



4-2012

Reclamation of Isopropyl Alcohol and N-Propyl Bromide

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Senior Design Reports (CBE). 38.
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Reclamation of Isopropyl Alcohol and N-Propyl Bromide

Abstract

The purpose of this design project is to recover a co-solvent mixture that is used to remove oil and water from metal machine parts. The cleansing solvents used are n-propylbromide (NPB) and isopropyl alcohol (IPA), which respectively remove oleic acid and water. The solvent mixture starts at an IPA/NPB molar ratio of 56/44 and can be used for cleaning machinery until the water reaches 7.5% by mole. This spent cleaning mixture is then delivered for reclamation of IPA and NPB so that it can be used for cleaning again. A 6,240 gallon truckload is delivered every two days, and the mixture to be cleaned has a molar composition of 47.6% IPA, 37.4% NPB, 7.5% oleic acid, and 7.5% water. The goals of the project are to completely remove the oleic acid, reduce the water molar composition to below 2.5%, maximize co-solvent recovery, and maximize profitability.

A major challenge of the project is the non-ideal behavior of the components, which includes multiple azeotropes and distillation boundaries. Another important characteristic of this design project is the unusually small scale: one 6,240 gallon quantity of used co-solvent mixture must be processed every two days. Due to this scale, batch processes were investigated as well as continuous processes.

The continuous alternative utilizes three major separation units: a 15-tray distillation column, a decanter for the distillate, and an evaporator for the bottoms. 93.8% of the original IPA and 99.2% of the original NPB is recovered. There is no oleic acid and 0.5% by mole of water in the product. Pure NPB and IPA are added at the end of the separation to compensate for the lost co-solvents, and to restore the IPA/NPB ratio to 56/44. A \$0.45/lb selling price of reclaimed co-solvent returns an IRR of 45.6% and an NPV of \$2,657,300 in year 10 of production.

The batch alternative utilizes a batch distillation column with multiple receivers and recovers 95.4% of the original IPA and 99.7% of the original NPB. There is 0.8% water by mole and no oleic acid in the product. Pure NPB and IPA also must be added to restore the original ratio. Because the composition of water is higher in the batch product than in the continuous, the co-solvent mixture is sold at a lower \$0.42/lb, resulting in an IRR of 37.2% and an NPV of \$2,452,500 in year 10. However, the batch process has significant down time and can potentially handle up to four times the solvent demand (2 trucks of solvent/day), resulting in an IRR of 130% and an NPV of \$22,494,500 at the same selling price. Because of the batch plant's ability to handle demand growth, its flexibility in separating different co-solvent ratios, and its robust economic potential, we recommend the construction of the batch co-solvent reclamation plant.

Reclamation of Isopropyl Alcohol and N-Propyl Bromide

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April 10, 2012

Professor Sean P. Holleran
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School of Engineering and Applied Science
Department of Chemical and Biomolecular Engineering
Philadelphia, PA 19104

April 10, 2012

Dear Professor Holleran and Professor Fabiano,

As per our senior design problem statement, we have designed a separation process that removes oleic acid and water from a co-solvent mixture of 56% isopropyl alcohol and 44% n-propyl bromide at an output of 4,600 gallons every two days. After investigating batch and continuous processes, we have found that both alternatives achieve the desired separation and are economically profitable. However, our final recommendation for this separation scheme is to construct a batch distillation plant.

With such a plant, we can price the co-solvent product at \$0.42/lb and make a very robust profit while operating at only one-fourth of maximum capacity. Over a ten-year production lifetime, the batch process predicts an internal rate of return of 37.2% and a net present value of \$2,452,500, which is a very sound economic return. The batch design also has the added capability of increasing operational capacity, so that it can process up to four times the quantity of its continuous counterpart. Finally, the batch plant can separate solvent mixtures of differing compositions, and is generally much more flexible. We therefore advocate the construction of the batch plant not because it is currently more profitable than a continuous plant, but rather because it has the potential to be, while also maintaining processing flexibility.

Sincerely,

Haoyu Deng

Angela Mu

Craig Schwait

Jamie Wessels

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Abstract

The purpose of this design project is to recover a co-solvent mixture that is used to remove oil and water from metal machine parts. The cleansing solvents used are n-propyl-bromide (NPB) and isopropyl alcohol (IPA), which respectively remove oleic acid and water. The solvent mixture starts at an IPA/NPB molar ratio of 56/44 and can be used for cleaning machinery until the water reaches 7.5% by mole. This spent cleaning mixture is then delivered for reclamation of IPA and NPB so that it can be used for cleaning again. A 6,240 gallon truck-load is delivered every two days, and the mixture to be cleaned has a molar composition of 47.6% IPA, 37.4% NPB, 7.5% oleic acid, and 7.5% water. The goals of the project are to completely remove the oleic acid, reduce the water molar composition to below 2.5%, maximize co-solvent recovery, and maximize profitability.

A major challenge of the project is the non-ideal behavior of the components, which includes multiple azeotropes and distillation boundaries. Another important characteristic of this design project is the unusually small scale: one 6,240 gallon quantity of used co-solvent mixture must be processed every two days. Due to this scale, batch processes were investigated as well as continuous processes.

The continuous alternative utilizes three major separation units: a 15-tray distillation column, a decanter for the distillate, and an evaporator for the bottoms. 93.8% of the original IPA and 99.2% of the original NPB is recovered. There is no oleic acid and 0.5% by mole of water in the product. Pure NPB and IPA are added at the end of the separation to compensate for the lost co-solvents, and to restore the IPA/NPB ratio to 56/44. A \$0.45/lb selling price of reclaimed co-solvent returns an IRR of 45.6% and an NPV of \$2,657,300 in year 10 of production.

The batch alternative utilizes a batch distillation column with multiple receivers and recovers 95.4% of the original IPA and 99.7% of the original NPB. There is 0.8% water by mole and no oleic acid in the product. Pure NPB and IPA also must be added to restore the original ratio. Because the composition of water is higher in the batch product than in the continuous, the co-solvent mixture is sold at a lower \$0.42/lb, resulting in an IRR of 37.2% and an NPV of \$2,452,500 in year 10. However, the batch process has significant down time and can potentially handle up to four times the solvent demand (2 trucks of solvent/day), resulting in an IRR of 130% and an NPV of \$22,494,500 at the same selling price. Because of the batch plant's ability

to handle demand growth, its flexibility in separating different co-solvent ratios, and its robust economic potential, we recommend the construction of the batch co-solvent reclamation plant.

INTRODUCTION

Co-solvents are commonly used in industry to clean metal machinery of oil and water build-up. Our client uses a co-solvent solution of isopropyl alcohol (IPA) and n-propyl bromide (NPB) to remove water and oleic acid from machinery. IPA is a widely accepted solvent for water in the medical and manufacturing fields, while NPB is a popular oil cleaning agent, especially since environmentally hazardous cleaning agents such as TCA and HFCs have become regulated and banned. Such a co-solvent mixture, however, is only effective up to a saturation point, above which it cannot capture any additional oil or water.

This project aims to design a process that removes oleic acid and water from the saturated co-solvent mixture, which is 47.6% IPA, 37.4% NPB, 7.5% oleic acid, and 7.5% water by mole, and reclaim it in its original proportions so that it can be reused for cleaning. Our company, Creative Trollers of America, seeks to find a solution that is both desirable to potential clients and profitable. Our process must therefore provide our clients with a service that is cheaper than simply purchasing a new co-solvent mixture of 56% IPA and 44% NPB by mole.

This project considers both a continuous separation scheme and a batch distillation process before making a final recommendation. There are advantages and disadvantages to each separation pathway, and our final conclusion is based on a number of considerations. One absolute requirement is the level of separation achieved by each process; we must take into account solvent recovery and final product purity. The project statement requires that the final product contain no more than 2.5% water by mole and no oleic acid. After designing the processes to meet these requirements, we analyze and compare the economic profitability of both alternatives. Finally, environmental effects, operational safety, and other miscellaneous factors will be investigated before making a final recommendation.

Additionally, our team is tasked with investigating other potential organic solvents that can substitute NPB. Although NPB is currently accepted as an environmentally safe and non-harmful chemical, there is anticipation that it will become regulated in the future due to health issues related to exposure. With this in mind, any solvent recommendation must have oil-cleaning qualities similar to NPB, yet must be less hazardous to remain unregulated. Our team uses the Pro-Pred molecular software to identify NPB's current solubility and toxicity parameters, which form the base criteria for discovering new oil-cleaning solvents using the Pro-CAMD software. Though this is an important consideration for the future, we stress it is a secondary goal of our project.

CONCEPT STAGE

Customer Requirements

After using the IPA/NPB co-solvent mixture to remove water and oil from machinery, our customer would like to reuse it for the same purpose in future cleanings. Thus, the customer's requirement is clear: restore this co-solvent mixture of IPA and NPB to its original quantity and composition (4,600 gallons in a 56/44 IPA to NPB molar ratio). To maximize cleaning potential, the client also requires that all of the oleic acid be removed and that only 2.5 percent by mole of water be present in the total reclaimed solvent. This process will be fitness to standard since we are restoring the used co-solvent to acceptable levels currently used in industry. Other customer and industry considerations include making the process plant safe and environmentally acceptable, allowing variability in customer cleaning schedules, and having the operational capacity to process at least one truckload every two days.

Market and Competitive Analysis

Our company, Creative Tollers of America, is contracted because other companies (including our client) believe that outsourcing co-solvent reclamation can reduce their costs and increase their profitability. To best decide where to locate our plant, it is important to note that the metal parts cleaned with IPA/NPB solvent are generally used for precision cutting, such as making bearings, drawn tubes, or coils for heat exchanger equipment. There is a market for this in any major metropolitan area, such as the Greater Philadelphia area; therefore, we have decided to locate our plant in New Jersey, which is close to multiple urban and industrial regions. However, it is important to note that the plant is designed to clean a quantity of 6,240 gallons every two days, so we can only service small to medium-sized customers. Likely candidates for our service include pharmaceutical companies, small industrial chemical plants, and configured consumer chemical plants, among others.

Parts Cleaning Technologies has a solvent-reclamation plant located in Cinnaminson, NJ and is an example of our competition. In order to successfully capture market share and compete with existing businesses, our value must be higher than theirs. We requested quotes from several tolling companies, but have not received responses about a comparable service; thus, we account for only our company's profitability in this project and have not done an intensive analysis on whether there are barriers to market entry. One competitive advantage of our proposed batch system is its flexibility: it can clean a range of different compositions of used co-solvent mixtures. Additionally, should NPB become regulated or banned in the future, the batch plant can potentially clean a substitute co-solvent mixture if it has similar properties to NPB. Later, we analyze how to lower the selling price of reclaimed co-solvent without sacrificing a positive return for our company.

Finally, Creative Tollers of America will also offer pick-up and drop-off service for our clients' co-solvents, allowing for flexibility in customer cleanup schedules. This limits our physical market access; by setting a constraint of 8 hours of driving per day, our truck service can cover a 180 mile radius from our plant (see Appendix C). After gauging the market size and the demand for our services in this area with the aid of our consultants, we conclude that receiving a 6,240 gallon truckload of spent co-solvent every two days is a fair market estimate. Therefore, we design both our continuous and batch processes to separate this amount of co-solvent.

Preliminary Process Synthesis

Since this is a separation process, our project team identified at an early stage the possibility for multiple separation pathways. Our client's original requirement of a recovered co-solvent product with less than a total of 2.5 mole percent water and no oleic acid eliminates many potential separation options. One such separation pathway appears promising and involves boiling up everything but oleic acid in the original co-solvent feed. This removes oleic acid from the separation problem and leaves only an IPA, NPB, and water system to be processed. However, utilizing a distillation column with this new 3-component feed produces a final water composition of approximately 2% by mole. Though this is allowable, it gives the client significantly less cleaning potential (our product from our final continuous process can be used 20% longer, while that from our final batch process can be used 15% longer). Additionally, this process has a massive utility requirement because of the initial heating as well as the substantial cooling necessary to bring the IPA/NPB/water mixture temperature back down to operating conditions for the second distillation column. Our project team therefore did not pursue this process pathway fully, and chose to concentrate on those discussed in the next section.

