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ECONOMIC RECOVERY OF PYRIDINE AND 3-METHYLPYRIDINE

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Abstract
The goal of this design project was to find the most cost effective way of recovering pyridine and 3-methylpyridine from a given impurity stream with a specific finished goods quality. Due to the multiple azeotropes that the organic components in the feed had with water, we had to first explore different methods of removing water. We explored two different approaches in depth – pervaporation and azeotropic distillation. Both processes allowed us to break the azeotropes with water by removing at least 98 wt% of the water and recover at least 88 wt% of pyridine.

To get a 15% return on investments (ROI) by the third year of production, we found that the pervaporation method allowed us to pay up to $0.71/lb for the necessary feed stream, while the azeotropic distillation method gave us a flexibility of up to $0.82/lb. Using a feed value of $0.71/lb for both processes, the total capital investment (TCI) for the pervaporation process is $10.7 million with a net present value (NPV) of $1.8 million, while the TCI for azeotropic distillation is $7.0 million with a NPV of $6.4 million. Taking both the finished goods quality specifications and economic profitability into account for our design project, we would recommend the azeotropic distillation process in recovering the most purified product.

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April 14, 2010

Dear Professor Fabiano and Dr. Holleran,

This project seeks to find the most cost effective method of recovering pyridine and 3-methylpyridine from a stream of impurities. We explored two different processes – pervaporation and azeotropic distillation with a benzene solvent – that were able to separate out water first to resolve the azeotropes the organic components in the feed had with water before continuing to recover the products. Following a detailed analysis of both processes, we believe that using an azeotropic distillation is the most economically profitable method of recovering pyridine and 3MP.

We are able to pay up to $0.82/lb for the feed stream and still get at least 15% on our return on investments (ROI) when using azeotropic distillation, while we can pay up to $0.71/lb for the feed for the same ROI when using pervaporation. Not only did we find azeotropic distillation to be the most cost effective method of recovering the products of interest, but we were also able to work around the azeotropes with water. Enclosed are our findings and analysis of the two aforementioned processes and reasoning as to why we would recommend the azeotropic distillation process over the use of pervaporation.

Sincerely,

Rita Cheng   Chi-Ho Cho   Stephanie Kirby   Bomyi Lim

ECONOMIC RECOVERY OF PYRIDINE AND 3-METHYLPYRIDINE

Rita Cheng

Chi-Ho Cho

Stephanie Kirby

Bomyi Lim

Senior Design Report

Spring 2010

Department of Chemical & Biomolecular Engineering

University of Pennsylvania

Faculty Advisor: Dr. Sean P. Holleran, University of Pennsylvania

Recommended by: Professor Leonard A. Fabiano, U. Penn

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ABSTRACT

The goal of this design project was to find the most cost effective way of recovering pyridine and 3-methylpyridine from a given impurity stream with a specific finished goods quality. Due to the multiple azeotropes that the organic components in the feed had with water, we had to first explore different methods of removing water. We explored two different approaches in depth – pervaporation and azeotropic distillation. Both processes allowed us to break the azeotropes with water by removing at least 98 wt% of the water and recover at least 88 wt% of pyridine.

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INTRODUCTION

Pyridine is an aromatic compound that exists as a colorless liquid with a distinctive fish-like odor. As seen in Figure 1, the compound is structurally related to benzene, but one of the –CH groups in the six-member ring is replaced by a nitrogen atom.

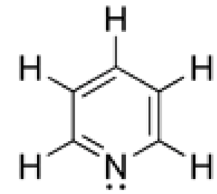

Figure 1. Molecular structure of pyridine.

There are various industrial applications for pyridine, where some of its more popular uses include roles as a chemical solvent and denaturant. As a polar but aprotic solvent, pyridine is miscible in multiple solvents and is used as a solvent in H NMR spectroscopy, for example. Additionally, pyridine can be used as a denaturant for antifreeze mixtures and ethyl alcohol. Other common applications, as seen in *Elvers et al., 2003,* include using pyridine in colorimetric determinations of cyanide in aqueous solutions and as a dyeing aide for textiles. With such a broad range of applications, the demand for pyridine is high and thus a process that can recover pyridine from impurities is worth looking into.

This project seeks to find the most cost effective process that will recover pyridine and 3-methylpyridine from a given impurity stream that also meets the specified criteria for waste disposal, minimal product losses and capital payback requirement.

Due to complications of azeotropes with organic components with water – pyridine, 3-methylpyridine and other light boiling impurities – various methods of removing water in the feed were explored. The first method used molecular sieves to selectively adsorb molecules based on size. Since water is the lightest and smallest (by size) component in the feed stream, molecular sieves would be able to successfully remove at least 99% of the water in the stream without any complications. However, the cost of this option would've been comparable to azeotropic distillation, and our goal was to find a cheaper alternative. The next method explored was the use of pervaporation, which separates liquid mixtures by partial vaporization through a membrane. The membrane acts as a selective barrier between a liquid phase feed and a vapor phase permeate, and the driving force for transport of different components is the chemical potential difference between the liquid retentate and vapor permeate on each side. Finally, the last method considered was the use of azeotropic distillation to remove water in the presence of a solvent that would not form an azeotrope with water.

Azeotropic distillation is a common method of separating mixtures used in the chemical engineering industry. For this design project we wanted to find a cheaper, but just as effective, method of removing water from the feed stream. A quick cost analysis on the use of molecular sieves versus pervaporation eliminated the former as an option due to the large expenses from the purchase of materials and regeneration cost of the sieves. As a result, this project compares the cost and efficiency between the use of pervaporation and azeotropic distillation in removing water and meeting the product quality requirements of pyridine and 3-methylpyridine.

CONCEPT STAGE

Market and Competitive Analysis

The pyridine product recovered in this design can be used in a range of applications and industries such as the textile sector, pharmaceuticals and daily-use chemicals such as pesticides. According to the China Chemical Report, China would be the main competitor to our processes since the country is one of the largest producers and consumers of pyridine. In 2002, China had six production pyridine producers with an average annual output of 4.2 kiloton, and the country's consumption amounted to roughly 10 kiloton.

In the azeotropic distillation process, we expect to recover roughly 6.3 million pounds of pyridine per year, and the sales projection at the third year of production is roughly $19.7 million. For the pervaporation process, we expect to recover slightly less pyridine – only 6.0 million pounds per year – and the sales projection for the same year of production would amount to $18.8 million total.

Existing Methods of Production

Currently there are industrial standards of separating pyridine from water using either azeotropic or azeotropic distillation. Engineers have found that methyl isoamyl ketone and propylene glycol dimethyl ether are effective agents in azeotropic distillation, while isophorone and sulfolane are effective in azeotropic distillation (Patent #5100514). The presence of these agents increases the relative volatility of pyridine to achieve a separation that normally would not happen because of the minimum boiling azeotrope pyridine has with water.

Customer Requirements

In designing a process that will recover pyridine and 3-methylpyridine from a given stream, the fitness-to-standard (FTS) and new-unique-and-difficult (NUD) requirements must be taken into consideration. FTS requirements for the recovered product include non-toxicity, low cost, environmentally friendly and one of five different quality requirements must be met before the product can be sold. The five quality requirements are:

a. Pyridine Finished Goods Quality Specifications (by weight):

Pyridine	99.75 % minimum
3-Methylpyridine	0.01 % maximum
N-butyronitrile	0.05% maximum
Water	0.1 % maximum

b. 3-Methylpyridine Finished Goods Quality Specifications:

3-Methylpyridine	98.0 % minimum
Sum of light boiling impurities	0.2% maximum
Water	0.2% maximum

c. Crude Quality Specifications:

Pyridine and 3-Methylpyridine	98.0% minimum
N-butyronitrile	0.03% maximum
Xylene	0.1% maximum
Water	1.0 % maximum

d. Pyridine Intermediate Quality Specifications:

Pyridine	98.0% minimum
3-Methylpyridine	1.0% maximum
N-butyronitrile	0.04% maximum
Xylene	0.1% maximum
Water	1.0% maximum

e. 3-Methylpyridine Intermediate Quality Specifications:

3-Methylpyridine	98.0% minimum
Pyridine	1.0% maximum
N-butyronitrile	0.04% maximum
Xylene	0.1% maximum
Water	1.0% maximum

The new-unique-and-difficult requirement for this design is lower cost through the use of pervaporation, which is able to remove 98 wt% of the water in a feed through the use of membrane technology, in place of an azeotropic distillation column.

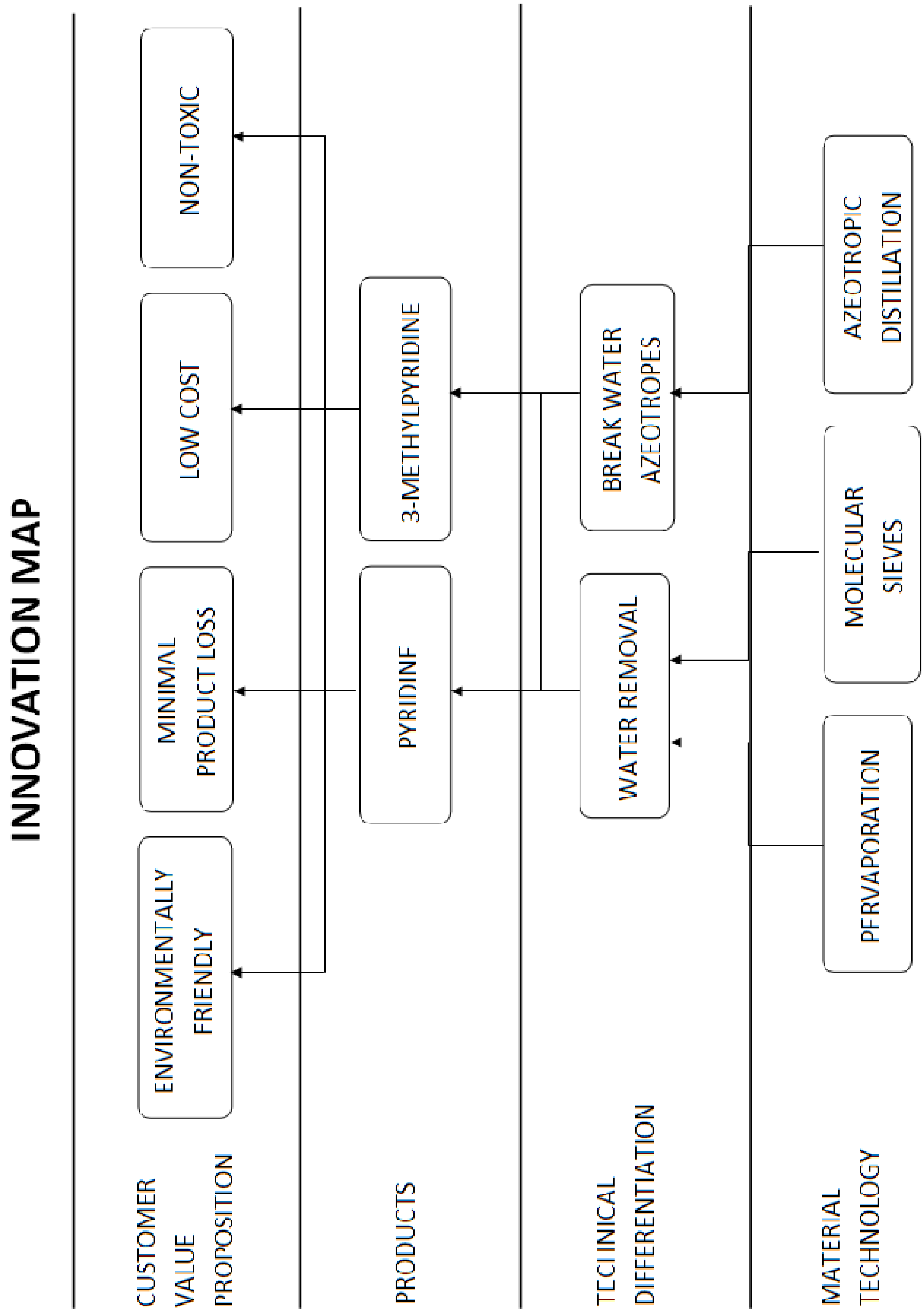
INNOVATION MAP
CUSTOMER VALUE PROPOSITION
ENVIRONMENTALLY FRIENDLY
MINIMAL PRODUCT LOSS
LOW COST
NON-TOXIC
PRODUCTS
PYRIDINF
3-METHYLPYRIDINE
TECIINICAL DIFFERENTIATION
WATER REMOVAL
BREAK WATER AZEOTROPES
MATERIAL TECHNOLOGY
PFRVAPORATION
MOLECULAR SIEVES
AZEOTROPIC DISTILLATION

Table 1: Relevant property data for each component in the stream

	acetonitrile	n-butyronitrile	methanol	3MP	pyridine	xylene	water
Chemical Formula	C_2H_3N	C_4H_7N	CH_4O	C_6H_7N	C_5H_5N	C_8H_{10}	H_2O
MW (g/mol)	41.05	69.11	32.04	93.13	79.1	106.17	18.02
Normal BP(C)	81.6	117.6	64.7	143.5	115.4	139.3	100.0
Solubility in H_2O	Soluble	Slightly soluble	Soluble	Soluble	Soluble	NOT soluble	N/A

Table 2: Temperatures at which each component forms an azeotrope with water

Temp (C)	METHANOL	ACN	PYRIDINE	3MP	N-BUTYRO	WATER	PXYLENE
63.58	x	x					
74.26		x				x	x
76.14						x	x
76.65		x				x	
86.08					x	x	
93.67			x			x	
93.90	x		x			x	
96.17				x		x	
138.12				x			x

Table 3: Temperatures at which certain components form azeotropes with benzene

Temp (C)	PYRIDINE	WATER	C6H6
93.67	x	x	
56.91		x	x

Preliminary Process Evaluations

The Azeotrope Problem

Various methods of separation were considered to recover pyridine and 3-methylpyridine (3MP). The first challenge that we faced was overcoming the various azeotropes that water formed with all the compounds in the feed stream except methanol, as seen in the Property Data on p8, Tables 1-3. The idea that the process could be completed using only ordinary distillation was eliminated; this also implied that water had to be removed before successful recovery of pyridine and 3MP could occur. We exploited various thermodynamic properties and solubilities so that the azeotrope problem could be solved.

The mixture of organic compounds with non-organic compounds presented opportunities for liquid-liquid separation. The first method explored was the use of a decanter, which took advantage of the solubility differences and did not conflict with the azeotropes in separating the organic compounds from the non-organic compounds. However, pyridine and 3MP were both soluble in water and made the separation difficult. A more rigorous approach was then taken using liquid-liquid extraction. Theoretically, organic components are more soluble in hydrocarbons than they are in water, so several solvents were explored, including benzene, octane and diethyl ether. Unfortunately, this approach was also unsuccessful because pyridine was relatively soluble in these solvents, and there was not a high enough degree of separation.

I. Using Molecular Sieves for Water Removal

An alternative water removal method that was considered for this design outside of pervaporation was the use of molecular sieves, which would remove most of the water and retain negligible amounts of any other component from our given feed stream. The size we would have used is 3A molecular sieves, which is the smallest available in the industry. Molecular sieves also have a high affinity for polar molecules, but polarity is only of concern when similar-sized molecules are present in a stream.

Additionally, molecular sieves must go through a regeneration process to reduce the moisture content to roughly 0.3 wt%, which can be done by heating to approximately 300ºC in a thermal swing process. With respect to the efficiency of this process, W.R. Grace & Co. state that the amount of water adsorbed is directly proportional to the weight or amount of sieves used; and the maximum amount is up to 22% of weight of the sieves. So while this option could potentially remove at least 99% of the water from the feed stream, the use of molecular sieves and the incurred costs from regeneration proved too costly compared to other alternatives.

II. Using Pervaporation to Remove Water

This method utilizes a hydrophilic membrane to withdraw the water from the organic stream. The membrane works both chemically and mechanically – the membrane is composed of cross-linked poly (vinyl alcohol), which attracts the polar water molecules in the solution. In addition, the smaller molecules diffuse through the membrane with greater fluxes. In this case, water was most favored for transport. Pervaporation transport is driven by a concentration and pressure gradient across the membrane, and therefore operates independently from the vapor-liquid equilibrium, avoiding the issue of the pyridine–water azeotrope. Pervaporation was able to remove 98% of the water from the feed stream, with a pyridine loss of 2%, and was one of the main processes investigated in this report.

III. Using Azeotropic Distillation to Remove Water

Azeotropic distillation was also considered as it was the conventional method of breaking azeotropes in distillation. Azeotropic distillation involves introducing a solvent that forms a heterogeneous low boiling azeotrope. A typical example of azeotropic distillation in industry involves the addition of benzene to water and ethanol. Benzene was introduced to our system to separate water from the rest of the components because water forms an azeotrope with benzene at a lower temperature than the lightest boiling component in the feed. This was confirmed in Aspen and was the other main process pursued in detail.

The Close Boiling Point Problem

Several components in the feed had boiling points close to each other. N-butyronitrile has a boiling point of 117.6ºC, which is very close to pyridine's boiling point of 115.4ºC, while xylene's boiling point of 139.3 ºC approached 3MP's boiling point of 143.5 ºC. This meant that ordinary distillation would not be effective in separating the components due to their low relative volatilities. Although there is a very small amount of n-butyronitrile in the feed, it becomes increasingly significant downstream when only pyridine and n-butyronitrile are left in the stream. Therefore, we needed to devise a method that would remove n-butyronitrile to meet the final product criteria for pyridine. Since both n-butyronitrile and xylene have limited solubility in water, we attempted to separate the two using a decanter. However, the decanter was unsuccessful because xylene and n-butyronitrile made up only 2 wt% of the entire stream.

In the process of eliminating light boiling impurities such as methanol and acetonitrile earlier in the process, we discovered that the various azeotropes with water could be used to our advantage. Water forms an azeotrope with xylene, acetonitrile, and n-butyronitrile at lower temperatures compared to the temperatures at which water forms azeotropes with pyridine and 3MP. Although there are other azeotropes between different components in the stream, the azeotrope with water affected the system the most because it was the dominant component in the stream (43 wt%). Although the azeotrope prevents perfect removal of these impurities, the separation was able to achieve a product stream that met the final product criteria. This separation was only obtained with the presence of the azeotrope with water. Therefore, n-butyronitrile and xylene were removed before water.

N-Butyronitrile Reaction

Another method that was explored to remove n-butyronitrile was converting the compound into a new material that was more easily separable from pyridine through a reaction. There were two different nitrile reactions (R-CN) that were researched – hydrolysis to acid and nucleophilic addition. The mechanisms and chemical equations for each reaction are as follows:

- Hydrolysis to Acid

$$RCN \xrightarrow{H+,\ \ heat} RCONH_2 \xrightarrow{water\ and\ heat} RCOOH$$

- Nucleophilic Addition

  Strong nucleophiles (Nu): RMgX, Rli, $LiAlH_4$

$$Nu - H + RCN \xrightarrow{yields} RCNH - Nu$$

This method was rejected because it would have introduced additional compounds that would have to be removed as well.

Bench Scale Lab Work

The most significant lab work that needs to be performed relates to the pervaporation process: the actual flux through the membrane and temperature drop across the modules need to be determined to more accurately design the pervaporation modules and inter-stage heaters.

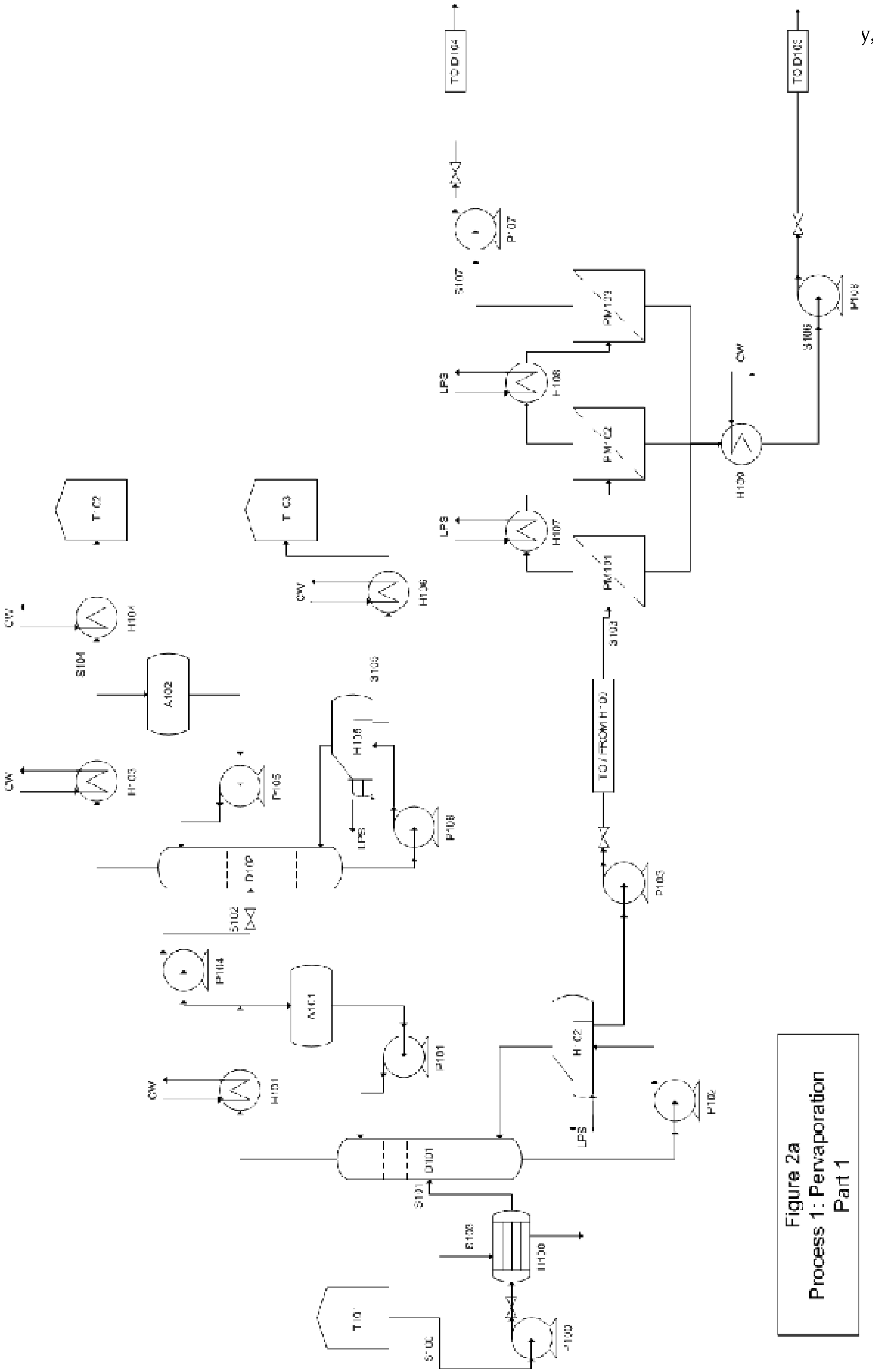

Figure 2a
Process 1: Pervaporation
Part 1

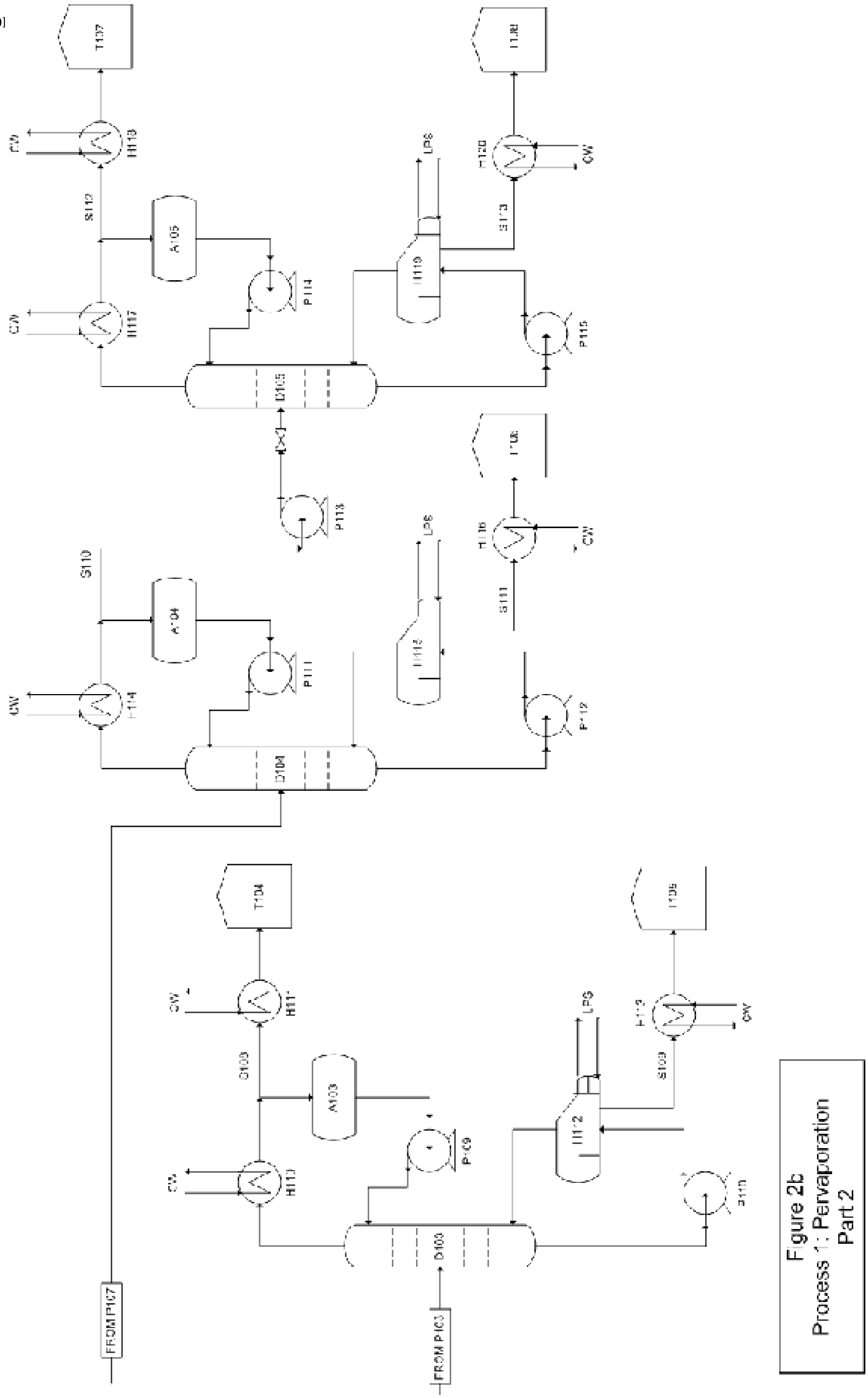

Figure 2b
Process 1: Pervaporation
Part 2

Table 4: Stream Data for Pervaporation

	S100	S101	S102	S103	S104	S105	S106
Temperature (F)	80.0	131.5	167.4	158.0	163.1	208.8	80.0
Pressure (psia)	15.0	15.0	15.0	31.0	15.0	17.7	15.0
Total Flow (lb/hr)	2600.0	2600.0	633.8	1966.2	497.0	135.7	1034.4
Mass Flow (lb/hr)							
Methanol	130.00	130.00	67.78	62.22	67.48	0.09	60.90
Acetonitrile	312.00	312.00	312.00	0.00	311.81	0.19	0.00
Pyridine	780.00	780.00	59.40	720.60	0.04	58.03	14.37
3-Methylpyridine	208.00	208.00	0.17	207.83	0.00	0.17	3.17
N-butyronitrile	26.00	26.00	25.94	0.06	17.04	8.91	0.00
Water	1118.00	1118.00	142.53	975.47	74.63	68.32	955.97
Xylene	26.00	26.00	26.00	0.00	26.00	0.00	0.00
Weight % by mass							
Methanol	5.0%	5.0%	10.7%	3.2%	13.6%	0.1%	5.9%
Acetonitrile	12.0%	12.0%	49.2%	0.0%	62.7%	0.1%	0.0%
Pyridine	30.0%	30.0%	9.4%	36.6%	0.0%	42.8%	1.4%
3-Methylpyridine	8.0%	8.0%	0.0%	10.6%	0.0%	0.1%	0.3%
N-butyronitrile	1.0%	1.0%	4.1%	0.0%	3.4%	6.6%	0.0%
Water	43.0%	43.0%	22.5%	49.6%	15.0%	50.3%	92.4%
Xylene	1.0%	1.0%	4.1%	0.0%	5.2%	0.0%	0.0%

	S107	S108	S109	S110	S111	S112	S113
Temperature (F)	140.0	167.9	223.5	224.8	307.9	198.8	242.9
Pressure (psia)	15.0	15.0	18.8	15.0	18.9	15.0	17.5
Total Flow (lb/hr)	930.8	101.6	932.8	730.0	200.8	31.6	698.4
Mass Flow (lb/hr)							
Methanol	1.25	57.66	3.24	1.25	0.00	1.17	0.08
Acetonitrile	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pyridine	706.29	9.80	4.57	705.18	1.11	18.09	687.09
3-Methylpyridine	203.67	2.62	0.55	3.99	199.68	0.00	3.99
N-butyronitrile	0.06	0.00	0.00	0.06	0.00	0.00	0.06
Water	19.52	31.50	924.47	19.52	0.00	12.37	7.15
Xylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Weight % by mass							
Methanol	0.1%	56.8%	0.3%	0.2%	0.0%	3.7%	0.0%
Acetonitrile	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Pyridine	75.9%	9.6%	0.5%	96.6%	0.6%	57.2%	98.4%
3-Methylpyridine	21.9%	2.6%	0.1%	0.5%	99.4%	0.0%	0.6%
N-butyronitrile	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Water	2.1%	31.0%	99.1%	2.7%	0.0%	39.1%	1.0%
Xylene	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%

