leading to the distillate | 1 | 2 | IV | |
| | High | Flow | Not directly in this section of the stream, | Residence time in the sequential heat | Flow sensor at exit of reflux drum to the distillate | 3 | 1 | IV | At higher flow rates the hot stream is not cooled below the flash point. |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | but does prove to be hazardous downstream | exchanger will be decreased. | | | | | |
| | No | Flow | None on this stream | No Acetonitrile product being made. Leaves the rest of the system in disarray | Flow rate sensor at the exit of the reflux drum to the distillate | 3 | 2 | III | Could indicate a malfunctioning reboiler which would result in only a liquid flow and no vapor flow to the condenser. |
| | Reverse | Flow | none | No Acetonitrile recovery. Possible damage to equipment | Differential pressure sensor to determine the direction of flow. | 3 | 1 | IV | Could be caused by a malfunctioning compressor |
| | Low | Pressure | If pressure is exceptionally low it is possible for the  to the ACN product | Lower capacity flow rate thus less heat transferred | Differential pressure sensor at the exit of the reflux drum leading to the distillate | 4 | 1 | III | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | leaving the exchanger to have lower flash point | | | | | | |
| | High | Pressure | none | Pressure exiting pump will be above 1 bar | Flow sensor at the exit of the reflux drum leading to the distillate | 1 | 2 | IV | |
| | Low | Temperatu re | none | More cooling utility will be used than needed. | Thermocou ple at the exit of the reflux drum leading to the distillate | 1 | 2 | IV | Not unsafe, but is operating less efficiently. |

| Name | Guide Word | Parameter | Potential Hazard | Effect | Safeguard | Consequence | Frequency | Risk | Actions/Comments |
|---|---|---|---|---|---|---|---|---|---|
| ACN PROD | High | Flow | Serious injury/death could result | Exit into container will be above flash point | Flow sensor and temperature sensor at the entrance and exit of the heat exchanger. Fail close valve will be needed. | 4 | 1 | III | Emphasize workplace safety precautions |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | Low | Flow | none | More utility will be used than needed | Flow sensor at inlet of heat exchanger | 2 | 1 | IV | |
| | No | Flow | none | No ACN is being produced | Flow sensor anywhere after the compressor pump. | 3 | 1 | IV | No revenue is made from the ACN product |
| | High | Temperature | Serious injury/death to any personnel. Possible damage to equipment and facility | ACN is above flash point | Use a control loop that utilizes a Thermocouple on the stream leaving the heat exchanger and a fail close valve before the exit | 4 | 1 | III | |
| | Low | Temperature | none | More cooling utility used than needed. | Thermocouple exiting the exchanger | 2 | 1 | IV | A lower temperature indicates less material used. This implies the bottoms of column 1 entering column 2 will have ACN that will make the toluene feed impure and non-profitable |
| | High | Pressure | Increased chance to | Indicates a block or valve | Include a pressure | 3 | 1 | IV | Schedule routine maintenance to |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | leak or rupture. Possible personnel contact to ACN | malfunction that is causing a pressure buildup. The pressure sensor earlier on in the stream could also be malfunctioning. | sensor after the heat exchanger, and implement a control loop to sound an alarm at different safety thresholds | | | | check for leaks and ruptures |
| | Low | Pressure | none | Malfunctioning compressor pump | Include pressure sensor as well as a flow meter before and after the compressor. Compare inlet and outlet values to determine pump power. | 1 | 2 | IV | |
| | | | | | | | | | |

| Name | Guide Word | Parameter | Potential Hazard | Effect | Safeguard | Consequence | Frequency | Risk | Actions/Comments |
|---|---|---|---|---|---|---|---|---|---|
| H-WASTE2 | High | Flow | none | Not enough cooling utility to meet required design specifications | Flow sensor before the entrance to the next heat exchanger | 4 | 2 | II | Could be a result of flash drum malfunction, or an issue earlier on in the process. Halt process if flow rate is too high |
| | No | Flow | None | Siloxane will appear in the recycle stream, and the entire process will no longer function up to specifications as well as damage to equipment. | Control loop equipped with two differential pressure transmitters. One will be place in the waste stream directly leaving the flash drum. The other will be in the H-WASTE2 stream. | 3 | 1 | IV | |
| | High | Temperature | none on this stream | Subsequent heat exchangers are not designed for this temperature which will result in higher temperatures further down the stream | Thermocouple and flow rate sensor | 4 | 1 | IV | If flow rate is within set tolerance it could indicate a malfunction in the previous heat exchanger. Or another error earlier in the process (Most |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | Likely condenser malfunction). |