None of the other distillation separation processes explored deliver the necessary solvent product specifications. Other separation schemes such as sorption, desiccation, or catalytic chemistry are explored later in Section 8: Other Separation Alternatives.

Assembly of Database

The Aspen Plus process simulation software is used for both the continuous and batch separation process designs. The components IPA, NPB, oleic acid, and water are readily available in Aspen's component database, and the NRTL-RK property method is used to determine binary interaction parameters for the chemicals. The non-random two-liquid model (NRTL) with Redlich-Kwong (RK) equation of state is selected for the process after speaking with consultants, and the UNIFAC group contribution model is used to estimate any remaining property parameters that are not given by the NRTL-RK method. These binary interaction parameters are listed in Table 3.1 below. The interaction coefficients between water and NPB and water and IPA help model the non-ideal behavior of the IPA-NPB-water system in the Aspen simulations for both the continuous and batch processes.

Component i	Water	Water	Water	Oleic acid	Oleic acid	NPB
Component j	NPB	IPA	Oleic acid	NPB	IPA	IPA
Temperature units	F	F	F	F	F	F
Source	LLE-ASPEN	VLE-IG	R-PCES	R-PCES	R-PCES	R-PCES
Property units:						
aij	8.3012	6.8284	0	0	0	0
aji	8.365	-1.3115	0	0	0	0
bij	-1139.509	-2670.223	8961.942	-787.7843	-466.5669	1224.464
bji	-1173.138	767.516	967.0927	1340.885	1141.201	38.70782
cij	0.2	0.3	0.3	0.3	0.3	0.3
dij	0	0	0	0	0	0
eij	0	0	0	0	0	0
eji	0	0	0	0	0	0
fij	0	0	0	0	0	0
fji	0	0	0	0	0	0
Tlower	32	77	77	77	77	77
Tupper	86	212	77	77	77	77

Table 3.1 Binary interaction coefficients calculated by the UNIFAC method in Aspen Plus

IPA is generally nonhazardous, and its material safety data sheet is attached in Appendix F. NPB, despite being an improvement over previous oil-removing solvents in terms of toxicity and ozone-depletion, has generated concerns of exposure-related health risks such as neurologic illnesses (Nemhauser 2008). In addition, laboratory testing of mice treated with NPB has revealed preliminary carcinogenic effects, but the chemical is not deemed to be a significant

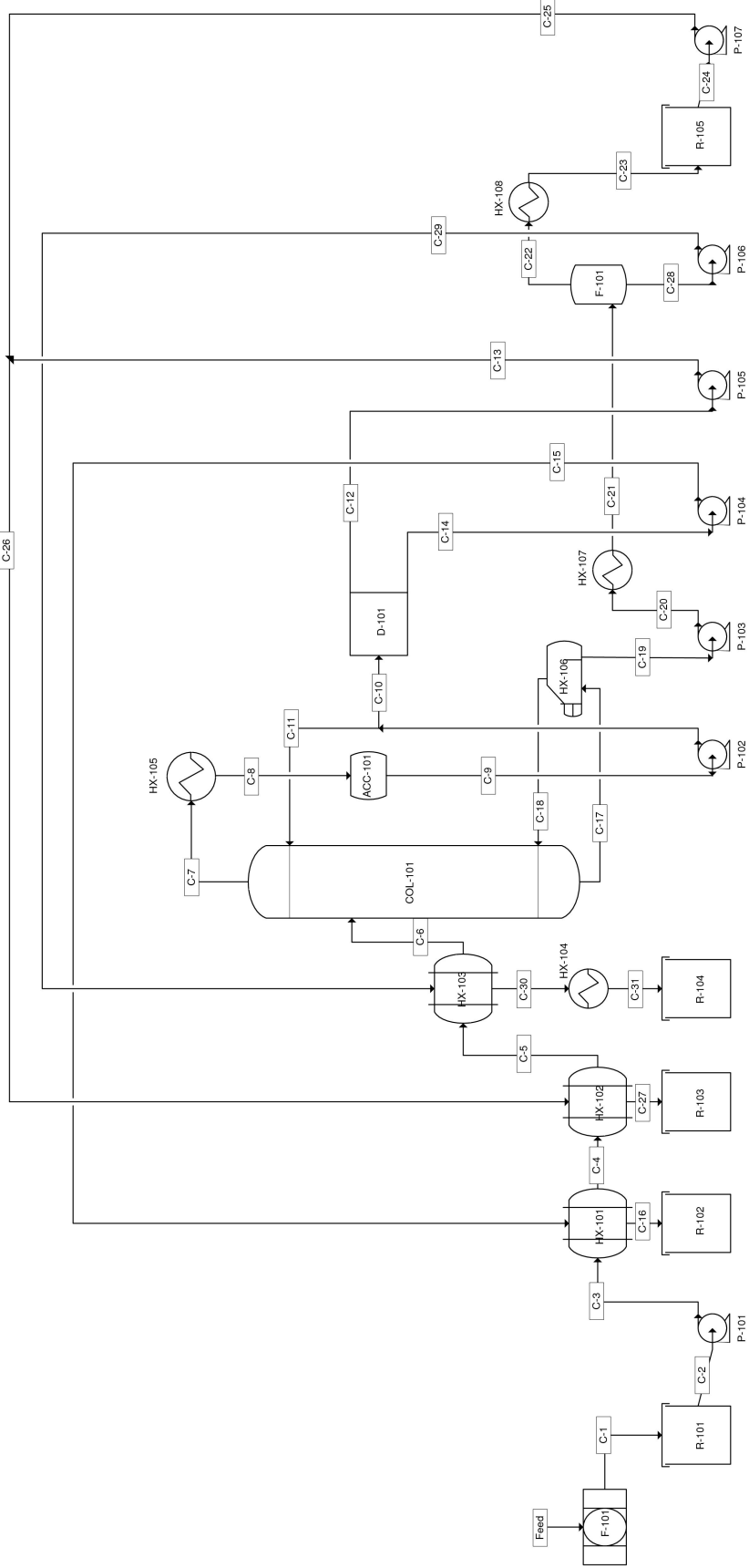
industrial risk by the EPA (Morgan 2011, EPA 2007). NPB's solvent properties and health and environmental impact will be analyzed more in depth in Section 9: Potential Co-solvent Alternatives, and its material safety data sheet is attached in Appendix F. Finally, the prices of IPA (lab grade), NPB, and oleic acid are listed in Table 3.2 below.

Chemical	Price
Isopropyl Alcohol (IPA)	\$0.68/lb
N-propyl Bromide (NPB)	\$2.10/lb
Oleic Acid	\$0.48/lb

Table 3.2: Prices of pure chemical components in our process. IPA's price is based on typical market prices ("IPA") NPB's price is given in the project statement, and oleic acid is priced at crude oil levels (Crude Oil Price 2012).

RECLAMATION OF IPA AND NPB -CONTINUOUS PROCESS-

Figure 4.1 Process Flowsheet



Material Balance

Streams Table									
Stream Number	Feed, C-1, C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10, C-11
Vapor fraction	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
Temperature (F)	70.0	70.5	71.7	105.6	125.0	142.0	125.0	125.0	125.1
Pressure (psia)	14.7	34.2	28.2	22.2	16.2	14.9	14.7	14.7	14.7
Composition (lb)									
isopropyl alcohol	324.4	324.4	324.4	324.4	324.4	215.7	215.7	143.8	71.9
n-propyl bromide	521.6	521.6	521.6	521.6	521.6	1337.1	1337.1	891.4	445.7
water	15.3	15.3	15.3	15.3	15.3	45.9	45.9	30.6	15.3
oleic acid	240.2	240.2	240.2	240.2	240.2	0.0	0.0	0.0	0.0
Total (lb)	1101.5	1101.5	1101.5	1101.5	1101.5	1598.7	1598.7	1065.8	532.9

Table 4.2: Mass and compositions for feed stream through C-11

Streams Table									
Stream Number	C-12	C-13	C-14	C-15	C-16	C-17	C-18	C-19	C-20
Vapor fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
Temperature (F)	125.0	125.2	125.0	125.1	100.0	179.4	179.4	179.4	179.4
Pressure (psia)	14.7	20.7	14.7	20.7	14.7	16.2	16.2	16.2	16.2
Composition (lb)									
isopropyl alcohol	59.5	59.5	12.4	12.4	12.4	252.5	565.0	565.0	565.0
n-propyl bromide	444.7	444.7	0.9	0.9	0.9	76.0	170.0	170.0	170.0
water	0.7	0.7	14.6	14.6	14.6	0.0	0.0	0.0	0.0
oleic acid	0.0	0.0	0.0	0.0	0.0	240.2	537.5	537.5	537.5
Total (lb)	504.9	504.9	27.9	27.9	27.9	568.7	1272.5	1272.5	1272.5

Table 4.3: Mass and compositions for streams C-12 through C-20

Streams Table									
Stream Number	C-22	C-23, C-24	C-25	C-26	C-27	C-28	C-29	C-30	C-31
Vapor fraction	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Temperature (F)	264.0	165.0	165.1	145.3	100.0	264.0	264.3	186.7	100.0
Pressure (psia)	14.7	14.7	20.7	20.7	14.7	14.7	26.7	20.7	14.7
Composition (lb)									
isopropyl alcohol	244.7	244.7	244.7	304.3	304.3	7.7	7.7	7.7	7.7
n-propyl bromide	72.7	72.7	72.7	517.4	517.4	3.2	3.2	3.2	3.2
water	0.0	0.0	0.0	0.8	0.8	0.0	0.0	0.0	0.0
oleic acid	0.1	0.1	0.1	0.1	0.1	240.2	240.2	240.2	240.2
Total (lb)	317.5	317.5	317.5	822.5	822.5	251.1	251.1	251.1	251.1

Table 4.4: Mass and compositions for streams C-22 through C-31

Process Description

To isolate NPB and IPA co-solvent from a co-solvent solution of NPB, IPA, water, and oleic acid, the continuous process primarily utilizes a distillation column, a rising film evaporator, and a decanter to take advantage of liquid-liquid and vapor-liquid equilibria. For a more technical description than is included here, please refer to Section 10: Other Considerations.

The project assumes that one 6,240 gallon truckload of used co-solvent is received every two days. The molar composition of the mixture is 47.6% IPA, 37.4% NPB, and 7.5 % of both oleic acid and water. The truck pumps the mixture into a 15,000 gallon storage tank. As the mixture is pumped into the storage tank, it is passed through a packed filter to remove any metallic particles from the parts the co-solvents were used to clean.

Distillation

The feed stream, C-2 is assumed to be at room temperature, or 70°F and has a mass flow of 1101.6 lb/hr. The feed stream, C-2, is fed to the distillation column, COL-101, using pump P-101 which increases the pressure from atmospheric to 19.5 psig in C-3. C-3 is heated to the operating temperature of the column, 125°F. The heating of the feed is achieved in three steps using C-16, C-27, and C-30 via heat exchangers HX-101, HX-102, and HX-103 respectively. The pressure drop across each of the heat exchangers is 6 psi. The duty required to heat the feed is 28,380 BTU/hr, with 2.2% provided by HX-101, 61.6% by HX-102, and 36.2% by HX-103.

C-6 enters a 15-tray distillation column above the seventh tray. COL-101 separates the four-component feed into two separate three-component streams. Oleic acid is significantly less volatile than the other three components, so the separation behaves essentially like a three-component distillation, with the heavy oleic acid leaving in the bottoms product. However, this pseudo three-component distillation is complicated by the presence of a ternary azeotrope and multiple azeotropic boundaries for the IPA, NPB, and water system. The column achieves the greatest possible separation of water into the distillate, such that the distillate stream mole composition is 21% IPA, 64% NPB, and 15% water. The bottoms stream has a composition of 74% IPA, 11% NPB, 15% oleic acid, and 144 ppm water. The distillate rate and bottoms rate are both 532.9 lb/hr. This split is chosen because it allows for the greatest separation of the water

and oleic acid at these operating conditions. The reflux ratio is two, and there is a 0.1 psi drop per tray.