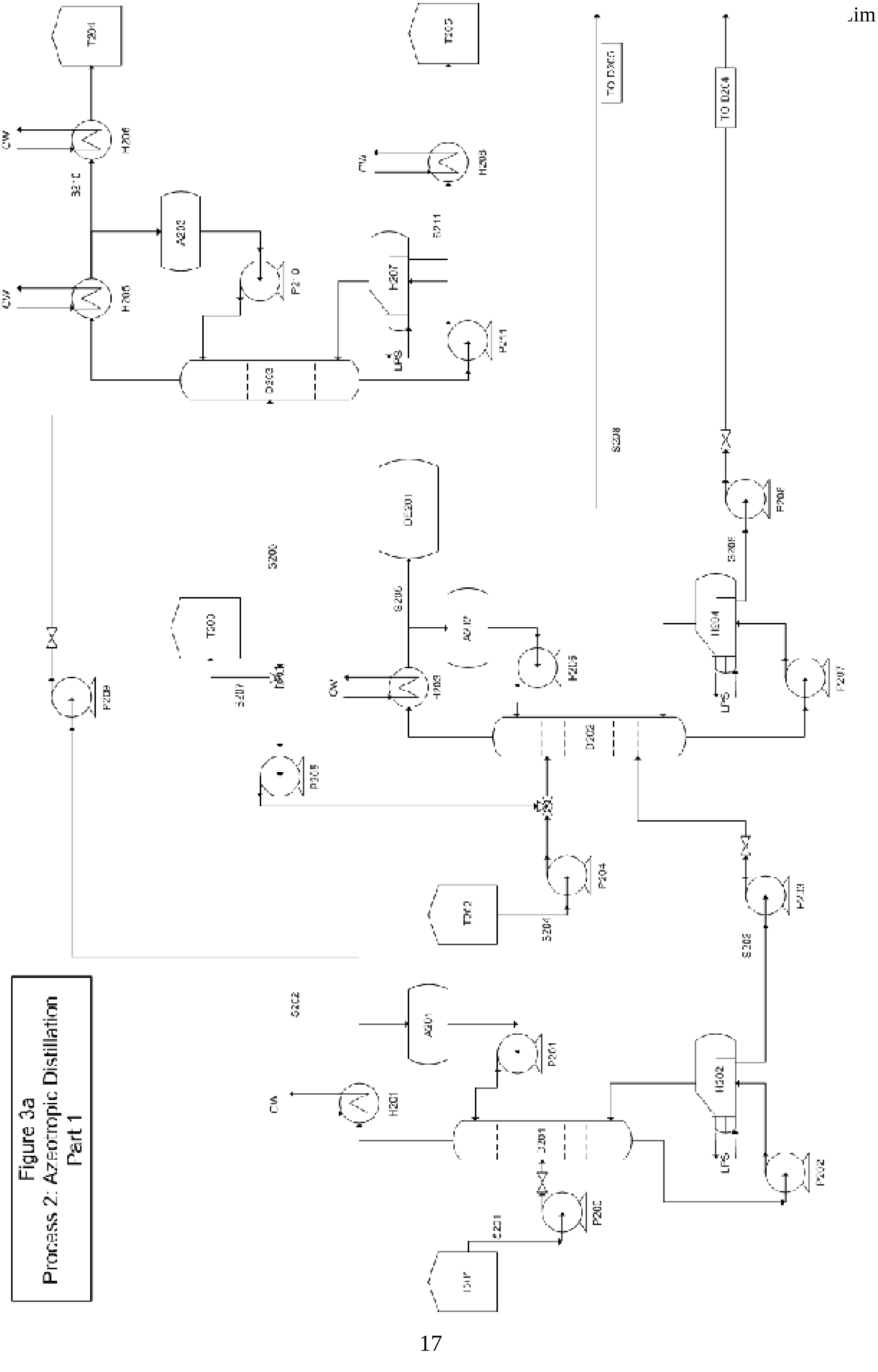

Figure 3a
Process 2: Azeotropic Distillation
Part 1

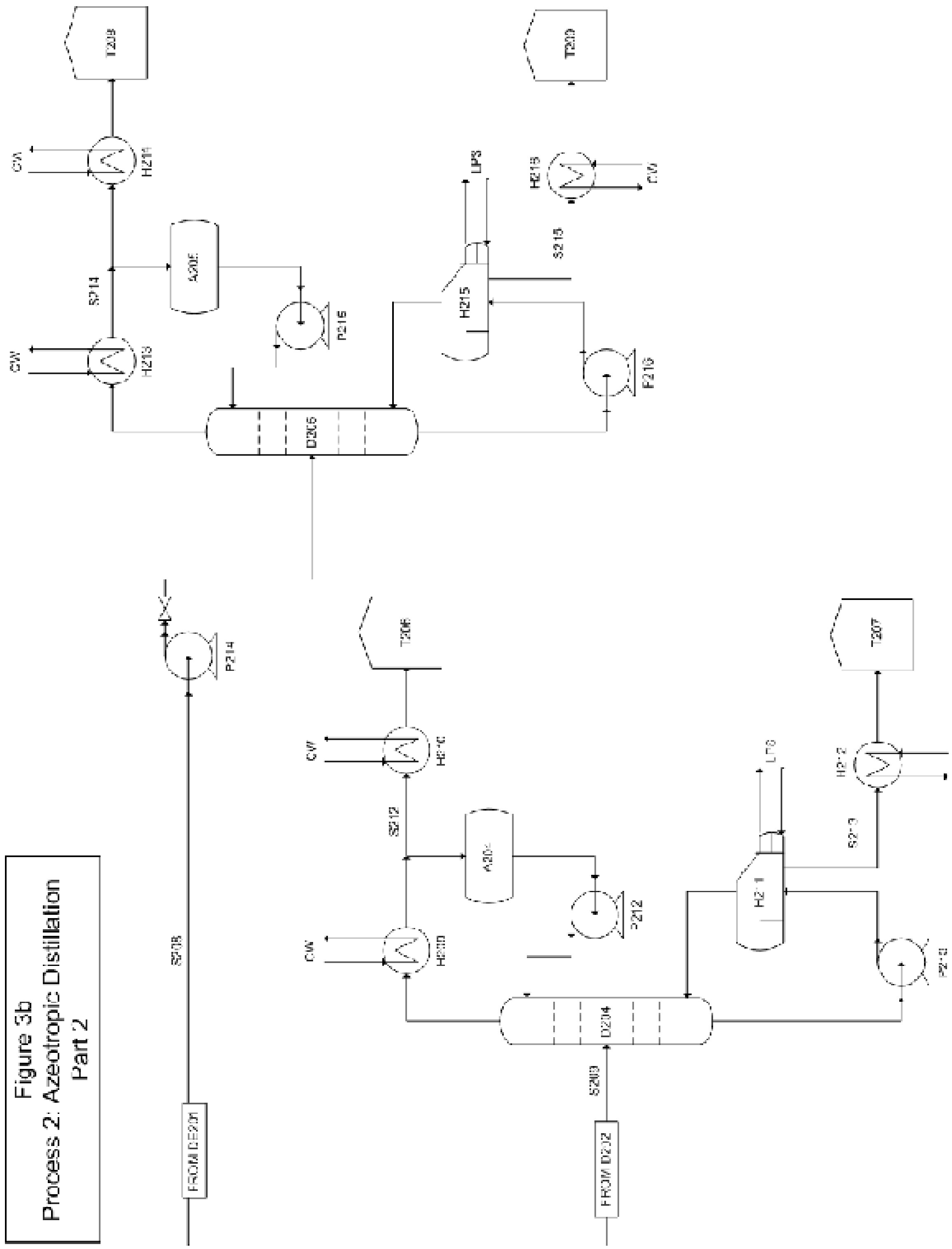

Figure 3b
Process 2: Azeotropic Distillation
Part 2

Table 5: Stream Data for Azeotropic Distillation

	S201	S202	S203	S204	S205	S206	S207
Temperature (F)	80.0	167.4	221.4	100.0	153.0	100.0	100.0
Pressure (psia)	15.0	15.0	21.6	30.0	22.0	15.0	30.0
Total Flow (lb/hr)	2600.0	632.7	1967.3	203.3	4937.5	3907.5	194.9
Mass Flow (lb/hr)							
Methanol	130.00	67.57	62.43	0.00	62.43	6.15	0.00
Acetonitrile	312.00	312.00	0.00	0.00	0.00	0.00	0.00
Pyridine	780.00	58.06	721.94	0.00	0.03	0.03	0.00
3-Methylpyridine	208.00	0.17	207.83	0.00	0.00	0.00	0.00
N-butyronitrile	26.00	25.94	0.06	0.00	0.00	0.00	0.00
Water	1118.00	142.95	975.05	0.00	975.05	4.09	0.00
Xylene	26.00	26.00	0.00	0.00	0.00	0.00	0.00
Benzene	0.00	0.00	0.00	203.29	3900.04	3897.25	194.86
Weight % by mass							
Methanol	5.0%	10.7%	3.2%	0.0%	1.3%	0.2%	0.0%
Acetonitrile	12.0%	49.3%	0.0%	0.0%	0.0%	0.0%	0.0%
Pyridine	30.0%	9.2%	36.7%	0.0%	0.0%	0.0%	0.0%
3-Methylpyridine	8.0%	0.0%	10.6%	0.0%	0.0%	0.0%	0.0%
N-butyronitrile	1.0%	4.1%	0.0%	0.0%	0.0%	0.0%	0.0%
Water	43.0%	22.6%	49.6%	0.0%	19.7%	0.1%	0.0%
Xylene	1.0%	4.1%	0.0%	0.0%	0.0%	0.0%	0.0%
Benzene	0.0%	0.0%	0.0%	100.0%	79.0%	99.7%	100.0%

	S208	S209	S210	S211	S212	S213	S214	S215
Temperature (F)	100.0	282.7	163.1	208.8	239.5	306.2	151.1	222.1
Pressure (psia)	15.0	25.7	15.0	17.7	15.0	18.6	15.0	18.4
Total Flow (lb/hr)	973.9	935.4	497.0	135.7	726.0	209.4	56.2	973.9
Mass Flow (lb/hr)								
Methanol	9.83	0.00	67.48	0.09	0.00	0.00	46.45	9.83
Acetonitrile	0.00	0.00	311.81	0.19	0.00	0.00	0.00	0.00
Pyridine	0.00	721.90	0.04	58.03	719.66	2.24	0.00	0.00
3-Methylpyridine	0.00	207.83	0.00	0.17	0.64	207.19	0.00	0.00
N-butyronitrile	0.00	0.06	17.04	8.91	0.05	0.00	0.00	0.00
Water	964.04	0.00	74.63	68.32	0.00	0.00	6.93	964.04
Xylene	0.00	0.00	26.00	0.00	0.00	0.00	0.00	0.00
Benzene	0.00	5.64	0.00	0.00	5.64	0.00	2.79	0.00
Weight % by mass								
Methanol	1.0%	0.0%	13.6%	0.1%	0.0%	0.0%	82.7%	1.0%
Acetonitrile	0.0%	0.0%	62.7%	0.1%	0.0%	0.0%	0.0%	0.0%
Pyridine	0.0%	77.2%	0.0%	42.8%	99.1%	1.1%	0.0%	0.0%
3-Methylpyridine	0.0%	22.2%	0.0%	0.1%	0.1%	98.9%	0.0%	0.0%
N-butyronitrile	0.0%	0.0%	3.4%	6.6%	0.0%	0.0%	0.0%	0.0%
Water	99.0%	0.0%	15.0%	50.3%	0.0%	0.0%	12.3%	99.0%
Xylene	0.0%	0.0%	5.2%	0.0%	0.0%	0.0%	0.0%	0.0%
Benzene	0.0%	0.6%	0.0%	0.0%	0.8%	0.0%	5.0%	0.0%

Process Descriptions – Overview

Process 1: Pervaporation

Process 1, as seen in Figure 2 on pages 14-15, contains five distillation columns and one pervaporation unit. The removal of n-butyronitrile was given the highest priority because it can only be removed with the presence of the water azeotropes, and was achieved in column D101, along with the near complete removal of acetonitrile and xylene. This organic waste stream was then sent to a second distillation column, D102, for further processing to meet the on-site fuel specifications. The bottoms stream from D101 contained a mixture of water, methanol, pyridine and 3MP; this was sent to the pervaporation unit, PM101-PM103, with the goal of removing water and methanol. The three pervaporation modules successfully separate 98% of the water and methanol with low energy and utility requirements. To meet the waste water requirements, the methanol was separated from the water in column D103. Finally, the permeate was sent to the last two columns, D104 and D105, to isolate our products.

Process 2: Azeotropic Distillation

Process 2 is shown on p17-18 in Figure 3. The first two distillation columns in process 2, D201 and D203, are identical to D101 and D102 in process 1. Instead of using a pervaporation unit to remove water, we used an azeotropic distillation column with a benzene solvent. This was achieved with high recovery of pyridine and 3MP. Additionally, benzene was separated from water through a decanter, DE201, and recycled back into the column, D202. The water stream was then sent to column D204 in order to meet the waste water specification, while the pyridine and 3MP stream was sent to D205 for separation.

Detailed Process Descriptions:

Process 1: Pervaporation

N-butyronitrile/Xylene Removal

The main purpose of the first distillation column is to remove n-butyronitrile and xylene from the feed stream. The low boiling azeotropes of water with acetonitrile (76.65ºC), xylene (76.14ºC), and n-butyronitrile (86.08ºC), aid the removal of these components. The K-values, or the vapor-liquid distribution ratios, of the components in the column are shown in Figures 4 and 5. A higher K-value indicates a higher relative volatility and a greater likelihood that the component will leave from the overhead stream. Industrial standards, as stated in *Perry's Chemical Engineer's Handbook,* dictate that the relative volatility, which is the ratio of the K-value of the light key to the K-value of the heavy key, must be greater than 1.05. Other than acetonitrile, xylene and n-butyronitrile, the other components all have relative volatilities of 1 or less, which explains why they fall mostly to the bottom stream.

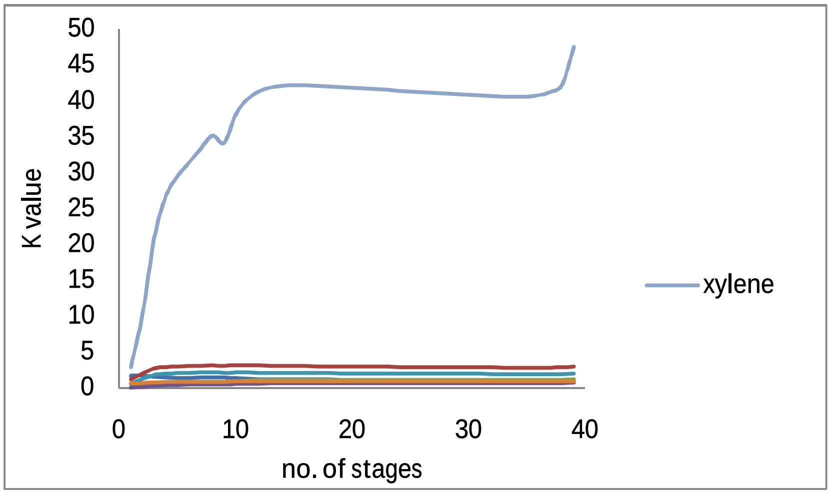

Figure 4: Xylene's K-value is much higher in comparison to all the other components in the system, and thus has the highest volatility.

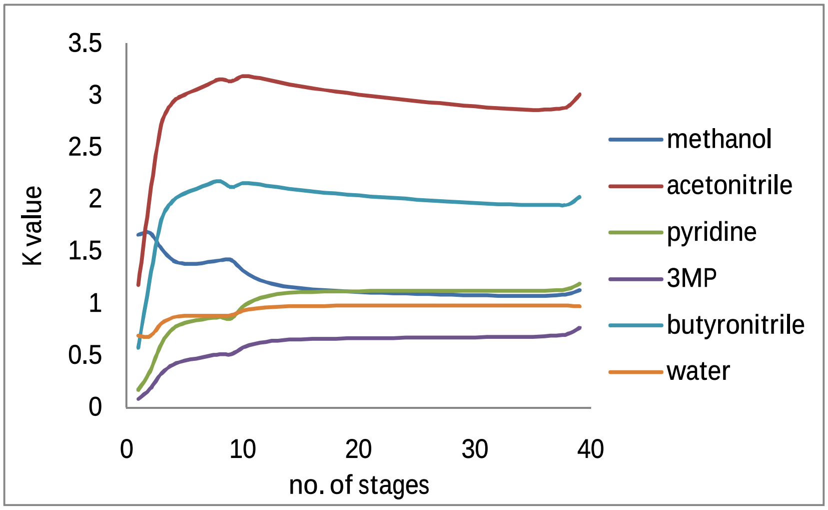

Figure 5: Figure 4 was rescaled to show the K-values of all the components minus xylene. N-butyronitrile and acetonitrile have the next 2 highest K-values, meaning they're relatively more volatile than the rest of the components.

In order to meet the intermediate finished goods specification for pyridine, the maximum amount of n-butyronitrile that could stay with the recovered pyridine in the bottom stream was 0.1 lb/hr. To meet this requirement, an iterative process was used to determine the appropriate distillate rate to be 634 lb/hr. Unfortunately, the large distillate rate also increased the amount of pyridine lost to the overhead. This unit resulted in the greatest loss of pyridine, almost 60 lb/hr, throughout the entire process.

Originally, the column was run with 50 stages. However, the composition profiles of the column, as seen in Figures 6 and 7, showed that some of the stages were unnecessary. The figures show the liquid composition of n-butyronitrile and xylene flattening out near the 40^{th} ideal stage; the very small composition of n-butyronitrile was again required to meet the specifications for pyridine. Thus the number of stages was set to 39.

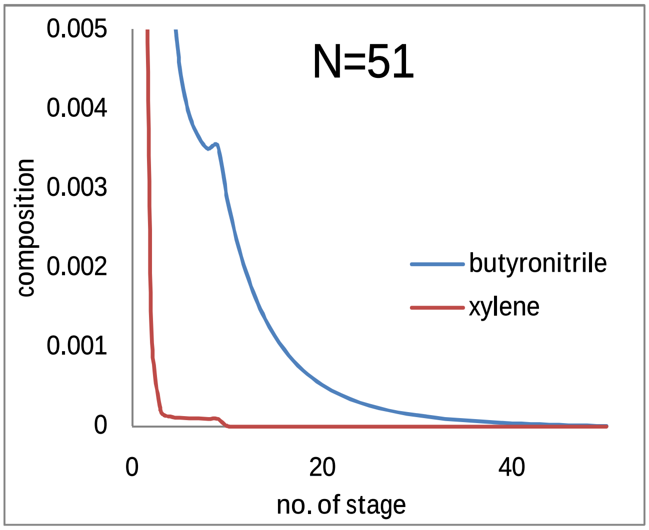

Figure 6: The liquid compositions of n-butyronitrile and xylene flatten out by the 40th stage.

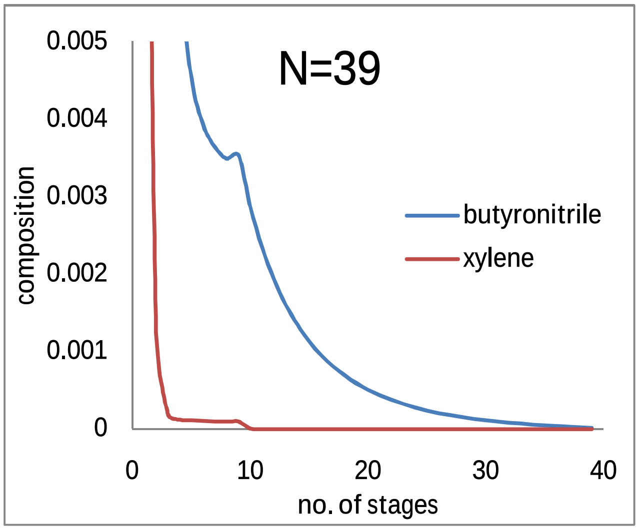

Figure 7: Only roughly 39 stages are necessary to achieve the desired separation.

The optimum combination of the number of stages and the reflux ratio had to be determined because it impacts the height and diameter of the column. Taking the number of stages to be 39, Aspen determined the reflux ratio of the column to be 3.5. Figure 8 shows the relationship between the reflux ratio and the number of ideal stages. As expected, the reflux ratio decreased with the increase in the number of stages. At a high number of stages, the reflux ratio stops decreasing and reaches an asymptote of 3. Thirty-nine stages is well before this asymptote; therefore it is a reasonable choice.

Additionally, tray sizing was done with sieve type trays with two passes; the resulting tray efficiency was found to be 56%, which meant that 66 real stages were required for this distillation column. The above method was used to optimize all the other distillation columns in this project.

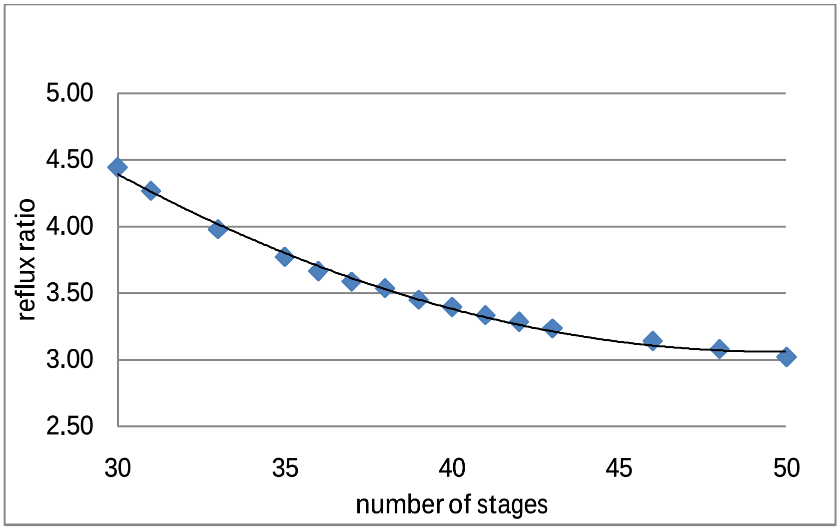

Figure 8: The plot of reflux ratio vs. the number of ideal stages flattens out as the number of stages increases beyond 40. 39 stages is taken as the optimum combination of the number of ideal stages and reflux ratio.

Our processes did not involve any manipulation of thermodynamic variables, and the selection of temperatures and pressures were chosen on a purely economic basis. The pressure of the top stage or the condenser was set to 15 psia. Although a higher pressure in the condenser and in the subsequent stages below would've resulted in a higher recovery of pyridine because of the higher reflux ratio that would've accompanied the new pressure. However, the relative gain in pyridine was inelastic to the increase in reflux ratio. In addition, the higher pressure in the condenser meant higher temperatures in the overhead and the bottoms stream, which is demonstrated in Figures 9 and 10.

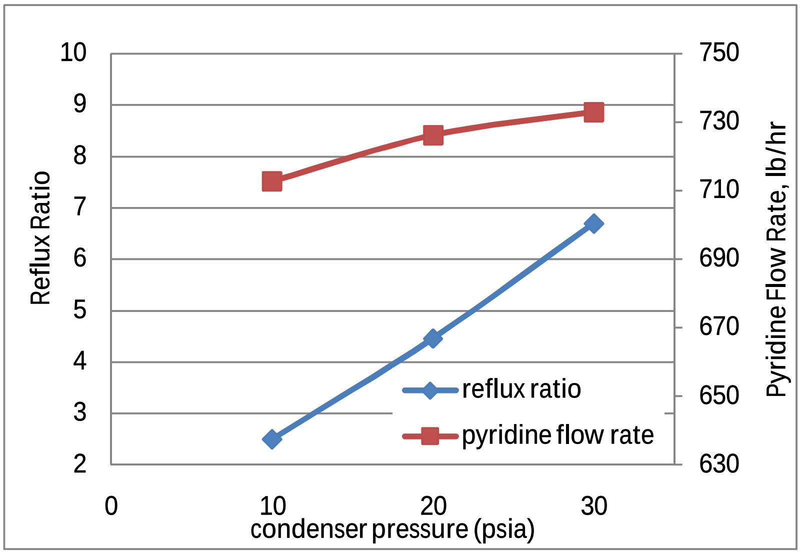

Figure 9: The rise in condenser pressure required relatively high reflux ratios to achieve similar or slightly improved separation.

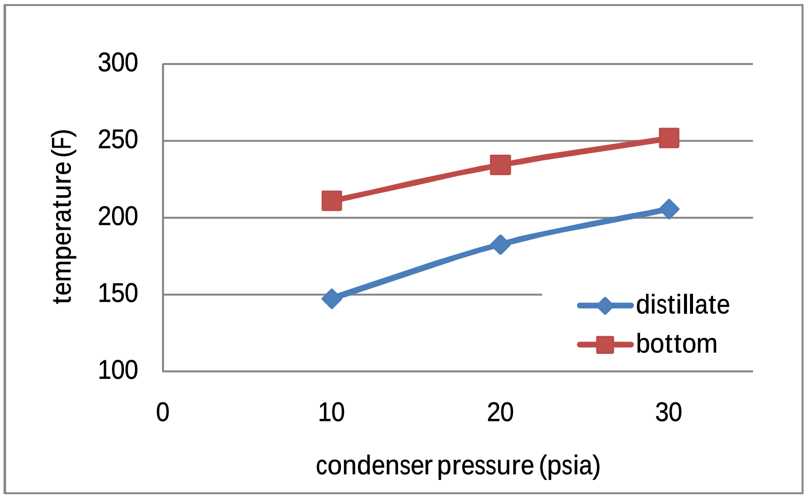

Figure 10: The rise in condenser pressure also increased the temperatures of the distillate and the bottom streams. This results in a higher utility cost.

Subsequently, the rise in pressure would've increased the utility cost of the condenser and the reboiler, as well as other heat exchangers needed to cool the product streams. The utility cost and the reflux ratio arising from the increase in pressure was not worth the additional recovery of pyridine. Therefore, the pressure was set to atmospheric pressure.

It was also found that an increase in feed temperature decreased the heat duty of the reboiler. The cost of adding a heater to preheat the feed stream before entering the distillation column was compared to the decrease in utility cost from the smaller heat duty. For example, heating the feed stream from 80°F to 170°F decreased the reboiler heat duty from 1.548 MBtu/hr to 1.375 MBtu/hr and resulted in a $5600 decrease in the annual utility cost. However, considering that the average bare module cost of the heat exchangers in our processes was $30,000, the money that could be saved by preheating the streams was not enough to offset the cost.

Organic Waste Treatment

The overhead from D101 consisted of a mixture of organic components and water. Because the concentration of water was so high in this stream, it would have been charged $0.20/lb if it was sent off site for disposal. This would amount to more than $1 million/year, which is far more than the bare module cost of a distillation column in our process. Therefore, a distillation column D102 was installed to purify the organic stream so that it could be used on site as fuel. This was done with relative ease as the only restriction to the distillate stream was to keep its water content below 15 wt% and pyridine below 5 wt%. The optimization process was performed in a manner similar to the other columns.

Pervaporation

Separation through pervaporation occurs through the selective adsorption of components through a membrane. To separate water from pyridine and 3MP, a hydrophilic membrane made out of poly(vinyl alcohol) was selected. The membrane preferentially forms hydrogen bonds with water and methanol in the feed solution; after adsorption, the compounds pass through the other side of the membrane as a vapor.

The flux of the compounds through the membrane is a function of the feed temperature and concentration, as well as the permeate pressure. The highest flux is obtained when the entering temperature and concentration of the permeating component are highest, and the pressure on the permeate side of the membrane is lowest. For this process a feed temperature of 158^{o}F was chosen, as it was sufficiently high to ensure a high flux, while not high enough to be in danger of membrane degradation, which occurs at temperatures above 300^{o}F. The concentration of water and methanol was fixed by the first distillation column. The permeate pressure was set to be a maximum 2.2 psia; lower pressures would not have significantly improved flux without adding heavily to the operating costs. The permeate pressure was achieved by immediately condensing the vapor permeate to a temperature that would yield a vapor pressure below 2.2 psia.

The mechanism of pervaporation results in a vapor permeate; the vaporization of the water and methanol results in a decrease in feed temperature across the membrane, as the energy required for vaporization must be taken from the feed stream. In order to prevent a large decrease in the flux towards the outlet end of the membrane, two inter-stage heaters were implemented to reheat the feed stream to its initial value. This was done by breaking the membrane into three separate modules with equal membrane area. It was assumed that the feed temperature dropped 15^{o}F across each membrane due to permeate vaporization, in accordance with values found by *Lipnizki, et al. 2002*. The inter-stage heaters require only 45lb/hr of low pressure steam combined to reheat the feed stream, and decrease the required membrane area by 5%, saving up to $30,520/year.

Permeate Water Waste Treatment

The permeate from the pervaporation unit consists mostly of water. However, the stream had to meet the condition of less than 1% organic and pH between 4 and 12. The pH requirement was easy to meet considering that the 92.4% of the stream was water which has a pH of 7. The main function of the water treatment was to remove more methanol from the stream so that the water in the bottom stream would be more than 99.0% pure. The distillation column was more rigorous than those that dealt with comparable amount of feed because of the tight purity requirement of water waste stream.

Recovery of 3MP and Pyridine from Retentate

The retentate from the pervaporation unit contained mostly pyridine and 3MP, which were separated through two distillation columns – the first removed 3MP in the bottom stream of D104, and the second removed pyridine in the bottom stream of D105. Since the azeotropes with water were no longer present in the system, the separation of our products was relatively easier to accomplish. We chose to first separate 3MP from the stream because its boiling point is much higher compared to the rest of the components. Its high boiling point also made 3MP the least volatile component in stream S107 and less likely to leave from the overhead of column D104. In order to achieve the greatest separation of 3MP from the rest of the stream, we used Apsen to create a liquid composition profile and were able to determine the number of ideal stages to be 21, which also gave the highest quality specification. We next proceeded to separate pyridine from the overhead of D104 but were unable to achieve the same finished goods specification as 3MP. The difference between water and pyridine's boiling points is not as great as that of 3MP and water and thus made the separation slightly more difficult. Since the relative volatilities of water and pyridine aren't as high, we would have lost a significant amount of pyridine to the overhead of D105 if we wanted to achieve the highest finished goods specification. Instead we met the intermediate quality specification with 98.4% pyridine purity. Had we met tried to purify to the highest standard, we would have lost 250 lb/hr of pyridine, or $8.5 million/year. Overall, we were able to recover 88.1% of the pyridine and 96% of the 3MP initially introduced into the system.

Process 2: Azeotropic Distillation

The removal of n-butyronitrile, xylene and acetonitrile for this process was the same as in Process 1.

Azeotropic Distillation

Benzene is often used in azeotropic distillation to overcome the azeotrope between water and an organic component such as ethanol. Benzene is highly immiscible with water, and causes water to be more volatile than it would be. The azeotrope between water and benzene is then the lightest boiler in the distillation column and both components are taken overhead,[3] leaving pyridine and 3MP at the bottom. The amount of benzene used in this column was approximately four times the amount of water in the system. Any less benzene would have produced an insufficient separation. Benzene was introduced to the upper part of the column, while the bottom stream from D201 entered the column towards the middle. Methanol was also taken out of the top as it is one of the lightest components in our system.

The distillate rate had to be high enough so that the maximum amount of water and benzene could be taken off the top; however, the distillate rate could not be higher than 4937 lb/hr, or additional pyridine would be lost in the overhead. The reflux ratio was set to return as much benzene back to the distillation column. The column had to take at least 98% of water in the feed stream to the overhead so that pyridine and 3MP could be purified to their product requirement.

The number of stages in the column was chosen in the same manner as that used in D101. After assuming a large number of stages, the liquid composition profile of the column was analyzed to deduce the unnecessary number of stages. Our finalized column had 20 ideal stages, or 34 real stages, and the liquid composition profile is shown in Figure 11.

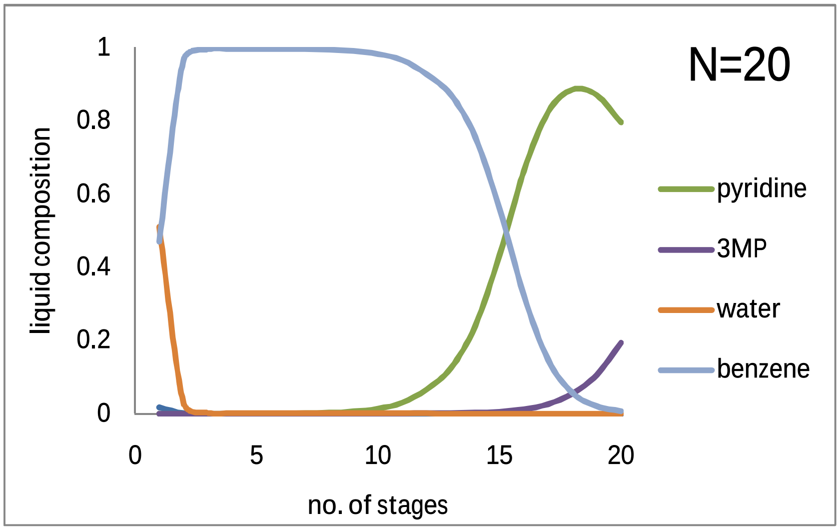

Figure 11: the liquid composition of benzene decreases sharply near the 15th stage.

The liquid composition of water decreases very rapidly near the bottom of the column while that of benzene needs many number of stages to achieve a low liquid composition.

The reflux ratio had to be high enough to ensure that a minimal amount of benzene would be found in the bottom stream of D202. It also had to take at least 98% of water in the feed stream to the overhead stream. Thus a high reflux ratio had to be set for a given a number of stages although it would increase the diameter of the column. The molar reflux ratio of 8 successfully removed almost all of the water and benzene to the overhead while leaving a bottom stream that consisted exclusively of pyridine and 3MP. Given the relatively small flow rate of our system, the increase in reflux ratio did not result in a significant increase in the column diameter.

The condenser pressure was set to 22 psia which was higher than the other columns in the process. A higher condenser pressure increases the amount of water and benzene in the overhead, which is necessary to achieve the desired separation; however, this comes at the cost of a relatively high reflux ratio. In addition, the benzene stream had to enter the column at a higher pressure to overcome the condenser pressure. Therefore, this solvent stream was set to 30 psia.

The benzene in the overhead had to be recycled back to the column with high purity to maintain a consistent input of benzene. The separation of benzene from water was achieved with relative ease with a decanter since the components are immiscible. The overhead of the azeotropic distillation column entered a decanter which successfully separated benzene from water and methanol. A purge stream of 5% was installed at the recycle stream to avoid build up of inerts. The recyle stream contained trace amounts of pyridine and 3MP, and thus their loss to the purge stream was insignificant. The water and methanol that left as the second liquid phase were separated by a later distillation column.

Water/Organic Waste Treatment

A distillation column treated the denser water phase from the decanter. The column had to separate the feed stream into a water stream and a methanol stream with enough purity to be stored and removed without an additional treatment cost. The column required 37 real stages and a molar reflux ratio of 3. The overhead was made mostly of methanol with 12.4% water, which qualified as on-site fuel. In order to dispose of the waste water at no additional cost, the stream had to contain no less than 99.0% water and trace amount of pyridine.

Separation of Pyridine and 3MP

The final step in this process was to separate pyridine and 3MP after leaving the azeotropic distillation column. Due to the high degree of purification, this stream only contained trace amounts of impurities and 5.6 lb/hr of benzene. The benzene is lighter than pyridine and therefore exits the overhead of D205 with the pyridine. This also prevents the pyridine from meeting the highest finished goods specification. Another rigorous distillation column could have been installed to separate the benzene from the pyridine, but this would not have been economically efficient. The separation of pyridine and 3MP was performed using 32 real stages and a molar reflux ratio of 4.8. The large reflux ratio was required to meet the purity specifications for the two key components. The overall process recovered 92.2% of the pyridine introduced to the system, and 99.7% of the 3MP.

UNIT DESCRIPTIONS

Process 1: Pervaporation

D101 (Distillation Column)

This unit is a non-foaming, carbon steel distillation column with sieve trays. The column takes in a feed of 2600 lb/hr, which enters at 131.5^oF. To account for possible entrainment flooding, only 85% of the flooding velocity was used in calculating the final diameter of 1.16 feet for the column. Additionally, taking into account a tray efficiency of 68% and assuming the ratio of downcomer area and cross-sectional area to be 0.2, the number of trays was calculated to be 66. The tray spacing is 2 feet, giving a length of 144 feet, and the shell thickness is 0.25 inch. The bare module cost of this column was calculated to be $433,000. The specification sheet is found on page 44.

D102(Distillation Column)

This unit is a non-foaming, carbon steel distillation column that uses sieve trays. The column takes in a stream of 1967 lb/hr from the bottom stream S203 at 221^oF in addition to the introduction of 207 lb/hr of a benzene solvent at 100 ^oF. The diameter of this unit is 5.32 feet and with a tray efficiency of 68%, the actual number of trays was found to be 34. This unit separates 99.3%, by mass fraction, of pyridine and 3-methylpyridine in the feed into this unit into the bottom, while about 77% of the distillate was made up of the benzene, which was recycled back into the column. The bare module cost of this column is $582,212. The specification sheet is found on page 46.