| Name | Guide Word | Parameter | Potential Hazard | Effect | Safeguard | Consequence | Frequency | Risk | Actions/Comments |
|---|---|---|---|---|---|---|---|---|---|
| MEK-IN | Low | Flow | Some Hot streams that are above their flash points will be open to the atmosphere | Not enough Cooling utility. Halt process until flow rate is resolved. | Implement a Control loop that utilizes a fail open valve on MEK stream inlet to the heat exchanger, and a fail close valve on the hot stream inlet to exchanger. | 3 | 1 | IV | Ensure the safeguard is installed, else there will be an increase in risk and possible liabilities |
| | Reverse | Flow | Some Hot streams that are above their flash points will be open to the atmosphere | Will violate the countercurrent design of the heat exchanger and decrease the amount of cooling utility. | Implement a differential pressure transducer to determine the magnitude and direction of flow | 4 | 1 | III | Unlikely, but if it occurs. The system will require shutdown until safe operating conditions can be met again |
| | High | Flow | None | Using more cooling utility than needed | Flow sensor at inlet to exchanger | 1 | 2 | IV | |
| | High | Temperature | Some Hot streams that are above their flash points will be open to the atmosphere | Lowers the log mean temperature difference which will decrease heat transfer | Thermocouple before the inlet to the heat exchanger | 4 | 1 | | Not likely, but if the thermocouple read a value higher than the accepted value shutdown operation until safe operating conditions are met. |

| Name | Guide Word | Parameter | Potential Hazard | Effect | Safeguard | Consequence | Frequency | Risk | Actions/Comments |
|---|---|---|---|---|---|---|---|---|---|
| CW-IN | Low | Flow | Hot stream doesn't get cooled past the flash point. | Not enough cooling utility will be supplied resulting in a higher hot stream outlet temperature than desired | PID control loop connected to a differential pressure transducer and a control valve | 4 | 1 | III | Emphasize importance in daily safety checklist |
| | No | Flow | Will most certainly result in errors further in the system | No cooling utility. | PID control loop connected to a differential pressure transducer and a control valve | 4 | 2 | II | Failure most likely resulting from a malfunctioning valve, or more severely an issue with the house water system |
| | Reverse | Flow | Will result in hazardous situations further in the system | Cooling duty (if any) will be insufficient | PID control loop connected to a differential pressure transducer and a control valve | 4 | 1 | III | Could have resulted from years of siloxane particulate buildup |
| | High | Temperature | Will result in | Cooling duty will be will | Thermocouple, control | 4 | 1 | III | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | hazardous situations further in the system, but this stream is not directly hazardous | be insufficient | loop, and alarm | | | | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Name | **Guide Word** | **Parameter** | **Potential Hazard** | **Effect** | **Safeguard** | **Consequence** | **Frequency** | **Risk** | **Actions/Comments** |
| High P Steam | low | flow | No immediate hazard, but will result in off spec recycle and waste that will be above the flash point | Column 2 reboiler does not vaporize enough of the liquid to stay at set specification leading to flooding | Flow rate sensor in the inlet to the reboiler in column 2 | 4 | 1 | III | |
| | High | flow | Toluene product stream will be above its flash point | Most material will end in the distillate. Increasing the capacity flow of the toluene product stream thus the change in temperature is less than specified in the design. | Flow rate sensors on steam entering the reboiler in column 2 | 4 | 1 | IIII | |