Decanter

C-10, the distillate product, leaves the column as a liquid at 125°F and is fed to the decanter, D-101. The decanter, operating at 125°F and atmospheric pressure, separates the IPA, NPB, and water mixture into two liquid phases. The residence time inside the decanter is 30 minutes, a time suggested as reasonable by our consultant. The product stream from the decanter, C-12, flows at 505 lb/hr and is only composed of 0.1% water by mass and 0.9% by mole. This is well below the customer's molar composition requirement of 2.5%. The product stream C-12 is 78% NPB and 21% IPA by mole.

The waste stream C-14, flowing at 28 lb/hr, contains 80.8% water by mole and 52.2% by mass. It is cooled in HX-101 to 100°F against the feed stream, which is an acceptable temperature for aqueous waste storage. Although this waste stream carries some IPA and NPB in it, only 3.8% of the original mass of IPA and 0.2% of the original mass of NPB is lost. Because the customer requires the recovery of a 56/44 ratio of co-solvent in the original 4,600 gallon quantity, both IPA and NPB is purchased and added to the final product in storage tank R-103.

Evaporation

The bottoms stream C-17 is 179°F and is pumped through P-103 to increase the pressure 6 psi. This accounts for the pressure drop in HX-107, which heats the bottoms to the operating temperature of F-101, 264°F. HX-107 is a rising film evaporator using low-pressure steam at 50.3 psig and is used to take advantage of the liquid-vapor equilibrium. The liquid and vapor are then separated in the vertical vessel, F-101. The more volatile IPA and the NPB are evaporated while the oleic acid remains a liquid. The product vapor stream C-22 has a mole flow of 4.7 lbmol/hr and mass flow of 318 lb/hr. C-22 is 87% IPA and 13% NPB by mole with oleic acid and water only present at 52 and 173 ppm respectively. It is then condensed and cooled to 165°F by HX-108 using cooling water.

The oleic acid waste stream from the vertical vessel, C-28, has a composition of 12.9% IPA, 2.6% NPB, and 85% oleic acid and a flow rate of 1.01 lbmol/hr or 251 lb/hr. This waste stream carries away 2.4% of the original mass of IPA and 0.6% of the original mass of NPB; this quantity of co-solvent product is also purchased and added to the product storage tank R-103. After being pumped, C-29 is then cooled to 187°F in HX-103 by the feed stream, and further cooled to 100°F in HX-104 using cooling water. The oleic acid can be safely handled and stored below this temperature.

Product Stream

The product streams from the decanter and the vertical vessel, C-12 and C-25, are pumped and mixed together into C-26. Stream C-26 is then cooled to 100°F by HX-102, at which point it can be safely stored and cooled by the atmosphere. This cooled product stream has a molar composition of 55.4% IPA, 45.1% NPB, and 0.5% water, well below the 2.5% water maximum. The amount of oleic acid in the product is negligible.

The final product stream from the process, C-27, is then stored in a closed 10,000 gallon receiver to await pick-up (a client will pick up reclaimed co-solvent while dropping off used co-solvent mixture every two days). The final product has 93.8% of the original IPA mass and 99.2% of the original NPB mass. As stated previously, fresh IPA and NPB must augment the final product in order to restore the original 56/44 co-solvent ratio and the total quantity to 4,600 gallons. To do this, 962 lb of IPA and 199 lb of NPB are added to storage tank R-103 every two days. When a client picks up recovered product every two days, 4,600 gallons of 56% IPA and 44% NPB are present, along with 4.38 gallons of water (36.5 lb).

Equipment List

Unit	Description
ACC-101	Reflux Drum Accumulator
COL-101	Distillation Tower
D-101	Decanter
F-101	Vertical Vessel
HX-101	Double Pipe Heat Exchanger
HX-102	Double Pipe Heat Exchanger
HX-103	Double Pipe Heat Exchanger
HX-104	Double Pipe Heat Exchanger
HX-105	Condenser (Double Pipe Heat Exchanger)
HX-106	Kettle Reboiler
HX-107	Rising Film Evaporator
HX-108	Condenser (Double Pipe Heat Exchanger)
P-101	Pump
P-102	Reflux Pump
P-103	Reboiler Pump
P-104	Pump
P-105	Pump
P-106	Pump
P-107	Pump
P-108	Pump
P-109	Pump
P-110	Pump
R-101	Storage Receiver
R-102	Storage Receiver
R-103	Storage Receiver
R-104	Storage Receiver
R-105	Condensate Collecting Tank

Table 4.5 Equipment list for continuous process

Unit Descriptions

All equipment is constructed from stainless steel unless otherwise specified. Unit costs are calculated from Warren Seider's spreadsheet *Capital Cost Estimation* and relevant sizing and costing factors are calculated from *Process and Product Design Principles* by Seider, Seader, Lewin, and Widagdo (2009). Reported costs are in 2011-2012 fiscal cycle values, and these will be used in the economic analysis.

Distillation Column

COL-101 - Specification sheet on page 37

The distillation column separates the preheated feed into a distillate stream of NPB, IPA, and water and a bottoms stream of NPB, IPA, and oleic acid. As stated earlier, oleic acid is considerably less volatile than the other components and will not vaporize easily. Thus, at temperatures less than oleic acid's boiling point, NPB, IPA, and water can be separated up to that three-component system's azeotropic boundaries. The distillate molar composition is 21% IPA, 64% NPB, and 15% water, and the bottoms molar composition is 74% IPA, 11% NPB, 15% oleic acid, and 144 ppm water.

The column was sized using the procedures described in chapter 19.6 of *Process and Product Design Principles* by Seider, et al. The number of theoretical stages was determined using Aspen Plus under the RadFrac subroutine, while the actual number of trays was found using the O'Connell correlation. From a sensitivity analysis on the column, increasing the number of theoretical trays past 6 does not noticeably increase the amount of water in the distillate.

The column is 28 ft tall and has an inner diameter of 1.02 ft. There are 15 stainless steel sieve trays, with a tray spacing of 1 ft, and an average tray efficiency of 0.41. The column operates at 125°F and 5 psig, and has a top tray pressure of 20 psia and a bottom tray pressure of 15.4 psia. The distillate is removed at a temperature of 141°F and the bottoms at 161°F. The feed stream enters the column at tray 6, and the molar reflux and boil-up ratio is 2:1. This unit has a purchase cost of \$44,100 and a bare module cost of \$183,300.

Reflux Drum Accumulator

ACC-101 – Specification sheet on page 37

This horizontal vessel functions as the reflux drum accumulator for the distillation column. It processes a volume of 179.5 gallons every hour, and the vessel has a diameter of 1.33 ft and a length of 2.66 ft. When half-full, the reflux accumulator has a residence time of 5 minutes. This unit has a bare module cost of \$29,400.

Decanter

D-101 – Specification sheet on page 38

This horizontal vessel is a decanter for the distillate product coming from the distillation column. Because it lies within the two-phase liquid envelope (see Appendix G), the totally condensed distillate is split into an organic stream with NPB and IPA and an aqueous stream with residual organics. Operating at 14.7 psia and 125°F, the decanter is 3.43 ft long, has a diameter of 1.71 ft, and has a residence time of 30 minutes. This unit has a purchase cost of \$17,700 and a bare module cost of \$54,000.

Vertical Vessel

F-101 – Specification sheet on page 39

This vertical 2-phase flash vessel separates the heated bottoms stream from heat exchanger HX-107 into a liquid oleic acid waste stream and a vapor organic co-solvent stream. Operating at 14.7 psia and 264°F, the flash drum has a length of 3.43 feet and a diameter of 1.71 feet. Designed to be adiabatic, the vessel nevertheless loses 3,013 BTU/hr of heat to the atmosphere. This unit has a purchase cost of \$4,700 and a bare module cost of \$19,500.

Heat Exchangers

HX-101 – Specification sheet on page 40

This double pipe heat exchanger is the first of a series of three heat exchangers to preheat the feed stream of dirty co-solvent. The outer heat-exchange surface area of the inner pipe is 0.10 ft², the fluid pressure drop is 6 psi, and the estimated heat transfer coefficient is 150.0 BTU/hr-ft²-°F, recommended by Professor Fabiano. The cold feed mixture is heated from 70.4°F to 71.6°F, and the heating fluid, aqueous waste stream C-15 from decanter D-101, is cooled from 125.1°F to 100°F so that it can be safely handled. There is a total heat transfer of

624 BTU/hr from the heating fluid to the cold stream. This unit has a purchase cost of \$900 and a bare module cost of \$3,500.

HX-102 – Specification sheet on page 41

This double pipe heat exchanger is the second of 3 heat exchangers that preheats the dirty feed stream to be cleaned. The outer heat-exchange surface area of the inner pipe is 3.47 ft², the fluid pressure drop is 6 psi, and the estimated heat transfer coefficient is 150.0 BTU/hr-ft²-°F, recommended by Professor Fabiano. The dirty mixture is heated from 71.6°F to 105.6°F, and the heating fluid, recovered NPB/IPA co-solvent product, is cooled from 145.3°F to 100°F so that it can be safely handled. There is a total heat transfer of 17,510 BTU/hr from the heating fluid to the cold stream. This unit has a purchase cost of \$1,500 and a bare module cost of \$5,900.

HX-103 – Specification sheet on page 42

This double pipe heat exchanger is the third of a series of 3 heat exchangers that preheats the dirty feed stream to be cleaned. The outer heat-exchange surface area of the inner pipe is 0.64 ft², the fluid pressure drop is 6 psi, and the estimated heat transfer coefficient is 150.0 BTU/hr-ft²-°F, recommended by Professor Fabiano. The dirty mixture is heated from 105.6°F to 125°F, and the heating fluid, oleic acid waste from flash drum F-101, is cooled from 264.3°F to 186.8°F. An additional heat exchanger is required to cool oleic acid to 100°F, at which point it can be safely handled. There is a total heat transfer of 10,266 BTU/hr from the heating fluid to the cold stream. This unit has a purchase cost of \$1,200 and a bare module cost of \$4,500.

HX-104 – Specification sheet on page 43

This double pipe heat exchanger finishes cooling the oleic acid waste from flash drum F-101 so that it can be stored safely. The outer heat-exchange surface area of the inner pipe is 2.32 ft², the fluid pressure drop is 6 psi, and the estimated heat transfer coefficient is 150.0 BTU/hr-ft²-°F, recommended by Professor Fabiano. The hot stream is cooled from 186.8°F to 100°F against 343 lb/hr of cooling water at a temperature of 90°F. A total of 10,390 BTU/hr is

removed from the hot oleic acid stream. This unit has a purchase cost of \$1,500 and a bare module cost of \$5,500.

HX-105 – Specification sheet on page 44

This double pipe heat exchanger serves as the total condenser to the distillation column. The outer heat-exchange surface area of the inner pipe is 111.9 ft² and it operates at 140°F, with a heat transfer coefficient of 150 BTU/°F-ft²-hr. This unit condenses distillate liquid by removing 250,900 BTU/hr against 8,549 lb/hr of cooling water at 90°F. This unit has a purchase cost of \$2,700 and a bare module cost of \$10,300.

HX-106 – Specification sheet on page 45

This kettle reboiler serves as the reboiler to the distillation column. The outer heat-exchange surface area of the inner pipe is 16.4 ft² and it operates at 174.7°F with a heat transfer coefficient of 150 BTU/°F-ft²-hr, vaporizing bottoms liquid by adding 277,000 BTU/hr. This unit utilizes 304 lb/hr of low pressure steam at 298 F and 50 psig. This unit has a purchase cost of \$2,000 and a bare module cost of \$8,200.