D103(Distillation Column)

This unit is a non-foaming, carbon steel distillation column that uses sieve trays and separates water and methanol out into storage tanks T104 and T105, respectively. The feed into this unit comes from the water/methanol mixture that pervaporation separated out from the bottoms stream of D101 and has a mass flow rate of 1034 lb/hr. The diameter of this unit is 1.14 feet and with a tray efficiency of 49%, the actual number of trays was found to be 37. The bare module cost of this column is $193,955. The specification sheet is found on page 48.

D104(Distillation Column)

This unit is a non-foaming, carbon steel distillation column that uses sieve trays. The feed into this column comes from stream S107, which contains our wanted products. The mass flow rate into this unit is 931 lb/hr. D104 separates out 99.6% of the 3MP in this stream out in the bottoms stream S111 and stores the product into tank T106. The diameter of this unit is 1.03 feet and with a tray efficiency of 53%, the actual number of trays was found to be 36. The bare module cost of this column is $244,984. The specification sheet is found on page 50.

D105(Distillation Column)

This unit is a non-foaming, carbon steel distillation column that uses sieve trays. The feed into this column comes from the distillate leaving D104, stream S110, which has a mass flow rate of 730 lb/hr. D105 separates out 97.4% of the pyridine that was in S110 into the bottoms stream, which is then sent to a storage tank T108. The distillate is a waste stream that will be sent to tank T107. The diameter of this unit is 0.35 feet and with a tray efficiency of

52%, the actual number of trays was found to be 19. The bare module cost of this column is $145,461. The specification sheet is found on page 52.

PM 101-103 (Pervaporation Modules)

These are three identical pervaporation modules, each containing 509m^2 of membrane for a total of 1526m^2. The feed stream enters at 158^oF with 52.7% methanol and water; the retentate leaves with only 2.2% methanol and water. There is a 2% loss of pyridine and 3MP through the membrane (14.4lb/hr pyridine, 4.15lb/hr 3MP). The vaporization of the permeate results in a 15^oF temperature drop through each module. The total bare module cost for all 3 modules is $2,839,007, assuming a bare module factor of 2.0. The specification sheet is found on page 54.

H100 (Heat Exchanger)

This shell-and-tube heat exchanger heats the feed stream S101 from 80^oF to 131.5^oF before it can enter the first distillation column D101, while cooling S103 from 221^oF to 158^oF before it enters the pervaporation modules. The bare module cost of the heat exchanger is $33,655. The specification sheet is found on page 63.

H107-H108(Heat Exchangers)

The heat exchangers reheat the retentate in between each pervaporation module back to 158^oF. H107 treats 1385.5lb/hr of retentate, while H108 treats 1034.6lb/hr. They require a combined of 45lb/hr of low pressure steam to achieve the 37,876Btu/hr of heating needed. Each heat exchanger has a bare module cost of approximately $43,746. The specification sheet is found on page 66.

H109(Heat Exchangers)

The heat exchanger condenses the permeate vapor to 131°F to create a pressure of 2.2psia. The mass flow rate through the condenser is 1035.5lb/hr, and requires a heat duty of -1,028,180 Btu/hr. The condensation is achieved by using 34,273lb/hr cooling water. The bare module cost of the heat exchanger is $38,651. The specification sheet is found on page 68.

For additional unit specifications, see p.44.

Process 2: Azeotropic Distillation

T201 (Storage Tank)

T201 is an API standard vertical coned-roof storage tank that contains 14 days worth of feed for continuous operation in the extractive distillation process. The carbon steel tank is 85% full with a volume of 132,817 gallons, which holds 874,000 lbs, and holds the fluids at a pressure of 15 psi and temperature of 80°F. The total mass flow rate of the given feed stream (S201) is 2600 lb/hr and the stream is composed of a mixture of methanol, pyridine, 3-methylpyridine, acetonitrile, n-butyronitrile, xylene (o, m and p) and water. The total bare module cost for this storage tank is $381,156, and a more complete specification sheet can be found on page 55.

P200 (Fluid Moving Pump)

P200 is a centrifugal single stage cast iron pump that pumps the feed stream (S201) of 2600 lb/hr into the first distillation column, D201, by increasing the pressure by 25 psi from 15 to 40 psi. At an efficiency of 70%, this pump has a head of approximately 177 feet, which needs a power requirement of about 20 hp. The total bare module cost of P200 is $12,286. More information can be found on the specification sheet on page 97.

D201 (Distillation Column)

This unit is a non-foaming, carbon steel distillation column with sieve trays. The column takes in a feed of 2600 lb/hr, which also enters at 80^{o}F. To account for possible entrainment flooding, only 85% of the flooding velocity was used in calculating the final diameter of 1.16 feet for the column. Additionally, taking into account a tray efficiency of 68% and assuming the ratio of downcomer area and cross-sectional area to be 0.2, the number of trays was calculated to be 66. The tray spacing is 2 feet, giving a length of 144 feet, and the shell thickness is 0.25 inch. The bare module cost of this column was calculated to be $433,099. The specification sheet is found on page 44.

H201 (Cooling Water)

The heat exchanger cools the stream leaving the condenser, S202, which has a mass flow rate of 4657.6 lb/hr and a heating duty of -12.94 MBtu/hr. The unit cools the stream from 167^{o}F to 120^{o}F. The amount of cooling water required for this unit is 412 gal/hr, which only costs approximately $0.03. The bare module cost of the heat exchanger is $33,900. The specification sheet is found on page 45.

P201 (Condenser Pump)

This pump takes in a portion of the distillate (S202) leaving D201 that goes through reflux accumulator A201, which has a mass flow rate of 2815.5 lb/hr. Acetonitrile makes up

40% (by mole fraction) of the stream, and the pump head is found to be 3.14 feet with a size factor of 13.6. The total bare module cost of this unit is $18,656. The specification sheet is found on page 45.

A201 (Reflux Accumulator)

This reflux accumulator is assumed to be a horizontal pressure vessel that is only 85% full and has a residence time of 0.25 hour. Additionally, with an aspect ratio of 2, the length and diameter were calculated to be 5.11 and 2.56 feet, respectively. The stream leaving the reflux accumulator feeds directly into pump P201, and the mass flow rate of this stream is 2815.5 lb/hr. The operating pressure inside this unit is 10 psig, and the total bare module cost is $15,057. The specification sheet is found on page 45.

P202 (Reboiler pump)

This centrifugal single stage cast iron pump increases the pressure of the bottoms stream S203 leaving the first distillation column D201, which has a mass flow rate of 4657.55 lb/hr, by 0.22 psi. With an efficiency of 68%, the pump head and size factor were found to be 8.41 feet and 10.5, respectively. The stream leaving this pump is then sent to a heat exchanger, H202, which is supplied with low pressure steam. The total bare module cost of P202 is $20,349. The specification sheet is found on page 45.

H202 (Low Pressure Steam)

This unit heats the stream, which has a mass flow rate of 1966 lb/hr, leaving the pump P202 with low pressure steam. The amount of steam required to heat this stream is 1691 lb/hr or

1.85 Btu/hr, and the total utility cost for this unit is about $44,000/year. Additionally, the bare module cost is $34,191. The specification sheet is found on page 45.

DE201 (Decanter)

The stream entering this decanter, S205, has a mass flow rate of 4938 lb/hr and separates out 99.2% of the benzene in the entering stream into a separate stream, S206, that is then recycled back into the second distillation column D202. The second stream leaving the decanter, S208, is then sent to distillation column D205, where methanol and water will be separated out and placed into storage tanks. The bare module cost of the decanter is $14,657. The specification sheet is found on page 86.

H208 (before storage)

This shell-and-tube heat exchanger cools the portion of stream S211 leaving H207 to 80^{o}F before the organic waste can be placed into storage tank T205. The amount of cooling water required for this unit is 56.3 gal/hr. The bare module cost of the heat exchanger is approximately $43,746. The specification sheet is found on page 65.

D202 (Distillation Column)

This unit is a non-foaming, carbon steel distillation column that uses sieve trays. The column takes in a stream of 1967 lb/hr from the bottom stream S203 at 221^{o}F in addition to the introduction of 207 lb/hr of a benzene solvent at 100 ^{o}F. The diameter of this unit is 5.32 feet and with a tray efficiency of 68%, the actual number of trays was found to be 34. This unit separates 99.3%, by mass fraction, of pyridine and 3-methylpyridine in the feed into this unit into the bottom, while about 77% of the distillate was made up of the benzene, which was recycled back into the column. The bare module cost of this column is $582,212. The specification sheet is found on page 80.

D203 (Distillation Column)

This unit is a non-foaming, carbon steel distillation column that uses sieve trays. The feed into this column comes from a portion of the distillate from column D201 and has a mass flow rate of 633 lb/hr at 167 ^{o}F. In this unit, the distillate stream S219 and the bottom stream S211 contain waste that can be used as fuel and an organic stream that needs to be sent away for treatment at a cost of $0.20/lb, respectively. The diameter of this unit is 1.16 feet and with a tray efficiency of 68%, the actual number of trays was found to be 19. There are 497 lb/hr that can be reused as fuel, while 136 lb/hr of the organic waste needs to be treated. The bare module cost of this column is $160,743. The specification sheet is found on page 46.

D204 (Distillation Column)

This unit is a non-foaming, carbon steel distillation column that uses sieve trays. The feed into this column comes from the bottom stream S209 leaving the distillation column D202 and has a mass flow rate of 935 lb/hr at 283^{o}F. This unit separates out pyridine and 3-methylpyridine from the top and bottom, respectively, and are then stored into tanks T206 and T207. The diameter of this unit is 1.34 feet and with a tray efficiency of 52%, the actual number of trays was found to be 13. The bare module cost of this column is $136,409. The specification sheet is found on page 82.

D205 (Distillation Column)

This unit is a non-foaming, carbon steel distillation column that uses sieve trays. The feed into this column comes from stream S208 leaving decanter DE201 after most of the benzene has been separated out. The mass flow rate of this unit is 1030 lb/hr at 100°F. D205 separates out methanol and water from the top and bottom, respectively, and are then stored into tanks T208 and T209. The diameter of this unit is 0.49 feet and with a tray efficiency of 49%, the actual number of trays was found to be 37. The bare module cost of this column is $189,543. The specification sheet is found on page 84.

For additional unit specifications, see p.44.

Approximations and Difficulties

The pervaporation modules required several assumptions to be made, including average flux, temperature drop through the membrane, membrane price, membrane lifetime, and feed temperature and pressure. Appropriate ranges for these values were obtained from *Drioli et al. 1993*, and from numbers suggested by Mr. Bruce Vrana, one of our industrial consultants. For the economic analysis, the values chosen were all on the conservative end of the ranges; a sensitivity analysis was later performed to obtain the dependence of profitability on the factors. The assumed values were: an inlet temperature of 158^{o}F, a temperature drop through each module of 15^{o}F, a permeate pressure of 2.2 psia, an average flux of 1.1 lb/m^2-hr, a membrane lifetime of 1 year, and a membrane cost of \$400/m^2.

Another difficulty encountered during the calculation was how many pervaporation modules to use. Ideally, we would have optimized the membrane area against the reheating cost for various numbers of modules; however, since the temperature drop was an assumed number, the optimization could not be performed. Three modules were chosen (with 2 inter-stage heaters) since many pervaporation processes in industry use three modules. The module design was chosen as a plate-in-frame model, again due to its overwhelming use in industry.

Finally, an issue that was present in nearly all pump calculations and some heat exchanger calculations was the size of the stream passing through the unit. The small flow rates resulted in sizing factors that were well below the lower limits for correlations found in *Seider et al., 2009*. In most cases, if the prices and sizes for the equipment seemed reasonable, the correlations were maintained. Several units, however, differed from average values by nearly two orders of magnitude; these units would need to be more precisely sized before moving forward with the design.

Heat Integration

Due to the presence of multiple distillation columns, heat integration is a viable method that could save on heating and cooling utility costs. A minor heat integration analysis was done on both processes, and H100 took advantage of the excess heat in S103 to preheat S101 before it entered the first distillation column. This saved a total of 107.6 lb/hr low pressure steam and 31,600 lb/hr cooling water. While there are other opportunities for heat integration in both processes, this was the largest opportunity to save on utilities.

PROCESS 1 - PERVAPORATION

DISTILLATION COLUMN

Identification:	Item	Distillation Column		
	Item No.	D-101/D-201	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	138,435	C_{BM}($):	542,344

Function: To separate n-butyronitrile from the product stream.
Operation: Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*Bottoms*	*Distillate*
Methanol	130.00	62.22	67.78
Acetonitrile	312.00	0.00	312.00
Pyridine	780.00	720.60	59.40
3-Methylpyridine	208.00	207.83	0.17
n-butyronitrile	26.00	0.06	25.94
Water	1118.00	975.47	142.53
Xylene	26.00	0.00	26.00
Total	2600.00	1966.18	633.82
Temperature(F):	80.0	223.7	167.4
Pressure(psia):	15.0	22.6	15.0
Vapor fraction	0.0	0.0	0.0

Design Data:

Number of stages:	66	Column Height:	144	ft
Feed Stage:	13	Inside Diameter:	1.34	ft
Reflux Ratio:	3.45	Tray spacing:	2	ft
Tray efficiency:	56.0%	Material:	carbon steel	
Tray type:	sieve			

Utilities:	Cooling water:	$	3,402	/yr
	Steam:	$	44,443	/yr

Associated Components:

Tower

Equip. type	Vertical Vessel		
Weight		6361.47	lb
Thickness		0.25	in
C_{BM}	$	433,099	

Condenser

Equip. type	Fixed Head heat exchanger		
Heat Duty		1,294,241	Btu/hr
Area		185.60	ft^2
Material	carbon steel		
C_{BM}	$	33,900	

Reboiler

Equip. type	Fixed Head heat exchanger		
Heat Duty		1,542,316	Btu/hr
Area		57.96	ft^2
Material	carbon steel		
C_{BM}	$	34,191	

Reflux Accumulator

Equip. type	Horizontal Vessel		
Res. Time		5.00	min
Length		2.58	ft
Depth		1.29	ft
Weight		151.54	lb
C_{BM}	$	15,057	

Reflux Pump

Equip. type	Centrifugal Pump		
Power Req'd		17.52	Hp
Pump Head		143.71	ft
Efficiency		70%	
C_{BM}	$	11,975	

Reboiler Pump

Equip. type	Centrifugal Pump		
Power Req'd		1.70	Hp
Pump Head		8.41	ft
Efficiency		70%	
C_{BM}	$	14,123	

Comments:

DISTILLATION COLUMN

Identification:	Item	Distillation Column		
	Item No.	D-102/D-203	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	76,557	C_{BM}($):	278,928

Function: To reduce the amount of organic waste in the process.

Operation: Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*Bottoms*	*Distillate*
Methanol	67.78	0.09	67.48
Acetonitrile	312.00	0.19	311.81
Pyridine	59.40	58.03	0.04
3-Methylpyridine	0.17	0.17	0.00
n-butyronitrile	25.94	8.91	17.04
Water	142.53	68.32	74.63
Xylene	26.00	0.00	26.00
Total	633.8	135.7	497.0
Temperature(F):	167.4	208.8	163.1
Pressure(psia):	15.0	17.7	15.0
Vapor fraction	0.0	0.0	0.0

Design Data:

Number of stages:	19	Column Height:	50	ft
Feed Stage:	6	Inside Diameter:	1.16	ft
Reflux Ratio:	3	Tray spacing:	2	ft
Tray efficiency:	58.3%	Material:	carbon steel	
Tray type:	sieve			

Utilities:	Cooling water:	$	2,191	/yr
	Steam:	$	24,050	/yr

Associated Components:

Tower

Equip. type	Vertical Vessel		
Weight		1767.48	lb
Thickness		0.25	in
C_{BM}	$	160,743	

Condenser

Equip. type Fixed Head heat exchanger

	Heat Duty	833,559	Btu/hr
	Area	119.56	ft^2
	Material	carbon steel	
	C_{BM}	$ 34,453	
Reboiler			
	Equip. type	Fixed Head heat exchanger	
	Heat Duty	834,636	Btu/hr
	Area	31.36	ft^2
	Material	carbon steel	
	C_{BM}	$ 37,906	
Reflux Accumulator			
	Equip. type	Horizontal Vessel	
	Res. Time	5.00	min
	Length	3.05	ft
	Depth	1.53	ft
	Weight	212.34	lb
	C_{BM}	$ 15,466	
Reflux Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	0.13	Hp
	Pump Head	50.79	ft
	Efficiency	70%	
	C_{BM}	$ 15,180	
Reboiler Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	0.53	Hp
	Pump Head	7.15	ft
	Efficiency	70%	
	C_{BM}	$ 15,180	
Comments:	Reflux pump bare module cost did not fall within the approriate range for the correlations		

DISTILLATION COLUMN

Identification:	Item	Distillation Column		
	Item No.	D-103	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	93,103	C_{BM}($):	342,175

Function:	To reduce the amount of organic waste in the process.
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*Bottoms*	*Distillate*
Methanol	60.90	3.24	57.66
Acetonitrile	0.00	0.00	0.00
Pyridine	14.37	4.57	9.80
3-Methylpyridine	3.17	0.55	2.62
n-butyronitrile	0.00	0.00	0.00
Water	955.97	924.47	31.50
Xylene	0.00	0.00	0.00
Total	1034.41	932.83	101.58
Temperature(F):	80.0	223.5	167.9
Pressure(psia):	15.0	18.8	15.0
Vapor fraction	0.0	0.0	0.0

Design Data:

Number of stages:	37	Column Height:	86	ft
Feed Stage:	8	Inside Diameter:	1.14	ft
Reflux Ratio:	5	Tray spacing:	2	ft
Tray efficiency:	49.1%	Material:	carbon steel	
Tray type:	sieve			

Utilities:	Cooling water:	$	277	/yr
	Steam:	$	14,581	/yr

Associated Components:

Tower

Equip. type	Vertical Vessel	
Weight	3228.50	lb
Thickness	0.25	in
C_{BM}	$ 193,955	

Condenser

Equip. type	Fixed Head heat exchanger	
Heat Duty	131,738	Btu/hr

	Area	10.85	ft^2
	Material	carbon steel	
	C_{BM}	$ 55,338	
Reboiler			
	Equip. type	Fixed Head heat exchanger	
	Heat Duty	506,015	Btu/hr
	Area	54.76	ft^2
	Material	carbon steel	
	C_{BM}	$ 35,304	
Reflux Accumulator			
	Equip. type	Horizontal Vessel	
	Res. Time	5.00	min
	Length	1.40	ft
	Depth	0.70	ft
	Weight	45.35	lb
	C_{BM}	$ 17,614	
Reflux Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	2.20	Hp
	Pump Head	83.28	ft
	Efficiency	70%	
	C_{BM}	$ 18,431	
Reboiler Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	0.50	Hp
	Pump Head	7.75	ft
	Efficiency	70%	
	C_{BM}	$ 21,533	

Comments:

DISTILLATION COLUMN

Identification:	Item	Distillation Column		
	Item No.	D-104	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	102,429	C_{BM}($):	383,595

Function:	To separate purified 3MP from organic stream
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*Bottoms*	*Distillate*
Methanol	1.25	0.00	1.25
Acetonitrile	0.00	0.00	0.00
Pyridine	706.29	1.11	705.18
3-Methylpyridine	203.67	199.68	3.99
n-butyronitrile	0.06	0.00	0.06
Water	0.00	0.00	0.00
Xylene	19.52	0.00	19.52
Total	930.79	200.79	730.00
Temperature(F):	140.0	307.9	224.8
Pressure(psia):	15.0	18.9	15.0
Vapor fraction	0.0	0.0	0.0

Design Data:

Number of stages:	36	Column Height:	84	ft
Feed Stage:	15	Inside Diameter:	1.03	ft
Reflux Ratio:	1.5	Tray spacing:	2	ft
Tray efficiency:	52.8%	Material:	carbon steel	
Tray type:	sieve			

Utilities:	Cooling water:	$	1,054	/yr
	Steam:	$	12,817	/yr

Associated Components:

Tower

Equip. type	Vertical Vessel		
Weight		2863.01	lb
Thickness		0.25	in
C_{BM}	$	244,984	

Condenser

Equip. type	Fixed Head heat exchanger		
Heat Duty		401,154	Btu/hr

	Area	12.85	ft^2
	Material	carbon steel	
	C_{BM}	$ 40,391	
Reboiler			
	Equip. type	Fixed Head heat exchanger	
	Heat Duty	444,784	Btu/hr
	Area	25.51	ft^2
	Material	carbon steel	
	C_{BM}	$ 51,399	
Reflux Accumulator			
	Equip. type	Horizontal Vessel	
	Res. Time	5.00	min
	Length	1.83	ft
	Depth	0.91	ft
	Weight	76.49	lb
	C_{BM}	$ 15,873	
Reflux Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	6.54	Hp
	Pump Head	82.84	ft
	Efficiency	70%	
	C_{BM}	$ 14,121	
Reboiler Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	0.95	Hp
	Pump Head	7.87	ft
	Efficiency	70%	
	C_{BM}	$ 16,829	

Comments:

DISTILLATION COLUMN

Identification:	Item	Distillation Column		
	Item No.	D-105	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	72,288	C_{BM}($):	264,051

Function:	To separate pyridine to obtain final product
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*Bottoms*	*Distillate*
Methanol	1.25	0.08	1.17
Acetonitrile	0.00	0.00	0.00
Pyridine	705.18	687.09	18.09
3-Methylpyridine	3.99	3.99	0.00
n-butyronitrile	0.06	0.06	0.00
Water	0.00	0.00	0.00
Xylene	19.52	7.15	12.37
Total	730.00	698.36	31.64
Temperature(F):	224.8	242.9	198.8
Pressure(psia):	15.0	17.5	15.0
Vapor fraction	0.0	0.0	0.0

Design Data:

Number of stages:	19	Column Height:	50	ft
Feed Stage:	10	Inside Diameter:	1.55	ft
Reflux Ratio:	2.6	Tray spacing:	2	ft
Tray efficiency:	51.8%	Material:	carbon steel	
Tray type:	sieve			

Utilities:	Cooling water:	$	157	/yr
	Steam:	$	1,874	/yr

Associated Components:

Tower

Equip. type	Vertical Vessel		
Weight		598.90	lb
Thickness		0.25	in
C_{BM}	$	145,461	

Condenser

Equip. type	Fixed Head heat exchanger		
Heat Duty		59,825	Btu/hr

	Area	2.52	ft^2
	Material	carbon steel	
	C_{BM}	$ 35,304	
Reboiler			
	Equip. type	Fixed Head heat exchanger	
	Heat Duty	65,046	Btu/hr
	Area	3.73	ft^2
	Material	carbon steel	
	C_{BM}	$ 37,602	
Reflux Accumulator			
	Equip. type	Horizontal Vessel	
	Res. Time	5.00	min
	Length	0.95	ft
	Depth	0.47	ft
	Weight	21.12	lb
	C_{BM}	$ 19,284	
Reflux Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	0.24	Hp
	Pump Head	48.71	ft
	Efficiency	70%	
	C_{BM}	$ 13,200	
Reboiler Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	0.32	Hp
	Pump Head	7.50	ft
	Efficiency	70%	
	C_{BM}	$ 13,200	
Comments:	The bare module cost of the reboiler pump and the reflux pump did not fall within the appropriate range for the correlations		

PERVAPORATION MODULES

Identification:	Item	Membrane Module		
	Item No.	PM101-PM103	Date:	4/13/2010
	No. required	3	By:	RC/CC/SK/BL
	C_{TPI}($):	1,456,328	C_{BM}($):	$2,912,656

Function:	To remove water and methanol from the pyridine product stream
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*Permeate*	*Retentate*
Methanol	62.27	61.02	1.25
Acetonitrile	0.00	0.00	0.00
Pyridine	720.70	14.41	706.29
3-Methylpyridine	207.83	4.16	203.67
n-butyronitrile	0.06	0.00	0.06
Water	975.42	955.91	19.51
Xylene	0.00	0.00	0.00
Total	1966.28	1035.51	930.77
Temperature(F):	158.0	144.0	131.0
Pressure(psia):	21.0	2.2	15.0
Vapor fraction	0.0	1.0	0.0

Design Data:

Module type	plate and frame		
Membrane Area	509	m^2 /module	1526.5 m^2 total
Membrane lifetime	1	years	
ΔT/module	15	F	

Comments: Several assumptions were made in the calculation of the module specs, including average flux, membrane lifetime, temperature loss, and permeate pressure.

FEED STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-101/T-201	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	$ 124,969	C_{BM}($):	$ 381,156
Function:	To store 14 days worth of feed.			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Feed*	*wt. %*		
Methanol	130.00	5.0		
Acetonitrile	312.00	12.0		
Pyridine	780.00	30.0		
3-Methylpyridine	208.00	8.0		
n-butyronitrile	26.00	1.0		
Water	1118.00	43.0		
Xylene	26.00	1.0		
Total	2600.00	100.0		
Temperature(F):	100.0			
Pressure(psia):	15.0			
Vapor fraction	0.0			
Design Data:				
Days Stored	14			
Total Volume	132,817	gal		
Material	Carbon Steel			
Pressure	15	psi		
Comments:				

ORGANIC WASTE STORAGE TANK (USED AS FUEL)

Identification:	Item	API Tank		
	Item No.	T-102/T-204	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	59,401	C_{BM}($):	181,173

Function:	To store 14 days worth of n-butyronitrile.
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*wt. %*
Methanol	67.48	13.6
Acetonitrile	311.81	62.7
Pyridine	0.04	0.0
3-Methylpyridine	0.00	0.0
n-butyronitrile	17.04	3.4
Water	74.63	15.0
Xylene	26.00	5.2
Total	497.0	100.00
Temperature(F):	100.0	
Pressure(psia):	15.0	
Vapor fraction	0.0	

Design Data:

Days Stored	14	
Total Volume	40,869	gal
Material	Carbon Steel	
Pressure	15	psi

Comments: The liquid organic waste stream is <5% pyridine and <15% water; therefore, it will be used on-site as fuel.

ORGANIC WASTE STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-103/T-205	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	26,891	C_{BM}($):	82,018

Function:	To store 14 days worth of organic waste.
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*wt. %*
Methanol	0.09	0.1
Acetonitrile	0.19	0.1
Pyridine	58.03	42.8
3-Methylpyridine	0.17	0.1
n-butyronitrile	8.91	6.6
Water	68.32	50.3
Xylene	0.00	0.0
Total	135.70	100.0
Temperature(F):	100.0	
Pressure(psia):	15.0	
Vapor fraction	0.0	

Design Data:

Days Stored	14	
Total Volume	11,677	gal
Material	Carbon Steel	
Pressure	15	psi

Comments: Because the liquid organic waste stream is >15% water it will be sent off site for disposal at a cost of $0.20/lb

METHANOL WASTE STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-104	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	24,066	C_{BM}($):	73,402

Function:	To store 14 days worth of methanol waste.
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*wt. %*
Methanol	57.66	56.8
Acetonitrile	0.00	0.0
Pyridine	9.80	9.6
3-Methylpyridine	2.62	2.6
n-butyronitrile	0.00	0.0
Water	31.50	31.0
Xylene	0.00	0.0
Total	101.58	100.0
Temperature(F):	100.0	
Pressure(psia):	15.0	
Vapor fraction	0.0	

Design Data:

Days Stored	14	
Total Volume	8,174	gal
Material	Carbon Steel	
Pressure	15	psi

Comments: Because the liquid organic waste stream is >15% water it will be sent off site for disposal at a cost of $0.20/lb

WATER STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-105	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	74,782	C_{BM}($):	228,084
Function:	To store 14 days worth of water.			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Feed*	*wt. %*		
Methanol	3.24	0.3		
Acetonitrile	0.00	0.0		
Pyridine	4.57	0.5		
3-Methylpyridine	0.55	0.1		
n-butyronitrile	0.00	0.0		
Water	924.47	99.1		
Xylene	0.00	0.0		
Total	932.83	100.0		
Temperature(F):	100.0			
Pressure(psia):	15.0			
Vapor fraction	0.0			
Design Data:				
Days Stored	14			
Total Volume	81,738	gal		
Material	Carbon Steel			
Pressure	15	psi		
Comments:	The water meets purity standards to be processed without additional cost			

3MP STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-106	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	35,640	C_{BM}($):	108,703

Function:	To store 14 days worth of 3-methylpyridine.
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*wt. %*
Methanol	0.00	0.0
Acetonitrile	0.00	0.0
Pyridine	1.11	0.6
3-Methylpyridine	199.68	99.4
n-butyronitrile	0.00	0.0
Water	0.00	0.0
Xylene	0.00	0.0
Total	200.79	100.0
Temperature(F):	100.0	
Pressure(psia):	15.0	
Vapor fraction	0.0	

Design Data:

Days Stored	14	
Total Volume	11,347	gal
Material	Carbon Steel	
Pressure	15	psi

Comments: The 3-methylpyridine meets the Finished Goods Quality Specifications.