| Name | Guide Word | Parameter | Potential Hazard | Effect | Safeguard | Consequence | Frequency | Risk | Actions/Comments |
|---|---|---|---|---|---|---|---|---|---|
| RADFRAC1 | High | Flow | none | Liquid level in column will rise gradually until the column ceases to work | High Flow alarm | 3 | 1 | IV | |
| | Low/zero | Flow | If flow rate is too small precipitation of siloxane may occur. | Temperature rise in column causing most components to go to the distillate | Flow sensors at both feeds | 3 | 1 | IV | If precipitation of siloxane occurs. Equipment will have to be cleaned at the least which costs money. Proving it is not economically viable to run the column at flow rates less than the design specification |
| | High | Level | Possible hazards later in column due to the large liquid flow rate | Flooding, and reboiler stops functioning | High level alarm, and shutdown | 2 | 1 | IV | Best to shut down the process, drain the column, and restart the process after determining the source of error. |
| | Low | Level | Column can get too hot | Possible chance stages will dry out | Low level alarm | 3 | 1 | IV | Will usually be detected by level sensors, but can also found from differential pressure transmitters and thermocouple readings of the |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | bottoms and distillate |
| | High | Pressure | Column become more susceptible to leaks | Separation of ACN will not reach required design specification | Pressure sensor in column | 3 | 1 | IV | Follow city regulations on environmental waste disposal |
| | Low | Pressure | | Vacuum is using more power than needed | Pressure sensor at inlet and exit of vacuum pump | 2 | 1 | IV | Costly to run at pressures lower than .1 bar |

| Name | Guide Word | Parameter | Potential Hazard | Effect | Safeguard | Consequence | Frequency | Risk | Actions/Comments |
|---|---|---|---|---|---|---|---|---|---|
| Heat Exchanger | High | Inlet cooling stream temperature | The stream itself is not hazardous, but the insufficient cooling of easily ignitable materials can be. | There is a decrease in the rate of cooling due to the lower value of the log mean temperature difference | Thermocouple at the Inlet of the cooling stream | 3 | 1 | IV | |
| | High | Exit hot stream temperature | Product is above its flash temperature, and exposed to open air | The hot exit stream stream is not cooled below its flash temperature, and exposed to open air | Thermocouples and Flow sensors placed at the hot stream entrance and exit as well as the inlet cooling stream. Also include a fail close valve on the hot stream exit | 4 | 1 | III | Use/write a program help in the automation process. Have it cross check measured values and design specific values, and if it is out of the accepted tolerance value actuate the fail close valve and sound an alarm. |
| | Equipment Malfunction | Ruptured tube | Outlet hot stream could be above flash and open to atmosphere | The cooling stream and heating stream cross contaminate | Include flow rate sensors at all inlets and exits of exchanger to | 4 | 1 | III | If cross contamination is allowed to continue or goes unnoticed; entire process streams |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | determine if there is crossover | | | | |

Appendix F: Utility Summary

The subsequent tables are a summary of the refrigerants used, and their annual cost assuming a working year of 8000 hours. Each calculation is based on the utility price displayed below in table G-1.

Table G-1: Cost of Cooling, Heating, and Electrical Utilities

| Utility Cost | | |
|---|---|---|
| **Cooling Water** | 0.000402 | $/kg |
| **MEK** | 0.000019706 | $/kJ |
| **Steam (P,T)** | | |
| *172 kPa, 115 C* | 0.0211 | $/kg |
| *1034 kPa, 181.4 C* | 0.0244 | $/kg |
| **Electricity** | 0.00002 | $/kJ |

*i. Electric Usage:*

Table G-2: Cost to Run Electrical Equipment

| Electricity Usage | | | |
|---|---|---|---|
| | **Electricity [kW]** | **$/kW** | **Annual Cost** |
| Pump -1 | 3.60E-02 | 7.19E-07 | $202 |
| Pump -2 | 3.39E-02 | 6.79E-07 | $19 |
| Vacuum Pump | 3.00E+01 | 4.60E-04 | $13,261 |
| | | Total | **$13,301** |

*ii. Cooling Water Usage*

Table G-3: Cooling Water

| Cooling Water Usage | | |
|---|---|---|
| **Unit** | **Mass Flow [kg/hr]** | **Annual Cost** |
| **E2-A** | 940.1 | $30,244.87 |

| | | |
|---|---|---|
| **E4-C** | 29.2 | $932.64 |
| **Condenser 2** | 2000 | $64,320.00 |
| | **Total** | **$95,497.51** |