HX-107 – Specification sheet on page 46

This rising film evaporator heats and partially vaporizes the bottoms product and leads directly to vertical vessel F-101. The desired co-solvent product present in the bottoms, NPB and IPA, vaporize in the evaporator, while oleic acid does not. As bottoms liquid is evaporated, the vapor pressure will press the remaining liquid as a thin film along the heat exchanger walls, which moves upwards with the vapor. The total heat-exchange surface area is 13.23 ft², and the unit operates at 274°F. Bottoms liquid is heated from 175°F to 274°F. The heat exchanger has a duty of 103,744 BTU/hr, an estimated heating coefficient of 150 BTU/°F -ft²-hr, and utilizes 112 lb/hr of low pressure steam at 298°F and 50 psig. This unit has a purchase cost of \$1,900 and a bare module cost of \$7,300

HX -108 – Specification sheet on page 47

This double pipe heat exchanger is a total condenser that converts the vapor product from the flash drum back into liquid. The outer heat-exchange surface area of the inner pipe is 3.84 ft²

with a heat transfer coefficient of 150 BTU/°F-ft²-hr, and it condenses the vapor product by removing 91,308 BTU/hr against 3016 lb/hr of cooling water at 90°F. This unit has a purchase cost of \$1,600 and a bare module cost of \$6,000.

Pumps

P-101 – Specification sheet on page 48

This gear pump delivers dirty feed to a series of 3 heat exchangers and the distillation column. It moves 2.34 gpm of feed, generates 48.1 ft of pump head, and increases the pressure of the feed by 19.5 psi. The pump's efficiency is 0.3 and it consumes 0.09 units of horsepower, requiring 212 BTU/hr of electricity. This unit has a purchase cost of \$700 and a bare module cost of \$2,100.

P-102 – Specification sheet on page 49

This gear pump acts as the reflux pump for the distillation column. Entering stream C-9 is pumped and then split into the reflux and distillate streams. It moves 4.5 gpm of condensed distillate, maintains the pump head, and raises the pressure of the distillate by 24.36 psi. The pump's efficiency is 0.3 and it consumes 0.09 units of horsepower, requiring 362 BTU/hr of electricity. This unit has a purchase cost of \$700 and a bare module cost of \$2,300.

P-103 – Specification sheet on page 50

This gear pump acts as the reboiler pump for the distillation column. Entering stream C-18 is pumped and then split into the boilup and bottoms streams. It moves 1.45 gpm of hot bottoms, generates 13.3 ft of pump head, and increases the pressure of the bottoms stream by 4.5 psi. The pump's efficiency is 0.3 and it consumes 0.013 units of horsepower, requiring 95 BTU/hr of electricity. This unit has a purchase cost of \$600 and a bare module cost of \$2,100.

P-104 – Specification sheet on page 51

This gear pump delivers the aqueous waste solution from the decanter to its storage tank. It moves 0.063 gpm of waste solution, generates 15.8 ft of pump head, and raises the pressure of the aqueous stream by 6 psi. The pump's efficiency is 0.3 and it consumes 0.00075 units of

horsepower, requiring 1.9 BTU/hr of electricity. This unit has a purchase cost of \$400 and a bare module cost of \$1,900.

P-105 – Specification sheet on page 52

This gear pump delivers the organic product from the decanter to the storage tank for the final product. It moves 0.96 gpm of co-solvent product, generates 13 ft of pump head, and raises the pressure of the aqueous stream by 6 psi. The pump's efficiency is 0.3 and it consumes 0.00083 units of horsepower, requiring 23.9 BTU/hr of electricity. This unit has a purchase cost of \$600 and a bare module cost of \$1,900.

P-106 – Specification sheet on page 53

This gear pump delivers the outlet oleic acid from the flash drum to its storage tank for sales. It moves 0.64 gpm of oleic acid, generates 34.7 ft of pump head, and raises the pressure of the aqueous stream by 12 psi. The pump's efficiency is 0.3 and it consumes 0.015 units of horsepower, requiring 37.5 BTU/hr of electricity. This unit has a purchase cost of \$600 and a bare module cost of \$1,800.

P-107 – Specification sheet on page 54

This gear pump moves the collected condensed product to the storage tank for the final product. It moves 0.73 gpm of waste solution, generates 17.4 ft of pump head, and raises the pressure of the aqueous stream by 6 psi. The pump's efficiency is 0.3 and it consumes 0.0094 units of horsepower, requiring 23.9 BTU/hr of electricity. This unit has a purchase cost of \$600 and a bare module cost of \$1,900.

Storage Tanks**R-101** - Specification sheet on page 58

This closed holding tank receives batches of the dirty solvent mixture every 2 days so that a continuous feed can be regulated. The tank is held at ambient temperature and 14.7 psia. This vertical vessel has a diameter of 10.6 ft, a height of 15 ft, and can hold a capacity of 15,000 gallons. This unit has a bare module cost of \$25,000.

R-102 - Specification sheet on page 60

This open holding tank stores the outlet water and IPA waste. The contents of the tank must be picked up and disposed of every 4 weeks. This tank is held at ambient temperature and 14.7 psia, and has a diameter of 7.15 ft, a height of 10 ft, and can hold a capacity of 3,000 gallons. This unit has a bare module cost of \$5,700.

R-103 – Specification sheet on page 59

This closed holding tank stores the final NPB and IPA co-solvent product. An additional 962 lb of IPA and 198 lb of NPB are added to the tank every two days to compensate for the lost co-solvents in the waste streams. This tank is held at ambient temperature and 14.7 psia, and has a diameter of 10.6 ft, a height of 15 ft, and a capacity of 10,000 gallons. Every two days, the recovered 4,600 gallon (plus ~4.5 gallons water) co-solvent product is gathered and delivered to the client. This unit has a bare module cost of \$20,000.

R-104 – Specification sheet on page 59

This closed holding tank stores the outlet oleic acid stream for sales. The oleic acid is not needed by the client and thus the contents of the tank are emptied and sold every 4 weeks to avoid overflow. This tank is held at ambient temperature and 14.7 psia, and has a diameter of 10.6 ft, a height of 15 ft, and holds a capacity of 10,000 gallons. This unit has a bare module cost of \$20,000.

R-105 – Specification sheet on page 61

This closed holding tank collects the condensate from HX-108. The liquid condensate is gathered in this tank so that its exit flow rate can be controlled and pumped in a continuous stream. This tank is held at ambient temperature and 14.7 psia, and has a diameter of 1.24 ft, a height of 2.5 ft, and can hold up to 23 gallons of liquid. This unit has a bare module cost of \$1,000.

Energy Balance

To ensure that energy is conserved, the following equation must be obeyed.

$$(Enthalpy\ of\ Streams)_{in} + Energy\ Added = (Enthalpy\ of\ Streams)_{out} + Energy\ Removed$$

Only the feed stream C-1 enters the continuous process. Energy is added to the system from the distillation reboiler HX-106 and the heater HX-107, which heats stream C-21, the bottoms product of the distillation column. The total enthalpy entering the system is summarized in Table 4.6 below.

Stream/Unit	Enthalpy Change (BTU/hr)
Stream C-2	-1,365,500
Unit HX-106	277,000
Unit HX-107	102,100
Total Heat In	-986,400 BTU/hr

Table 4.6 Enthalpy added to the system

Three streams exit the system: C-17, C-28, and C-32. Energy is removed from the system using cooling water in units HX-104, HX-105, and HX-108. The total enthalpy leaving the system is summarized in Table 4.7.

Stream/Unit	Enthalpy Change (BTU/hr)
Stream C-17	-127,700
Stream C-28	-905,900
Stream C-32	-316,600
HX-104	10,400
HX-105	258,800
HX-108	91,300
Total Heat Out	-989,700 BTU/hr

Table 4.7 Enthalpy removed from the system

There is a slight difference between enthalpy in and enthalpy out, but the error in the calculations is as low as 0.4%. We believe that this difference is reasonable because of rounding

error. Additionally, the enthalpy that is added and lost from pumps and pressure drops is nearly negligible compared to the much larger heat duties and enthalpies of the other units and streams.

Utility Summary

The annual cost of utilities for the continuous process is only a small contribution to the overall process costs. This is partly due to the fact that the process runs at relatively low temperatures. Aside from the bottoms stream from COL-101 that is heated to 264°F, the remainder of the process is kept at temperatures below 180°F, which is significantly lower than the boiling point of water. The low flow rates present in this process also contribute to the low utility costs. Smaller pumps are able to be used for these low flows, reducing the cost of electricity. Heating and cooling these small volumes is also achieved with lower steam and cooling water flow rates, reducing their annual cost requirement.

The continuous process requires three utilities: low pressure steam, cooling water, and electricity. The prices for these utilities were taken from the cost sheet outline in Table 23.1 of *Product and Process Design Principles* (Seider, 604). Since the table provides utility prices from 1995, the current utility prices were estimated using the Chemical Engineering Plant Cost Indexes (CEPCI) for 1995 and 2011 as a scaling factor. The CEPCIs used for 1995 and 2011 are 381 and 564, respectively. Table 4.8 below is a summary of the prices for each utility.

Utility	1995 Prices	2011 Prices
Low Pressure Steam (per 1000 lb)	\$3.00	\$4.44
Cooling Water (per 1000 lb)	\$0.0094	\$0.014
Electricity (per 1000 BTU)	\$0.018	\$0.026

Table 4.8 Market utility prices for low pressure steam (50.3 psig, 298°F), cooling water (90°F), and electricity in 1995 and 2011. The CEPCI indexes for 1995 and 2011 are 381 and 564, respectively.

The greatest contribution to utility costs, \$14,600/yr, comes from low pressure steam used to heat the column reboiler and HX-107, which is the exchanger that heats the inlet stream to flash vessel F-101. Steam at a low pressure of 50.3 psig and 298°F is sufficient for the reboiler and HX-107 because the outlet (cold) streams only need to be heated to 175°F and 264°F, respectively, and are at very low flow rates. The second greatest contributor is cooling water at 90°F, which totals to approximately \$1,300/yr. The lowest contributor to utility costs is the electricity needed for pumps, totaling only \$500/yr. The low requirement is due to the fact that most of the pumps handle very small volumes, requiring little power. Table 4.9 summarizes the utility requirements for each process unit in the continuous scheme.

UTILITY COSTS				
Utility	Unit	Quantity	Price	Annual Cost (\$/yr)
Low Pressure Steam		(lb/hr)	(\$/1000lb)	
	HX-106	304	\$4.40	\$10,700
	HX-107	112	\$4.40	\$3,900
Cooling Water		(lb/hr)	(\$/1000lb)	
	HX-104	343	\$0.014	\$38
	HX-105	8550	\$0.014	\$940
	HX-108	3020	\$0.014	\$330
Electricity		(BTU/hr)	(\$/1000BTU)	
	P-101	211.5	\$0.026	\$44
	P-102	362.2	\$0.026	\$75
	P-103	44.4	\$0.026	\$10
	P-104	1.9	\$0.026	\$0
	P-105	28.3	\$0.026	\$6
	P-106	37.5	\$0.026	\$8
	P-107	23.9	\$0.026	\$5
	P-108	1.7	\$0.026	\$0
	P-109	495.5	\$0.026	\$102
	P-110	1467.1	\$0.026	\$303
			Total	\$16,500

Table 4.9 Per-unit utility requirements for the continuous facility

The continuous process requires a total of 416 lb/hr of low pressure steam, 11,900 lb/hr of cooling water, and 2700 BTU/hr of electricity. The annual cost of utilities total \$16,500. Table 4.10 below summarizes the consumption of each utility per pound of reclaimed co-solvent mixture, which is produced at approximately 823 lb/hr.

Utility	Total Amount	Per lb Reclaimed Co-solvent
Low Pressure Steam (lb/hr)	416	0.51
Cooling Water (lb/hr)	11913	14.6
Electricity (BTU/hr)	2674	3.3

Table 4.10 Hourly and per-pound-of-product utility consumption for the continuous process

Equipment Specification Sheets

DISTILLATION COLUMN

Identification:	<i>Distillation Column</i>	<i>April, 2012</i>
Item No.	COL-101	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$231,100

Function: Separate H₂O from oleic acid in a four-component mixture of H₂O, oleic acid, n-propyl bromide, and isopropyl alcohol.