WASTE STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-107	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	13,193	C_{BM}($):	40,239

Function:	To store 14 days worth of pyridine waste.
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*wt. %*
Methanol	1.17	3.7
Acetonitrile	0.00	0.0
Pyridine	18.09	57.2
3-Methylpyridine	0.00	0.0
n-butyronitrile	0.00	0.0
Water	12.37	39.1
Xylene	0.00	0.0
Total	31.63	100.0
Temperature(F):	100.0	
Pressure(psia):	15.0	
Vapor fraction	0.0	

Design Data:

Days Stored	14	
Total Volume	1,617	gal
Material	Carbon Steel	
Pressure	15	psi

Comments: Because the liquid organic waste stream is >15% water it will be sent off site for disposal at a cost of $0.20/lb

PYRIDINE STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-108	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	65,212	C_{BM}($):	198,897

Function:	To store 14 days worth of pyridine.
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*wt. %*
Methanol	0.08	0.0
Acetonitrile	0.00	0.0
Pyridine	687.09	98.4
3-Methylpyridine	3.99	0.6
n-butyronitrile	0.06	0.0
Water	7.15	1.0
Xylene	0.00	0.0
Total	698.37	100.0

Temperature(F):	100.0
Pressure(psia):	15.0
Vapor fraction	0.0

Design Data:

Days Stored	14	
Total Volume	37,101	gal
Material	Carbon Steel	
Pressure	15	psi

Comments: The pyridine meets the Intermediate Quality Specifications

HEAT EXCHANGER

Identification:	Item	Heat Exchanger		
	Item No.	H-100	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	10,617	C_{BM}($):	33,655

Function:	To cool S103 before entering PM-101 and preheat S101 before entering D101
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol	130.00	130.00	62.27	62.27
Acetonitrile	312.00	312.00	0.00	0.00
Pyridine	780.00	780.00	720.70	720.70
3-Methylpyridine	208.00	208.00	207.83	207.83
n-butyronitrile	26.00	26.00	0.06	0.06
Water	1118.00	1118.00	975.42	975.42
Xylene	26.00	26.00	0.00	0.00
Total	2600.00	2600.00	1966.28	1966.28
Temperature(F):	80.0	131.5	221.0	158.0
Pressure(psia):	20.0	15.0	36.0	31.0
Vapor fraction	0.0	0.0	0.0	0.0

Design Data:

Q	1444168.7	Btu/hr	Thi	221.0 F
Uo	100.0	Btu/hr-ft2-F	Tho	158.0 F
A	172.7	ft2	Tci	80.0 F
Material	carbon steel		Tco	131.5 F
			ΔTLM	83.6 F

Utilities:	Cooling water:	0
	Steam:	0
	Electricity:	0

Comments:

CONDENSER

Identification:	Item	Heat Exchanger		
	Item No.	H-104/H-206	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	19,476	C_{BM}($):	61,740

Function: To cool organic fuel stream to storage.
Operation: Continuous

Materials Handled:

Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol			67.48	67.48
Acetonitrile			311.81	311.81
Pyridine			0.04	0.04
3-Methylpyridine			0.00	0.00
n-butyronitrile			17.04	17.04
Water	27813.11	27813.11	74.63	74.63
Xylene			26.00	26.00
Total	27813.11	27813.11	497.00	497.00
Temperature(F):	90.0	120.0	163.1	100.0
Pressure(psia):	15.0	15.0	15.0	10.0
Vapor fraction	0.0	0.0	0.0	0.0

Design Data:

Q	833,559	Btu/hr	Thi	163.1 F
Uo	250	Btu/hr-ft2-F	Tho	100.0 F
A	147.2	ft2	Tci	90.0 F
Material			Tco	120.0 F
			ΔTLM	22.7 F

Utilities: Cooling water: 1378.8 lb/hr

Comments:

CONDENSER

Identification:	Item	Heat Exchanger		
	Item No.	H-106/H-208	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	13,800	C_{BM}($):	43,746

Function:	To cool organic waste stream to storage
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol			0.09	0.09
Acetonitrile			0.19	0.19
Pyridine			58.03	58.03
3-Methylpyridine			0.17	0.17
n-butyronitrile			8.91	8.91
Water	16884.06	16884.06	68.32	68.32
Xylene			0.00	0.00
Total	16884.06	16884.06	135.70	135.70
Temperature(F):	90.0	120.0	208.8	100.0
Pressure(psia):	15.0	15.0	15.0	10.0
Vapor fraction	0.0	0.0	0.0	0.0

Design Data:

Q	506,015	Btu/hr	Thi	208.8	F
Uo	250	Btu/hr-ft2-F	Tho	100.0	F
A	56.1	ft2	Tci	90.0	F
Material			Tco	120.0	F
			ΔTLM	36.1	F

Utilities:	Cooling water:	4177.2	lb/hr

Comments: The bare module cost of this heat exchanger did not fall in the appropriate range of the correlation

HEAT EXCHANGER

Identification:	Item	Heat Exchanger		
	Item No.	H-107	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	13,800	C_{BM}($):	43,746

Function:	To reheat the retentate from the first pervaporation module
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol	25.04	25.04		
Acetonitrile	0.00	0.00		
Pyridine	711.91	711.91		
3-Methylpyridine	205.29	205.29		
n-butyronitrile	0.06	0.06		
Water	392.28	392.28	28.00	28.00
Xylene	0.00	0.00		
Total	1334.59	1334.59	28.00	28.00
Temperature(F):	131.0	158.0	298.0	293.0
Pressure(psia):	29.0	24.0	64.7	64.7
Vapor fraction	0.0	0.0	1.0	0.0

Design Data:

Q	24478.6	Btu/hr	Thi	298.0 F
Uo	250.0	Btu/hr-ft2-F	Tho	293.0 F
A	0.7	ft2	Tci	131.0 F
Material	carbon steel		Tco	158.0 F
			ΔTLM	150.7 F

Utilities:	Cooling water:	0	
	Steam:	28	lb/hr low pressure steam
	Electricity:	0	

Comments: The bare module cost did not fall within the appropriate range for the correlations

HEAT EXCHANGER

Identification:	Item	Heat Exchanger		
	Item No.	H-108	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	13,800	C_{BM}($):	43,746

Function:	To reheat the retentate from the second pervaporation module.
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol	7.05	7.05		
Acetonitrile	0.00	0.00		
Pyridine	707.66	707.66		
3-Methylpyridine	204.07	204.07		
n-butyronitrile	0.06	0.06		
Water	110.37	110.37	17.00	17.00
Xylene	0.00	0.00		
Total	1029.20	1029.20	17.00	17.00
Temperature(F):	131.0	158.0	298.0	293.0
Pressure(psia):	22.0	17.0	64.7	64.7
Vapor fraction	0.0	0.0	1.0	0.0

Design Data:

Q	14330.4	Btu/hr	Thi	298.0 F
Uo	250.0	Btu/hr-ft2-F	Tho	293.0 F
A	0.4	ft2	Tci	131.0 F
Material	carbon steel		Tco	158.0 F
			ΔTLM	150.7 F

Utilities:	Cooling water:	0	
	Steam:	17	lb/hr low pressure steam
	Electricity:	0	

Comments:	The bare module cost did not fall within the appropriate range for the correlations

CONDENSER

Identification:	Item	Heat Exchanger		
	Item No.	H-109	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	12,193	C_{BM}($):	38,651

Function:	To condense the permeate vapor.
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol			61.02	61.02
Acetonitrile			0.00	0.00
Pyridine			14.41	14.41
3-Methylpyridine			4.16	4.16
n-butyronitrile			0.00	0.00
Water	34273.00	34273.00	955.91	955.91
Xylene			0.00	0.00
Total	34273.00	34273.00	1035.51	1035.51
Temperature(F):	90.0	120.0	144.0	120.0
Pressure(psia):	15.0	10.0	3.0	2.2
Vapor fraction	0.0	0.0	1.0	0.0

Design Data:

Q	1028180.9	Btu/hr	Thi	144.0 F
Uo	100.0	Btu/hr-ft2-F	Tho	120.0 F
A	172.7	ft2	Tci	90.0 F
Material	carbon steel		Tco	120.0 F
			ΔTLM	83.6 F

Utilities:	Cooling water:	34273 lb/hr
	Steam:	0
	Electricity:	0

Comments:

CONDENSER

Identification:	Item	Heat Exchanger			
	Item No.	H-111	Date:	4/13/2010	
	No. required	1	By:	RC/CC/SK/BL	
	C_{TPI}($):	13,800	C_{BM}($):	43,746	

Function:	To cool methanol stream to storage
Operation:	Continuous

Materials Handled:				
Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol			57.66	57.66
Acetonitrile			0.00	0.00
Pyridine			9.80	9.80
3-Methylpyridine			2.62	2.62
n-butyronitrile			0.00	0.00
Water	242.19	242.19	31.50	31.50
Xylene			0.00	0.00
Total	242.19	242.19	101.58	101.58
Temperature(F):	90.0	120.0	167.9	100.0
Pressure(psia):	15.0	15.0	15.0	10.0
Vapor fraction	0.0	0.0	0.0	0.0

Design Data:					
Q	7,280	Btu/hr	Thi	167.9	F
Uo	250	Btu/hr-ft2-F	Tho	100.0	F
A	1.21	ft2	Tci	90.0	F
Material			Tco	120.0	F
			ΔTLM	24.2	F

Utilities:	Cooling water:	242.2	lb/hr

Comments: The bare module cost of this heat exchanger did not fall in the appropriate range of the correlation

CONDENSER

Identification:	Item	Heat Exchanger		
	Item No.	H-113	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	12,526	C_{BM}($):	39,708

Function:	To cool waste water stream to storage			
Operation:	Continuous			

Materials Handled:				
Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol			3.24	3.24
Acetonitrile			0.00	0.00
Pyridine			4.57	4.57
3-Methylpyridine			0.55	0.55
n-butyronitrile			0.00	0.00
Water	4382.50	4382.50	924.47	924.47
Xylene			0.00	0.00
Total	4382.50	4382.50	932.83	932.83
Temperature(F):	90.0	120.0	223.5	100.0
Pressure(psia):	15.0	15.0	15.0	10.0
Vapor fraction	0.0	0.0	0.0	0.0

Design Data:					
Q	131,738	Btu/hr	Thi	223.5	F
Uo	250	Btu/hr-ft2-F	Tho	100.0	F
A	13.17	ft2	Tci	90.0	F
Material			Tco	120.0	F
			ΔTLM	40.0	F

Utilities:	Cooling water:	4382.5	lb/hr

Comments:

CONDENSER

Identification:	Item	Heat Exchanger			
	Item No.	H-116	Date:	4/13/2010	
	No. required	1	By:	RC/CC/SK/BL	
	C_{TPI}($):	13,800	C_{BM}($):	43,746	

Function:	To cool 3MP stream to storage
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol			0.00	0.00
Acetonitrile			0.00	0.00
Pyridine			1.11	1.11
3-Methylpyridine			199.68	199.68
n-butyronitrile			0.00	0.00
Water	680.20	680.20	0.00	0.00
Xylene			0.00	0.00
Total	680.20	680.20	200.79	200.79
Temperature(F):	90.0	120.0	307.9	100.0
Pressure(psia):	15.0	15.0	15.0	10.0
Vapor fraction	0.0	0.0	0.0	0.0

Design Data:

Q	20,445	Btu/hr	Thi	307.9	F
Uo	100	Btu/hr-ft2-F	Tho	100.0	F
A	3.37	ft2	Tci	90.0	F
Material			Tco	120.0	F
			ΔTLM	60.6	F

Utilities:	Cooling water:	680.2	lb/hr

Comments: The bare module cost of this heat exchanger did not fall in the appropriate range of the correlation

CONDENSER

Identification:	Item	Heat Exchanger		
	Item No.	H-118	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	13,800	C_{BM}($):	43,746

Function:	To cool organic waste stream S112 to storage
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol			1.17	1.17
Acetonitrile			0.00	0.00
Pyridine			18.09	18.09
3-Methylpyridine			0.00	0.00
n-butyronitrile			0.00	0.00
Water	96.51	96.51	0.00	0.00
Xylene			12.37	12.37
Total	96.51	96.51	31.64	31.64
Temperature(F):	90.0	120.0	198.8	100.0
Pressure(psia):	15.0	15.0	15.0	10.0
Vapor fraction	0.0	0.0	0.0	0.0

Design Data:

Q	2,499	Btu/hr	Thi	198.8	F
Uo	100	Btu/hr-ft2-F	Tho	100.0	F
A	0.75	ft2	Tci	90.0	F
Material			Tco	120.0	F
			ΔTLM	33.3	F

Utilities:	Cooling water:	96.5	lb/hr

Comments: The bare module cost of this heat exchanger did not fall in the appropriate range of the correlation

CONDENSER

Identification:	Item	Heat Exchanger		
	Item No.	H-120	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	18,692	C_{BM}($):	59,255

Function:	To cool pyridine stream to storage
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol			0.08	0.08
Acetonitrile			0.00	0.00
Pyridine			687.09	687.09
3-Methylpyridine			3.99	3.99
n-butyronitrile			0.06	0.06
Water	1638.20	1638.20	0.00	0.00
Xylene			7.15	7.15
Total	1638.20	1638.20	698.36	698.36
Temperature(F):	90.0	120.0	242.9	100.0
Pressure(psia):	15.0	15.0	15.0	10.0
Vapor fraction	0.0	0.0	0.0	0.0

Design Data:

Q	49,244	Btu/hr	Thi	242.9	F
Uo	100	Btu/hr-ft2-F	Tho	100.0	F
A	10.94	ft2	Tci	90.0	F
Material			Tco	120.0	F
			ΔTLM	45.0	F

Utilities:	Cooling water:	1638.2	lb/hr

Comments:

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-100	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CTPI($):	3,672	CBM($):	12,117

Function:	To pump S201 stream from 15psia to 89.2psia
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Inlet*	*Outlet*
Methanol	130.00	130.00
Acetonitrile	312.00	312.00
Pyridine	780.00	780.00
3-Methylpyridine	208.00	208.00
n-butyronitrile	26.00	26.00
Water	1118.00	1118.00
Xylene	26.00	26.00
benzene	0.00	0.00
Total	2600.00	2600.00
Temperature(F):	80.0	80.0
Pressure(atm):	15.0	40.0
Vapor fraction	0.0	0.0

Design Data:

Flow rate	2600.00	lb/hr	Material	carbon steel	
ΔP	74.17	psia	Enclosure		
Pump Head	189.74	ft	Power Req'd	21.36	Hp

Utilities:	Electricity:	15.93	kW

Comments:

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-103	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	4,205	C_{BM}($):	13,878
Function:	To pump S103 stream from 22.6 psia to 56 psia			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Inlet*	*Outlet*		
Methanol	62.22	62.22		
Acetonitrile	0.00	0.00		
Pyridine	720.60	720.60		
3-Methylpyridine	207.83	207.83		
n-butyronitrile	0.06	0.06		
Water	975.47	975.47		
Xylene	0.00	0.00		
Total	1966.18	1966.18		
Temperature(F):	223.7	223.7		
Pressure(psia):	22.6	46.0		
Vapor fraction	0.0	0.0		
Design Data:				
Flow rate	1966.18	lb/hr	Material	Carbon Steel
ΔP	33.4	psi	Enclosure	
Pump Head	84.73	ft	Power Req'd	7.21 Hp
Utilities:	Electricity:	5.38	kW	
Comments:				

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-104/P-209	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CTPI($):	5,155	CBM($):	17,012

Function:	To pump S202 stream from 15 psia to 50.5psia
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Inlet*	*Outlet*
Methanol	67.57	67.57
Acetonitrile	312.00	312.00
Pyridine	58.06	58.06
3-Methylpyridine	0.17	0.17
n-butyronitrile	25.94	25.94
Water	142.95	142.95
Xylene	26.00	26.00
benzene	0.00	0.00
Total	632.70	632.70
Temperature(F):	167.0	167.0
Pressure(atm):	15.0	40.0
Vapor fraction	0.0	0.0

Design Data:

Flow rate	632.70 lb/hr		Material	carbon steel
ΔP	35.50 psia		Enclosure	
Pump Head	111.55 ft		Power Req'd	3.06 Hp

Utilities:	Electricity:	2.28 kW

Comments:

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-107	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	4,965	C_{BM}($):	16,384
Function:	To pump S107 stream from 15 psia to 60 psia			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Inlet*	*Outlet*		
Methanol	1.25	1.25		
Acetonitrile	0.00	0.00		
Pyridine	706.29	706.29		
3-Methylpyridine	203.67	203.67		
n-butyronitrile	0.06	0.06		
Water	0.00	0.00		
Xylene	19.52	19.52		
Total	930.79	930.79		
Temperature(F):	140.0	140.0		
Pressure(psia):	15.0	40.0		
Vapor fraction	0.0	0.0		
Design Data:				
Flow rate	930.79 lb/hr		Material	Carbon Steel
ΔP	45.06 psi		Enclosure	
Pump Head	110.08 ft		Power Req'd	4.44 Hp
Utilities:	Electricity:	3.31 kW		
Comments:				

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-108	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	4,536	C_{BM}($):	14,969
Function:	To pump S106 stream from 2.175 psia to 65.625 psia			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Inlet*	*Outlet*		
Methanol	60.90	60.90		
Acetonitrile	0.00	0.00		
Pyridine	14.37	14.37		
3-Methylpyridine	3.17	3.17		
n-butyronitrile	0.00	0.00		
Water	955.97	955.97		
Xylene	0.00	0.00		
Total	1034.41	1034.41		
Temperature(F):	80.0	80.0		
Pressure(psia):	2.18	40.00		
Vapor fraction	0.0	0.0		
Design Data:				
Flow rate	1034.41	lb/hr	Material	Carbon Steel
ΔP	63.45	psi	Enclosure	
Pump Head	160.96	ft	Power Req'd	7.22 Hp
Utilities:	Electricity:	5.38	kW	
Comments:				

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-113	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	5,444	C_{BM}($):	17,965

Function:	To pump S110 stream from 15 psia to 49.8 psia
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Inlet*	*Outlet*
Methanol	1.25	1.25
Acetonitrile	0.00	0.00
Pyridine	705.18	705.18
3-Methylpyridine	3.99	3.99
n-butyronitrile	0.06	0.06
Water	0.00	0.00
Xylene	19.52	19.52
Total	730.00	730.00
Temperature(F):	224.8	224.8
Pressure(psia):	15.0	40.0
Vapor fraction	0.0	0.0

Design Data:

Flow rate	730.00	lb/hr	Material	Carbon Steel	
ΔP	34.77	psi	Enclosure		
Pump Head	88.95	ft	Power Req'd	2.81	Hp

Utilities:	Electricity:	2.10	kW

Comments:

PROCESS 2 - AZEOTROPIC DISTILLATION

DISTILLATION COLUMN

Identification:	Item	Distillation Column		
	Item No.	D-202	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	196,539	C_{BM}($):	761,916

Function: To separate water/benzene stream from pyridine/3MP stream
Operation: Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*Recycle*	*Solvent*	*Bottoms*	*Distillate*
Methanol	62.43	6.15	0.00	0.00	62.43
Acetonitrile	0.00	0.00	0.00	0.00	0.00
Pyridine	721.94	0.03	0.00	721.90	0.03
3-Methylpyridine	207.83	0.00	0.00	207.83	0.00
n-butyronitrile	0.06	0.00	0.00	0.06	0.00
Water	975.05	4.09	0.00	0.00	975.05
Xylene	0.00	0.00	0.00	0.00	0.00
Benzene	0.00	3702.39	203.29	5.64	3900.04
Total	1967.30	3712.65	203.29	935.43	4937.55
Temperature(F):	80.0	100.0	100.0	282.7	153.0
Pressure(psia):	15.0	22.0	22.0	25.7	22.0
Vapor fraction	0.0	0.0	0.0	0.0	0.0

Design Data:

Number of stages:	34	Column Height:	80	ft
Feed Stage:	20	Inside Diameter:	5.324	ft
Solvent Feed Stage:	2	Tray spacing:	2	ft
Reflux Ratio:	8	Material:	carbon steel	
Tray efficiency:	53.6%			
Tray type:	sieve			

Utilities:	Cooling water:	$	36,809	/yr
	Steam:	$	409,302	/yr

Associated Components:

Tower

	Equip. type	Vertical Vessel		
	Weight		14409.97	lb
	Thickness		0.25	in
	C_{BM}	$	582,212	

Condenser			
	Equip. type	Fixed Head heat exchanger	
	Heat Duty	14,003,737	Btu/hr
	Area	2783.03	ft^2
	Material	carbon steel	
	C_{BM}	$ 93,425	
Reboiler			
	Equip. type	Fixed Head heat exchanger	
	Heat Duty	14,204,083	Btu/hr
	Area	814.71	ft^2
	Material	carbon steel	
	C_{BM}	$ 49,305	
Reflux Accumulator			
	Equip. type	Horizontal Vessel	
	Res. Time	5.00	min
	Length	5.11	ft
	Depth	2.56	ft
	Weight	591.27	lb
	C_{BM}	$ 14,293	
Reflux Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	153.21	Hp
	Pump Head	79.64	ft
	Efficiency	70%	
	C_{BM}	$ 11,581	
Reboiler Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	25.47	Hp
	Pump Head	7.57	ft
	Efficiency	70%	
	C_{BM}	$ 11,100	
Comments:			

DISTILLATION COLUMN

Identification:	Item	Distillation Column		
	Item No.	D-204	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	67,723	C_{BM}($):	247,602

Function:	To separate pyridine and 3MP stream to obtain final product
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*Bottoms*	*Distillate*
Methanol	0.00	0.00	0.00
Acetonitrile	0.00	0.00	0.00
Pyridine	721.90	2.24	719.66
3-Methylpyridine	207.83	207.19	0.64
n-butyronitrile	0.06	0.00	0.05
Water	0.00	0.00	0.00
Xylene	0.00	0.00	0.00
Benzene	5.64	0.00	5.64
Total	935.43	209.43	726.00
Temperature(F):	282.7	306.2	239.5
Pressure(psia):	25.7	18.6	15.0
Vapor fraction	0.0	0.0	0.0

Design Data:

Number of stages:	32	Column Height:	76	ft
Feed Stage:	23	Inside Diameter:	1.34	ft
Reflux Ratio:	4.8	Tray spacing:	2	ft
Tray efficiency:	52.4%	Material:	carbon steel	
Tray type:	sieve			

Utilities:	Cooling water:	$	2,122	/yr
	Steam:	$	22,852	/yr

Associated Components:

Tower

Equip. type	Vertical Vessel		
Weight		3076.89	lb
Thickness		0.25	in
C_{BM}	$	136,409	

Condenser

	Equip. type	Fixed Head heat exchanger	
	Heat Duty	807,317	Btu/hr
	Area	60.15	ft^2
	Material	carbon steel	
	C_{BM}	$ 34,041	
Reboiler			
	Equip. type	Fixed Head heat exchanger	
	Heat Duty	793,058	Btu/hr
	Area	45.49	ft^2
	Material	carbon steel	
	C_{BM}	$ 35,423	
Reflux Accumulator			
	Equip. type	Horizontal Vessel	
	Res. Time	5.00	min
	Length	2.70	ft
	Depth	1.35	ft
	Weight	165.93	lb
	C_{BM}	$ 15,077	
Reflux Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	13.85	Hp
	Pump Head	75.98	ft
	Efficiency	70%	
	C_{BM}	$ 12,143	
Reboiler Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	1.66	Hp
	Pump Head	7.96	ft
	Efficiency	70%	
	C_{BM}	$ 14,510	
Comments:			

DISTILLATION COLUMN

Identification:	Item	Distillation Column		
	Item No.	D-205	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_P($):	89,306	C_{BM}($):	328,709

Function:	To purify the water and organic stream
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*Bottoms*	*Distillate*
Methanol	56.28	9.83	46.45
Acetonitrile	0.00	0.00	0.00
Pyridine	0.01	0.00	0.00
3-Methylpyridine	0.00	0.00	0.00
n-butyronitrile	0.00	0.00	0.00
Water	970.96	964.04	6.93
Xylene	0.00	0.00	0.00
Benzene	2.79	0.00	2.79
Total	1030.04	973.87	56.17
Temperature(F):	100.0	222.1	151.1
Pressure(psia):	15.0	18.4	15.0
Vapor fraction	0.0	0.0	0.0

Design Data:

Number of stages:	37	Column Height:	86	ft
Feed Stage:	18	Inside Diameter:	1.0	ft
Reflux Ratio:	3	Tray spacing:	2	ft
Tray efficiency:	42.8%	Material:	carbon steel	
Tray type:	sieve			

Utilities:	Cooling water:	$	309	/yr
	Steam:	$	6,524	/yr

Associated Components:

Tower

Equip. type	Vertical Vessel		
Weight		1411.93	lb
Thickness		0.25	in
C_{BM}	$	189,543	

Condenser

	Equip. type	Fixed Head heat exchanger	
	Heat Duty	117,580	Btu/hr
	Area	22.45	ft^2
	Material	carbon steel	
	C_{BM}	$ 41,950	
Reboiler			
	Equip. type	Fixed Head heat exchanger	
	Heat Duty	226,393	Btu/hr
	Area	12.99	ft^2
	Material	carbon steel	
	C_{BM}	$ 49,242	
Reflux Accumulator			
	Equip. type	Horizontal Vessel	
	Res. Time	5.00	min
	Length	1.15	ft
	Depth	0.57	ft
	Weight	30.74	lb
	C_{BM}	$ 17,614	
Reflux Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	0.64	Hp
	Pump Head	87.99	ft
	Efficiency	70%	
	C_{BM}	$ 15,180	
Reboiler Pump			
	Equip. type	Centrifugal Pump	
	Power Req'd	0.47	Hp
	Pump Head	8.85	ft
	Efficiency	70%	
	C_{BM}	$ 15,180	

Comments:

DECANTER

Identification:	Item	Vertical Vessel		
	Item No.	DE-201	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	4,179	C_{BM}($):	14,657

Function:	To separate benzene from water
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*Outlet 1*	*Outlet 2*
Methanol	62.43	6.15	56.28
Acetonitrile	0.00	0.00	0.00
Pyridine	0.03	0.03	0.01
3-Methylpyridine	0.00	0.00	0.00
n-butyronitrile	0.00	0.00	0.00
Water	975.05	4.09	970.96
Xylene	0.00	0.00	0.00
benzene	3900.04	3897.25	2.79
Total	4937.55	3907.51	1030.04
Temperature(F):	153.0	100.0	100.0
Pressure(atm):	22.0	15.0	15.0
Vapor fraction	0.0	0.0	0.0

Design Data:

Days Stored				
Length	5.11 ft		Material	carbon steel
Diameter	2.56 ft		Pressure	10.00 psi
Total Volume	26.22 ft3		Weight	591.27 lb

Comments:

BENZENE STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-202	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CP($):	68,510	CBM($):	208,956
Function:	To store 14 days worth of benzene.			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Feed*	*wt. %*		
Methanol	0.00	0.0		
Acetonitrile	0.00	0.0		
Pyridine	0.00	0.0		
3-Methylpyridine	0.00	0.0		
n-butyronitrile	0.00	0.0		
Water	0.00	0.0		
Xylene	0.00	0.0		
Benzene	203.29	100.0		
Total	203.29	100.0		
Temperature(F):	100.0			
Pressure(psia):	15.0			
Vapor fraction	0.0			
Design Data:				
Days Stored	14			
Total Volume	10,708	gal		
Material	Carbon Steel			
Pressure	15	psi		
Comments:				

PURGE STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-203	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CP($):	59,401	CBM($):	18,117

Function:	To store 14 days worth of purge from the benzene recycle stream.
Operation:	Continuous

Materials Handled:		
Quantity (lb/hr):	*Feed*	*wt. %*
Methanol	0.00	0.0
Acetonitrile	0.00	0.0
Pyridine	0.00	0.0
3-Methylpyridine	0.00	0.0
n-butyronitrile	0.00	0.0
Water	0.00	0.0
Xylene	0.00	0.0
Benzene	194.86	100.0
Total	194.86	100.0
Temperature(F):	100.0	
Pressure(psia):	15.0	
Vapor fraction	0.0	

Design Data:		
Days Stored	14	
Total Volume	10,758	gal
Material	Carbon Steel	
Pressure	15	psi

Comments:	The liquid organic waste stream is <5% pyridine and <15% water; therefore, it will be used on-site as fuel.

PYRIDINE STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-206	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CP($):	65,212	CBM($):	215,200
Function:	To store 14 days worth of 3-methylpyridine.			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Feed*	*wt %*		
Methanol	0.00	0.0		
Acetonitrile	0.00	0.0		
Pyridine	719.66	99.1		
3-Methylpyridine	0.64	0.1		
n-butyronitrile	0.05	0.0		
Water	0.00	0.0		
Xylene	0.00	0.0		
Benzene	5.64	0.8		
Total	726.00	100.0		
Temperature(F):	100.0			
Pressure(psia):	15.0			
Vapor fraction	0.0			
Design Data:				
Days Stored	14			
Total Volume	38,933	gal		
Material	Carbon Steel			
Pressure	15	psi		
Comments:	The pyridine meets the Intermediate Quality Specifications.			

3MP STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-207	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CP($):	35,640	CBM($):	117,613
Function:	To store 14 days worth of 3-methylpyridine.			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Feed*	*wt %*		
Methanol	0.00	0.0		
Acetonitrile	0.00	0.0		
Pyridine	2.24	1.1		
3-Methylpyridine	207.19	98.9		
n-butyronitrile	0.00	0.0		
Water	0.00	0.0		
Xylene	0.00	0.0		
Benzene	0.00	0.0		
Total	209.43	100.0		
Temperature(F):	100.0			
Pressure(psia):	15.0			
Vapor fraction	0.0			
Design Data:				
Days Stored	14			
Total Volume	11,829	gal		
Material	Carbon Steel			
Pressure	15	psi		
Comments:	The 3-methylpyridine meets the Finished Goods Quality Specifications.			

METHANOL WASTE STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-208	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CP($):	24,063	CBM($):	79,407

Function:	To store 14 days worth of methanol waste.
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Feed*	*wt %*
Methanol	46.45	82.7
Acetonitrile	0.00	0.0
Pyridine	0.00	0.0
3-Methylpyridine	0.00	0.0
n-butyronitrile	0.00	0.0
Water	6.93	12.3
Xylene	0.00	0.0
Benzene	2.79	5.0
Total	56.17	100.0

Temperature(F):	100.0
Pressure(psia):	15.0
Vapor fraction	0.0

Design Data:

Days Stored	14	
Total Volume	3,467	gal
Material	Carbon Steel	
Pressure	15	psi

Comments: The liquid organic waste stream is <5% pyridine and <15% water; therefore, it will be used on-site as fuel.

WATER STORAGE TANK

Identification:	Item	API Tank		
	Item No.	T-209	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CP($):	74,782	CBM($):	246,779
Function:	To store 14 days worth of methanol waste.			
Operation:	Continuous			

Materials Handled:		
Quantity (lb/hr):	*Feed*	*wt %*
Methanol	9.83	1.0
Acetonitrile	0.00	0.0
Pyridine	0.00	0.0
3-Methylpyridine	0.00	0.0
n-butyronitrile	0.00	0.0
Water	964.04	99.0
Xylene	0.00	0.0
Benzene	0.00	0.0
Total	973.87	100.0
Temperature(F):	100.0	
Pressure(psia):	15.0	
Vapor fraction	0.0	

Design Data:		
Days Stored	14	
Total Volume	50,385	gal
Material	Carbon Steel	
Pressure	15	psi

Comments: The water meets purity standards to be processed without additional cost.

CONDENSER

Identification:	Item	Heat Exchanger			
	Item No.	H-210	Date:	4/13/2010	
	No. required	1	By:	RC/CC/SK/BL	
	CTPI($):	18,511	CBM($):	58,681	
Function:	To cool pyridine stream to storage tank				
Operation:	Continuous				
Materials Handled:					
Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*	
Methanol			0.00	0.00	
Acetonitrile			0.00	0.00	
Pyridine			719.66	719.66	
3-Methylpyridine			0.64	0.64	
n-butyronitrile			0.05	0.05	
Water	1659.51	1659.51	0.00	0.00	
Xylene			0.00	0.00	
Benzene			5.64	5.64	
Total	1659.51	1659.51	726.0	726.0	
Temperature(F):	90.0	120.0	239.5	100.0	
Pressure(atm):	15.0	15.0	15.0	15.0	
Vapor fraction	0.0	0.0	0.0	0	
Design Data:					
Q	49,884	Btu/hr	Thi	239.5	F
Uo	100	Btu/hr-ft2-F	Tho	100.0	F
A	9.56	ft2	Tci	90.0	F
Material	carbon steel		Tco	120.0	F
			ΔTLM	44.1	F
Utilities:	Cooling water:	1659.5	lb/hr		
	Steam:				
	Electricity:				
Comments:					

CONDENSER

Identification:	Item	Heat Exchanger			
	Item No.	H-212	Date:	4/13/2010	
	No. required	1	By:	RC/CC/SK/BL	
	CTPI($):	13,800	CBM($):	43,746	
Function:	To cool 3MP stream to storage				
Operation:	Continuous				
Materials Handled:					
Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*	
Methanol			0.00	0.00	
Acetonitrile			0.00	0.00	
Pyridine			2.24	2.24	
3-Methylpyridine			207.19	207.19	
n-butyronitrile			0.00	0.00	
Water	653.40	653.40	0.00	0.00	
Xylene			0.00	0.00	
Benzene			0.00	0.00	
Total	653.40	653.40	209.4	209.4	
Temperature(F):	90.0	120.0	306.2	100.0	
Pressure(atm):	15.0	15.0	18.6	15.0	
Vapor fraction	0.0	0.0	0.0	0.0	
Design Data:					
Q	19,641	Btu/hr	Thi	306.2	F
Uo	100	Btu/hr-ft2-F	Tho	100.0	F
A	2.07	ft2	Tci	90.0	F
Material	carbon steel		Tco	120.0	F
			ΔTLM	60.3	F
Utilities:	Cooling water:	653.4	lb/hr		
	Steam:				
	Electricity:				
Comments:	the bare module cost did not fall within the appropriate range of the correlations				

CONDENSER

Identification:	Item	Heat Exchanger		
	Item No.	H-214	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CTPI($):	13,800	CBM($):	42,090

Function:	To cool organic fuel stream to storage
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*
Methanol			46.45	46.45
Acetonitrile			0.00	0.00
Pyridine			0.00	0.00
3-Methylpyridine			0.00	0.00
n-butyronitrile			0.00	0.00
Water	107.58	107.58	6.93	6.93
Xylene			0.00	0.00
Benzene			2.79	2.79
Total	107.58	107.58	56.2	56.2
Temperature(F):	90.0	120.0	151.1	100.0
Pressure(atm):	15.0	15.0	15.0	15.0
Vapor fraction	0.0	0.0	0.0	0.0

Design Data:

Q	3,234	Btu/hr	Thi	151.1	F
Uo	100	Btu/hr-ft2-F	Tho	100.0	F
A	0.89	ft2	Tci	90.0	F
Material	carbon steel		Tco	120.0	F
			ΔTLM	18.6	F

Utilities:	Cooling water:	1042.0	lb/hr
	Steam:		
	Electricity:		

Comments:

CONDENSER

Identification:	Item	Heat Exchanger			
	Item No.	H-216	Date:	4/13/2010	
	No. required	1	By:	RC/CC/SK/BL	
	CTPI($):	12,494	CBM($):	38,106	
Function:	To cool orgnic waste stream to storage				
Operation:	Continuous				
Materials Handled:					
Quantity (lb/hr):	*Cold In*	*Cold Out*	*Hot In*	*Hot Out*	
Methanol			9.83	9.83	
Acetonitrile			0.00	0.00	
Pyridine			0.00	0.00	
3-Methylpyridine			0.00	0.00	
n-butyronitrile			0.00	0.00	
Water	4177.18	4177.18	964.04	964.04	
Xylene			0.00	0.00	
Benzene			0.00	0.00	
Total	4177.18	4177.18	973.9	973.9	
Temperature(F):	90.0	120.0	222.1	100.0	
Pressure(atm):	15.0	15.0	18.4	15.0	
Vapor fraction	0.0	0.0	0.0	0.0	
Design Data:					
Q	125,566	Btu/hr	Thi	222.1	F
Uo	100	Btu/hr-ft2-F	Tho	100.0	F
A	27.39	ft2	Tci	90.0	F
Material	carbon steel		Tco	120.0	F
			ΔTLM	39.6	F
Utilities:	Cooling water:	421.1	lb/hr		
	Steam:				
	Electricity:				
Comments:					

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-200	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	C_{TPI}($):	3,723	CBM($):	12,286
Function:	To pump S201 stream from 15psia to 84.2psia			
Operation:	Continuous			

Materials Handled:		
Quantity (lb/hr):	*Inlet*	*Outlet*
Methanol	130.00	130.00
Acetonitrile	312.00	312.00
Pyridine	780.00	780.00
3-Methylpyridine	208.00	208.00
n-butyronitrile	26.00	26.00
Water	1118.00	1118.00
Xylene	26.00	26.00
benzene	0.00	0.00
Total	2600.00	2600.00
Temperature(F):	80.0	80.0
Pressure(atm):	15.0	40.0
Vapor fraction	0.0	0.0

Design Data:				
Flow rate	2600.00 lb/hr	Material	carbon steel	
ΔP	79.17 psia	Enclosure		
Pump Head	176.95 ft	Power Req'd	19.92	Hp

Utilities:	Electricity:	14.85 kW

Comments:

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-203	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CTPI($):	4,060	CBM($):	13,398

Function:	To pump S203 stream from 21.55psia to 59.9psia
Operation:	Continuous

Materials Handled:

Quantity (lb/hr):	*Inlet*	*Outlet*
Methanol	62.43	62.43
Acetonitrile	0.00	0.00
Pyridine	721.94	721.94
3-Methylpyridine	207.83	207.83
n-butyronitrile	0.06	0.06
Water	975.05	975.05
Xylene	0.00	0.00
benzene	0.00	0.00
Total	1967.30	1967.30
Temperature(F):	221.4	221.4
Pressure(atm):	21.6	40.0
Vapor fraction	0.0	0.0

Design Data:

Flow rate	1967.30 lb/hr	Material	carbon steel	
ΔP	38.39 psia	Enclosure		
Pump Head	103.86 ft	Power Req'd		8.84 Hp

Utilities:	Electricity:	6.60 kW

Comments:

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-204	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CTPI($):	4,600	CBM($):	15,180
Function:	To pump S204 stream from 15psia to 74.2psia			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Inlet*	*Outlet*		
Methanol	0.00	0.00		
Acetonitrile	0.00	0.00		
Pyridine	0.00	0.00		
3-Methylpyridine	0.00	0.00		
n-butyronitrile	0.00	0.00		
Water	0.00	0.00		
Xylene	0.00	0.00		
benzene	203.29	203.29		
Total	203.29	203.29		
Temperature(F):	100.0	100.0		
Pressure(atm):	15.0	55.0		
Vapor fraction	0.0	0.0		
Design Data:				
Flow rate	203.29 lb/hr		Material	carbon steel
ΔP	59.22 psia		Enclosure	
Pump Head	158.83 ft		Power Req'd	1.34 Hp
Utilities:	Electricity:	1.00 kW		
Comments:				

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-205	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CTPI($):	3,554	CBM($):	11,728
Function:	To pump S206 stream from 15psia to 74.2psia			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Inlet*	*Outlet*		
Methanol	6.15	6.15		
Acetonitrile	0.00	0.00		
Pyridine	0.03	0.03		
3-Methylpyridine	0.00	0.00		
n-butyronitrile	0.00	0.00		
Water	4.09	4.09		
Xylene	0.00	0.00		
benzene	3897.25	3897.25		
Total	3907.51	3907.51		
Temperature(F):	100.0	100.0		
Pressure(atm):	15.0	55.0		
Vapor fraction	0.0	0.0		
Design Data:				
Flow rate	3907.51	lb/hr	Material	carbon steel
ΔP	59.22	psia	Enclosure	
Pump Head	158.83	ft	Power Req'd	25.52 Hp
Utilities:	Electricity:	19.03	kW	
Comments:				

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-208	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CTPI($):	5,216	CBM($):	17,213
Function:	To pump S209 stream from 15psia to 38.5psia			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Inlet*	*Outlet*		
Methanol	0.00	0.00		
Acetonitrile	0.00	0.00		
Pyridine	721.90	721.90		
3-Methylpyridine	207.83	207.83		
n-butyronitrile	0.06	0.06		
Water	0.00	0.00		
Xylene	0.00	0.00		
benzene	5.64	5.64		
Total	935.43	935.43		
Temperature(F):	282.70	282.70		
Pressure(atm):	25.7	40.0		
Vapor fraction	0.0	0.0		
Design Data:				
Flow rate	935.43 lb/hr		Material	carbon steel
ΔP	23.54 psia		Enclosure	
Pump Head	63.69 ft		Power Req'd	2.58 Hp
Utilities:	Electricity:	5216.09 kW		
Comments:				

PUMP

Identification:	Item	Centrifugal Pump		
	Item No.	P-214	Date:	4/13/2010
	No. required	1	By:	RC/CC/SK/BL
	CTPI($):	4,600	CBM($):	15,180
Function:	To pump S208 stream from 15psia to 58.9psia			
Operation:	Continuous			
Materials Handled:				
Quantity (lb/hr):	*Inlet*	*Outlet*		
Methanol	56.28	56.28		
Acetonitrile	0.00	0.00		
Pyridine	0.01	0.01		
3-Methylpyridine	0.00	0.00		
n-butyronitrile	0.00	0.00		
Water	970.96	970.96		
Xylene	0.00	0.00		
benzene	2.79	2.79		
Total	1030.04	1030.04		
Temperature(F):	100.0	100.0		
Pressure(atm):	15.0	40.0		
Vapor fraction	0.0	0.0		
Design Data:				
Flow rate	1030.04	lb/hr	Material	carbon steel
ΔP	43.86	psia	Enclosure	
Pump Head	104.65	ft	Power Req'd	4891.13 Hp
Utilities:	Electricity:	3.48	kW	
Comments:				

ECONOMIC ANALYSIS

Equipment Cost Summary:

TABLE 6: Equipment List Process 1 – Pervaporation

Unit	Unit Description	C_{BM}($)	Unit	Unit Description	C_{BM}($)
T-101	API Tank	$381,156	H-112	Reboiler	$35,304
P-100	Centrifugal Pump	$12,223	P-109	Reflux Pump	$18,594
H-100	Shell & Tube Heat Exchanger	$33,655	P-110	Reboiler Pump	$21,533
D-101	Distillation Column	$433,099	A-103	Reflux Accumulator	$17,614
H-101	Condenser	$33,048	H-111	Shell & Tube Heat Exchanger	$43,746
H-102	Reboiler	$33,976	T-104	API Tank	$73,402
P-101	Reflux Pump	$11,975	H-113	Shell & Tube Heat Exchanger	$39,708
P-102	Reboiler Pump	$14,123	T-105	API Tank	$228,084
A-101	Reflux Accumulator	$15,057	D-104	Distillation Column	$244,984
P-104	Centrifugal Pump	$17,021	H-114	Condenser	$40,391
D-102	Distillation Column	$160,743	H-115	Reboiler	$51,399
H-103	Condenser	$34,453	P-111	Reflux Pump	$14,121
H-105	Reboiler	$37,906	P-112	Reboiler Pump	$16,829
P-105	Reflux Pump	$13,904	A-104	Reflux Accumulator	$15,873
P-106	Reboiler Pump	$20,908	H-116	Shell & Tube Heat Exchanger	$43,746
A-102	Reflux Accumulator	$15,466	T-106	API Tank	$108,703
H-104	Shell & Tube Heat Exchanger	$61,740	P-113	Centrifugal Pump	$17,965
T-102	API Tank	$181,173	D-105	Distillation Column	$145,461
H-106	Shell & Tube Heat Exchanger	$43,746	H-117	Condenser	$35,304
T-103	API Tank	$82,018	H-119	Reboiler	$37,602
P-103	Centrifugal Pump	$13,868	P-114	Reflux Pump	$15,180
PM-101-103	Pervaporation Modules	$2,912,656	P-115	Reboiler Pump	$15,180
H-107	Interstage-Heater	$43,746	A-105	Reflux Accumulator	$19,284
H-108	Interstage-Heater	$43,746	H-118	Shell & Tube Heat Exchanger	$43,746
H-109	Condenser	$38,651	T-107	API Tank	$40,239
P-107	Centrifugal Pump	$16,384	H-120	Shell & Tube Heat Exchanger	$59,255
P-108	Centrifugal Pump	$14,969	T-108	API Tank	$198,897
D-103	Distillation Column	$193,955		Spare Pumps (5)	$75,900
H-110	Condenser	$55,338		Total	$6,688,744

TABLE 7: Equipment List Process 2 -- Azeotropic Distillation					
Unit	Unit Description	C_{BM}($)	Unit	Unit Description	C_{BM}($)
T-201	API Tank	$381,156	A-203	Reflux Accumulator	$15,466
P-200	Centrifugal Pump	$12,287	H-206	Shell & Tube Heat Exchanger	$59,771
D-201	Distillation Column	$433,099	T-204	API Tank	$181,173
H-201	Condenser	$33,900	H-208	Shell & Tube Heat Exchanger	$43,746
H-202	Reboiler	$34,191	T-205	API Tank	$88,741
P-201	Reflux Pump	$11,975	D-204	Distillation Column	$136,409
P-202	Reboiler Pump	$14,123	H-209	Condenser	$34,041
A-201	Reflux Accumulator	$15,057	H-211	Reboiler	$35,423
P-203	Centrifugal Pump	$13,401	P-212	Reflux Pump	$12,143
T-202	API Tank	$208,956	P-213	Reboiler Pump	$14,510
P-204	Centrifugal Pump	$15,180	A-204	Reflux Accumulator	$15,077
D-202	Distillation Column	$582,212	H-210	Shell & Tube Heat Exchanger	$58,681
H-203	Condenser	$93,425	T-206	API Tank	$215,200
H-204	Reboiler	$49,305	H-212	Shell & Tube Heat Exchanger	$43,746
P-206	Reflux Pump	$11,581	T-207	API Tank	$117,613
P-207	Reboiler Pump	$11,100	P-214	Centrifugal Pump	$16,141
A-202	Reflux Accumulator	$14,293	D-205	Distillation Column	$189,543
DE-201	Decanter	$14,657	H-213	Condenser	$41,950
T-203	API Tank	$40,239	H-215	Reboiler	$49,242
P-205	Centrifugal Pump	$11,727	P-215	Reflux Pump	$15,180
P-208	Centrifugal Pump	$17,213	P-216	Reboiler Pump	$15,180
P-209	Centrifugal Pump	$17,012	A-205	Reflux Accumulator	$17,614
D-203	Distillation Column	$160,743	H-214	Shell & Tube Heat Exchanger	$42,090
H-205	Condenser	$34,453	T-208	API Tank	$79,407
H-207	Reboiler	$37,906	H-216	Shell & Tube Heat Exchanger	$38,106
P-210	Reflux Pump	$15,180	T-209	API Tank	$246,779
P-211	Reboiler Pump	$15,180		Spare Pumps(5)	$75,900
				Total	$4,198,423

The bare module costs of the equipment for both processes are shown in Table 6 and Table 7. The equipment costs were calculated using the correlations presented in ***Seider, et al. 2009,*** with the final values scaled up to 2010 costs using a CE Index of 575. Process 1 had a total equipment cost of $6,689,000, while Process 2 had a total cost of $4,198,000. The difference in the equipment prices was $2,491,000, which was largely due to the $2,913,000 spent on the pervaporation modules for Process 1. Included in the total equipment cost is the price for 5 spare pumps, one for each distillation column, to minimize downtime in the event of unexpected pump failure.

Additional equipment is required for the start-up period, including a vacuum pump to generate the low pressure on the permeate side of the pervaporation membrane, as well as an additional heat exchanger for Process 1 to heat S101with 107.6 lb/hr low pressure steam.

Working Capital

The estimation of working capital was performed using the definition:

$$C_{wc} = \textit{cash reserves} + \textit{inventory} + \textit{accounts receivable} - \textit{accounts payable}$$

These funds are needed to cover the operating costs required during early operation of the plant, before payment has been received for the products. It was assumed that 30 days of cash reserves were needed (excluding raw materials), as well as 30 days for accounts payable and accounts receivable. Seven days of raw materials and product storage were also assumed to allow for weekly delivery. The total working capital during full scale production for Process 1 was calculated to be $961,291; Process 2 had a total of $882,294. Tables 8 and 9 show the contributions of each of the components to these values. The difference in working capital stems from two sources: Process 1 has a smaller accounts receivable due to the smaller amount of pyridine and 3MP produced, while Process 2 has a larger accounts payable due to the benzene used in azeotropic distillation.

TABLE 8: Working Capital Process 1

	2011	2012	2013
Accounts Receivable	$ 773,834	$ 386,917	$ 386,917
Cash Reserves	$ 93,676	$ 46,838	$ 46,838
Accounts Payable	$ (564,800)	$ (282,400)	$ (282,400)
Pyridine Inventory	$ 180,561	$ 90,281	$ 90,281
Raw Materials	$ 126,531	$ 63,265	$ 63,265
Total	$ 609,803	$ 304,902	$ 304,902
Present Value at 15%	*$ 530,264*	*$ 230,549*	*$ 200,478*
		Total:	$ 961,291

TABLE 9: Working Capital Process 2

	2011	2012	2013
Accounts Receivable	$ 810,653	$ 405,327	$ 405,327
Cash Reserves	$ 78,827	$ 39,413	$ 39,413
Accounts Payable	$ (670,524)	$ (335,262)	$ (335,262)
Pyridine Inventory	$ 189,152	$ 94,576	$ 94,576
Raw Materials	$ 151,583	$ 75,791	$ 75,791
Total	$ 559,691	$ 279,846	$ 279,846
Present Value at 15%	*$ 486,688*	*$ 211,603*	*$ 184,003*
		Total:	$ 882,294

Total Capital Investment

The total capital investment of each process is a summation of all costs involved in the building of the plant: the working capital, the total depreciable capital (which includes the bare module investment as well as the cost of site preparation, service facilities, allocated costs, and contingencies) and the startup cost. Tables 10 and 11 show the progressive summation of costs to obtain a total capital investment of $10,685,000 for Process 1 and $6,986,000 for Process 2. Both values seem reasonable, with Process 1 requiring a larger capital investment due to the large cost of the membrane.

TABLE 10: Total Capital Investment Process 1			
Bare Module Costs			
Fabricated Equipment		$	4,981,102
Process Machinery	+	$	338,071
Spares	+	$	75,900
Storage	+	$	1,293,672
Total Bare Module Costs:		$	6,688,745
Direct Permanent Investment			
Cost of Site Preparations:	+	$	334,437
Cost of Service Facilities:	+	$	334,437
Direct Permanent Investment		$	7,357,619
Total Depreciable Capital			
Contingencies & Contractor Fees	+	$	1,324,371
Total Depreciable Capital		$	8,681,991
Total Permanent Investment			
Cost of Land:	+	$	173,640
Cost of Plant Start-Up:	+	$	868,199
Total Permanent Investment		$	9,723,829
Total Working Capital	+	$	961,291
Total Capital Investment		$	10,685,120

TABLE 11: Total Capital Investment Process 2			
Bare Module Costs			
Fabricated Equipment		$	2,231,981
Process Machinery	+	$	331,277
Spares	+	$	75,900
Storage	+	$	1,559,264
Total Bare Module Costs:		$	4,198,423
Direct Permanent Investment			
Cost of Site Preparations:	+	$	209,921
Cost of Service Facilities:	+	$	209,921
Direct Permanent Investment		$	4,618,265
Total Depreciable Capital			
Contingencies & Contractor Fees	+	$	831,288
Total Depreciable Capital		$	5,449,553
Total Permanent Investment			
Cost of Land:	+	$	108,991
Cost of Plant Start-Up:	+	$	544,955
Total Permanent Investment		$	6,103,499
Total Working Capital	+	$	882,294
Total Capital Investment		$	6,985,793

Operating Costs

The estimated annual costs of operation of both the pervaporation and azeotropic distillation processes are shown in Tables 12 and 13, respectively. The cost of the feed solution was manipulated in both processes to achieve a 15% return on investment: Process 1 could afford a feed cost of $0.712/lb, and Process 2 could afford $0.822/lb. In order to directly compare the annual costs, however, both processes were given a feed price of $0.71/lb. The values in Table 7 were obtained using very conservative estimates of flux, membrane cost, and membrane lifetime: an average flux of 1.1lb/m^2-h, a membrane cost of $400/m^2, and a lifetime of one year. When applying more optimistic values (2.2 lb/m^2-h flux, $200/m^2 membrane, and a lifetime of 2 years), Process 1 could absorb a feed cost of up to $0.76/lb.

The two annual costs are very similar; Process 1 has a slightly higher annual cost than Process 2, indicating that the replacement cost of the pervaporation membrane (using conservative estimates) was more expensive than the annual purchase cost of benzene.

TABLE 12: Annual Cost Summary Process 1	
Variable Cost Summary (at 100% Capacity)	
General Expenses	
Selling / Transfer Expenses:	$627,666
Direct Research:	$1,004,265
Allocated Research:	$104,611
Administrative Expense:	$418,444
Mgmt. Incentive Comp.	$261,527
Total General Expenses	$2,416,513
Raw Materials	$14,620,320
Byproducts	($2,819,315)
Utilities	$609,004
Total Variable Costs	$15,519,969

TABLE 13: Annual Cost Summary Process 2	
Variable Cost Summary (at 100% Capacity)	
General Expenses	
Selling / Transfer Expenses:	$657,530
Direct Research:	$1,052,048
Allocated Research:	$109,588
Administrative Expense:	$438,353
Mgmt. Incentive Comp.	$273,971
Total General Expenses	$2,531,490
Raw Materials	$15,258,062
Byproducts	($3,030,620)
Utilities	$564,623
Total Variable Costs	$15,323,554

The prices obtained for the products, pyridine and 3-methylpyridine, as well as the cost of the benzene used in azeotropic distillation were obtained from old ICIS price reports from 2004. Pyridine was priced at $3.85/lb, taking into account the $0.04/lb required to convert the pyridine produced to the Finished Goods quality specifications. 3-methylpyridine was priced at $2.05/lb, and benzene at $0.39/lb.

Utilities:

A summary of the utility requirements for each process can be found in Tables 14 and 15. The majority of the cost is from the high amounts of low pressure steam used in the distillation columns. Process 1 requires only 20% of the utilities needed for Process 2, due to the low energy requirements of pervaporation.

TABLE 14: Utility costs Process 1

Utility	Unit#	Utility Amount	Price	Annual Cost
Electricity		(kW)	($/kW-hr)	($/yr)
	P100	15.928	0.06	8371.85
	P101	13.065	0.06	6866.80
	P102	1.265	0.06	665.12
	P103	5.378	0.06	2825.89
	P104	2.278	0.06	1197.38
	P105	3.200	0.06	1681.82
	P106	0.366	0.06	192.44
	P107	3.311	0.06	1740.22
	P108	5.380	0.06	2827.85
	P109	1.637	0.06	860.31
	P110	0.371	0.06	194.79
	P111	4.880	0.06	2564.86
	P112	0.708	0.06	372.34
	P113	2.096	0.06	1101.75
	P114	0.180	0.06	94.85
	P115	0.239	0.06	125.42
	Total	60.281	0.06	31683.69
Cooling Water		(lb/hr)	($/1000lb)	($/yr)
	H100	0.0	0.009	0.00
	H101	43184.5	0.009	3401.94
	H103	27813.1	0.009	2191.03
	H104	1378.8	0.009	108.62
	H106	4177.2	0.009	329.07
	H109	34723.0	0.009	2735.37
	H110	4395.7	0.009	346.28
	H111	242.2	0.009	19.08
	H113	4382.5	0.009	345.24
	H114	13385.2	0.009	1054.45
	H116	680.2	0.009	53.58
	H117	1996.2	0.009	157.25
	H118	96.5	0.009	7.60
	H120	1638.2	0.009	129.05
	Total	138093.3	0.009	10878.57
Low Pressure Steam		(lb/hr)	($/lb)	($/yr)
	H102	1691.1	0.003	44442.11
	H105	915.2	0.003	24051.46
	H107	28.0	0.003	735.84
	H108	17.0	0.003	446.76
	H112	554.8	0.003	14580.14
	H115	487.7	0.003	12816.76
	H119	71.3	0.003	1873.76
	Total	3765.1	0.003	98946.83
Total			$	141,509.09

TABLE 15: Utility Costs Process 2

Utility	Unit#	Utility Amount	Price	Annual Cost
Electricity		(kW)	($/kW-hr)	($/yr)
	P200	14.852	0.06	7806.21
	P201	6.596	0.06	3466.60
	P202	1.002	0.06	526.49
	P203	19.033	0.06	10003.90
	P204	114.250	0.06	60049.80
	P205	18.994	0.06	9983.14
	P206	1.923	0.06	1010.83
	P207	2.278	0.06	1197.47
	P208	0.094	0.06	49.41
	P209	0.398	0.06	209.35
	P210	10.329	0.06	5428.66
	P211	1.239	0.06	651.22
	P212	3.480	0.06	1829.09
	P213	0.479	0.06	251.55
	P214	0.350	0.06	183.91
	P215	13.060	0.06	6864.34
	P216	1.265	0.06	664.88
	Total	209.621	0.06	110176.85
Cooling Water		(lb/hr)	($/1000gal)	($/yr)
	H201	43184.5	0.009	3401.95
	H203	467258.5	0.009	36809.21
	H205	914.1	0.009	72.01
	H206	1042.0	0.009	82.09
	H208	421.1	0.009	33.17
	H209	26937.5	0.009	2122.06
	H210	1659.5	0.009	130.73
	H212	653.4	0.009	51.47
	H213	3923.3	0.009	309.06
	H214	107.6	0.009	8.47
	H216	4177.2	0.009	329.07
	Total	550278.6	0.009	43349.29
Low Pressure Steam		(lb/hr)	($/lb)	($/yr)
	H202	1691.1	0.003	44443.07
	H204	15574.7	0.003	409301.87
	H207	915.3	0.003	24053.39
	H211	869.6	0.003	22852.59
	H215	248.2	0.003	6523.69
	Total	19298.9	0.003	507174.60
Total			$	660,700.74

Fixed Costs

Several fixed costs must also be accounted for. Table 16 summarizes the cost factors used, as obtained from ***Seider et al. 2009,*** p604. Tables 17 and 18 summarize the total cost values. The factors chosen are independent of production level, and are the same for both processes. The total fixed cost value for Process 1 is $1,940,000, and the value for Process 2 is $1,577,000.

TABLE 16: Fixed Costs

Operations		
Operators per Shift:	3	(assuming 3 shifts)
Direct Wages and Benefits:	$35	/operator hour
Direct Salaries and Benefits:	15%	of Direct Wages and Benefits
Operating Supplies and Services:	6%	of Direct Wages and Benefits
Maintenance		
Wages and Benefits:	3.5%	of Total Depreciable Capital
Salaries and Benefits:	25.0%	of Maintenance Wages and Benefits
Materials and Services:	100.0%	of Maintenance Wages and Benefits
Maintenance Overhead:	5.0%	of Maintenance Wages and Benefits
Operating Overhead		
General Plant Overhead:	7.1%	of Maintenance and Operations Wages and Benefits
Mechanical Department Services:	2.4%	of Maintenance and Operations Wages and Benefits
Employee Relations Department:	5.9%	of Maintenance and Operations Wages and Benefits
Business Services:	7.4%	of Maintenance and Operations Wages and Benefits
Property Taxes and Insurance		
Property Taxes and Insurance:	2.0%	of Total Depreciable Capital
Straight Line Depreciation		
Direct Plant:	8.0%	of Total Depreciable Capital, less 1.18 times the Allocated Costs for Utility Plants
Allocated Plant:	6.0%	of 1.18 times the Allocated Costs for Utility Plants and Related Facilities

TABLE 17: Fixed Cost Summary Process 1		TABLE 18: Fixed Cost Summary Process 2	
Operations		Operations	
Direct Wages and Benefits	$ 655,200	Direct Wages and Benefits	$ 655,200
Direct Salaries and Benefits	$ 98,280	Direct Salaries and Benefits	$ 98,280
Operating Supplies and Services	$ 39,312	Operating Supplies and Services	$ 39,312
Total Operations	$ 792,792	Total Operations	$ 792,792
Maintenance		Maintenance	
Wages and Benefits	$ 303,870	Wages and Benefits	$ 190,734
Salaries and Benefits	$ 75,967	Salaries and Benefits	$ 47,684
Materials and Services	$ 303,870	Materials and Services	$ 190,734
Maintenance Overhead	$ 15,193	Maintenance Overhead	$ 9,537
Total Maintenance	$ 698,900	Total Maintenance	$ 438,689
Operating Overhead		Operating Overhead	
General Plant Overhead:	$ 80,466	General Plant Overhead:	$ 70,425
Mechanical Department Services:	$ 27,200	Mechanical Department Services:	$ 23,806
Employee Relations Department:	$ 66,866	Employee Relations Department:	$ 58,522
Business Services:	$ 83,865	Business Services:	$ 73,400
Total Operating Overhead	$ 258,396	Total Operating Overhead	$ 226,153
Property Taxes and Insurance		Property Taxes and Insurance	
Property Taxes and Insurance:	$ 173,640	Property Taxes and Insurance:	$ 108,991
Total Fixed Costs	$ 1,923,728	Total Fixed Costs	$ 1,566,625

Profitability Analysis

The main indicators of profitability are the internal rate of return, return on investment, and net present value. A discount rate of 15% was chosen for the NPV calculation. The depreciation was determined using the 5-year MACRS schedule which can be found in Appendix D. An income tax rate of 40% was used, as suggested in *Seider et al., 2009.*

The profitability of both processes depends heavily on the chosen price for the feed stream. In order to directly compare the profitability of the two processes, both were given a feed cost of $0.71/lb. For the pervaporation process, this resulted in a 15% ROI, an 18.68% IRR, and a NPV of $1,779,200. For the azeotropic distillation process, this resulted in a 31.36% ROI, 32.45% IRR, and $6,444,100 NPV. A sensitivity analysis was performed to illustrate the impact of feed cost on NPV for both processes, as shown in Figure 12.

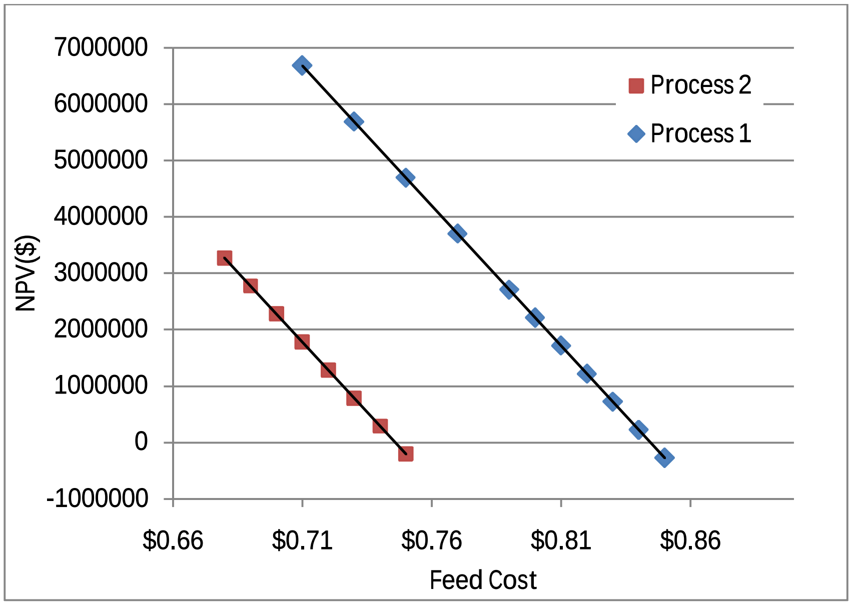

Figure 12: Illustrates the effect of feed cost on the NPV for process 1 and 2. Process 1 is profitable below a feed cost of \$0.745/lb, while Process 2 is profitable below \$0.845/lb.

Additional analysis was also required for the pervaporation process, as the calculations required a significant number of assumptions. The effect of average flux, membrane cost, and membrane lifetime on NPV can be seen in Figure 13.

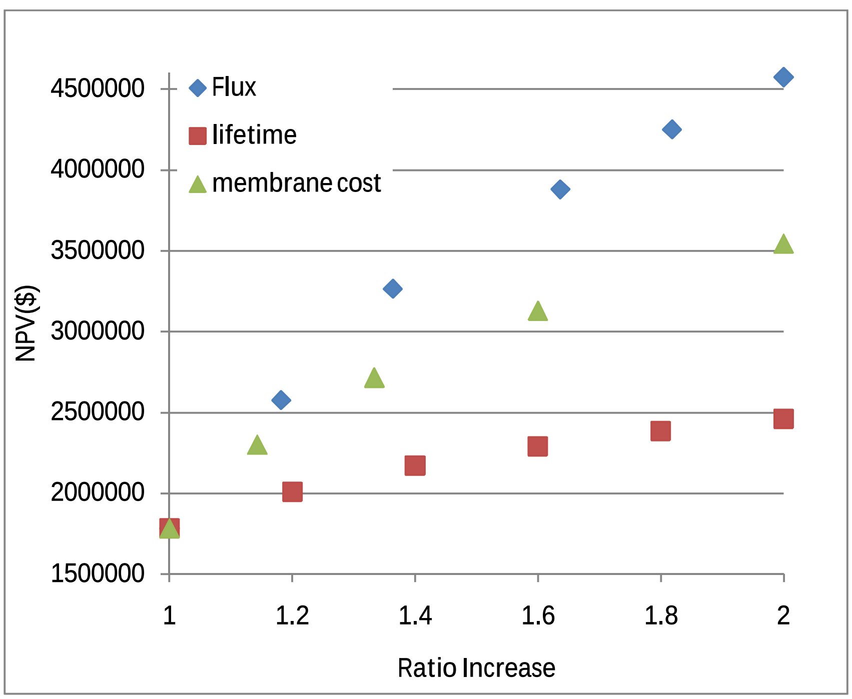

Figure 13: Shows the relative impact of flux, membrane cost, and lifetime on NPV for pervaporation. Each factor was scaled up to double the conservative estimate. The flux has the greatest impact on NPV, shown in blue.

OTHER CONSIDERATIONS

Environmental problems and fixes

Several of the chemicals in our processes require caution when dealing with large quantities. Pyridine, 3MP, methanol, and benzene are all flammable and must be kept away from heat and ignition sources. Both of our processes are run well below auto ignition temperatures. Some chemicals such as pyridine and 3MP are not biodegradable when released into water. Pyridine and methanol are toxic to aquatic life. Most chemicals except water have specific regulations set by the federal and state laws for disposal. Prolonged exposure to airborne benzene, pyridine and 3MP are hazardous, so adequate ventilation becomes important.

Safety and Health Concerns

Pyridine, 3MP, methanol, benzene and n-butyronitrile are very harmful if swallowed, absorbed through skin, or inhaled. 3MP, pyridine and n-butyronitrile can be fatal if swallowed. In addition, prolonged exposure to pyridine, 3MP, and benzene has chronic effects including carcinogenic and mutagenic effects.

Startup and Process Controllability

All units require some degree of control to maintain proper separation. The azeotropic distillation column is very sensitive to changes in composition within the column; therefore the benzene and feed flow rates to the column should be carefully controlled. The pervaporation unit must operate with a permeate pressure at or below the specified 2.2 psia; higher pressures would decrease the flux through the membrane and lead to incomplete separation. Therefore, strict control must be placed on the permeate condenser to ensure the pressure remains below the threshold.

Start-up requires special considerations in both processes. In process 2, under steady state conditions only 207 lb/hr of benzene is being fed to the system, to make up for the loss to in the decanter and purge streams. During start up, however, 3900 lb must be fed to the azeotropic distillation column until steady state is reached.

Process 1 requires extra equipment for start-up, including a vacuum pump to generate the pressure differential across the pervaporation membrane before there is any vapor to condense. In addition, a heat exchanger is needed to preheat S101 before it enters D101 with low pressure steam until S103 can be used to do so.

CONCLUSIONS AND RECOMMENDATIONS

The processes outlined in this report offer two competing methods to recover pyridine and 3-methylpyridine from a given impure stream. The design had to meet quality specifications set by the potential clients. Although there are other existing industry methods, the new processes enclosed sought to be more cost efficient and environmentally friendly.

The design was complicated by multiple azeotropes with water. Therefore, the key element in each of our processes is centered around the removal of water. The first process employed pervaporation, using a hydrophilic membrane to withdraw water and methanol from the product stream. The benefits of pervaporation include low utility requirements relative to conventional methods, and operation independent of vapor liquid equilibrium. One drawback is the high replacement cost for the membrane, which needs to be replaced every year.

The second process utilized azeotropic distillation with a benzene solvent to break the water azeotropes. Benzene forms a low boiling heterogeneous azeotrope with water and changes the chemical interaction of the system, allowing for separation of water from the stream. The water benzene mixture is separated easily with a decanter. Although a large amount of benzene needs to be circulating the system, the majority is recycled. The benefit of this process is high recovery of pyridine and 3-methylpyridine; however, the process incurs high utility costs and the additional purchasing cost of benzene.

The main measure of profitability for the two processes is the feed cost that could be absorbed to give a 15% return on investment. Process 1 could afford $0.71/lb feed, while Process 2 could afford up to $0.82/lb. For a set feed cost of $0.71/lb in both processes, the total capital investment for Process 1 and Process 2 is $ 10,685,000, and $6,986,000 respectively. Assuming a 15 year lifetime, the net present value is $1,779,000 for Process 1, and $6,444,000 for Process

2. The investor's rate of return is 18.68% for the pervaporation process and 32.45% for the azeotropic distillation process. In both processes, the removal of n-butyronitrile in the first distillation column resulted in a large loss of product and decreased the profitability of the processes; the removal of water was the most expensive step in both.

Further investigation to confirm the assumptions made in calculating the pervaporation module parameters is recommended. The more significant parameters include flux, temperature drop across a module, and membrane cost. In addition, the pump sizing and heat exchanger designs were performed using correlations found in ***Seider et al., 2009***. Due to the small stream flow rates, many of the units did not fall into the acceptable size ranges. The accuracy of the calculations could be improved by the use of more appropriate correlations.

Overall, Process 1 recovers 88.1% of the original amount of pyridine introduced to the system, and 96.0% of 3MP. Meanwhile, Process 2 recovers 92.2% of the pyridine and 99.7% of 3MP originally introduced to the system. Although both processes have their benefits and drawbacks, we would recommend the implementation of Process 2 for the economic recovery of pyridine and 3-methylpyridine.

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APPENDIX A: PROBLEM STATEMENT

Economic Recovery of Pyridine

(recommended by Leonard A. Fabiano, U. Penn)

Introduction and Scope

The pyridine manufacturing process consists of a vapor phase catalyzed reaction and purification processes. Pyridine and 3-methylpyridine are synthetically co-produced in a circulating fluidized bed reactor. Impurities are also produced in the reaction process. These impurities are removed based on customer needs. During separation processes to make finished goods, useful product is lost to various streams and must be recovered. The subject of this project is to recover the pyridine and 3-methylpyridine from an impurity stream for recycle back to the process at the lowest processing cost that meets targeted capital payback criteria.

You are the design engineering team from an engineering consulting firm that has been hired to evaluate potential separation technologies and make a recommendation on the most cost effective new process for recovery of pyridine and 3-methylpyridine from this stream. The design must meet the specified criteria for waste disposal, minimal product losses, and capital payback requirement.

General Process Description

A stream containing light boiling impurities, water, pyridine and 3–methylpyridine are processed to remove the light boiling impurities through separation technologies. The current process generates recycle streams that need further processing. The current operating cost for recovering pyridine from these streams is $0.04/lb of recycle (pyridine + 3methylpyridine + water + light boiling impurities), approximately $800,000 per year.