*iii. MEK Usage*

Table G-4: MethylEthylKetone Usage

| MEK Usages | | | | |
|---|---|---|---|---|
| **Unit** | kW Required | Annual Energy Consumption (kJ) | Cost of MEK | True Cost |
| **E1** | 1.4 | 40320000 | $794 | $3,971 |
| **E2-B** | 0.7 | 20160000 | $397. | $1,588 |
| **E3-B** | 8.76 | 252288000 | $4,970 | $19,880 |
| **ED-4** | 0.325 | 9360000 | $184 | $737 |
| **Cond 1** | 160 | 4608000000 | $90,777 | $363,110 |
| | | | Total | **$389,288** |

*iv. Steam Usage*

Table G-5: Steam Consumption

| Steam Usage | | | |
|---|---|---|---|
| Unit | Steam Flow [kg/hr] | Cost [$/kg] | Annual Cost |
| Reboiler 1 | 300 | 0.0211 | $50,640 |
| Reboiler 2 | 300 | 0.0244 | $58,560 |
| Flash Drum | 12.35 | 0.0244 | $2,411 |
| | | **Total Cost** | **$111,611** |

Appendix G: Inherently Safer Design Checklist

I. Minimize

A. Inventory Reduction (Calibri body)

1. Can hazardous raw materials inventory be reduced?
   No. All profit comes from the recycling of hazardous materials back into the process.
2. Can in-process storage and inventory be reduced?
   No. Already taken into consideration
3. Can finished product inventory be reduced?
   No.

B. Process Considerations

1. Can the use of alternate equipment with reduced hazardous material inventory requirement be done? Such as:
   a) Continuous in-line mixers in place of mixing vessels
      Yes. It would be costly, and would severely alter the process
   b) Compact heat exchangers (higher heat transfer area per unit volume) in place of shell-and tube
      No. The flow rate is too high for a feasible compact exchanger.
   c) Combine unit operations (such as reactive distillation in place of separate reactor with multi-column fractionation train; installing internal reboilers or heat exchangers) to reduce overall system volume
      No. No stream would provide adequate heat duty to replace a reboiler.
2. Has piping been designed for reducing the piping diameters?
   Will be considered in later design. The only exception being the gravity driven cooling streams.
3. Can pipeline inventory be reduced by using the hazardous material as a gas rather than a liquid (e.g., chlorine)?
   No.
4. Can process conditions be changed to reduce production of hazardous waste or by-products?

   No. The process is currently operating at the minimum allowable concentration of p-xylene in the waste.

II. Substitute

A. Is it possible to completely eliminate hazardous raw materials, process intermediates, or by-products by using an alternative process or chemistry?
No. The process is chemical specific.

B. Is it possible to completely eliminate in-process solvents and flammable heat transfer media by changing chemistry or processing conditions?
No. The addition of p-xylene is needed to separate toluene from acetonitrile.

C. Is it possible to substitute less hazardous raw materials?
No.

III. Moderate

A. Is it possible to limit the supply pressure of raw materials to less than the maximum allowable working pressure of the vessels they are delivered to?
No. All pressures are set and decreasing pressure would just tax the system further.

B. Is it possible to make reaction conditions (temperature, pressure) less severe by using a catalyst, or a better catalyst?
No. Already taken into consideration with the addition of p-xylene to increase the ease of separation.

C. Can the process be operated at less severe conditions?
No. All temperatures and pressures are set to meet separation specifications.

D. Is it possible to dilute hazardous raw materials to reduce the hazard potential?
No.

E. Is it possible to design operating conditions such that materials that become unstable at elevated temperatures or freeze at low temperatures heating and cooling medium will not be operating in those ranges?
No. Sharp Separation, in this case, can only be achieved at elevated temperatures.

F. Can process conditions be changed to avoid handling flammable liquids above their flash points?
Yes. The changes have already been implemented.

G. Is equipment designed to totally contain the materials that might be present inside at ambient temperature or the maximum attainable process temperature (i.e., higher maximum allowable working temperature to accommodate loss of cooling, simplify reliance of external systems such as refrigeration systems to control temperature such that vapor pressure is less than equipment design pressure)?
Yes.