Operation: Continuous

Materials Handled:	<i>Feed</i>	<i>Liquid Dist.</i>	<i>Bottoms</i>
Quantity (lb/h):	1106	533	569
Molar Composition:			
<i>IPA</i>	0.374	0.640	0.108
<i>NPB</i>	0.476	0.210	0.742
<i>H₂O</i>	0.075	0.150	420 PPB
<i>Oleic Acid</i>	0.075	TRACE	0.150
Temperature (°F):	60	140.5	175.7

Design Data:

Number of Trays:	15	Molar Reflux Ratio:	2
Tray Type:	Seive	Tray Spacing (ft):	1
Pressure (psig):	5		
Material:	Stainless Steel		
Height (ft):	28		
Inside Diameter (ft):	1.07		
Average Tray Efficiency:	0.41		
Feed Stage:	6		
Condenser Temperature (°F):	140		

REFLUX ACCUMULATOR

Item No.	ACC-101
Type	Horizontal
Reflux Ratio:	2
Volume (gal/hr)	179.5
Diameter (ft):	1.33
Length (ft):	2.66
Material:	Stainless Steel
Residence Time (min):	5

Controls:

Tolerances:

Comments and Drawings:

DECANTER

Identification: *Horizontal Flash 3 Vessel* *April, 2012*
 Item No. D-101 JW/ CS/ HD/ AM
 No. required 1

Cost of Bare Module: \$54,000
Function: Separates column distillate stream into two liquid phases.
Operation: Continuous

Materials Handled:	<i>Inlet</i>	<i>Liquid 1, Outlet</i>	<i>Liquid 2, Outlet</i>
Quantity (lb/h):	533	505	27.9
Molar Composition:			
<i>IPA</i>	0.211	0.213	0.202
<i>NPB</i>	0.639	0.778	0.008
<i>H₂O</i>	0.150	0.009	0.791
<i>Oleic Acid</i>	TRACE	0.000	0.000
Temperature (°F):	125.1	125	125

Design Data:

Temperature (°F):	125
Pressure (psia):	14.7
Length (ft):	3.43
Diameter (ft):	1.71
Material:	Stainless Steel
Residence time (min)	30

Utilities:
Controls: *level, temperature*
Tolerances:
Comments and Drawings:

VERTICAL VESSEL

Identification: *Vertical, Flash 2 Vessel* *April, 2012*
 Item No. F-101 JW/ CS/ HD/ AM
 No. required 1

Cost of Bare Module: \$19,500
Function: To separate oleic acid from the bottoms product of COL-101 through flash vaporization.
Operation: Continuous

Materials Handled:	<i>Feed to Flash</i>	<i>Outlet Liquid</i>	<i>Outlet Vapor</i>
Quantity (lb/h):	568	251	317
Molar Composition:			
<i>IPA</i>	0.742	0.128	0.874
<i>NPB</i>	0.108	0.026	0.125
<i>H₂O</i>	136 PPM	13 PPM	162 PPM
<i>Oleic Acid</i>	0.150	0.846	52 PPM
Temperature (°F):	274	264	264

Design Data:

Temperature (°F): 264
 Pressure (psia): 14.7
 Length (ft): 2.57
 Diameter (ft): 0.64
 Heat Duty (BTU/hr) -3013
 Residence Time (min): 5
 Material: Carbon Steel

Utilities:
 Controls: *temperature*
 Tolerances:
 Comments and Drawings:

HEAT EXCHANGER

Identification:	<i>Double Pipe Heat Exchanger</i>	<i>April, 2012</i>
Item No.	HX-101	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$3,400

Function: To heat inlet feed stream from 70.4°F to 71.6°F using the hot, 2nd liquid stream from the decanter.

Operation: Continuous

Materials Handled:	<i>Cold Stream</i>	<i>Hot Stream</i>
Quantity (lb/h):	1102	28
Molar Composition:		
<i>IPA</i>	0.476	0.2
<i>NPB</i>	0.374	0.007
<i>H₂O</i>	0.075	0.792
<i>Oleic Acid</i>	0.075	0
Inlet Temperature (°F):	70.4	125.1
Outlet Temperature (°F):	71.6	100

Design Data:

Pressure (psig):	6
Heat Transfer Coefficient (BTU/°F-ft ² - hr):	150
Outer Surface Area of Inner Pipe (ft ²):	0.10
Heat Duty (BTU/hr):	624
Pipe Material:	Stainless Steel/ Stainless Steel

Utilities:

Comments & Drawings:

HEAT EXCHANGER

Identification:	<i>Double Pipe Heat Exchanger</i>	<i>April, 2012</i>
Item No.	HX-102	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$5,900

Function: To heat inlet feed stream from 71.6°F to 105.6°F using the hot, co-solvent product stream from the decanter.

Operation: Continuous

Materials Handled:	<i>Cold Stream</i>	<i>Hot Stream</i>
Quantity (lb/h):	1102	823
Molar Composition:		
<i>IPA</i>	0.476	0.544
<i>NPB</i>	0.374	0.452
<i>H₂O</i>	0.075	0.004
<i>Oleic Acid</i>	0.075	26 PPM
Inlet Temperature (°F):	71.6	145.3
Outlet Temperature (°F):	105.6	100

Design Data:

Pressure (psig):	6
Heat Transfer Coefficient (BTU/°F-ft ² - hr):	150
Outer Surface Area of Inner Pipe (ft ²):	3.47
Heat Duty (BTU/hr):	17,510
Pipe Material:	Stainless Steel/ Stainless Steel

Utilities:

Comments & Drawings:

HEAT EXCHANGER

Identification:	<i>Double Pipe Heat Exchanger</i>	<i>April, 2012</i>
Item No.	HX-103	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$4,500

Function: To heat inlet feed stream to 125°F, the column's operating temperature, using the outlet liquid stream from the flash vessel (F-101).

Operation: Continuous

Materials Handled:	<i>Cold Stream</i>	<i>Hot Stream</i>
Quantity (lb/h):	1102	251
Molar Composition:		
<i>IPA</i>	0.476	0.128
<i>NPB</i>	0.374	0.026
<i>H₂O</i>	0.075	13 PPM
<i>Oleic Acid</i>	0.075	0.846
Inlet Temperature (°F):	105.6	264.3
Outlet Temperature (°F):	125	186.8

Design Data:

Pressure (psig):	6
Heat Transfer Coefficient (BTU/°F-ft ² - hr):	150
Outer Surface Area of Inner Pipe (ft ²):	0.64
Heat Duty (BTU/hr):	10,266
Pipe Material:	Stainless Steel/ Stainless Steel

Utilities:

Comments & Drawings:

HEAT EXCHANGER

Identification:	<i>Double Pipe Heat Exchanger</i>	<i>April, 2012</i>
Item No.	HX-104	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module:	\$5,500
Function:	To cool outlet oleic acid stream from 186.8°F to 100°F so it is cool enough to be safely collected.
Operation:	Continuous

Materials Handled:	<i>Hot Stream</i>
Quantity (lb/h):	251
Molar Composition:	
<i>IPA</i>	0.128
<i>NPB</i>	0.026
<i>H₂O</i>	13 PPM
<i>Oleic Acid</i>	0.846
Inlet Temperature (°F):	186.8
Outlet Temperature (°F):	100

Design Data:	Pressure (psig):	6
	Heat Transfer Coefficient (BTU/°F-ft ² - hr):	150
	Outer Surface Area of Inner Pipe (ft ²):	2.32
	Heat Duty (BTU/hr):	-10,390
	Pipe Material:	Stainless Steel/ Stainless Steel
	Cooling Material:	Cooling Water (90°F - 120°F)

Utilities:	Cooling water (90°F - 120°F) at 343 lb/hr
Comments & Drawings:	

CONDENSER

Identification:	<i>Double Pipe Heat Exchanger</i>	<i>April, 2012</i>
Item No.	HX-105	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module:	\$10,300
Function:	Total condenser for column vapor distillate.
Operation:	Continuous

Materials Handled:	<i>Hot Inlet, Vapor</i>	<i>Hot Outlet, Liquid</i>
Quantity (lb/h):	1599	1599
Molar Composition:		
<i>IPA</i>	0.211	0.211
<i>NPB</i>	0.639	0.639
<i>H₂O</i>	0.150	0.150
<i>Oleic Acid</i>	TRACE	TRACE
Temperature (°F):	142	125

Design Data:

Pressure (psig):	6
Heat Duty (BTU/hr):	250,900
Heat Transfer Coefficient (BTU/°F-ft ² - hr):	150
Heat Transfer Area (ft ²):	111.9
Cooling Material:	Cooling Water (90°F - 120°F)
Pipe Material:	Stainless Steel/ Stainless Steel

Utilities:	Cooling water, 8549 lb/hr at 90°F - 120°F
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Comments & Drawings:	
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REBOILER

Identification:	<i>Kettle Reboiler</i>	<i>April, 2012</i>
Item No.	HX-106	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$7,500

Function: Serves as column reboiler. Partially reboils the bottoms product back into column, which will optimize separation.

Operation: Continuous

Materials Handled:	<i>Cold Inlet</i>	<i>Cold Outlet, Vapor</i>	<i>Cold Outlet, Liquid</i>
Quantity (lb/h):	1841	1272	569
Molar Composition:			
IPA	0.726	0.721	0.741
NPB	0.235	0.279	0.109
H ₂ O	0.0002	0.0003	145 PPM
Oleic Acid	0.0386	.19 ppm	0.15
Temperature (°F):	164.1	179.4	179.4

Design Data:

Temperature (°F):	174.7
Pressure (psig):	6
Heat Duty (BTU/hr):	277,000
Heat Transfer Coefficient (BTU/°F-ft ² - hr):	150
Heat Transfer Area (ft ²):	16.4
Heating Material:	50 psig steam at 298°F
Pipe Material:	Stainless Steel/ Stainless Steel

Utilities: Steam (50 psig, 298°F) at 304 lb/hr

Comments & Drawings:

HEAT EXCHANGER

Identification:	<i>Rising Film Evaporator</i>	<i>April, 2012</i>
Item No.	HX-107	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$7,300
Function: To heat bottoms liquid to 274°F, the operating temperature of flash vessel F-101.

Operation: Continuous

Materials Handled:	<i>Cold Stream</i>
Quantity (lb/h):	568
Molar Composition:	
<i>IPA</i>	0.742
<i>NPB</i>	0.108
<i>H₂O</i>	136 PPM
<i>Oleic Acid</i>	0.15
Inlet Temperature (°F):	175
Outlet Temperature (°F):	274

Design Data:

Pressure (psig):	6
Heat Transfer Coefficient (BTU/°F-ft ² - hr):	150
Outer Surface Area of Inner Pipe (ft ²):	13.23
Heat Duty (BTU/hr):	103,744
Pipe Material:	Stainless Steel/ Stainless Steel
Heating Material:	50 psig steam at 298°F

Utilities: Steam (50 psig, 298°F) at 112 lb/hr
Comments & Drawings:

HEAT EXCHANGER

Identification:	<i>Double Pipe Heat Exchanger</i>	<i>April, 2012</i>
Item No.	HX-108	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module:	\$6,000
Function:	To condense the outlet vapor stream from flash vessel F-101.
Operation:	Continuous

Materials Handled:	<i>Hot Stream</i>
Quantity (lb/h):	317
Molar Composition:	
<i>IPA</i>	0.874
<i>NPB</i>	0.125
<i>H₂O</i>	162 PPM
<i>Oleic Acid</i>	52 PPM
Inlet Temperature (°F):	264.6
Outlet Temperature (°F):	165.1

Design Data:	Pressure (psig):	6
	Heat Transfer Coefficient (BTU/°F-ft ² -hr):	150
	Outer Surface Area of Inner Pipe (ft ²):	3.84
	Heat Duty (BTU/hr):	-91,308
	Pipe Material:	Stainless Steel/ Stainless Steel
	Cooling Material:	Cooling Water (90°F - 120°F)

Utilities:	Cooling water (90°F - 120°F) at 3016 lb/hr
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Comments & Drawings:

PUMP

Identification:	<i>Gear Pump</i>	<i>April, 2012</i>
Item No.	P-101	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module:	\$2,100
Function:	To pump the feed from the feed storage tank to column.
Operation:	Continuous

Materials Handled:

Inlet Stream ID:	
Quantity (lb/h):	1102
Molar Composition:	
IPA	0.476
NPB	0.374
H ₂ O	0.075
Oleic Acid	0.075
Temperature (°F):	70

Design Data:

Volumetric Flow Rate (gpm):	2.34
Head Developed (ft):	48.1
Single Stage:	Yes
Material:	Stainless Steel
Efficiency	0.3
Work Required (HP):	0.09
Pressure Change (psi):	19.5
Electricity (kW):	0.067

Utilities:	Electricity; 212 BTU/hr
Cost of Utilities:	\$29/ yr
Comments & Drawings:	

REFLUX PUMP

Identification:	<i>Gear Pump</i>	<i>April, 2012</i>
Item No.	P-102	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$2,250
Function: To pump the reflux back to distillation column and distillate stream to decanter.