An energy efficient, low capital means of recovering the pyridine and 3-methylpyridine from water and the light boiling impurities is preferred.

Alternatives to be Considered

Pyridine and 3-methylpyridine must be separated from water and light impurities. This is complicated by azeotropes of the organic components with water (pyridine, 3-methylpyridine and the light boiling impurities azeotrope with water). Potential alternatives to be considered, but not limited to, are shown below:

a. Removal of water followed by separation of light impurities from the products

b. Chemical treatment of water + lights + pyridine stream with caustic to form two layers, layer separation of organics, followed by separation of light impurities from pyridine

c. Removal of water using membrane technology, followed by separation of light impurities from pyridine

d. Adsorption of water on molecular sieves, followed by separation of light impurities from pyridine

Design Keys

a. Composition of Stream Requiring Pyridine and 3-Methylpyridine Recovery

Components	MW	Flows, lb/hr	Weight %
METHANOL	32.04	130	5
ACETONITRILE	41.05	312	12
PYRIDINE	79.1	780	30
3-METHYLPYRIDINE	93.13	208	8
n-BUTYRONITRILE	69.11	26	1
XYLENE (o,m, & p)	106.17	26	1
WATER	18.02	1,118	43
Total		2,600	100

b. Equipment Sizing Basis

Equipment should be sized for the specified stream requiring pyridine and 3-methylpyridine recovery + 20% contingency to allow for maintenance downtime. So, the unit should be designed to process an instantaneous feed rate of 3,120 lb/hr.

c. Utilities

The following utilities are available at the manufacturing site within 200 ft of where the proposed pyridine recovery process will be installed:

Steam: 180 psig, 380ºF saturated

Cooling water: 85ºF supply temperature, maximum 120ºF return temperature, 40 psig

Nitrogen: > 98% purity, 100 psig

Plant and instrument air: 80ºF, 100 psig, dew point = -22ºF

City water: 40 psig, 55-65ºF

Purified water (boiler feed water quality): 200ºF, 40 psig

Electric power: 480 V, 3 phase, 60 Hz

Natural gas: 30 psig

d. Process Conditions and Constraints

The process is to be designed with sufficient automation that a minimum of operating personnel will be required – to be discussed with the industrial consultants and faculty. A detailed design of the control system is not required. A Distributed Control System is available for controlling the process instrumentation. While a continuous process is preferred for ease of operations, would a batch process be preferable?

Tanks are available in the area where the new process equipment will be installed within 200 ft for storage of the stream requiring pyridine and 3-methylpyridine recovery, the recovered pyridine stream, the recovered 3-methylpyridine, and the waste streams.

A preliminary plant layout, footprint and elevations, are to be proposed in order to assess the total area required for this facility.

e. Heat Generation and Removal

Heat input could be provided through electrical heating, steam, or a natural gas fired furnace with circulating heat transfer oil. Cooling could be provided through air cooled exchangers or cooling water cooled exchangers. Provide the basis for your design team's selection.

f. Waste Water Processing Capabilities

Water with organic concentrations up to a maximum of 1% and a pH of 4-12 can be processed on-site at the facilities waste water treatment plant for removal of organics and pH adjustment. If the new process generates waste water with > 1% organics, a pH < 4 or pH > 12, it must be sent off-site for treatment at $4.00/gal.

g. Liquid Waste Fuel Processing Capabilities

Liquid organic waste streams must be < 5% pyridine and < 15% water in order to be used on-site as fuel to be equivalent with the existing process. If the liquid organic waste stream is > 15% water, it must be sent off site for disposal at a cost of $0.20/lb.

Environmental/Health/Safety

The proposed design must comply with U.S. environmental laws and protect the safety and health of the manufacturing site personnel and the community. All equipment should be designed using good engineering practice and meet or exceed applicable U.S. codes and standards. Your design team should indicate the most serious environmental problems, provide references, and identify the applicable codes.

Quality Requirements

The recovered pyridine and 3-methylpyridine streams from the new process must be capable of being purified to meet finished goods specifications. The recovered material from the new process would have to be incorporated into one of the following streams based on its quality as specified. The additional processing costs for these streams are included below:

a. Pyridine Finished Goods Quality Specifications:

Pyridine	99.75% minimum
3-Methylpyridine	0.01% maximum
N-butyronitrile	0.05% maximum
Water	0.1% maximum

No additional processing necessary

b. 3-Methylpyridine Finished Goods Quality Specifications:

3-Methylpyridine	98.0% minimum
Sum of light boiling impurities	0.2% maximum
Water	0.2% maximum

No additional processing necessary

c. Crude Quality Specifications:

Pyridine and 3-Methylpyridine	98.0% minimum

N-butyronitrile	0.03% maximum
Xylene	0.1% maximum
Water	1.0 % maximum

Additional processing energy cost = $0.07/lb of crude

d. Pyridine Intermediate Quality Specifications:

Pyridine	98.0% minimum
3-Methylpyridine	1.0% maximum
N-butyronitrile	0.04% maximum
Xylene	0.1% maximum
Water	1.0% maximum

Additional processing energy cost = $0.04/lb of pyridine intermediate cut

e. 3-Methylpyridine Intermediate Quality Specifications:

3-Methylpyridine	98.0% minimum
Pyridine	1.0% maximum
N-butyronitrile	0.04% maximum
Xylene	0.1% maximum
Water	1.0% maximum

Additional processing energy cost = $0.04/lb of 3-methylpyridine intermediate cut

Cost Data

	$/Unit	Units
Natural gas	11.00	MCF(Std)
Electricity	35.00	KWH
City water	1.00	MGAL
Steam	17.00	MLB

Nitrogen	2.25	MCF(Std)
50% Caustic	0.125	LB

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APPENDIX B: DETAILED DESIGN CALCULATIONS

Sample Calculation: Pump
Unit ID: P-100

Flow Rate	2600	lb/hr		
Pressure Rise	30	psi	10681.13	lb/ft2
Liquid Density	56.29317	lb/ft3	74.1745	psi
Pump Head	189.7411	ft		
Volumetric Rate	5.758351	gpm		
Size Factor	79.31929			
HP	21.35614	Hp		
CB	3220.882	(400<S<100000)		
FM	1	cast iron	(Table 22.21, p562)	
FT	1	(Table 22.20, p561)		
Cp	3220.882			
Scaled to 2010 Price:	3704.014			

Sample Calculation: Storage Tank
Unit ID: T-101

Hours required	336		
Flow Rate	2600	lb/hr	
Density	57.88188	lb/ft3	
Fluid Volume	15092.81	ft3	
Tank Volume	17756.24	ft3	(85% capacity)
	132816.7	gal	
Cp	108668.8		
Scaled to 2010 Price:	124969.1		

Sample Calculation: Reflux Accumulator
Unit ID: A-101

Horizontal Pressure Vessel				
Residence Time	0.083333	hr	(50% full)	
Aspect Ratio = L/D	2			
Flow Rate	1491	lb/hr		
Density	44.39854	lb/ft3		
Vol. Flow rate	33.58218	ft3/hr		Density Material
Holdup	2.798515	ft3		490 lb/ft3
Volume (50%full)	5.597031	ft3		(carbon steel)
Diameter	1.527376	ft		
Length	3.054752	ft		
Weight	212.3432	lb		
Operating Pressure	0	psig	(IF operating Pressure is between 0 and 5 psig,	
Design Pressure	10	psig	DESIGN PRESSURE = 10 psig)	
Maximum Stress (S)	13750	psi	(for carbon steel, T up to 650 F)	
Fractional Weld Efficiency	0.85			
Wall thickness	0.000654	ft	(if this value is too small,	
	0.007845	in	use correlations on p 575)	
Modified Thickness:	0.25	in		
	0.020833	ft		
Cv	2224.523	(for 1000<W<920,000 lb)		
CPL	2184.964	(for 3<Di<12 ft)		
Cp	4409.488			
Scaled to 2010 Price:	5070.911			

Sample Calculation: Distillation Column
Unit ID: D-201

PROPERTIES

L (liq flow rate)	4661	lb/hr
G (gas flow rate)	2819	lb/hr
ρ (liq)	56.8313	lb/ft^3
ρ (gas)	0.07482	lb/ft^3
surface tension	48.20225	dyne/cm

CAPACITY PARAMETER

C_{SB} (Fair correlation*)	0.37	ft/s
Tray Spacing	24	inch
F_{LG} (flow ratio)	0.0600	

*See p.505 in Product and Process Design Principles textbook for Fair correlation graph

F_{ST} (surf tension factor)	1.19				
F_F (foaming factor)	1		(non-foaming)		
F_{HA} (hole area factor)	1		(sieve tray)		
$C = C_{SB}*F_{ST}*F_F*F_{HA}$	0.44	ft/s			

FLOODING VELOCITY

U_f	12.2	ft/s	=	43743	ft/hr
f (% flooding)	0.8				
$U = f*U_f$	34995	ft/hr			

DIAMETER

A_d/A_T	0.2				
D	1.34	feet	=	16.13	inch

PURCHASE & INSTALLATION				
Tray Input into Aspen		39	trays	
Tray Efficiency		69%		
Actual No. of trays		66	trays	
Length		144	feet	
t_S (shell thickness)		0.25	inch	(up to 4 ft diameters)
Tower Weight (W)		6361	lb	
P_d (internal P)		15	psi	
S (max allowable stress)		15000	psi	(up to T = 750F)
E (frac weld efficiency)		0.85		
ρ (density of carbon steel)		0.284	lb/in^3	
F_M (material factor)		1		(carbon steel)
C_{PL} (platforms & ladders)	$	19,496.53		
C_V (empty vessel)	$	32,011.16	4200<W<1000000	
C_P (purchase cost)	$	51,507.69		
PURCHASE COST OF TRAYS				
N_T (number of trays)		66		
F_{NT} (number factor)		1		
F_{TT} (type factor)		1		(sieve)
F_{TM} (materials factor)		1		(carbon steel)
C_{BT} (base cost)	$	591.26		
$C_T = N_T*F_{NT}*F_{TT}*F_{TM}*C_{BT}$	$	39,023.00		
TOTAL COST OF COLUMN				
C_P	$	90,530.69		
INSTALLATION COST OF COLUMN				
F_{BM} (bare module factor)		4.16		(Vertical Pressure Vessel)
C_{BM} (column)	$	376,607.68		
Scale to Year 2010 (CE index = 575)	$	433,098.83		

Sample Calculation: Heat Exchanger
Unit ID: H-201

U	100	Btu/°F-ft^2-hr
Shell side: organic solvent		
Tube side: water solvent		
Range of U: 50 - 120 Btu/°F-ft^2-hr		
?T_{LM}	69.7221082	°F
Q	1294240.7	Btu/hr
A	185.628452	ft^2

<u>Shell-and-Tube Cost</u>

C_B	$ 7,516.45	
F_M	1	
Assume shell and tube both use carbon steel material		
a = 0 inch		
b = 0 inch		
F_L	1.25	
Length = 8 feet		
P	50	psi
F_P	0.989725	
$C_P=C_B*F_M F_L*F_P$	$ 9,299.03	
F_{BM}	3.17	
C_{BM}	$29,477.92	
Scale to Year 2010 (CE index = 575)	$33,899.61	

Sample Calculation: Pervaporation Modules
Unit ID: PM-101-103

FEED	FLUX1	RETENT 1	FLUX 2	RETENT 2	FLUX 3	PRODUCT
1966.28 lb/hr total		1334.59 total		1029.20 total		930.79 total
1037.69 lb/hr water	1.33	417.33 water	0.69	117.41 water	0.23	20.75 water
0.53 frac water	lb/m^2-hr	0.31 frac water	lb/m^2-hr	0.11 frac water	lb/m^2-hr	0.02 frac water

PERM1	PERM2	PERM3
631.69 lb/hr total	305.39 lb/hr total	98.41 lb/hr total
620.36 lb/hr water+meOH	299.91 lb/hr water+meOH	96.64 lb/hr water+meOH
0.98 wat frac water+meOH	0.98 wate frac water+meOH	0.98 wat frac water+meOH

Overall mass balance:
1035.49 1035.49

Overall Water Balance:
1037.69 1037.6738

Overall Water removal:
0.98

Box 1 Water balance:
417.3252 417.32519
Box 2 Water bal:
117.4119 117.41185

In box 1,	
start flux	1.8
ending flux	0.8599252
AVERAGE	1.3299626
In box 2	
start flux	1.0583695
ending flux	0.3125154
average	0.6854425
In box 3	
start flux	0.3846344
ending flux	0.0869565
average	0.2357954

Area balance:
509 509 509
Total Area: 1526.45 m^2

Weighted Average Flux
1.09 lb/m^2-hr

Module Cost:
Area 16419.76 ft2
Cp $623,951
Scaled to 2010 Price:
$717,544

APPENDIX C:

ASPEN SPLIT ANALYSIS

AZEOTROPE SEARCH REPORT

Physical Property Model: NRTL-RK Valid Phase: VAP-LIQ

Mixture Investigated For Azeotropes At A Pressure Of 101325 N/SQM

Comp ID	Component Name	Classification	Temperature
METHANOL	METHANOL	Saddle	64.53 C
ACN	ACETONITRILE	Saddle	81.48 C
PYRIDINE	PYRIDINE	Saddle	115.16 C
3MP	3-METHYLPYRIDINE	Stable Node	144.15 C
N-BUTYRO	BUTYRONITRILE	Saddle	117.37 C
WATER	WATER	Stable Node	100.02 C
PXYLENE	P-XYLENE	Stable Node	138.37 C

9 Azeotropes Sorted by Temperature

01

Number Of Components: 2 Temperature 63.58 C
Homogeneous Classification: Unstable Node

	MOLE BASIS	MASS BASIS
METHANOL	0.8000	0.7574
ACN	0.2000	0.2426

02

Number Of Components: 2 Homogeneous	Temperature 76.65 C Classification: Saddle	
	MOLE BASIS	**MASS BASIS**
ACN	0.6748	0.8255
WATER	0.3252	0.1745

03

Number Of Components: 3 Homogeneous	Temperature 74.26 C Classification: Saddle	
	MOLE BASIS	**MASS BASIS**
ACN	0.3485	0.3463
WATER	0.4782	0.2085
PXYLENE	0.1733	0.4452

04

Number Of Components: 2 Homogeneous	Temperature 93.67 C Classification: Saddle	
	MOLE BASIS	**MASS BASIS**
PYRIDINE	0.2526	0.5974
WATER	0.7474	0.4026

05

Number Of Components: 3	**Temperature 93.90 C**	
Homogeneous	**Classification: Saddle**	
	MOLE BASIS	**MASS BASIS**
METHANOL	0.0372	0.0372
PYRIDINE	0.2220	0.5471
WATER	0.7407	0.4157

06

Number Of Components: 2	**Temperature 96.17 C**	
Homogeneous	**Classification: Saddle**	
	MOLE BASIS	**MASS BASIS**
3MP	0.1280	0.4314
WATER	0.8720	0.5686

07

Number Of Components: 2	**Temperature 138.12 C**	
Homogeneous	**Classification: Saddle**	
	MOLE BASIS	**MASS BASIS**
3MP	0.1992	0.1791
PXYLENE	0.8008	0.8209

08

Number Of Components: 2 Homogeneous	Temperature 86.08 C Classification: Saddle	
	MOLE BASIS	MASS BASIS
N-BUTYRO	0.3609	0.6841
WATER	0.6391	0.3159

09

Number Of Components: 2 Homogeneous	Temperature 76.14 C Classification: Saddle	
	MOLE BASIS	MASS BASIS
WATER	0.6751	0.2607
PXYLENE	0.3249	0.7393

APPENDIX D: PROFITABILITY ANALYSIS WORKSHEET

	MACRS Depreciation Schedule:				
	5 year	*7 year*	*10 year*	*15 year*	*20 year*
1	20.00%	14.29%	10.00%	5.00%	3.75%
2	32.00%	24.49%	18.00%	9.50%	7.22%
3	19.20%	17.49%	14.40%	8.55%	6.68%
4	11.52%	12.49%	11.52%	7.70%	6.18%
5	11.52%	8.93%	9.22%	6.93%	5.71%
6	5.76%	8.92%	7.37%	6.23%	5.29%
7		8.93%	6.55%	5.90%	4.89%
8		4.46%	6.55%	5.90%	4.52%
9			6.56%	5.91%	4.46%
10			6.55%	5.90%	4.46%
11			3.28%	5.91%	4.46%
12				5.90%	4.46%
13				5.91%	4.46%
14				5.90%	4.46%
15				5.91%	4.46%
16				2.95%	4.46%
17					4.46%
18					4.46%
19					4.46%
20					4.46%
21					2.23%

General Information

Process Title:	Pyridine Recovery, Process 1
Product:	Pyridine
Plant Site Location:	Gulf Coast
Site Factor:	1.00
Operating Hours per Year:	7920
Operating Days Per Year:	330
Operating Factor:	0.9041

Product Information

This Process will Yield

	686	lb of Pyridine per hour
	16,468	lb of Pyridine per day
	5,434,335	lb of Pyridine per year
Price	$3.85	/lb

Chronology

Year	Action	Distribution of Permanent Investment	Production Capacity	Depreciation 5 year MACRS	Product Price
2010	Design		0.0%		
2011	Construction	100%	0.0%		
2012	Production	0%	45.0%	20.00%	$3.85
2013	Production	0%	67.5%	32.00%	$3.85
2014	Production	0%	90.0%	19.20%	$3.85
2015	Production		90.0%	11.52%	$3.85
2016	Production		90.0%	11.52%	$3.85
2017	Production		90.0%	5.76%	$3.85
2018	Production		90.0%		$3.85
2019	Production		90.0%		$3.85
2020	Production		90.0%		$3.85
2021	Production		90.0%		$3.85
2022	Production		90.0%		$3.85
2023	Production		90.0%		$3.85
2024	Production		90.0%		$3.85
2025	Production		90.0%		$3.85
2026	Production		90.0%		$3.85

Raw Materials

	Raw Material:	Unit:	Required Ratio:		Cost of Raw Material:	
1	Feed	lb	3.7892398	lb per lb of Pyridine	$0.712	per lb
	Total Weighted Average:				$2.698	per lb of Pyridine

Byproducts

	Byproduct:	Unit:	Ratio to Product		Byproduct Selling Price	
1	3MP	lb	0.2913342	lb per lb of Pyridine	$2.050	per lb
2	Organic Waste	lb	0.392193	lb per lb of Pyridine	-$2.000E-01	per lb
	Total Weighted Average:				$0.519	per lb of Pyridine

Utilities

	Utility:	Unit:	Required Ratio		Utility Cost	
1	Low Pressure Steam	1 lb	1.5523131	1 lb per lb of Pyridine	$3.000E-03	per 1 lb
2	Cooling Water	1 gal	7.8164535	1 gal per lb of Pyridine	$7.500E-05	per 1 gal
3	Electricity	kWh	0.0878535	kWh per lb of Pyridine	$0.060	per kWh
4	Membrane replacement	m2	0.0002539	m2 per lb of Pyridine	$400.00	per m2
	Total Weighted Average:				$0.112	per lb of Pyridine

Variable Costs

General Expenses:

Selling / Transfer Expenses:	3.00%	of Sales
Direct Research:	4.80%	of Sales
Allocated Research:	0.50%	of Sales
Administrative Expense:	2.00%	of Sales
Management Incentive Compensation:	1.25%	of Sales

Working Capital

Accounts Receivable	a	30	Days
Cash Reserves (excluding Raw Materials)	a	30	Days
Accounts Payable	a	30	Days
Pyridine Inventory	a	7	Days
Raw Materials	a	7	Days

Total Permanent Investment

Cost of Site Preparations:	5.00%	of Total Bare Module Costs
Cost of Service Facilities:	5.00%	of Total Bare Module Costs
Allocated Costs for utility plants and related facilities:	$0	
Cost of Contingencies and Contractor Fees:	18.00%	of Direct Permanent Investment
Cost of Land:	2.00%	of Total Depreciable Capital
Cost of Royalties:	$0	
Cost of Plant Start-Up:	10.00%	of Total Depreciable Capital

Fixed Costs

Operations

Operators per Shift:	3	(assuming 3 shifts)
Direct Wages and Benefits:	$35	/operator hour
Direct Salaries and Benefits:	15%	of Direct Wages and Benefits
Operating Supplies and Services:	6%	of Direct Wages and Benefits
Technical Assistance to Manufacturing:	$0.00	per year, for each Operator per Shift
Control Laboratory:	$0.00	per year, for each Operator per Shift

Maintenance

Wages and Benefits:	3.50%	of Total Depreciable Capital
Salaries and Benefits:	25%	of Maintenance Wages and Benefits
Materials and Services:	100%	of Maintenance Wages and Benefits
Maintenance Overhead:	5%	of Maintenance Wages and Benefits

Operating Overhead

General Plant Overhead:	7.10%	of Maintenance and Operations Wages and Benefits
Mechanical Department Services:	2.40%	of Maintenance and Operations Wages and Benefits
Employee Relations Department:	5.90%	of Maintenance and Operations Wages and Benefits
Business Services:	7.40%	of Maintenance and Operations Wages and Benefits

Property Taxes and Insurance

Property Taxes and Insurance:	2%	of Total Depreciable Capital

Straight Line Depreciation

Direct Plant:	8.00%	of Total Depreciable Capital, less 1.18 times the Allocated Costs for Utility Plants and Related Facilities
Allocated Plant:	6.00%	of 1.18 times the Allocated Costs for Utility Plants and Related Facilities

Other Annual Expenses

Rental Fees (Office and Laboratory Space):	$0
Licensing Fees:	$0
Miscellaneous:	$0

Depletion Allowance

Annual Depletion Allowance:	$0

Cash Flow Summary

Year	Percentage of Design Capacity	Product Unit Price	Sales	Capital Costs	Working Capital	Var Costs	Fixed Costs	Depreciation	Depletion Allowance	Taxible Income	Taxes	Net Earnings
2010	0%		-	-	-	-	-	-	-	-	-	-
2011	0%		-	(9,723,800)	(609,800)	-	-	-	-	-	-	-
2012	45%	$3.85	9,415,000	-	(304,900)	(6,690,500)	(1,923,700)	(1,736,400)	-	(935,600)	374,200	(561,400)
2013	68%	$3.85	14,122,500	-	(304,900)	(10,035,700)	(1,923,700)	(2,778,200)	-	(615,200)	246,100	(369,100)
2014	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	(1,666,900)	-	1,858,400	(743,300)	1,115,000
2015	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	(1,000,200)	-	2,525,100	(1,010,100)	1,515,100
2016	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	(1,000,200)	-	2,525,100	(1,010,100)	1,515,100
2017	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	(500,100)	-	3,025,200	(1,210,100)	1,815,100
2018	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	-	-	3,525,300	(1,410,100)	2,115,200
2019	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	-	-	3,525,300	(1,410,100)	2,115,200
2020	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	-	-	3,525,300	(1,410,100)	2,115,200
2021	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	-	-	3,525,300	(1,410,100)	2,115,200
2022	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	-	-	3,525,300	(1,410,100)	2,115,200
2023	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	-	-	3,525,300	(1,410,100)	2,115,200
2024	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	-	-	3,525,300	(1,410,100)	2,115,200
2025	90%	$3.85	18,830,000	-	-	(13,380,900)	(1,923,700)	-	-	3,525,300	(1,410,100)	2,115,200
2026	90%	$3.85	18,830,000	-	1,219,600	(13,380,900)	(1,923,700)	-	-	3,525,300	(1,410,100)	2,115,200

Profitability Measures

The Internal Rate of Return (IRR) for this project is 18.68%

The Net Present Value (NPV) of this project in 2010 is $ 1,779,200

ROI Analysis (Third Production Year)

Annual Sales	18,829,972
Annual Costs	(15,304,664)
Depreciation	(777,906)
Income Tax	(1,098,961)
Net Earnings	1,648,441
Total Capital Investment	10,943,436
ROI	15.06%

Sensitivity Analyses

Note: The Sensitivity Analyses section below takes quite a bit of memory to update each time a cell is changed; therefore, automatic calculations are turned off. After making your axis selections, press "F9" to recalculate the IRR values. (These two lines may be deleted before printing.)

	Vary Initial Value by +/-
x-axis	50%
y-axis	50%

Variable Costs (columns); Product Price (rows)

Product Price	$7,433,853	$8,920,624	$10,407,395	$11,894,165	$13,380,936	*$14,867,707*	$16,354,477	$17,841,248	$19,328,019	$20,814,789	$22,301,560
$1.93	-0.37%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$2.31	14.79%	5.04%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$2.70	25.01%	17.81%	9.23%	-3.33%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.08	33.59%	27.37%	20.57%	12.76%	2.62%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.47	41.30%	35.60%	29.60%	23.12%	15.87%	7.07%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.85	48.43%	43.09%	37.54%	31.72%	25.51%	18.68%	10.74%	0.17%	Negative IRR	Negative IRR	Negative IRR
$4.24	55.16%	50.06%	44.82%	39.40%	33.75%	27.76%	21.27%	13.95%	4.91%	Negative IRR	Negative IRR
$4.62	61.56%	56.65%	51.64%	46.50%	41.20%	35.69%	29.90%	23.69%	16.83%	8.75%	-2.33%
$5.01	67.69%	62.94%	58.11%	53.18%	48.14%	42.94%	37.57%	31.94%	25.97%	19.47%	12.06%
$5.39	73.59%	68.98%	64.29%	59.53%	54.68%	49.72%	44.63%	39.37%	33.90%	28.12%	21.92%
$5.78	79.30%	74.80%	70.24%	65.62%	60.92%	56.14%	51.26%	46.26%	41.12%	35.78%	30.18%

General Information

Process Title:	Pyridine Recovery, Process 2
Product:	Pyridine
Plant Site Location:	Gulf Coast
Site Factor:	1.00
Operating Hours per Year:	7920
Operating Days Per Year:	330
Operating Factor:	0.9041

Product Information

This Process will Yield

	719	lb of Pyridine per hour
	17,251	lb of Pyridine per day
	5,692,898	lb of Pyridine per year
Price	$3.85	/lb

Chronology

Year	Action	Distribution of Permanent Investment	Production Capacity	Depreciation 5 year MACRS	Product Price
2010	Design		0.0%		
2011	Construction	100%	0.0%		
2012	Production	0%	45.0%	20.00%	$3.85
2013	Production	0%	67.5%	32.00%	$3.85
2014	Production	0%	90.0%	19.20%	$3.85
2015	Production		90.0%	11.52%	$3.85
2016	Production		90.0%	11.52%	$3.85
2017	Production		90.0%	5.76%	$3.85
2018	Production		90.0%		$3.85
2019	Production		90.0%		$3.85
2020	Production		90.0%		$3.85
2021	Production		90.0%		$3.85
2022	Production		90.0%		$3.85
2023	Production		90.0%		$3.85
2024	Production		90.0%		$3.85
2025	Production		90.0%		$3.85
2026	Production		90.0%		$3.85

Raw Materials

	Raw Material:	Unit:	Required Ratio:		Cost of Raw Material:	
1	Feed	lb	3.6171383	lb per lb of Pyridine	$0.822	per lb
2	Benzene	lb	0.2879799	lb per lb of Pyridine	$0.39	per lb
	Total Weighted Average:				$3.085	per lb of Pyridine

Byproducts

	Byproduct:	Unit:	Ratio to Product		Byproduct Selling Price	
1	3MP	lb	0.2781023	lb per lb of Pyridine	$2.050	per lb
2	Organic waste	lb	0.1887932	lb per lb of Pyridine	-$2.000E-01	per lb
	Total Weighted Average:				$0.532	per lb of Pyridine

Utilities

	Utility:	Unit:	Required Ratio		Utility Cost	
1	Low Pressure Steam	1 lb	26.848737	1 lb per lb of Pyridine	$3.000E-03	per 1 lb
2	Cooling Water	1 gal	15.152359	1 gal per lb of Pyridine	$7.500E-05	per kWh
3	Electricity	kWh	0.2916262	kWh per lb of Pyridine	$0.060	per kWh
	Total Weighted Average:				$0.099	per lb of Pyridine

Variable Costs

General Expenses:

Selling / Transfer Expenses:	3.00%	of Sales
Direct Research:	4.80%	of Sales
Allocated Research:	0.50%	of Sales
Administrative Expense:	2.00%	of Sales
Management Incentive Compensation:	1.25%	of Sales

Working Capital

Accounts Receivable	a	30	Days
Cash Reserves (excluding Raw Materials)	a	30	Days
Accounts Payable	a	30	Days
Pyridine Inventory	a	7	Days
Raw Materials	a	7	Days

Total Permanent Investment

Cost of Site Preparations:	5.00%	of Total Bare Module Costs
Cost of Service Facilities:	5.00%	of Total Bare Module Costs
Allocated Costs for utility plants and related facilities:	$0	
Cost of Contingencies and Contractor Fees:	18.00%	of Direct Permanent Investment
Cost of Land:	2.00%	of Total Depreciable Capital
Cost of Royalties:	$0	
Cost of Plant Start-Up:	10.00%	of Total Depreciable Capital

Fixed Costs

Operations

Operators per Shift:	3	(assuming 3 shifts)
Direct Wages and Benefits:	$35	/operator hour
Direct Salaries and Benefits:	15%	of Direct Wages and Benefits
Operating Supplies and Services:	6%	of Direct Wages and Benefits
Technical Assistance to Manufacturing:	$0.00	per year, for each Operator per Shift
Control Laboratory:	$0.00	per year, for each Operator per Shift

Maintenance

Wages and Benefits:	3.50%	of Total Depreciable Capital
Salaries and Benefits:	25%	of Maintenance Wages and Benefits
Materials and Services:	100%	of Maintenance Wages and Benefits
Maintenance Overhead:	5%	of Maintenance Wages and Benefits

Operating Overhead

General Plant Overhead:	7.10%	of Maintenance and Operations Wages and Benefits
Mechanical Department Services:	2.40%	of Maintenance and Operations Wages and Benefits
Employee Relations Department:	5.90%	of Maintenance and Operations Wages and Benefits
Business Services:	7.40%	of Maintenance and Operations Wages and Benefits

Property Taxes and Insurance

Property Taxes and Insurance:	2%	of Total Depreciable Capital

Straight Line Depreciation

Direct Plant:	8.00%	of Total Depreciable Capital, less 1.18 times the Allocated Costs for Utility Plants and Related Facilities
Allocated Plant:	6.00%	of 1.18 times the Allocated Costs for Utility Plants and Related Facilities

Other Annual Expenses

Rental Fees (Office and Laboratory Space):	$0
Licensing Fees:	$0
Miscellaneous:	$0

Depletion Allowance

Annual Depletion Allowance:	$0

Cash Flow Summary

Year	Percentage of Design Capacity	Product Unit Price	Sales	Capital Costs	Working Capital	Var Costs	Fixed Costs	Depreciation	Depletion Allowance	Taxible Income	Taxes	Net Earnings
2010	0%		-	-	-	-	-	-	-	-	-	-
2011	0%		-	(6,103,500)	(559,700)	-	-	-	-	-	-	-
2012	45%	$3.85	9,862,900	-	(279,800)	(7,933,400)	(1,566,600)	(1,089,900)	-	(727,000)	290,800	(436,200)
2013	68%	$3.85	14,794,400	-	(279,800)	(11,900,200)	(1,566,600)	(1,743,900)	-	(416,200)	166,500	(249,700)
2014	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	(1,046,300)	-	1,246,100	(498,400)	747,600
2015	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	(627,800)	-	1,664,600	(665,800)	998,800
2016	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	(627,800)	-	1,664,600	(665,800)	998,800
2017	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	(313,900)	-	1,978,500	(791,400)	1,187,100
2018	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	-	-	2,292,400	(917,000)	1,375,400
2019	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	-	-	2,292,400	(917,000)	1,375,400
2020	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	-	-	2,292,400	(917,000)	1,375,400
2021	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	-	-	2,292,400	(917,000)	1,375,400
2022	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	-	-	2,292,400	(917,000)	1,375,400
2023	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	-	-	2,292,400	(917,000)	1,375,400
2024	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	-	-	2,292,400	(917,000)	1,375,400
2025	90%	$3.85	19,725,900	-	-	(15,866,900)	(1,566,600)	-	-	2,292,400	(917,000)	1,375,400
2026	90%	$3.85	19,725,900	-	1,119,400	(15,866,900)	(1,566,600)	-	-	2,292,400	(917,000)	1,375,400

Profitability Measures

The Internal Rate of Return (IRR) for this project is 18.03%

The Net Present Value (NPV) of this project in 2010 is $ 975,800

ROI Analysis (Third Production Year)

Annual Sales	19,725,892
Annual Costs	(17,433,497)
Depreciation	(488,280)
Income Tax	(721,646)
Net Earnings	1,082,469
Total Capital Investment	7,222,881
ROI	14.99%

Sensitivity Analyses

Note: The Sensitivity Analyses section below takes quite a bit of memory to update each time a cell is changed; therefore, automatic calculations are turned off. After making your axis selections, press "F9" to recalculate the IRR values. (These two lines may be deleted before printing.)