H. For processes handling flammable materials, is it possible to design the layout to minimize the number and size of confined areas and to limit the potential for serious overpressure in the event of a loss of containment and subsequent ignition?
Yes. Will be a major consideration in plant design.

I. Can process units be located to eliminate or minimize adverse effects from adjacent hazardous installations?
Yes. Install splash guards on drains to reduce contamination. Isolate the exits of the high volatility liquids in one section to reduce risk to the rest of plant.

J. Can process units be designed to limit the magnitude of process deviations:
Yes. Already taken into consideration.

K. Can hazardous material liquid spill be prevented from entering drainage system/sewer?

Yes. Install splash guards over waste water gutters. All flammable stream exits/containment should be at a lower height than the rest of the process to reduce contamination.

L. For flammable materials, can spills be directed away from the storage vessel to reduce the risk of a boiling liquid expanding vapor explosion (BLEVE) in the event of a fire?

Yes. Design the plant on a slight incline, and implement different levels of drains.

M. Passive safety design is preferred. Can passive design be implemented? For example, to prevent or reduce fire damage, an active method is automatic water spray actuated by flame or heat detector; a procedural method by having an operator turn on the water spray, or passive method by using fire insulation.

Yes. Can see implications an implementations in the P&ID diagram.

IV. Simplify

A. Can equipment be designed such that it is difficult or impossible to create a potential hazardous situation due to an operating or maintenance error? Such as:

1. Easy operation of valves designed to prevent inadvertent errors
   Yes. Most of the valve actuators will be run autonomously.
2. Simplified control displays
   Yes. Will be a consideration when deciding on the control software to use.
3. Operate at lower pressure to limit release
   No.
4. Operate at lower temperature to prevent run away reactions or material failure
   Not possible. All temperatures are set to meet design specifications.
5. Use passive rather than active controls
   Yes. Currently implementing both.
6. Use buried or shielded tanks
   Yes. Already taken into consideration.
7. Use fail-safe controls if utilities are lost
   Yes. Fail open valves on cooling utilities, and fail close valves on streams entering the atmosphere containing liquids above their flash point.
8. Limit the complexity and degree of instrumentation redundancy
   Yes. There are some instrumentation redundancies, but these redundancies help locate errors quickly.
9. Use refrigerated storage vs. pressurized storage
   Yes. Already taken into consideration.
10. Minimize connections, paths and number of flanges in hazardous processes
    Yes. Needs to be considered in further design.
11. Use fewer bends in piping
    Yes. Should be considered later in the design process.

12. Use expansion loops in piping rather than bellows
    Yes. Space is not an issue, so an expansion loop should be used.
13. Design into the process, equipment isolation mechanism for maintenance
    Yes. Already taken into consideration, but should still be investigated further as the design evolves.
14. Limit manual operations such as filter cleaning, manual sampling, hose handling for loading/unloading operations, etc.
    Yes. The process is automated as much as possible.
15. Design vessels for full vacuum eliminating risk of vessel collapse
    Yes. Already taken into consideration, i.e. of the vacuum pump.
16. Design both shell and tube side of heat exchangers to contain the maximum attainable pressure, eliminating the need for pressure relief
    Yes.
17. Can the equipment be designed to make incorrect assembly impossible?
    Use equipment that clearly identifies status

B. Can passive leak-limiting technology be used to limit potential loss of containment? Some examples include the following:

We are not at this point in the design process. A leak of a stream containing a liquid above its flash point is still a serious safety concern, thus this section should be taken into further consideration at a later point.

1. Blowout resistant gaskets
   Yes.
2. Increasing wall strength
   Yes.
3. Using fewer seams and joints
   Yes.
4. Providing extra corrosion/erosion allowance
   No. None of the materials used are considered very corrosive.
5. Reducing vibration
   Yes. Should at least be considered
6. Minimizing the use of open-ended, quick-opening valves
   Yes.
7. Eliminating open-ended, quick-opening valves in hazardous service
   Yes.
8. Improving valve seating reliability
   Yes.
9. Eliminating unnecessary expansion joints, hoses, and rupture disks
   Yes.
10. Eliminating unnecessary sight glasses/glass rotameters
    Yes.