Operation: Continuous

Materials Handled:

Inlet Stream ID:	C-9
Quantity (lb/h):	1599
Molar Composition:	
<i>IPA</i>	0.211
<i>NPB</i>	0.639
<i>H₂O</i>	0.150
<i>Oleic Acid</i>	TRACE
Temperature (°F):	125.1

Design Data:

Volumetric Flow Rate (gpm):	4.5
Head Developed (ft):	0
Single Stage:	Yes
Material:	Stainless Steel
Efficiency	0.3
Work Required (HP):	0.14
Pressure Change:	24.36

Utilities: Electricity; 362 BTU/hr

Cost of Utilities: \$50/ yr

Comments & Drawings:

REBOILER PUMP

Identification:		<i>Gear Pump</i>	<i>April, 2012</i>
	Item No.	P-103	JW/ CS/ HD/ AM
	No. required	1	

Cost of Bare Module: \$2,100

Function: To pump the bottom liquids from reboiler to the rising film evaporator and vertical vessel.

Operation: Continuous

Materials Handled:

Inlet Stream ID:	C-18
Quantity (lb/h):	569
Molar Composition:	
<i>IPA</i>	0.741
<i>NPB</i>	0.109
<i>H₂O</i>	0.150
<i>Oleic Acid</i>	145 PPM
Temperature (°F):	179.4

Design Data:

Volumetric Flow Rate (gpm):	1.45
Head Developed (ft):	13.3
Single Stage:	Yes
Material:	Stainless Steel
Efficiency	0.3
Work Required (HP):	0.013
Pressure Change (psi):	4.5
Electricity (kW):	0.01

Utilities: Electricity; 95 BTU/hr

Cost of Utilities: \$13/ yr

Comments & Drawings:

PUMP

Identification:	<i>Gear Pump</i>	<i>April, 2012</i>
Item No.	P-104	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$1,900

Function: To pump 2nd liquid (water +IPA waste) from decanter to Heat Exchanger 1.

Operation: Continuous

Materials Handled:

Inlet Stream ID:	
Quantity (lb/h):	27.9
Molar Composition:	
<i>IPA</i>	0.202
<i>NPB</i>	0.008
<i>H₂O</i>	0.791
<i>Oleic Acid</i>	0.000
Temperature (°F):	125

Design Data:

Volumetric Flow Rate (gpm):	0.063
Head Developed (ft):	15.8
Single Stage:	Yes
Material:	Stainless Steel
Efficiency	0.3
Work Required (HP):	0.00075
Pressure Change (psi):	6
Electricity (kW):	0.00056

Utilities: Electricity; 1.9 BTU/hr

Cost of Utilities: \$0/ yr

Comments & Drawings:

PUMP

Identification:	<i>Gear Pump</i>	<i>April, 2012</i>
Item No.	P-105	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$1,900

Function: To pump the 1st liquid phase from the decanter to Heat Exchanger 2.

Operation: Continuous

Materials Handled:

Inlet Stream ID:

Quantity (lb/h): 505

Molar Composition:

IPA 0.213*NPB* 0.778*H₂O* 0.009*Oleic Acid* 0.000

Temperature (°F): 125

Design Data:

Volumetric Flow Rate (gpm):	0.96
Head Developed (ft):	13
Single Stage:	Yes
Material:	Stainless Steel
Efficiency	0.3
Work Required (HP):	0.011
Pressure Change (psi):	6
Electricity (kW):	0.0083

Utilities: Electricity; 23.9 BTU/hr

Cost of Utilities: \$4/ yr

Comments & Drawings:

PUMP

Identification:	<i>Gear Pump</i>	<i>April, 2012</i>
Item No.	P-106	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$1,800

Function: To pump oil from flash vessel to Heat Exchanger 3.

Operation: Continuous

Materials Handled:

Inlet Stream ID:

Quantity (lb/h): 251

Molar Composition:

IPA 0.128

NPB 0.026

H₂O 14 PPM

Oleic Acid 0.846

Temperature (°F): 264

Design Data:

Volumetric Flow Rate (gpm): 0.64

Head Developed (ft): 34.7

Single Stage: Yes

Material: Stainless Steel

Efficiency 0.3

Work Required (HP): 0.015

Pressure Change (psi): 12

Electricity (kW): 0.011

Utilities: Electricity; 37.5 BTU/hr

Cost of Utilities: \$5/ yr

Comments & Drawings:

PUMP

Identification:	<i>Gear Pump</i>	<i>April, 2012</i>
Item No.	P-107	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module:	\$1,900
Function:	To pump condensed vapor product stream from flash vessel to Heat Exchanger HX-102.
Operation:	Continuous

Materials Handled:

Inlet Stream ID:	
Quantity (lb/h):	317
Molar Composition:	
IPA	0.873
NPB	0.127
H ₂ O	173 PPM
Oleic Acid	52 PPM
Temperature (°F):	165

Design Data:

Volumetric Flow Rate (gpm):	0.73
Head Developed (ft):	17.4
Single Stage:	Yes
Material:	Stainless Steel
Efficiency	0.3
Work Required (HP):	0.0094
Pressure Change (psi):	6
Electricity (kW):	0.007

Utilities:	Electricity; 23.9 BTU/hr
Cost of Utilities:	\$3/ yr
Comments & Drawings:	

PUMP

Identification:	<i>Gear Pump</i>	<i>April, 2012</i>
Item No.	P-108	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$1,300**Function:** To pump cooling water through Heat Exchanger HX-104 to cool outlet oleic acid.**Operation:** Continuous**Materials Handled:**

Inlet Stream ID:

Quantity (lb/h): 343

Molar Composition:

 H_2O 1.000

Temperature (°F): 90-120

Design Data:

Volumetric Flow Rate (gpm): 0.06

Head Developed (ft):

Single Stage: Yes

Material: Stainless Steel

Efficiency

Work Required (HP):

Pressure Change:

Utilities: Electricity; 1.7 BTU/hr**Cost of Utilities:** \$0/ yr**Comments & Drawings:**

PUMP

Identification:	<i>Gear Pump</i>	<i>April, 2012</i>
Item No.	P-109	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$2,300

Function: To pump cooling water through Heat Exchanger HX-108 to condense outlet vapor from flash vessel F-101.

Operation: Continuous

Materials Handled:

Inlet Stream ID:	
Quantity (lb/h):	3016
Molar Composition:	
<i>H₂O</i>	1.00
Temperature (°F):	90-120

Design Data:

Volumetric Flow Rate (gpm):	6.02
Head Developed (ft):	
Single Stage:	Yes
Material:	Stainless Steel
Efficiency	
Work Required (HP):	
Pressure Change:	

Utilities: Electricity; 496 BTU/hr

Cost of Utilities: \$69/ yr

Comments & Drawings:

PUMP

Identification:	<i>Gear Pump</i>	<i>April, 2012</i>
Item No.	P-110	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module:	\$2,500
Function:	To pump cooling water through the column condenser HX-105.
Operation:	Continuous

Materials Handled:	
Inlet Stream ID:	
Quantity (lb/h):	8549
Molar Composition:	
<i>H₂O</i>	1.000
Temperature (°F):	90-120

Design Data:	
Volumetric Flow Rate (gpm):	16.6
Head Developed (ft):	
Single Stage:	Yes
Material:	Stainless Steel
Efficiency	
Work Required (HP):	
Pressure Change:	

Utilities:	Electricity; 1467 BTU/hr
Cost of Utilities:	\$204/ yr
Comments & Drawings:	

STORAGE TANK

Identification:

Item No. *Closed, 15,000 gal Storage Tank*
 R-101
 No. required 1

April, 2012
 JW/ CS/ HD/ AM

Cost of Bare Module:

\$25,000

Function:

Used to collect and store feed mixture.

Operation:**Materials Handled:**

Molar Composition:

<i>IPA</i>	<i>Feed Tank</i>	0.476
<i>NPB</i>		0.374
<i>H₂O</i>		0.075
<i>Oleic Acid</i>		0.075

Design Data:

Type:	Vertical vessel, Closed
Volume (gal):	15,000
Temperature (°F):	<100
Pressure (psi):	14.7
Height (ft):	21.9
Diameter (ft):	10.8
Material:	Carbon Steel

Utilities:

none

Controls:**Comments and Drawings:**

STORAGE TANK

Identification: *Closed, 10,000 gal Storage Tank* *April, 2012*
Item No. R-103, 104 JW/ CS/ HD/ AM
No. required 2

Cost of Bare Module: \$20,000
Function: R-103 for co-solvent product and R-104 for oleic acid byproduct.

Operation:

Materials Handled:	<i>Product Tank</i>	<i>Oleic Acid</i>
Molar Composition:		
<i>IPA</i>	0.544	0.128
<i>NPB</i>	0.452	0.026
<i>H₂O</i>	0.005	0.846
<i>Oleic Acid</i>	26 PPM	14 PPM

Design Data:

Type:	Vertical vessel, Closed
Volume (gal):	10,000
Temperature (°F):	<100
Pressure (psi):	14.7
Height (ft):	15
Diameter (ft):	10.6
Material:	Carbon Steel

Utilities: none

Controls:

Comments and Drawings: Oil storage tank must be emptied every 4 weeks.

STORAGE TANK

Identification:

Item No.	<i>Open, 3000 gallon storage tank</i>	<i>April, 2012</i>
No. required	R-102	JW/ CS/ HD/ AM
	1	

Cost of Bare Module:

\$5,700

Function:

To collect aqueous liquid phase from decanter as waste.

Operation:**Materials Handled:**

Molar Composition:

<i>IPA</i>	0.202
<i>NPB</i>	0.008
<i>H₂O</i>	0.791
<i>Oleic Acid</i>	0.000

Design Data:

Type:	Vertical vessel, Open
Temperature (°F):	<100
Pressure (psi):	14.7
Volume (gal):	3000
Length (ft):	10
Diameter (ft):	7.15
Material:	Carbon Steel

Utilities:

none

Controls:**Comments and Drawings:**

Must be emptied every 4 weeks.

COLLECTING TANK

Identification:	<i>Vertical pressure vessel</i>	<i>April, 2012</i>
Item No.	R-105	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module: \$1,000

Function: To collect liquid condensate from heat exchanger HX-108.