	Vary Initial Value by +/-
x-axis	50%
y-axis	50%

Variable Costs (columns) vs. Product Price (rows)

Product Price	$8,814,929	$10,577,915	$12,340,901	$14,103,887	$15,866,872	*$17,629,858*	$19,392,844	$21,155,830	$22,918,816	$24,681,801	$26,444,787
$1.93	-3.50%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$2.31	20.12%	3.23%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$2.70	34.63%	22.85%	7.99%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.08	46.84%	36.60%	25.36%	11.83%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.47	57.86%	48.43%	38.48%	27.68%	15.11%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.85	68.08%	59.17%	49.95%	40.27%	29.85%	18.03%	2.24%	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$4.24	77.69%	69.17%	60.44%	51.41%	41.97%	31.90%	20.67%	6.63%	Negative IRR	Negative IRR	Negative IRR
$4.62	86.81%	78.61%	70.24%	61.66%	52.82%	43.60%	33.83%	23.10%	10.26%	Negative IRR	Negative IRR
$5.01	95.53%	87.58%	79.50%	71.27%	62.84%	54.17%	45.17%	35.67%	25.36%	13.40%	Negative IRR
$5.39	103.89%	96.16%	88.32%	80.36%	72.26%	63.99%	55.48%	46.67%	37.42%	27.47%	16.21%
$5.78	111.94%	104.39%	96.77%	89.04%	81.20%	73.23%	65.09%	56.74%	48.12%	39.09%	29.47%

APPENDIX E: MSDS

Material Safety Data Sheet

N-Butyronitrile, 98%

ACC# 96789

Section 1 - Chemical Product and Company Identification

MSDS Name: N-Butyronitrile, 98%
Catalog Numbers: AC108140000, AC108140010, AC108140025
Synonyms: N-Butanenitrile; 1-Cyanopropane; Propyl Cyanide.
Company Identification:

Acros Organics N.V.
One Reagent Lane
Fair Lawn, NJ 07410

For information in North America, call: 800-ACROS-01
For emergencies in the US, call CHEMTREC: 800-424-9300

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
109-74-0	N-Butyronitrile	98	203-700-6

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: Clear liquid. Flash Point: 16 deg C.
Danger! May be fatal if swallowed. Highly flammable. Harmful if absorbed through the skin. Causes eye and skin irritation. May cause respiratory and digestive tract irritation.
Target Organs: None known.

Potential Health Effects

Eye: Causes eye irritation.
Skin: Causes skin irritation. Harmful if absorbed through the skin.
Ingestion: May be fatal if swallowed. May cause irritation of the digestive tract. Forms cyanide in the body. Cyanide in the body is capable of producing cyanosis.
Inhalation: May cause respiratory tract irritation.
Chronic: Not available. None

Section 4 - First Aid Measures

Eyes: Flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid immediately.
Skin: Get medical aid immediately. Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes.
Ingestion: If victim is conscious and alert, give 2-4 cupfuls of milk or water. Never give anything by mouth to an unconscious person. Get medical aid immediately.
Inhalation: Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.
Notes to Physician: Treat symptomatically.

Section 5 - Fire Fighting Measures

General Information: As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Vapors may form an explosive mixture with air. Vapors can travel to a source of ignition and flash back. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. Use water spray to keep fire-exposed containers cool. Water may be ineffective. Material is lighter than water and a fire may be spread by the use of water. Flammable liquid and vapor. Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas. Containers may explode when heated.
Extinguishing Media: For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam. Water may be ineffective. For large fires, use water spray, fog or alcohol-resistant foam. Do NOT use straight streams of water. Cool containers with flooding quantities of water until well after fire is out.
Flash Point: 16 deg C (60.80 deg F)
Autoignition Temperature: 501 deg C (933.80 deg F)
Explosion Limits, Lower:1.65 vol %
Upper: .00 vol %
NFPA Rating: (estimated) Health: ; Flammability: ; Instability:

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks: Absorb spill with inert material (e.g. vermiculite, sand or earth), then place in suitable container. Use water spray to dilute spill to a non-flammable mixture. Avoid runoff into storm sewers and ditches which lead to waterways. Clean up spills immediately, observing precautions in the Protective Equipment section. Scoop up with a nonsparking tool, then place into a suitable container for disposal. Use water spray to disperse the gas/vapor. Remove all sources of ignition. Provide ventilation.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Ground and bond containers when transferring material. Do not get on skin and clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep container tightly closed. Keep away from heat, sparks and flame. Do not ingest or inhale. Use only in a chemical fume hood. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames.
Storage: Keep away from heat, sparks, and flame. Keep away from sources of ignition. Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances. Keep away from acids.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Use only under a chemical fume hood.
Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
N-Butyronitrile	none listed	8 ppm TWA; 22 mg/m3 TWA	none listed

OSHA Vacated PELs: N-Butyronitrile: No OSHA Vacated PELs are listed for this chemical.
Personal Protective Equipment
Eyes: Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard

EN166.
Skin: Wear appropriate protective gloves to prevent skin exposure.
Clothing: Wear appropriate protective clothing to prevent skin exposure.
Respirators: Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Section 9 - Physical and Chemical Properties

Physical State: Liquid
Appearance: Clear
Odor: suffocating odor, sharp odor
pH: Not available.
Vapor Pressure: 19.5 mm Hg @25C
Vapor Density: 2.4
Evaporation Rate:Not available.
Viscosity: 624@15C
Boiling Point: 117.5 deg C
Freezing/Melting Point:-112 deg C
Decomposition Temperature:Not available.
Solubility: 33 g/l (25 c)
Specific Gravity/Density:.7940g/cm3
Molecular Formula:C4H7N
Molecular Weight:69.11

Section 10 - Stability and Reactivity

Chemical Stability: Stable under normal temperatures and pressures.
Conditions to Avoid: Incompatible materials, ignition sources, excess heat, strong acids, strong oxidants.
Incompatibilities with Other Materials: Strong acids - strong bases - strong oxidizing agents - strong reducing agents.
Hazardous Decomposition Products: Hydrogen cyanide, nitrogen oxides, carbon monoxide, irritating and toxic fumes and gases, carbon dioxide, nitrogen.
Hazardous Polymerization: Has not been reported.

Section 11 - Toxicological Information

RTECS#:

CAS# 109-74-0: ET8750000
LD50/LC50:
CAS# 109-74-0:
- Draize test, rabbit, eye: 500 mg/24H Mild;
- Inhalation, mouse: LC50 = 249 ppm/1H;
- Oral, mouse: LD50 = 27689 ug/kg;
- Oral, rat: LD50 = 50 mg/kg;
- Skin, rabbit: LD50 = 500 uL/kg;

.

Carcinogenicity:
CAS# 109-74-0: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No information available.
Teratogenicity: No information available.
Reproductive Effects: No information available.
Mutagenicity: No information available.
Neurotoxicity: No information available.
Other Studies:

Section 12 - Ecological Information

Ecotoxicity: No data available. No information available.
Environmental: Major fate processes are biodegradation and volatilization. Not expected to bioconcentrate.
Physical: No information available.
Other: No information available.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.
RCRA P-Series: None listed.
RCRA U-Series: None listed.

Section 14 - Transport Information

	US DOT	Canada TDG
Shipping Name:	BUTYRONITRILE	No information available.
Hazard Class:	3	
UN Number:	UN2411	
Packing Group:	II	

Section 15 - Regulatory Information

US FEDERAL

TSCA
CAS# 109-74-0 is listed on the TSCA inventory.
Health & Safety Reporting List
None of the chemicals are on the Health & Safety Reporting List.
Chemical Test Rules
None of the chemicals in this product are under a Chemical Test Rule.
Section 12b
None of the chemicals are listed under TSCA Section 12b.
TSCA Significant New Use Rule
None of the chemicals in this material have a SNUR under TSCA.
CERCLA Hazardous Substances and corresponding RQs
None of the chemicals in this material have an RQ.
SARA Section 302 Extremely Hazardous Substances
None of the chemicals in this product have a TPQ.
SARA Codes
CAS # 109-74-0: immediate, fire.
Section 313 No chemicals are reportable under Section 313.
Clean Air Act:
This material does not contain any hazardous air pollutants.
This material does not contain any Class 1 Ozone depletors.
This material does not contain any Class 2 Ozone depletors.
Clean Water Act:
None of the chemicals in this product are listed as Hazardous Substances under the CWA.
None of the chemicals in this product are listed as Priority Pollutants under the CWA.
None of the chemicals in this product are listed as Toxic Pollutants under the CWA.
OSHA:
None of the chemicals in this product are considered highly hazardous by OSHA.
STATE
CAS# 109-74-0 can be found on the following state right to know lists: New Jersey, Pennsylvania, Minnesota, Massachusetts.

California Prop 65

California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives
Hazard Symbols:
T
Risk Phrases:
R 11 Highly flammable.
R 23/24/25 Toxic by inhalation, in contact with skin and if swallowed.

Safety Phrases:
S 45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

WGK (Water Danger/Protection)
CAS# 109-74-0: No information available.
Canada - DSL/NDSL
CAS# 109-74-0 is listed on Canada's DSL List.
Canada - WHMIS
WHMIS: Not available.
This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.
Canadian Ingredient Disclosure List
CAS# 109-74-0 is listed on the Canadian Ingredient Disclosure List.

Section 16 - Additional Information

MSDS Creation Date: 9/23/1998
Revision #3 Date: 10/03/2005

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall Fisher be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if Fisher has been advised of the possibility of such damages.

MATERIAL SAFETY DATA SHEET

Date-Issued: 08/08/2000
MSDS Ref. No: 211120
Date-Revised: 02/26/2001
Revision No: 2

Xylene

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1. PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME: Xylene
PRODUCT DESCRIPTION: Xylene
PRODUCT CODE: 211120
PRODUCT FORMULATION NAME: Xylene
CHEMICAL FAMILY: Aromatic Hydrocarbon Solvent
GENERIC NAME: Xylol, Dimethyl Benzene

MANUFACTURER

Americhem Sales Corporation
340 North Street
Mason, MI 48854
Contact: Americhem Sales Corporation
Product Stewardship: 517-676-9363
Transportation: 517-676-9363

24 HR. EMERGENCY TELEPHONE NUMBERS

CHEMTREC (U.S.): (800) 424-9300
Canutec (613) 996-6666
Emergency Phone: 800-424-9300

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2. COMPOSITION / INFORMATION ON INGREDIENTS

Chemical Name	Wt.%	CAS#	EINECS#
Xylenes (o-,m-,p- isomers)	75 - 90	1330-20-7	
Ethyl Benzene	10 - 25	100-41-4	

---

3. HAZARDS IDENTIFICATION

EMERGENCY OVERVIEW

PHYSICAL APPEARANCE: Clear, Colorless liquid.

IMMEDIATE CONCERNS: CAUTION! May cause eye and skin irritation.

POTENTIAL HEALTH EFFECTS

EYES: May cause moderate burning, tearing, redness and swelling.

SKIN: Moderate irritation and discomfort. Defatting of skin and redness are possible. Toxic systemic effects from absorbtion are expected to be minor.

INGESTION: Gastrointestinal tract irritation and/or discomfort is possible.

INHALATION:Dizziness, impaired coordination, headaches and loss of consciousness. Severe respiratory tract irritation. Toxic systemic effects are possible.

MEDICAL CONDITIONS AGGRAVATED: Disorders of the skin, respiratory and central nervous system.

ROUTES OF ENTRY: Absorption, Inhalation

TARGET ORGAN STATEMENT:Reports have associated repeated and prolonged occupational overexposure to solvents with permanent brain and nervous system damage (sometimes referred to as Solvent or Painters' Syndrome). Intentional misuse by deliberately concentrating and inhaling this material may be harmful or fatal.

CANCER STATEMENT: This material and components above 0.1% are not listed as carcinogens by IARC, NTP or OSHA.

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4. FIRST AID MEASURES

EYES: Immediately flush eyes with plenty of water for 15 minutes. If irritation persists, seek medical attention.

SKIN: Wash exposed area with mild soap and water. Get medical attention if irritation develops or persists.

INGESTION: Do not Induce Vomiting. Get immediate medical attention.

INHALATION:Remove victim from area of exposure. If unconscious, give oxygen. Give artificial respiration if not breathing. Get immediate medical attention.

NOTES TO PHYSICIAN:Exposure to high concentrations of this material (e.g., in enclosed spaces or with deliberate abuse) may be associated with cardiac arrhythmias. Epinephrine and other sympathomimetic drugs may initiate cardiac arrhythmias in persons exposed to this material. If sympathomimetic drugs are administered, observe for the development of cardiac arrhythmias.

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5. FIRE FIGHTING MEASURES

FLASHPOINT AND METHOD: (81°F)ASTM D56

FLAMMABLE LIMITS: 1.0 to 7.0

AUTOIGNITION TEMPERATURE: (810°F) to (984°F)

EXTINGUISHING MEDIA: Use dry chemical, foam, or carbon dioxide.

EXPLOSION HAZARDS: Vapor accumulations may flash and/or explode if ignited. Keep ignition sources, open flames, ect., away from thse fumes.

FIRE FIGHTING PROCEDURES:Proper respiratory equipment to protect against the hazardous effects of combustion products is recommended. Water in a straight hose stream may cause fire to spread and should be used as a cooling medium only.

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6. ACCIDENTAL RELEASE MEASURES

SMALL SPILL:

Extinguish possible sources of ignition. Evacuate all unprotected personnel and ventilate area. Only personnel equipped with proper respiratory, skin/eye protection should enter spill area. Dike area to contain spill and clean up by absorbing on an inert absorbant or other means. Don't flush into sewers or natural waterways.

LARGE SPILL:

Contain material as described above and call the local fire or police department for immediate emergency assistance.

7. HANDLING AND STORAGE

HANDLING:

Open container slowly to relieve any pressure. Bond and ground all equipment when transferring from one vessel or container to another. This material can accumulate static charge by flow or agitation. Vapors can be ignited by static discharge. Use explosion proof equipment as directed by local fire codes.

STORAGE:

Store unopened containers under cool, dry and ventilated conditions. Keep away from heat, sparks and flame.

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE GUIDELINES:

OSHA HAZARDOUS COMPONENTS (29 CFR 1910.1200)

		EXPOSURE LIMITS					
		OSHA PEL		ACGIH TLV		Supplier OEL	
		ppm	mg/m^3	ppm	mg/m^3	ppm	mg/m^3
Xylenes (o-,m-,p- isomers)	TWA	100		100			
	STEL			150			
Ethyl Benzene	TWA			100			
	STEL			150			

ENGINEERING CONTROLS: If current ventilation practices are not adequate to maintain airborne concentrations below the established exposure guidelines, additional ventilation or exhaust systems may be required. Where explosive mixtures may be present, electrical systems safe for such locations must be used.

PERSONAL PROTECTIVE EQUIPMENT

EYES AND FACE: Wear safety glasses with side shields or goggles when handling this material.

SKIN:To prevent any contact, wear impervious protective clothing such as neoprene or butyl rubber gloves, apron, boots or whole bodysuit, as appropriate.

RESPIRATORY: Use NIOSH/MSHA approved respirators when vapors or mist concentrations exceed permissible exposure limits.

PROTECTIVE CLOTHING: Chemical resistant boots, apron, etc. as necessary to prevent contamination of clothing and skin contact.

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9. PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE: Liquid

ODOR: Light Aromatic

APPEARANCE: Clear

COLOR: Colorless

pH: Not Applicable

PERCENT VOLATILE: 100

VAPOR PRESSURE: 7 mmHg at 20°C

VAPOR DENSITY: 3.7 (Air=1)

BOILING POINT: (276°F) to (284°F)

FREEZING POINT: Not Determined

MELTING POINT: Not Determined

SOLUBILITY IN WATER: Negligible

EVAPORATION RATE: 0.6 (n-Butyl Acetate=1)

SPECIFIC GRAVITY: 0.87 (water=1) at (60°F)

MOLECULAR FORMULA: C8H10

MOLECULAR WEIGHT: 106

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10. STABILITY AND REACTIVITY

STABLE: YES

HAZARDOUS POLYMERIZATION: NO

CONDITIONS TO AVOID: Exposure to excessive heat, open flames and sparks. Avoid conditions that favor the formation of excessive mists and/or fumes.

STABILITY: Stable

POLYMERIZATION: Will not occur

HAZARDOUS DECOMPOSITION PRODUCTS: Oxides of Carbon when burned.

INCOMPATIBLE MATERIALS: Strong oxidizing agents.

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11. TOXICOLOGICAL INFORMATION

TARGET ORGANS: A six week inhalation study with xylene produced hearing loss in rats.

REPRODUCTIVE EFFECTS:Both mixed xylenes and the individual isomers produced limited evidence of fetal toxicity in laboratory animals. Inhalation and oral administration of xylene resulted in decreased fetal weight, increased incidences of delayed bone development, skeletal variations and missed abortions.

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12. ECOLOGICAL INFORMATION

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13. DISPOSAL CONSIDERATIONS

DISPOSAL METHOD:Conditions of use may cause this material to become a hazardous waste as defined by state or federal law. Use approved treatment, transporters and disposal sites.

FOR LARGE SPILLS:Extinguish possible sources of ignition. Evacuate all unprotected personnel and ventilate area. Only personnel equipped with proper respiratory, skin/eye protection should enter spill area. Dike area to contain spill and clean up by absorbing on an inert absorbent or other means. Don't flush into sewers or natural waterways.

---

14. TRANSPORT INFORMATION

DOT (DEPARTMENT OF TRANSPORTATION)

PROPER SHIPPING NAME: Xylene

PRIMARY HAZARD CLASS/DIVISION: 3

UN/NA NUMBER: UN1307

PACKING GROUP: III

LABEL: Flammable Liquid

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15. REGULATORY INFORMATION

UNITED STATES

SARA TITLE III (SUPERFUND AMENDMENTS AND REAUTHORIZATION ACT)

311/312 HAZARD CATEGORIES:

FIRE: YES PRESSURE GENERATING: NO REACTIVITY: NO ACUTE: YES CHRONIC: YES

313 REPORTABLE INGREDIENTS: Xylene (CAS No. 1330-20-7) - 75 to 90%
Ethyl benzene (CAS No. 100-41-4) - 10 to 25%

CERCLA (COMPREHENSIVE RESPONSE, COMPENSATION, AND LIABILITY ACT)

CERCLA REGULATORY: Xylene (CAS No. 1330-20-7) - 75 to 90%
Ethyl benzene (CAS No. 100-41-4) - 10 to 25%

TSCA (TOXIC SUBSTANCE CONTROL ACT)

TSCA REGULATORY: This material or its components are listed in the TSCA inventory.

PROPOSITION 65 STATEMENT:This material contains the following chemicals which are known to the State of California to cause cancer, birth defects or other reproductive harm, and are subject to the requirments of California Proposition 65 (CA Health & Safety Code Section 25249.5):

ComponentEffect
BenzeneCancer
TolueneDevelopmental Toxicant

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16. OTHER INFORMATION

REVISION SUMMARY

Revision #: 2

This MSDS replaces the February 21, 2001 MSDS. Any changes in information are as follows:
In Section 14
DOT UN/NA Number

NFPA CODES

HEALTH: 2 FIRE: 3 REACTIVITY: 0

HMIS CODES

HEALTH: *2 FIRE: 3 REACTIVITY: 0 PROTECTION: X

MSDS Number: P7456 * * * * * *Effective Date: 09/22/09* * * * * * *Supercedes: 08/24/07*

24 Hour Emergency Telephone: 908-859-2151
CHEMTREC: 1-800-424-9300

MSDS *Material Safety Data Sheet*

National Response in Canada
CANUTEC: 613-996-6666

Outside U.S. and Canada
Chemtrec: 703-527-3887

From: Mallinckrodt Baker, Inc.
222 Red School Lane
Phillipsburg, NJ 08865

Mallinckrodt CHEMICALS J.T.Baker

NOTE: CHEMTREC, CANUTEC and National Response Center emergency numbers to be used only in the event of chemical emergencies involving a spill, leak, fire, exposure or accident involving chemicals.

All non-emergency questions should be directed to Customer Service (1-800-582-2537) for assistance.

PYRIDINE

1. Product Identification

Synonyms: Azabenzene
CAS No.: 110-86-1
Molecular Weight: 79.10
Chemical Formula: C5H5N
Product Codes:
J.T. Baker: 3348, 9105, 9393
Mallinckrodt: 7180, 7181

2. Composition/Information on Ingredients

Ingredient	CAS No	Percent	Hazardous

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  Pyridine                                  110-86-1        99 - 100%
Yes
```

3. Hazards Identification

Emergency Overview

WARNING! FLAMMABLE LIQUID AND VAPOR. HARMFUL IF SWALLOWED, INHALED OR ABSORBED THROUGH SKIN. AFFECTS CENTRAL NERVOUS SYSTEM, LIVER AND KIDNEYS. CAUSES SEVERE IRRITATION TO EYES, SKIN AND RESPIRATORY TRACT.

SAF-T-DATA(tm) Ratings (Provided here for your convenience)

Health Rating: 3 - Severe (Life)
Flammability Rating: 2 - Moderate
Reactivity Rating: 2 - Moderate
Contact Rating: 3 - Severe
Lab Protective Equip: GOGGLES & SHIELD; LAB COAT & APRON; VENT HOOD; PROPER GLOVES; CLASS B EXTINGUISHER
Storage Color Code: Red (Flammable)

Potential Health Effects

Inhalation:
Inhalation causes severe irritation to the respiratory tract. Symptoms of overexposure include headache, dizziness, nausea, shortness of breath, coughing, insomnia, diarrhea, gastrointestinal disturbances, and back pain with urinary frequency. Liver and kidney damage may occur. May be fatal.
Ingestion:
Toxic effects parallel those of inhalation. May be fatal if swallowed.
Skin Contact:
Causes severe irritation, possibly burns, to the skin. Symptoms include redness and severe pain. Absorption through the skin may occur, resulting in toxic effects similar to inhalation. May act as a photosensitizer.
Eye Contact:
Vapors cause eye irritation. Splashes cause severe irritation, possible corneal burns and eye damage.
Chronic Exposure:
Liver and kidney damage has been reported.
Aggravation of Pre-existing Conditions:

Persons with pre-existing skin, eye or central nervous system disorders, or impaired liver, kidney, or pulmonary function may be more susceptible to the effects of this substance.

4. First Aid Measures

Inhalation:
Remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention immediately.
Ingestion:
If swallowed, give large quantities of water to drink and get medical attention immediately. Never give anything by mouth to an unconscious person.
Skin Contact:
Immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Get medical attention immediately. Wash clothing before reuse. Thoroughly clean shoes before reuse.
Eye Contact:
Immediately flush eyes with plenty of water for at least 15 minutes, lifting lower and upper eyelids occasionally. Get medical attention immediately.

5. Fire Fighting Measures

Fire:
Flash point: 20C (68F) CC
Autoignition temperature: 482C (900F)
Flammable limits in air % by volume:
lel: 1.8; uel: 12.4
Flammable Liquid Contact with strong oxidizers may cause fire.
Explosion:
Above flash point, vapor-air mixtures are explosive within flammable limits noted above. Vapors can flow along surfaces to distant ignition source and flash back. Sensitive to static discharge.
Fire Extinguishing Media:
Dry chemical, foam or carbon dioxide. Water spray may be used to keep fire exposed containers cool. Water may be ineffective.
Special Information:
In the event of a fire, wear full protective clothing and NIOSH-approved self-contained breathing apparatus with full facepiece operated in the pressure demand or other positive pressure mode. Water may be used to flush spills away from exposures and to dilute spills to non-flammable mixtures.

6. Accidental Release Measures

Ventilate area of leak or spill. Remove all sources of ignition. Wear appropriate personal protective equipment as specified in Section 8. Isolate hazard area. Keep unnecessary and unprotected personnel from entering. Contain and recover liquid when possible. Use non-sparking tools and equipment. Collect liquid in an appropriate container or absorb with an inert material (e. g., vermiculite, dry sand, earth), and place in a chemical waste container. Do not use combustible materials, such as saw dust. Do not flush to sewer! If a leak or spill has not ignited, use water spray to disperse the vapors, to protect personnel attempting to stop leak, and to flush spills away from exposures. US Regulations (CERCLA) require reporting spills and releases to soil, water and air in excess of reportable quantities. The toll free number for the US Coast Guard National Response Center is (800) 424-8802.

J. T. Baker SOLUSORB� solvent adsorbent is recommended for spills of this product.

7. Handling and Storage

Protect against physical damage. Store in a cool, dry well-ventilated location, away from any area where the fire hazard may be acute. Outside or detached storage is preferred. Separate from incompatibles. Containers should be bonded and grounded for transfers to avoid static sparks. Storage and use areas should be No Smoking areas. Use non-sparking type tools and equipment, including explosion proof ventilation. Containers of this material may be hazardous when empty since they retain product residues (vapors, liquid); observe all warnings and precautions listed for the product. Do Not attempt to clean empty containers since residue is difficult to remove. Do not pressurize, cut, weld, braze, solder, drill, grind or expose such containers to heat, sparks, flame, static electricity or other sources of ignition: they may explode and cause injury or death.

8. Exposure Controls/Personal Protection

Airborne Exposure Limits:
For Pyridine:
- OSHA Permissible Exposure Limit (PEL) -
5 ppm (TWA).
- ACGIH Threshold Limit Value (TLV) -
1 ppm (TWA), A3 - Confirmed animal carcinogen with unknown relevance to humans

- NIOSH Recommended Exposure Limit (REL) -
5 ppm (Ceiling).
Ventilation System:
A system of local and/or general exhaust is recommended to keep employee exposures below the Airborne Exposure Limits. Local exhaust ventilation is generally preferred because it can control the emissions of the contaminant at its source, preventing dispersion of it into the general work area. Please refer to the ACGIH document, *Industrial Ventilation, A Manual of Recommended Practices*, most recent edition, for details.
Personal Respirators (NIOSH Approved):
If the exposure limit is exceeded and engineering controls are not feasible, a full facepiece respirator with organic vapor cartridge may be worn up to 50 times the exposure limit or the maximum use concentration specified by the appropriate regulatory agency or respirator supplier, whichever is lowest. For emergencies or instances where the exposure levels are not known, use a full-facepiece positive-pressure, air-supplied respirator. WARNING: Air purifying respirators do not protect workers in oxygen-deficient atmospheres. Where respirators are required, you must have a written program covering the basic requirements in the OSHA respirator standard. These include training, fit testing, medical approval, cleaning, maintenance, cartridge change schedules, etc. See 29CFR1910.134 for details.
Skin Protection:
Wear impervious protective clothing, including boots, gloves, lab coat, apron or coveralls, as appropriate, to prevent skin contact.
Eye Protection:
Use chemical safety goggles and/or a full face shield where splashing is possible. Maintain eye wash fountain and quick-drench facilities in work area.

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9. Physical and Chemical Properties

Appearance:
Colorless to yellow liquid.
Odor:
Penetrating, sickening.
Solubility:
Miscible in water.
Specific Gravity:
0.98 @ 25C/4C
pH:
8.5
% Volatiles by volume @ 21C (70F):
100
Boiling Point:
115.3C (239F)

Melting Point:
-42C (-44F)
Vapor Density (Air=1):
2.72
Vapor Pressure (mm Hg):
18 @ 20C (68F)
Evaporation Rate (BuAc=1):
No information found.

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10. Stability and Reactivity

Stability:
Stable under ordinary conditions of use and storage. Heat will contribute to instability.
Hazardous Decomposition Products:
May form cyanide fumes and oxides of carbon and nitrogen if heated to decomposition.
Hazardous Polymerization:
Will not occur.
Incompatibilities:
Heat, flame, maleic anhydride, perchromates, strong acids, strong oxidizers. Will attack some forms of plastics, rubber, and coatings.
Conditions to Avoid:
Heat, flames, ignition sources and incompatibles.

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11. Toxicological Information

Oral rat LD50: 891 mg/kg; inhalation rat LC50: 28500 mg/m3/1-hour; skin rabbit LD50: 1121 mg/kg; Irritation data: skin rabbit, open Draize, 10 mg/24H mild; eye rabbit, standard Draize, 2 mg severe. Investigated as a tumorigen and mutagen.