V. Transport of Hazardous Materials

A. Can the plant be located to minimize need for transportation of hazardous materials?

Yes. The plant is supplying most of the hazardous materials back to itself. The waste is the only material leaving the plant and is composed of mostly p-xylene which can flash at temperatures slightly above room temperatures. Plant location should be considered, but is not mandatory.

B. Can materials be transported:

1. In a less hazardous form
   Yes. The waste should be kept refrigerated
2. In a safer transport method.
   Yes. Consider using trains instead of semi-trucks to transport waste
3. In a safer route
   Should be considered depending on location

Appendix H: Sample Calculations

*i. Economics*

a. Delivered Equipment Cost

This method is used to cost all equipment using values given by EconExpert

$$DEC = [Base\ Cost] \cdot [M_{factor}] \cdot [P_{factor}] \cdot [Delivery\ Fee]$$

Where:

$$DEC \equiv Delievered\ Equipment\ Cost$$
$$M_{factor} \equiv Material\ Factor\ [From\ EconExpert]$$
$$P_{factor} \equiv Pressure\ Feactor[From\ EconExpert]$$
$$Delivery\ Fee = 1.1\ (10\%\ Fee)$$
$$DEC_{ACNTower} = [\$8{,}886] * (1.7 * 4.0) * 1.1 = \$66{,}467$$

b. Fixed Capital Investment

$$FCI = Total\ Plant\ Cost = Total\ Direct\ Cost\ (TDC) + Total\ Indirect\ Cost\ (TIC) + Contracting$$

Where:

$$TDC \equiv 244\%\ of\ DEC_{total}$$
$$TIC \equiv 80\%\ of\ DEC_{total}$$
$$Contracting \equiv 63\%\ of\ DEC_{total}$$

Percentages Given by Peters and Timmerhaus (1981)

$$FCI = (2.44 + 0.8 + 0.63) \cdot [\$531{,}819]$$
$$FCI = \$2{,}058{,}140$$

c. Total Product Cost

$$Total\ Product\ Cost = Manufacturing\ Cost + General\ Expenses$$

Where:

$$Mfg\ Cost = 24.2\%\ of\ FCI + 15\% of\ Labor\ Cost + 55\% of\ (Labor + Superv. + Maint.)$$
$$General\ Expenses \equiv 15\%\ of\ Mfg\ Cost + 15\%\ of\ (Labor + Superv. + Maint.)$$
$$Total\ Product\ Cost = \$1{,}144{,}360 + \$320{,}100 = \$1{,}464{,}000$$

d. Working Capital Investment (WCI)

$$WCI = 86\%\ of\ DEC_{total}$$
$$WCI = \$457{,}360 \text{ [Recovered at year 20]}$$

e. Total Capital Investment (TCI)

$$TCI = WCI + FCI$$
$$TCI = \$457{,}360 + \$2{,}060{,}000$$
$$TCI = \$2{,}520{,}000$$

f. Labor Costs

$$\text{Labor Cost} = \frac{1}{4} \cdot \left(\frac{8000\ \text{hr}}{\text{year}}\right) \cdot [\#\ \text{Workers}] \cdot \left[\frac{\$}{\text{hr} \cdot \text{Worker}}\right] * [\text{Benefits}]$$

Where

$$\#\ \text{Workers} = 8$$

$$\frac{\$}{\text{hr}} = \$25$$

$$\text{Benefits} = 1.7$$

$$Labor\ Cost = \frac{1}{4} \cdot \left(8000 \frac{hr}{year}\right) \cdot (8\ Workers) \cdot \left(\frac{\$25}{hr \cdot Worker}\right) \cdot 1.7$$

$$Labor\ Cost = \frac{\$680{,}000}{yr}$$

g. Annual Operating Cost (Total)

$$Operating\ Cost = Total\ Product\ Cost + Utility\ Costs + Labor + Raw\ Materials$$

Where

$$Utility\ Cost \equiv \Sigma[Heating + Cooling + Electric]_{costs}$$

$$Utility\ Cost \equiv \$637{,}280\ (see\ utility\ summary)$$

$$Raw\ Materials \equiv Xylene\ Purchased, Waste\ Disposed = \left[\dot{m}_i \cdot \left[\frac{\$}{kg}\right]_i\right] - 1.5 * \dot{m}_{waste}$$