Operation:

Materials Handled: *Condensate*

Quantity (lb/hr): 317

Molar Composition:

IPA 0.874

NPB 0.125

H₂O 162 PPM

Oleic Acid 52 PPM

Temperature (°F): 165.100

Design Data:

Type: Vertical vessel, Closed

Volume (gal): 23

Temperature (°F): 165

Pressure (psi): 14.7

Height (ft): 2.5

Diameter (ft): 1.24

Material: Carbon Steel

Utilities: none

Controls: level

Tolerances:

Comments and Drawings:

**RECLAMATION OF IPA AND NPB
-BATCH PROCESS-**

Process Flow Diagram

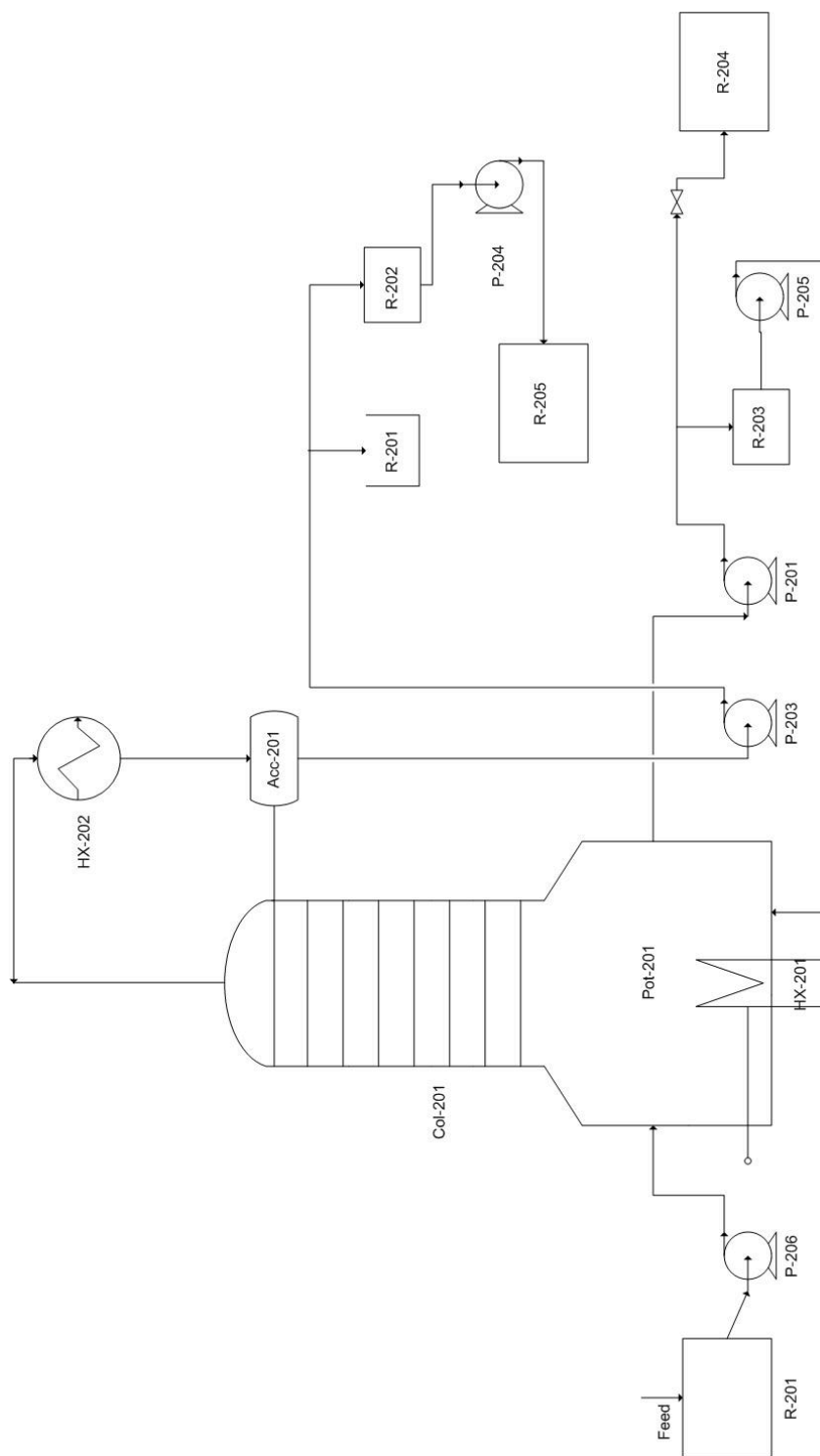


Figure 5.1: Process Flow Diagram for the batch process

Process Description

In addition to the continuous process design, a batch alternative was also prepared and analyzed. Batch production is usually carried out for particularly low-volume, expensive products (such as fine chemicals or pharmaceutical drugs). In this scenario, batch distillation is considered because of low-volume limitations—first, because each client demands only a small product volume at a time (4,600 gallons), and second, because our clients are limited to companies within a drivable distance. In addition, this batch distillation requires only a standard column, which could be easily adapted if future EPA constraints change the composition of our feed components.

To achieve the desired separation of IPA, NPB, water, and oleic acid, two main separations are carried out using a single batch distillation column. At the bottom of the system is a pot, where the feed is first charged. The pot is surrounded by a steam-heated carbon-steel jacket that supplies the required heat for boilup. An eleven-tray rectifying column stands on top of the pot. As the still is heated, the vapor stream that leaves the top of the column enters a total condenser, through which 90°F cooling water is constantly run. Main-cuts (desired products) and off-cuts (intermediate fractions) are taken at various points in the process. Analysis was done using ASPEN Batch Distillation V7.3 software.

Recipe (See Figs. 5.2 & 5.3)

Startup

The first batch recipe begins with the charging of the 6,240 gallon feed (47.6% NPB, 37.4% IPA, 7.5% oleic acid, and 7.5% water) to the pot. The stainless steel jacket is turned on and circulates high-pressure steam at 150 psia and 350°F to boil the contents. The contents begin to boil, and the vapor rises through the trays and reaches the condenser. When this happens, cooling water starts to run through the condenser and condenses the vapor stream. The reflux valve is then opened when the liquid begins to fill the condenser holdup tank, and the liquid is sent back to the top plate. When the liquid fills the holdup on the top tray, it falls to the plate below, and the process is repeated until the reboiler is reached. At this point, the process is in total reflux. It is estimated this startup process will take approximately one hour.

Operation

After the column reaches steady state at total reflux, the reflux ratio is set to one for an hour, and most of the water, some IPA, and a small amount of NPB are quickly boiled off the top and sent to waste receiver R-201. R-201's molar composition is 83.9% water, 15.6% IPA, and 0.4% NPB, and withdraws 89.8% of the system's water content, satisfying the rest of the system's water purity specifications. After this off-cut is removed, the reflux ratio is increased to two, and the main cut is taken over the next five hours. The contents of this stream are collected in product receiver R-202 (37.0% IPA, 61.8% NPB, 0% oleic acid, and 1.2% water). At this point in the process, 65% of the product has been collected, enough so that only IPA and oleic acid remain in the pot, which can be easily separated in a binary batch distillation.

Over the next hour, the column is shut down and prepped for the second batch. The valve to product receiver R-202 is closed, and the column is brought back to total reflux. The contents of the pot are quickly pumped to an intermediate receiver, R-203. Then, the heat and cooling water are shut off to the column, and the contents of the column are allowed to collapse into the pot. The pot and reflux drum holdups, which meet oleic acid and water specifications, are then pumped to product receiver R-202. At this point, the column is devoid of any solvents, and the only product to be separated is held in intermediate receiver R-203 (68.0% IPA, 31.9% oleic acid). This mixture can be handled in a simple binary distillation.

The contents of R-203 are then pumped back into the pot. The column is restarted and brought to steady state total reflux after an hour. After that point, the column is distilled at a constant reflux ratio of one to send pure IPA to product receiver R-202. At total reflux, the contents of the pot are then pumped to waste oleic acid receiver R-204. The column is shut down, and the column and reflux drum contents, both 100% IPA, are pumped to product receiver R-202.

Shutdown—At the end of the process, three receivers are occupied: water waste receiver R-201 (15.7% IPA, 0.4% oleic acid, and 83.9% water), product receiver R-202 (54.4% IPA, 44.8% NPB, 0% oleic acid, 0.8% water), and oleic acid waste receiver R-204 (11.0% IPA and 89.0% oleic acid).

To prep for the startup of the first batch again, the contents of product receiver R-202 are pumped to a large product holding tank, R-205, which is sized to hold the equivalent of two batches. (When a truck is ready to deliver the product to a customer, it will transfer the requisite

amount from the holding tank.) A new feed charge is subsequently transferred to the distillation column from a large feed holding tank R-206 to begin the process again.

Batch Distillation Schedule

"Reclamation of Co-Solvents"

Tollers of America

WBS	Tasks	Start	End	Duration
	1 Operation - 1st Batch	0:00:00	7:00:00	7:00:00
	1.1 Start up column at total reflux	0:00:00	1:00:00	1:00:00
	1.2 Distill at reflux ratio of 1 to withdraw H2O to REC-201	1:00:00	2:00:00	1:00:00
	1.3 Distill at reflux ratio of 2 to withdraw IPA/NPB to REC-202	2:00:00	7:00:00	5:00:00
	2 Draining and Shutdown	7:00:00	8:00:00	1:00:00
	2.1 Drain OLE/IPA pot contents at total reflux to REC-203	7:00:00	7:10:00	0:10:00
	2.2 Shut off heat, allow column contents to collapse into pot	7:10:00	7:30:00	0:20:00
	2.3 Drain new pot contents and pump to REC-202	7:30:00	7:50:00	0:20:00
	2.4 Pump REC-203 contents back into still	7:50:00	8:00:00	0:10:00
	3 Operation - 2nd Batch	8:00:00	10:00:00	2:00:00
	3.1 Start up column at total reflux	8:00:00	9:00:00	1:00:00
	3.2 Distill at reflux ratio of 1 to withdraw IPA to REC-202	9:00:00	10:00:00	1:00:00
	4 Draining and Shutdown	10:00:00	10:30:00	0:30:00
	4.1 Drain OLE pot contents at total reflux to REC-204	10:00:00	10:10:00	0:10:00
	4.2 Shut off heat, allow column contents to collapse into pot	10:10:00	10:20:00	0:10:00
	4.3 Pump pot contents to product REC-202	10:20:00	10:30:00	0:10:00
	5 Transfer	10:30:00	12:00:00	1:30:00
	5.1 Pump REC-202 contents to product holding tank REC-205	10:30:00	11:00:00	0:30:00
	5.2 Transfer contents from feed holding tank REC-206 to still	11:00:00	11:30:00	0:30:00
	(5.3) Transfer contents from REC-205 to truck (once every 2 days)	11:30:00	12:00:00	0:30:00

Figure 5.2: Batch Schedule

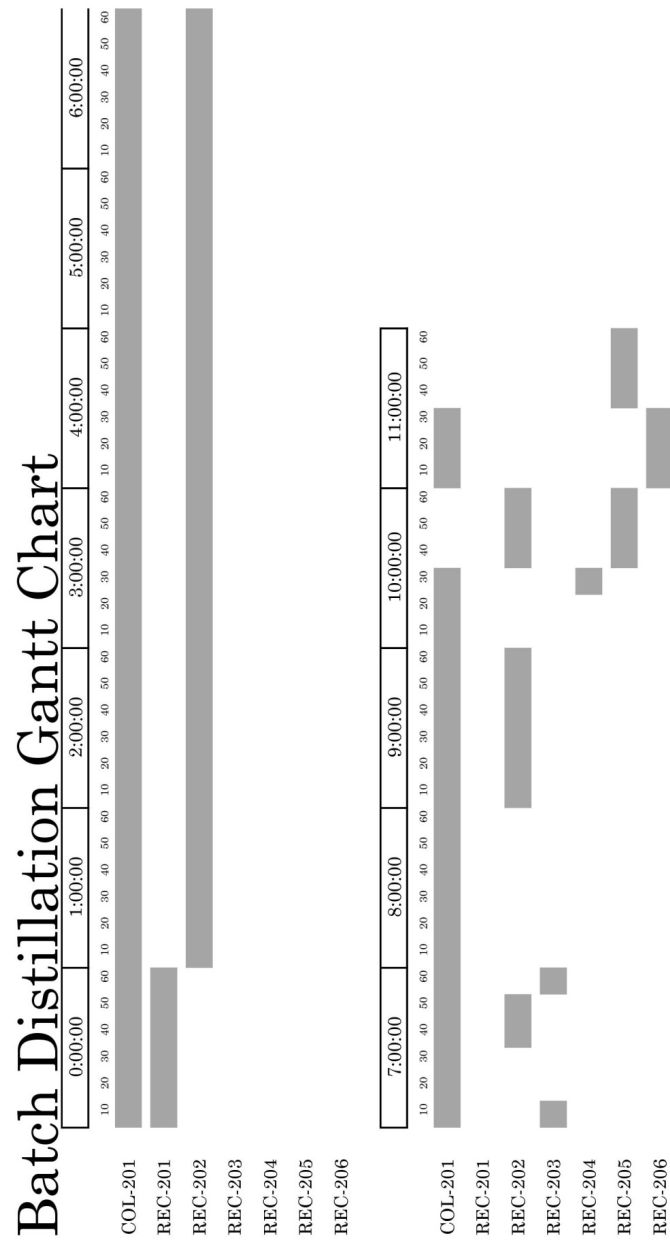


Figure 5.3: Batch Equipment Gantt Chart

Material Balance

At hour 0 (initial feed):