```
  --------\Cancer Lists\------------------------------------------------------
-
                                         ---NTP Carcinogen---
  Ingredient                             Known    Anticipated    IARC
Category
  ------------------------------------   -----    -----------    ------------
-
  Pyridine (110-86-1)                     No          No              3
```

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12. Ecological Information

Environmental Fate:
When released into the soil, this material is expected to readily biodegrade. When released into the soil, this material is expected to leach into groundwater. When released into the soil, this material is expected to have a half-life between 1 and 10 days. When released into water, this material may biodegrade to a moderate extent. When released into water, this material may evaporate to a moderate extent. This material is not expected to significantly bioaccumulate. When released into the air, this material may be moderately degraded by reaction with photochemically produced hydroxyl radicals. When released into the air, this material may be removed from the atmosphere to a moderate extent by wet deposition.
Environmental Toxicity:
This material may be toxic to aquatic life.

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13. Disposal Considerations

Whatever cannot be saved for recovery or recycling should be handled as hazardous waste and sent to a RCRA approved incinerator or disposed in a RCRA approved waste facility. Processing, use or contamination of this product may change the waste management options. State and local disposal regulations may differ from federal disposal regulations. Dispose of container and unused contents in accordance with federal, state and local requirements.

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14. Transport Information

Domestic (Land, D.O.T.)

Proper Shipping Name: PYRIDINE
Hazard Class: 3
UN/NA: UN1282
Packing Group: II
Information reported for product/size: 441LB

International (Water, I.M.O.)

Proper Shipping Name: PYRIDINE
Hazard Class: 3
UN/NA: UN1282

Packing Group: II
Information reported for product/size: 441LB

15. Regulatory Information

--------\Chemical Inventory Status - Part 1\---------------------------------

Ingredient	TSCA	EC	Japan	Australia
Pyridine (110-86-1)	Yes	Yes	Yes	Yes

--------\Chemical Inventory Status - Part 2\---------------------------------

Ingredient	Korea	--Canada-- DSL	--Canada-- NDSL	Phil.
Pyridine (110-86-1)	Yes	Yes	No	Yes

--------\Federal, State & International Regulations - Part 1\----------------

Ingredient	-SARA 302- RQ	-SARA 302- TPQ	------SARA 313------ List	------SARA 313------ Chemical Catg.
Pyridine (110-86-1)	No	No	Yes	No

--------\Federal, State & International Regulations - Part 2\----------------

Ingredient	CERCLA	-RCRA- 261.33	-TSCA- 8(d)
Pyridine (110-86-1)	1000	U196	No

Chemical Weapons Convention: No TSCA 12(b): No CDTA: No
SARA 311/312: Acute: Yes Chronic: Yes Fire: Yes Pressure: No
Reactivity: No (Pure / Liquid)

WARNING:
THIS PRODUCT CONTAINS A CHEMICAL(S) KNOWN TO THE STATE OF CALIFORNIA TO CAUSE CANCER.

Australian Hazchem Code: 2WE
Poison Schedule: None allocated.
WHMIS:
This MSDS has been prepared according to the hazard criteria of the Controlled Products Regulations (CPR) and the MSDS contains all of the information required by the CPR.

16. Other Information

NFPA Ratings: Health: 3 Flammability: 3 Reactivity: 0
Label Hazard Warning:
WARNING! FLAMMABLE LIQUID AND VAPOR. HARMFUL IF SWALLOWED, INHALED OR ABSORBED THROUGH SKIN. AFFECTS CENTRAL NERVOUS SYSTEM, LIVER AND KIDNEYS. CAUSES SEVERE IRRITATION TO EYES, SKIN AND RESPIRATORY TRACT.
Label Precautions:
Keep away from heat, sparks and flame.
Keep container closed.
Use only with adequate ventilation.
Avoid breathing vapor.
Avoid contact with eyes, skin and clothing.
Wash thoroughly after handling.
Label First Aid:
If swallowed, give large amounts of water to drink. Never give anything by mouth to an unconscious person. If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. In case of contact, immediately flush eyes or skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. In all cases get medical attention immediately.
Product Use:
Laboratory Reagent.
Revision Information:
No Changes.
Disclaimer:
****

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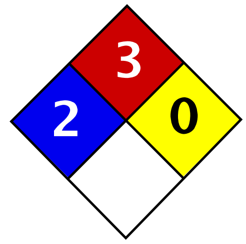

Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
Acetonitrile MSDS

Section 1: Chemical Product and Company Identification

Product Name: Acetonitrile

Catalog Codes: SLA3625, SLA1279, SLA1942

CAS#: 75-05-8

RTECS: AL7700000

TSCA: TSCA 8(b) inventory: Acetonitrile

CI#: Not applicable.

Synonym: Methyl Cyanide

Chemical Name: Acetonitrile

Chemical Formula: CH3CN

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Acetonitrile	75-05-8	100

Toxicological Data on Ingredients: Acetonitrile: ORAL (LD50): Acute: 2460 mg/kg [Rat.]. 269 mg/kg [Mouse]. DERMAL (LD50): Acute: 1250 mg/kg [Rabbit.].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (permeator). Severe over-exposure can result in death.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.
DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female, Reproductive system/toxin/male [SUSPECTED].
The substance is toxic to blood, kidneys, lungs, liver, mucous membranes, gastrointestinal tract, upper respiratory tract, skin, eyes, central nervous system (CNS).
The substance may be toxic to the reproductive system.
Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure to a

highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Get medical attention.

Skin Contact:
In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Cover the irritated skin with an emollient. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention immediately.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention immediately.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
If swallowed, do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 524°C (975.2°F)

Flash Points: CLOSED CUP: 2°C (35.6°F). OPEN CUP: 5.6°C (42.1°F) (Cleveland).

Flammable Limits: LOWER: 4.4% UPPER: 16%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Highly flammable in presence of open flames and sparks, of heat, of oxidizing materials.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available.
Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water.
SMALL FIRE: Use DRY chemical powder.
LARGE FIRE: Use alcohol foam, water spray or fog.

Special Remarks on Fire Hazards: Store under nitrogen.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill:
Dilute with water and mop up, or absorb with an inert dry material and place in an appropriate waste disposal container.

Large Spill:
Flammable liquid. Poisonous liquid.
Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up.. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, reducing agents, acids, alkalis, moisture.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Do not store above 23°C (73.4°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
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.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 40 (ppm) from ACGIH (TLV) [United States] [1999]
STEL: 60 from ACGIH (TLV) [United States] [1999]
TWA: 20 (ppm) from NIOSH
TWA: 40 STEL: 60 (ppm) from OSHA (PEL) [United States]
Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Liquid.)

Odor: Aromatic; Ether-like (Strong.)

Taste: Burning, sweetish

Molecular Weight: 41.05 g/mole

Color: Colorless.

pH (1% soln/water): 7 [Neutral.]

Boiling Point: 81.6 (178.9°F)

Melting Point: -46°C (-50.8°F)

Critical Temperature: Not available.

Specific Gravity: 0.783 (Water = 1)

Vapor Pressure: 9.7kPa (@ 20°C)

Vapor Density: 1.42 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, methanol.

Solubility: Soluble in cold water, hot water, methanol.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Reactive with oxidizing agents, reducing agents, acids, alkalis, moisture.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: High dielectric constant; high polarity; strongly reactive.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE.
Acute oral toxicity (LD50): 269 mg/kg [Mouse].

Acute dermal toxicity (LD50): 1250 mg/kg [Rabbit.].
Acute toxicity of the vapor (LC50): 7551 8 hours [Rat.].

Chronic Effects on Humans:
DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female, Reproductive system/toxin/male [SUSPECTED].
Causes damage to the following organs: blood, kidneys, lungs, liver, mucous membranes, gastrointestinal tract, upper respiratory tract, skin, eyes, central nervous system (CNS).
May cause damage to the following organs: the reproductive system.

Other Toxic Effects on Humans:
Hazardous in case of skin contact (irritant), of ingestion, of inhalation.
Slightly hazardous in case of skin contact (permeator).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Material is irritating to mucous membranes and upper respiratory tract.

Section 12: Ecological Information

Ecotoxicity: Ecotoxicity in water (LC50): 1020 mg/l 96 hours [Fish (Fathead Minnow)]. 1850 mg/l 96 hours [Fish (bluegill)].

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Acetonitrile UNNA: UN1648 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
New York release reporting list: Acetonitrile
Rhode Island RTK hazardous substances: Acetonitrile
Pennsylvania RTK: Acetonitrile
Florida: Acetonitrile
Minnesota: Acetonitrile
Massachusetts RTK: Acetonitrile
New Jersey: Acetonitrile

TSCA 8(b) inventory: Acetonitrile
TSCA 8(a) PAIR: Acetonitrile
TSCA 8(d) H and S data reporting: Acetonitrile: 1992
SARA 313 toxic chemical notification and release reporting: Acetonitrile
CERCLA: Hazardous substances.: Acetonitrile: 5000 lbs. (2268 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).
EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F).
CLASS D-1B: Material causing immediate and serious toxic effects (TOXIC).
CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R11- Highly flammable.
R23/24/25- Toxic by inhalation, in contact with skin and if swallowed.
S16- Keep away from sources of ignition - No smoking.
S27- Take off immediately all contaminated clothing.
S45- In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves.
Lab coat.
Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate.
Splash goggles.

Section 16: Other Information

References:

-Hawley, G.G.. The Condensed Chemical Dictionary, 11e ed., New York N.Y., Van Nostrand Reinold, 1987.
-Material safety data sheet emitted by: la Commission de la SantÃ© et de la SÃ©curitÃ© du Travail du QuÃ©bec.
-SAX, N.I. Dangerous Properties of Indutrial Materials. Toronto, Van Nostrand Reinold, 6e ed. 1984.
-The Sigma-Aldrich Library of Chemical Safety Data, Edition II.
-Guide de la loi et du rÃ¨glement sur le transport des marchandises dangeureuses au canada. Centre de conformitÃ© internatinal LtÃ©e. 1986.

Other Special Considerations: Not available.

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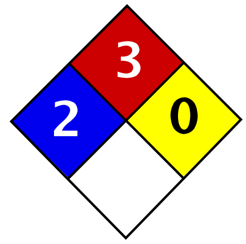
Last Updated: 11/06/2008 12:00 PM



Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
Benzene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Benzene

Catalog Codes: SLB1564, SLB3055, SLB2881

CAS#: 71-43-2

RTECS: CY1400000

TSCA: TSCA 8(b) inventory: Benzene

CI#: Not available.

Synonym: Benzol; Benzine

Chemical Name: Benzene

Chemical Formula: C6-H6

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Benzene	71-43-2	100

Toxicological Data on Ingredients: Benzene: ORAL (LD50): Acute: 930 mg/kg [Rat]. 4700 mg/kg [Mouse]. DERMAL (LD50): Acute: >9400 mg/kg [Rabbit]. VAPOR (LC50): Acute: 10000 ppm 7 hours [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of eye contact (irritant), of inhalation. Hazardous in case of skin contact (irritant, permeator), of ingestion. Inflammation of the eye is characterized by redness, watering, and itching.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC.
MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast.
TERATOGENIC EFFECTS: Not available.
DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE].
The substance is toxic to blood, bone marrow, central nervous system (CNS).
The substance may be toxic to liver, Urinary System.
Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. WARM water MUST be used. Get medical attention immediately.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention if symptoms appear.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 497.78°C (928°F)

Flash Points: CLOSED CUP: -11.1°C (12°F). (Setaflash)

Flammable Limits: LOWER: 1.2% UPPER: 7.8%

Products of Combustion: These products are carbon oxides (CO, CO_2).

Fire Hazards in Presence of Various Substances:
Highly flammable in presence of open flames and sparks, of heat.
Slightly flammable to flammable in presence of oxidizing materials.
Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available.
Risks of explosion of the product in presence of static discharge: Not available.
Explosive in presence of oxidizing materials, of acids.

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water.
SMALL FIRE: Use DRY chemical powder.
LARGE FIRE: Use alcohol foam, water spray or fog.

Special Remarks on Fire Hazards:
Extremely flammable liquid and vapor. Vapor may cause flash fire.
Reacts on contact with iodine heptafluoride gas.

Dioxygenyl tetrafluoroborate is as very powferful oxidant. The addition of a small particle to small samples of benzene, at ambient temperature, causes ignition.
Contact with sodium peroxide with benzene causes ignition.
Benzene ignites in contact with powdered chromic anhydride.
Virgorous or incandescent reaction with hydrogen + Raney nickel (above 210 C) and bromine trifluoride.

Special Remarks on Explosion Hazards:
Benzene vapors + chlorine and light causes explosion.
Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate.
Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion.
Interaction of nitryl perchlorate with benzene gave a slight explosion and flash.
The solution of permanganic acid (or its explosive anhydride, dimaganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene.
Peroxodisulfuric acid is a very powferful oxidant. Uncontrolled contact with benzene may cause explosion.
Mixtures of peroxomonsulfuric acid with benzene explodes.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Flammable liquid.
Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up.. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
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.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:

TWA: 0.5 STEL: 2.5 (ppm) from ACGIH (TLV) [United States]
TWA: 1.6 STEL: 8 (mg/m3) from ACGIH (TLV) [United States]
TWA: 0.1 STEL: 1 from NIOSH
TWA: 1 STEL: 5 (ppm) from OSHA (PEL) [United States]
TWA: 10 (ppm) from OSHA (PEL) [United States]
TWA: 3 (ppm) [United Kingdom (UK)]
TWA: 1.6 (mg/m3) [United Kingdom (UK)]
TWA: 1 (ppm) [Canada]
TWA: 3.2 (mg/m3) [Canada]
TWA: 0.5 (ppm) [Canada]Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor:
Aromatic. Gasoline-like, rather pleasant.
(Strong.)

Taste: Not available.

Molecular Weight: 78.11 g/mole

Color: Clear Colorless. Colorless to light yellow.

pH (1% soln/water): Not available.

Boiling Point: 80.1 (176.2°F)

Melting Point: 5.5°C (41.9°F)

Critical Temperature: 288.9°C (552°F)

Specific Gravity: 0.8787 @ 15 C (Water = 1)

Vapor Pressure: 10 kPa (@ 20°C)

Vapor Density: 2.8 (Air = 1)

Volatility: Not available.

Odor Threshold: 4.68 ppm

Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 2.1

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, diethyl ether, acetone.

Solubility:
Miscible in alcohol, chloroform, carbon disulfide oils, carbon tetrachloride, glacial acetic acid, diethyl ether, acetone.
Very slightly soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, ignition sources, incompatibles.

Incompatibility with various substances: Highly reactive with oxidizing agents, acids.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Benzene vapors + chlorine and light causes explosion.
Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate.
Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion.
Interaction of nitryl perchlorate with benzene gave a slight explosion and flash.
The solution of permanganic acid (or its explosive anhydride, dimaganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene.
Peroxodisulfuric acid is a very powferful oxidant. Uncontrolled contact with benzene may cause explosion.
Mixtures of peroxomonsulfuric acid with benzene explodes.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE.
Acute oral toxicity (LD50): 930 mg/kg [Rat].
Acute dermal toxicity (LD50): >9400 mg/kg [Rabbit].
Acute toxicity of the vapor (LC50): 10000 7 hours [Rat].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC.
MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast.
DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE].
Causes damage to the following organs: blood, bone marrow, central nervous system (CNS).
May cause damage to the following organs: liver, Urinary System.

Other Toxic Effects on Humans:
Very hazardous in case of inhalation.
Hazardous in case of skin contact (irritant, permeator), of ingestion.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects (female fertility, Embryotoxic and/or foetotoxic in animal) and birth defects.
May affect genetic material (mutagenic).
May cause cancer (tumorigenic, leukemia))
Human: passes the placental barrier, detected in maternal milk.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects:
Skin: Causes skin irritation. It can be absorbed through intact skin and affect the liver, blood, metabolism,and urinary system.
Eyes: Causes eye irritation.
Inhalation: Causes respiratory tract and mucous membrane irritation. Can be absorbed through the lungs. May affect behavior/Central and Peripheral nervous systems (somnolence, muscle weakness, general anesthetic, and

other symptoms similar to ingestion), gastrointestinal tract (nausea), blood metabolism, urinary system.
Ingestion: May be harmful if swallowed. May cause gastrointestinal tract irritation including vomiting. May affect behavior/Central and Peripheral nervous systems (convulsions, seizures, tremor, irritability, initial CNS stimulation followed by depression, loss of coordination, dizziness, headache, weakness, pallor, flushing), respiration (breathlessness and chest constriction), cardiovascular system, (shallow/rapid pulse), and blood.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Benzene UNNA: 1114 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: Benzene
California prop. 65 (no significant risk level): Benzene: 0.007 mg/day (value)
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer which would require a warning under the statute: Benzene
Connecticut carcinogen reporting list.: Benzene
Connecticut hazardous material survey.: Benzene
Illinois toxic substances disclosure to employee act: Benzene
Illinois chemical safety act: Benzene
New York release reporting list: Benzene
Rhode Island RTK hazardous substances: Benzene
Pennsylvania RTK: Benzene
Minnesota: Benzene
Michigan critical material: Benzene
Massachusetts RTK: Benzene
Massachusetts spill list: Benzene
New Jersey: Benzene
New Jersey spill list: Benzene
Louisiana spill reporting: Benzene
California Director's list of Hazardous Substances: Benzene

TSCA 8(b) inventory: Benzene
SARA 313 toxic chemical notification and release reporting: Benzene
CERCLA: Hazardous substances.: Benzene: 10 lbs. (4.536 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).
EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F).
CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

DSCL (EEC):
R11- Highly flammable.
R22- Harmful if swallowed.
R38- Irritating to skin.
R41- Risk of serious damage to eyes.
R45- May cause cancer.
R62- Possible risk of impaired fertility.
S2- Keep out of the reach of children.
S26- In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
S39- Wear eye/face protection.
S46- If swallowed, seek medical advice immediately and show this container or label.
S53- Avoid exposure - obtain special instructions before use.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves.
Lab coat.
Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate.
Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 08:35 PM

Last Updated: 11/06/2008 12:00 PM

Material Safety Data Sheet
Instant FAME/Instant Anaerobe Methods
Methanol

SECTION 1 – CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

MSDS Name: Methanol
MSDS Preparation Date: 06/19/2009
Synonyms or Generic ID for Methanol: Carbinol; Methyl alcohol; Methyl hydroxide; Monohydroxymethane; Wood alcohol; Wood naptha; Wood spirits; Columbian spirits; Methanol.
Chemical Family: Methanol Family
Formula: CH_3OH
Molecular Weight: N/A
PIN (UN#/ NA#): UN1230
Company Identification:
Microbial ID.
125 Sandy Drive
Newark, DE 19713
For Information, call: (800)276-8068, (302)737-4297
For Domestic CHEMTREC assistance, call: 800-424-9300
For International CHEMTREC assistance, call: 703-527-3887

SECTION 2 – COMPOSITION, INFORMATION ON INGREDIENTS

67-56-1	Methanol	<99%	200-659-6	Irritant, Flammable

NFPA Rating: (estimated) Health: 1; Flammability: 3; Instability: 0

State: Liquid	Appearance: colorless	Odor: Alcohol-like, weak odor
Boiling Point: 64.7°C@760mmHg	pH: Not available	Specific Gravity: 7910g/cm3@20°C
Vapor Pressure (mm Hg): 128mmHg @20°C	Vapor Density (AIR=1): 1.11	
Flash Point: 12°C	Solubility in Water: miscible	

SECTION 3 – HAZARDS IDENTIFICATION

Appearance: Colorless liquid, Flash Point: 12°C, 53.6°F.

Danger! Poison! May be fatal or cause blindness if swallowed. Vapor harmful. **Flammable liquid and vapor.** Harmful if swallowed, inhaled, or absorbed through the skin. Causes eye, skin, and respiratory tract irritation. May cause central nervous system depression. Cannot be made non-poisonous.
Target Organs: Eyes, nervous system, optic nerve.

Potential Health Effects
Eye: May cause painful sensitization to light. Methanol is a mild to moderate eye irritant. Inhalation, ingestion or skin absorption of methanol can cause significant disturbance in vision, including blindness.
Skin: Causes moderate skin irritation. May be absorbed through the skin in harmful amounts. Prolonged and or repeated contact may cause defatting of skin and dermatitis. Methanol can be absorbed through the skin, producing systemic effects that include visual disturbances.
Ingestion: May be fatal or cause blindness if swallowed. Aspiration hazard. Cannot be made non-poisonous. May cause gastrointestinal irritation with nausea, vomiting and diarrhea. May cause systematic toxicity with acidosis. May cause central nervous system depression, characterized by excitement, followed by headache, dizziness, drowsiness, and nausea. Advanced stages may cause collapse, unconsciousness, coma, and possible death due to failed respiratory failure. May cause cardiopulmonary system effects.

Inhalation: Methanol is toxic and can very readily form extremely high vapor concentrations at room temperature. Inhalation is the most common route of occupational exposure. At first, methanol causes CNS depression with nausea, headache, vomiting, dizziness and incoordination. A time period with no obvious symptoms follows (typically 8-24 hrs). This latent period is followed by metabolic acidosis and severe visual effects which may include reduced reactivity and/or increased sensitivity to light, blurred, doubl and/or snowy vision, and blindness. Depending on the severity of exposure and the promptness of treatment, survivors may recover completely or may have permanent blindness, vision disturbances and/or nervous system effects.
Chronic: Prolonged or repeated skin contact may cause dermatitis. Chronic exposure may cause effects similar to those of acute exposure. Methanol is only very slowly eliminated from the body. Because of this slow elimination, methanol should be regarded as a cumulative poison. Though a single exposure may cause no effect, daily exposures may result in the accumulation of a harmful amount. Methanol has produced fetotoxicity in rats and teratogenicity in mice exposed by inhalation to high concentrations that did not produce significant maternal toxicity.

SECTION 4 – FIRST AID MEASURES

Eyes: In case of contact, immediately flush eyes with plenty of water for a t least 15 minutes. Get medical aid.
Skin: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Get medical aid immediately. Wash clothing before reuse.
Ingestion: Potential for aspiration if swallowed. Get medical aid immediately. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If vomiting occurs naturally, have victim lean forward.
Inhalation: If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.
Notes to Physician: Effects may be delayed.
Antidote: Ethanol may inhibit methanol metabolism.

SECTION 5 – FIRE FIGHTING MEASURES

General Information: Ethanol may inhibit methanol metabolism. As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. Use water spray to keep fire-exposed containers cool. Water may be ineffective. Material is lighter than water and a fire may be spread by the use of water. Vapors are heavier than air and may travel to a source of ignition and flash back. Vapors can spread along the ground and collect in low or confined areas.
Extinguishing Media: For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam. Water may be ineffective. For large fires, use water spray, fog or alcohol-resistant foam. Do NOT use straight streams of water.
Flash Point: 12 deg C (53.60 deg F)
Autoignition Temperature: 455 deg C (851.00 deg F)
Explosion Limits, Lower:6.0 vol %
Upper: 31.00 vol %
NFPA Rating: (estimated) Health: 1; Flammability: 3; Instability: 0

SECTION 6 – ACCIDENTAL RELEASE MEASURES

General Information: Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks: Use water spray to disperse the gas/vapor. Remove all sources of ignition. Absorb spill using an absorbent, non-combustible material such as earth, sand, or vermiculite. Do not use combustible materials such as sawdust. Use a spark-proof tool. Provide ventilation. A vapor suppressing foam may be used to reduce vapors. Water spray may reduce vapor but may not prevent ignition in closed spaces.

SECTION 7-HANDLING AND STORAGE

Handling: Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Ground and bond containers when transferring material. Use spark-proof tools and explosion proof equipment. Avoid contact with eyes, skin, and clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep container tightly closed. Do not ingest or inhale. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames. Use only with adequate ventilation. Keep away from heat, sparks and flame. Avoid use in confined spaces.
Storage: Keep away from heat, sparks, and flame. Keep away from sources of ignition. Store in a cool, dry, well-ventilated area away from incompatible substances. Flammables-area. Keep containers tightly closed.

SECTION 8 – EXPOSURE CONTROL/ PERSONAL PROTECTION

Engineering Controls: Use explosion-proof ventilation equipment. Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use adequate general or local exhaust ventilation to keep airborne concentrations below the permissible exposure limits.

Chemical Name	ACGIH	NIOSH	OSHA – Final PELs
Methanol	200 ppm TWA; 250 ppm STEL; Skin - potential significant contribution to overall exposure by the cutaneous route	200 ppm TWA; 260 mg/m3 TWA 6000 ppm IDLH	200 ppm TWA; 260 mg/m3 TWA

OSHA Vacated PELs: Methanol: 200 ppm TWA; 260 mg/m3 TWA
Personal Protective Equipment
Eyes: Wear chemical splash goggles.
Skin: Wear butyl rubber gloves, apron, and/or clothing.
Clothing: Wear appropriate protective clothing to prevent skin exposure.
Respirators: Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

SECTION 9 – PHYSICAL AND CHEMICAL PROPERTIES

Physical State: Clear liquid
Appearance: clear, colorless - APHA: 10 max
Odor: alcohol-like - weak odor
pH: Not available.
Vapor Pressure: 128 mm Hg @ 20 deg C
Vapor Density: 1.11 (Air=1)
Evaporation Rate:5.2 (Ether=1)
Viscosity: 0.55 cP 20 deg C
Boiling Point: 64.7 deg C @ 760 mmHg
Freezing/Melting Point:-98 deg C
Decomposition Temperature: Not available.
Solubility: miscible
Specific Gravity/Density:.7910 g/cm3 @ 20°C
Molecular Formula:CH4O
Molecular Weight:32.04

SECTON 10 – STABILITY AND REACTIVITY

Chemical Stability: Stable under normal temperatures and pressures.
Conditions to Avoid: High temperatures, ignition sources, confined spaces.
Incompatibilities with Other Materials: Oxidizing agents, reducing agents, acids, alkali metals, potassium, sodium, metals as powders (e.g. hafnium, raney nickel), acid anhydrides, acid chlorides, powdered aluminum, powdered magnesium.
Hazardous Decomposition Products: Carbon monoxide, irritating and toxic fumes and gases, carbon dioxide, formaldehyde.
Hazardous Polymerization: Will not occur.

SECTION 11 – TOXICOLOGICAL INFORMATION

RTECS#:
CAS# 67-56-1: PC1400000
LD50/LC50:
CAS# 67-56-1:
Draize test, rabbit, eye: 40 mg Moderate;
Draize test, rabbit, eye: 100 mg/24H Moderate;
Draize test, rabbit, skin: 20 mg/24H Moderate;
Inhalation, rabbit: LC50 = 81000 mg/m3/14H;
Inhalation, rat: LC50 = 64000 ppm/4H;
Oral, mouse: LD50 = 7300 mg/kg;
Oral, rabbit: LD50 = 14200 mg/kg;
Oral, rat: LD50 = 5600 mg/kg;
Skin, rabbit: LD50 = 15800 mg/kg;

Human LDLo Oral: 143 mg/kg; Human LDLo Oral: 428 mg/kg; Human TCLo Inhalation; 300 ppm caused visual field changes & headache; Monkey LDLo Skin: 393 mg/kg. Methanol is significantly less toxic to most experimental animals than humans, because most animal species metabolize methanol differently. Non-primate species do not ordinarily show symptoms of metabolic acidosis or the visual effects which have been observed in primates and humans.
Carcinogenicity:
CAS# 67-56-1: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No information found
Teratogenicity: There is no human information available. Methanol is considered to be a potential developmental hazard based on animal data. In animal experiments, methanol has caused fetotoxic or teratogenic effects without maternal toxicity.
Reproductive Effects: See actual entry in RTECS for complete information.
Mutagenicity: See actual entry in RTECS for complete information.
Neurotoxicity: ACGIH cites neuropathy, vision and CNS under TLV basis.

SECTION 12 – ECOLOGICAL INFORMATION

Ecotoxicity: Fish: Fathead Minnow: 29.4 g/L; 96 Hr; LC50 (unspecified)Fish: Goldfish: 250 ppm; 11 Hr; resulted in deathFish: Rainbow trout: 8000 mg/L; 48 Hr; LC50 (unspecified)Fish: Rainbow trout: LC50 = 13-68 mg/L; 96 Hr.; 12 degrees CFish: Fathead Minnow: LC50 = 29400 mg/L; 96 Hr.; 25 degrees C, pH 7.63Fish: Rainbow trout: LC50 = 8000 mg/L; 48 Hr.; UnspecifiedBacteria: Phytobacterium phosphoreum: EC50 = 51,000-320,000 mg/L; 30 minutes; Microtox test No data available.
Environmental: Dangerous to aquatic life in high concentrations. Aquatic toxicity rating: TLm 96>1000 ppm. May be dangerous if it enters water intakes. Methyl alcohol is expected to biodegrade in soil and water very rapidly. This product will show high soil mobility and will be degraded from the ambient atmosphere by the reaction with photochemically produced hyroxyl radicals with an estimated half-life of 17.8 days. Bioconcentration factor for fish (golden ide) < 10. Based on a log Kow of -0.77, the BCF value for methanol can be estimated to be 0.2.
Physical: No information available.
Other: No information available.

SECTION 13 – DISPOSAL CONSIDERATIONS

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.

RCRA P-Series: None listed.
RCRA U-Series:
CAS# 67-56-1: waste number U154 (Ignitable waste).

SECTION 14 – TRANSPORT INFORMATION

	US DOT	CANADA TDG
Shipping Name:	Methanol	Methanol
Hazard Class:	3	3
UN Number:	UN1230	UN1230
Packing Group:	II	II
Additional Information		Flash Point 12°C

SECTION 15 – REGULATORY INFORMATION

US FEDERAL

TSCA
CAS# 67-56-1 is listed on the TSCA inventory.
Health & Safety Reporting List
None of the chemicals are on the Health & Safety Reporting List.
Chemical Test Rules
None of the chemicals in this product are under a Chemical Test Rule.
Section 12b
None of the chemicals are listed under TSCA Section 12b.
TSCA Significant New Use Rule
None of the chemicals in this material have a SNUR under TSCA.
CERCLA Hazardous Substances and corresponding RQs
CAS# 67-56-1: 5000 lb final RQ; 2270 kg final RQ
SARA Section 302 Extremely Hazardous Substances
None of the chemicals in this product have a TPQ.
SARA Codes
CAS # 67-56-1: immediate, fire.
Section 313
This material contains Methanol (CAS# 67-56-1, > 99%),which is subject to the reporting requirements of Section 313 of SARA Title III and 40 CFR Part 373.
Clean Air Act:
CAS# 67-56-1 is listed as a hazardous air pollutant (HAP).
This material does not contain any Class 1 Ozone depletors.
This material does not contain any Class 2 Ozone depletors.
Clean Water Act:
None of the chemicals in this product are listed as Hazardous Substances under the CWA.
None of the chemicals in this product are listed as Priority Pollutants under the CWA.
None of the chemicals in this product are listed as Toxic Pollutants under the CWA.
OSHA:
None of the chemicals in this product are considered highly hazardous by OSHA.
STATE
CAS# 67-56-1 can be found on the following state right to know lists: California, New Jersey, Pennsylvania, Minnesota, Massachusetts.

California Prop 65
California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives
Hazard Symbols:
T F
Risk Phrases:
R 11 Highly flammable.
R 23/24/25 Toxic by inhalation, in contact with skin and if swallowed.
R 39/23/24/25 Toxic : danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed.

Safety Phrases:
S 16 Keep away from sources of ignition - No smoking.
S 36/37 Wear suitable protective clothing and gloves.
S 45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).
S 7 Keep container tightly closed.

WGK (Water Danger/Protection)
CAS# 67-56-1: 1
Canada - DSL/NDSL
CAS# 67-56-1 is listed on Canada's DSL List.
Canada - WHMIS
This product has a WHMIS classification of B2, D1B, D2B.
This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.
Canadian Ingredient Disclosure List
CAS# 67-56-1 is listed on the Canadian Ingredient Disclosure List.

SECTION 16 – Other Information

This Material Safety Data Sheet has been prepared in accordance with 29 CFR 1910.1200 and contains information believed to be accurate and complete at the date of preparation. The statements contained herein are offered for informational purposes only and are based upon technical data. MIDI Inc. believes them to be accurate but does not purport to be all-inclusive. The above-stated product is intended for use only by persons having the necessary technical skills and facilities for handling the product at their discretion and risk. Since conditions and manner of use are outside our control, we (MIDI Inc.) make no warranty of merchantability or any such warranty, express or implied with respect to information and we assume no liability resulting from the above product or its use. Users should make their own investigations to determine suitability of information and product for their particular purposes.

MATERIAL SAFETY DATA SHEET

1. CHEMICAL PRODUCT & MANUFACTURER'S DETAILS

PRODUCT NAME : 3-Aminopyridine

MANUFACTURER

FACTORY & REGISTERED OFFICE:	*HEAD OFFICE:*
Jubilant Organosys Limited Bhartiagram, Gajraula District: Jyotiba Phuley Nagar Uttar Pradesh-244223 , India PHONE NO: +91-5924-252353 upto 60 Contact Department-Safety: Extension 298 FAX NO : 91-5924-252352 EMERGENCY PHONE: +91-5924-268141	Jubilant Organosys Limited Plot 1-A, Sector 16-A, Institutional Area, Noida, Uttar Pradesh-201301 India. PHONE NO: +91-120-2516601 Contact department: EHS FAX NO : +91-120-2516629 Email: support@jubl.com

2. CHEMICAL IDENTIFICATION

- *CHEMICAL NAME* : 3-Aminopyriine
- *SYNONYMS* : 3-Pyridinamine,beta-Aminopyridine
- *CHEMICAL CLASSIFICATION* : Aromatic Hetrocyclic Compound
- *CHEMICAL FORMULA* : $(C_5H_4N)NH_2$
- *C.A.S. NO.* : 462-08-8

3. HAZARD IDENTIFICATION & HEALTH HAZARD

- Fatal if swallowed
- May be fatal in contact with skin
- May be fatal if inhaled
- Combustible
- Route of entry: inhalation, skin, ingestion
- Irritating to eyes and respiratory system

4. FIRST AID MEASURES

Eye:
Immediately flush eyes with plenty of water for at least 15 minutes by separating eyelids with fingers. Get medical help.

Skin:
Immediately remove contaminated clothings and shoes. Flush skin with copious amount of water for atleast fifteen minutes. Wash contaminated clothing before reuse.

Inhalation:
Remove the affected person (s) to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen.

Ingestion:
If swallowed, wash mouth with water if conscious. Make victim drink plenty of water and induce vomiting. Call a physician

5. FIRE FIGHTING MEASURES

***Extinguishing media*:**
Water spray, dry chemical powder, carbon dioxide, and chemical foam.

***Special fire fighting procedure*:**
Wear protective clothing, wear self contained breathing apparatus.

Unusual fire and explosion hazard:
Emits toxic fumes under fire conditions.

6. ACCIDENTAL RELEASE MEASURES

- Evacuate the area
- Wear self-contained breathing apparatus, protective clothing (single piece suit) rubber boots and heavy rubber gloves
- Sweep up, place in a bag and hold for disposal. Ventilate area (if incident has occurred in-door) and wash spill site after material pick up is complete.
- Avoid raising dust

7. HANDLING AND STORAGE

- Keep containers tightly closed
- Wear suitable protective clothing, breathing apparatus, gloves and eye/face protection
- Use only in a chemical fume hood
- Do not breathe dust, vapour, mist or gas

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

- Avoid inhalation of Dust
- Avoid contact with eyes, skin and clothing
- Avoid prolonged/repeated exposure
- Wash thoroughly after handling
- Use only in a chemical fume hood
- Wear appropriate NIOSH/MSHA approved respirator, chemical resistant gloves/safety goggles and protective clothing (single piece suit)
- In case of contact use safety showers and eye bath for washing

9. PHYSICOCHEMICAL PROPERTIES & FIRE/ EXPLOSION HAZARD DATA

PHYSICAL STATE	: Solid
APPEARANCE	: Yellow to brown
ODOUR	: Characteristic
BOILING POINT	: 248 °C
MELTING POINT	: 60-63 °C
FLASH POINT	: 124°C
VAPOUR PRESSURE	: Data not relevant
BULK DENSITY	: 0.75 g/cm^3
VAPOR DENSITY (AIR=1)	: Data not relevant
SOLUBILITY IN WATER	: Soluble
pH	: 8.5 (10% solution in water)
LEL	: Data not applicable
UEL	: Data not applicable
AUTO IGNITION TEMPERATURE	: 628°C
EXPLOSIVE SENSITIVITY TO IMPACTS	: Data not available
EXPLOSIVE SENSITIVITY TO STATIC ELECTRICITY	: Data not available
COMBUSTIBLE LIQUID	: No
FLAMMABLE MATERIAL	: No
PYROPHORIC MATERIAL	: No
EXPLOSIVE MATERIAL	: No
OXIDISER	: No
ORGANIC PEROXIDE	: No
CORROSIVE MATERIAL	: No
MOLECULAR WEIGHT	: 94.12

10. STABILITY AND REACTIVITY

- Stable under normal temperature & pressures
- Incompatible with oxidising agents, strong acids, acid chlorides, acid anhydrides
- Conditions to avoid - incompatible materials, dust generation
- Hazardous combustion or decomposition products:
  thermal decomposition may produce carbon monoxide and oxides of nitrogen

11. TOXICOLOGICAL INFORMATION

- ***Acute effects:***
  May be fatal if swallowed, inhaled or absorbed through skin.
  High concentrations are extremely destructive to tissues of the mucous membranes and upper respiratory tract, eyes and skin. May cause convulsions
- ***Target organs:***
  Damage to the Nervous system

11. TOXICOLOGICAL INFORMATION

- ***Toxicity***:
  ORAL RAT LD50 : 21 mg/kg

- ***Carcinogenicity***:
  Not list by ACGIH, IARC, NIOSH, NTP or OSHA

RTECS # : US1650000

12. ECOLOGICAL INFORMATION

- ***Ecotoxicity***: Bioaccumulation – none or low
- ***Environmental***: Not readily biodegradable.

13. DISPOSAL CONSIDERATION

- Dissolve in a combustible liquid and burn in a chemical incinerator equipped with an afterburner and scrubber.
- Observe all federal, state and local environmental regulations

14. TRANSPORT INFORMATION

PROPER SHIPPING NAME	:	Aminopyridine
UN/ID NUMBER	:	2671
UN HAZARD CLASS	:	6.1
UN PACKING GROUP	:	II

15. REGULATORY INFORMATION

European information

- EC NO. : 207-322-2
- R-23/24/25 (Toxic by inhalation/ contact with skin/ swallowed)
- S-36/37/39 (wear suitable protective clothing/gloves and eye/face protection)
- S-45 (in case of accident, if you feel unwell, seek medical advice immediately)

US information

- Is listed in EPA TSCA chemical inventory.
- None of the chemicals in this product are listed under TSCA section 12b
- None of the chemicals in this product have an RQ under SARA Section 302 RQ
- None of the chemicals in this product have an TPQ under SARA Section 302 TPQ
- None of the chemicals in this product are reported under SARA Section 313
- None of the chemicals in this product contain any class1 & class2 ozone depletors , neither contain any hazardous air pollutants under ‘Clean Air Act’
- None of the chemicals in this product are listed as Hazardous substances or priority pollutants or Toxic substances list under ‘Clean Water Act’

16. OTHER INFORMATION

Information contained in this MSDS is believed to be correct but no representation, guarantee or warranties of any kind are made as to its accuracy, suitability for a particular application or results to be obtained from them. This MSDS shall be used as a guide only. JUBILANT ORGANOSYS LIMITED makes no warranties expressed or implied of the adequacy of this document for any particular purpose.

Document Name: 0151A02 Div 05 msds 3-Aminopyridine
Date: 02-Nov-04
Revision Number: 02