Where

$$\dot{m}_i \equiv Mass\ Flow\ Rate\ of\ Xylene$$

$$\left[\frac{\$}{kg}\right]_i = Price\ Per\ Kilogram\ \ of\ Xylene$$

$$Operating\ Cost = \$1{,}464{,}460 + \$637{,}280 + \$680{,}000 + \$795{,}280$$

$$Annual\ Operating\ Cost = \frac{\$3.57Mil}{year}\ with\ a\ 1^{st}\ year\ cost\ of\ \$3.93\ Mil$$

h. SOYD Depreciation Value

$$SOYD\ Depreciation\ (year\ 20) = \frac{0.85 \cdot TCI}{SOYD}$$

Where

SOYD= 210

$$Year_{20}\ Depreciation = \left(\frac{0.85}{210}\right) * \$2{,}515{,}000 = \$10{,}182$$

$$Year_{12}\ Depreciation = Year_{20}\ Depreciation * [11\ Useful\ Years\ Remaining]$$

$$Year_{10} Depreciation = \$122{,}182$$

i. After Tax Cash Flow

$$ATCF = 0.6 \cdot [BTCF - Year_n Depreciation]$$

Where

$$BTCF \equiv Revenue - Total\ Product\ Cost$$
$$ACTF_{yr12} = 0.6 * [\$6{,}102{,}760 - \$91{,}640] = \$3{,}698{,}300$$

j. ROR

The rate of return was calculated in excel using the built-in IRR function with our after tax cash flow as input.

*ii. Equipment Sample Calculations*

a. Liquid Ring Vacuum Pump

$$Installed\ Cost = \$28{,}000 \left(\frac{HP}{10}\right)^{0.5} * 2.62$$
$$2.62 \equiv Factor\ to\ adjust\ cost\ from\ 1981\ to\ 2015$$
$$Installed\ Cost = \$88{,}600$$

b. Mixer:

$$Volume_{70\%} = Vol.Flow\ in * Holding\ Time$$
$$Volume_{70\%} = 3.94 \frac{L}{min} * 5\ \mathrm{min} * \left(\frac{1\mathrm{m}^3}{1000L}\right) = 0.0256m^3$$
$$\frac{Height}{Diameter} = 4\ (assumed)$$
$$\therefore H = 0.36m \qquad D = 0.09m$$

c. Column Height

$$Height_{Column} = n_{theoretical} * HETP_{packing} * 1.15$$
$$H_{ACN\ Column} = 23 * 0.08m * 1.15 = 2.39m$$

d. Flash Drum

$$Flv = \frac{W_l}{W_v} * \left(\frac{\rho_v}{\rho_l}\right)^{.5}$$
$$K_{drum} = e^{A+Bln(Flv)+C(\ln(flv))^2+D*(\ln(Flv))^3+E*(\ln(Flv))^4}$$
$$u_{perm} = K_{drum} * \left(\frac{(\rho_l - \rho_v)}{\rho_v}\right)^{.5}$$
$$V = \frac{u_{perm} A_c \rho_v}{MW_{vap}}$$

| Constant | Value |
|---|---|
| A | -1.877478097 |
| B | -.8145804597 |
| C | -.1870744085 |
| D | -.0145228667 |
| E | -.0010148518 |

ρ = density
W = mass flow rate
Flv = empirical ratio

A-E = constants
$K_{drum}$ = case specific constant
$U_{perm}$= Max velocity at max diameter of flash drum. (Ft/s)
V = Molar flow rate
$A_c$ = Cross sectional error
$MW_{vap}$ = Molecular weight of the vapor

e. Storage Tank Volume

$$Volume_{tank} = 2 * V_{50\%}$$

Where:

$$V_{50\%} = \dot{V}_{in} * Fill\ Time$$

For the ACN Product Tank

$$V_{tank} = 2 \cdot \left(\frac{4.7m^3}{day}\right) \cdot (2\ Days) = 18.8m^3$$

Appendix I: References

References


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