Pot			
	Mass (lb)	Mole (lbmol)	Composition (mole frac)
IPA	15,658	261	0.476
NPB	24,984	205	0.374
WATER	740	41	0.075
Oleic Acid	11,595	41	0.075

Table 5.4: Time 0h

After five hours of Batch 1 main-cut distillation:

		R-201	R-202	Pot	Column	Drum
Holdup (lbmol)		44.0	326.5	129.7	17.9	29.9
Composition (mole frac)	IPA	0.157	0.370	0.681	0.994	0.903
	NPB	0.004	0.618	0.000	0.005	0.094
	Oleic Acid	0.000	0.000	0.319	0.000	0.000
	WATER	0.839	0.012	0.000	0.001	0.003

Table 5.5: Time 7h

Collapsed column contents following Batch 1 completion:

		R-201	R-202	Pot
Holdup (lbmol)		44.0	374.4	129.6
Composition (mole frac)	IPA	0.157	0.443	0.681
	NPB	0.004	0.547	0.000
	Oleic Acid	0.000	0.000	0.319
	WATER	0.839	0.010	0.000

Table 5.6: Time 8h

After one hour of Batch 2 main-cut distillation:

		R-201	R-202	Pot	Column	Drum
Holdup (lbmol)		44.0	409.9	46.3	17.9	29.9
Composition (mole frac)	IPA	0.157	0.491	0.110	1.000	1.000
	NPB	0.004	0.500	0.000	0.000	0.000
	Oleic Acid	0.000	0.000	0.890	0.000	0.000
	WATER	0.839	0.009	0.000	0.000	0.000

Table 5.7: Time 10h

Collapsed column contents following Batch 2 completion:

		R-201 (waste water)	R-202 (product receiver)	R-204 (waste oleic)
End function		Dispose	Sell	Sell
Holdup (lbmol)		44.0	457.7	46.3
Composition (mole frac)	IPA	0.157	0.544	0.110
	NPB	0.004	0.448	0.000
	Oleic Acid	0.000	0.000	0.890
	WATER	0.839	0.008	0.000

Table 5.8: Hour 12

Optimization

The entire process takes place over 12 hours and is based on the premise of optimizing operation time for each cut. This is due to the fact that our steam utilities are the most expensive operating cost. To optimize operation time, we follow an experiment-based algorithm (Greaves et al. 2001) for finding the minimum batch time for the column and mixture (Figure 5.3). For a given separation task, we begin with a low reflux ratio and gradually increase it to the point where the main cuts and off-cuts meet specifications. This is based on the fact that as reflux ratio increases, batch time also increases as a non-linear function of the column and operating conditions.

To govern Greaves' algorithm, two controlling parameters for this experiment are determined. The first is provided in the problem statement—the concentration of water must not be greater than 2.5%. The second parameter was selected by the team to allow for the binary separation between oleic acid and IPA. In order for that Batch 2 binary distillation to be possible, all of the NPB has to first be removed in the Batch 1 main-cut separation. This effectively sets a lower bound for the product holdup in the main-cut distillation. Combined, the two parameters work to determine the optimal reflux ratio and batch times for this process.

The first hour-long off-cut separation of R-201 is the easiest, as water easily comes out the top and operates at a reflux ratio of one. The main cut, which needs a higher reflux ratio of two, is determined to have a minimum batch time of five hours. The last separation, which is a binary separation between oleic acid and IPA, is very simple and only takes one hour at a reflux ratio of one. See cut compositions for Batch 1 (Fig. 5.5) and Batch 2 (Fig. 5.6).

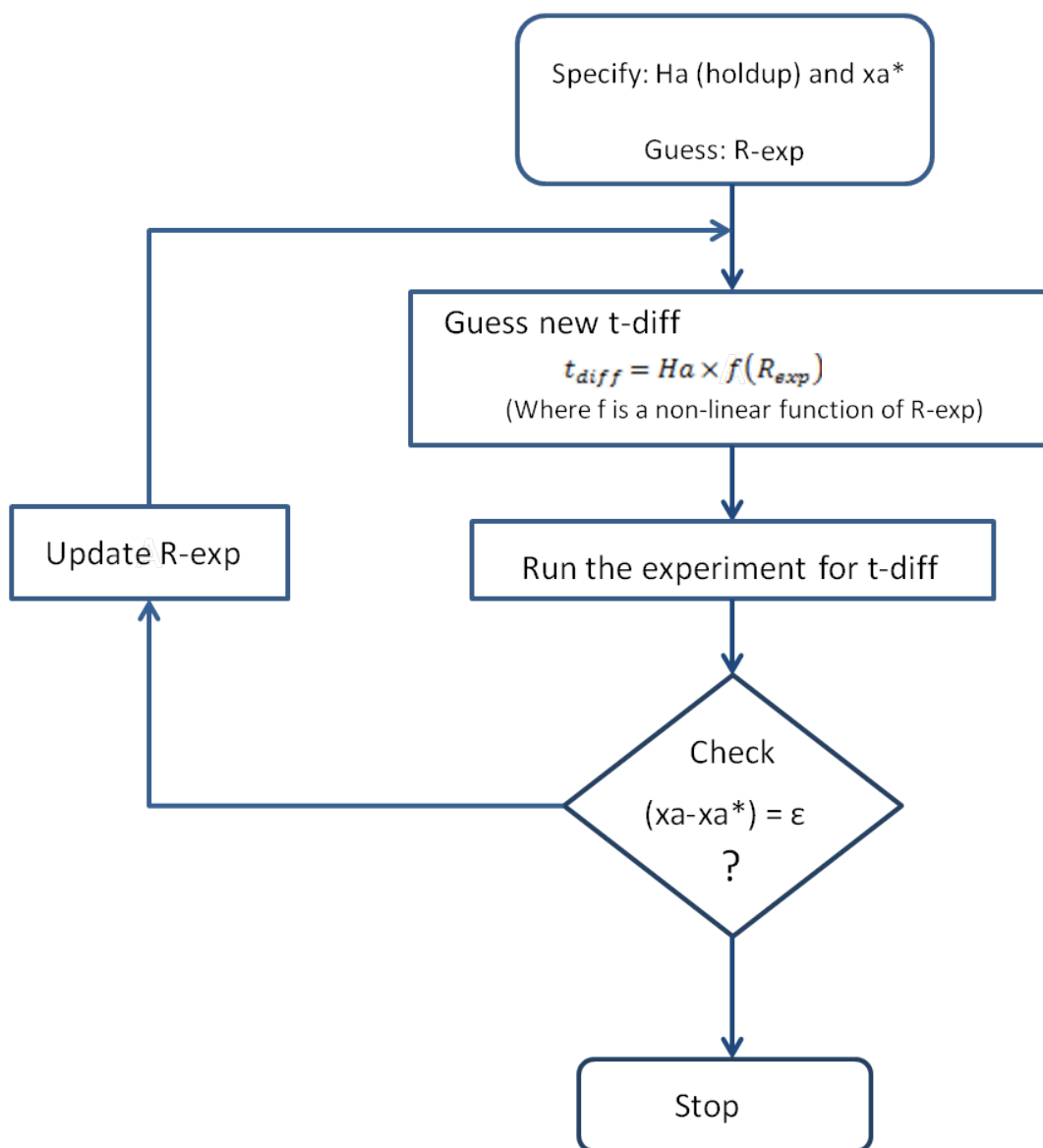


Fig. 5.9: Greaves et al. (2001) method for optimizing batch reflux ratios

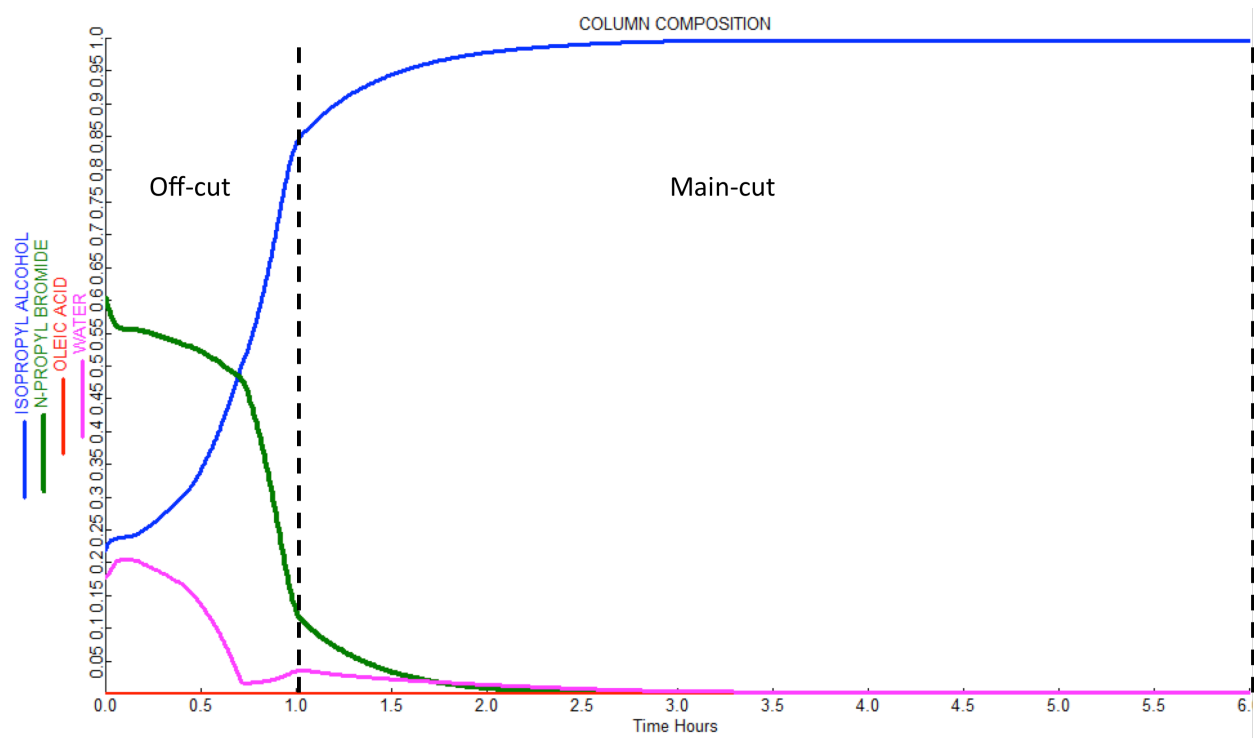


Fig. 5.10: Column Composition for Batch 1 distillation. Off-cut 1 removes 89.8% of the system’s water content at a reflux ratio of one. Main-cut 1 accumulates 65% of the eventual IPA/NPB product and operates until all of the NPB is removed from the pot.

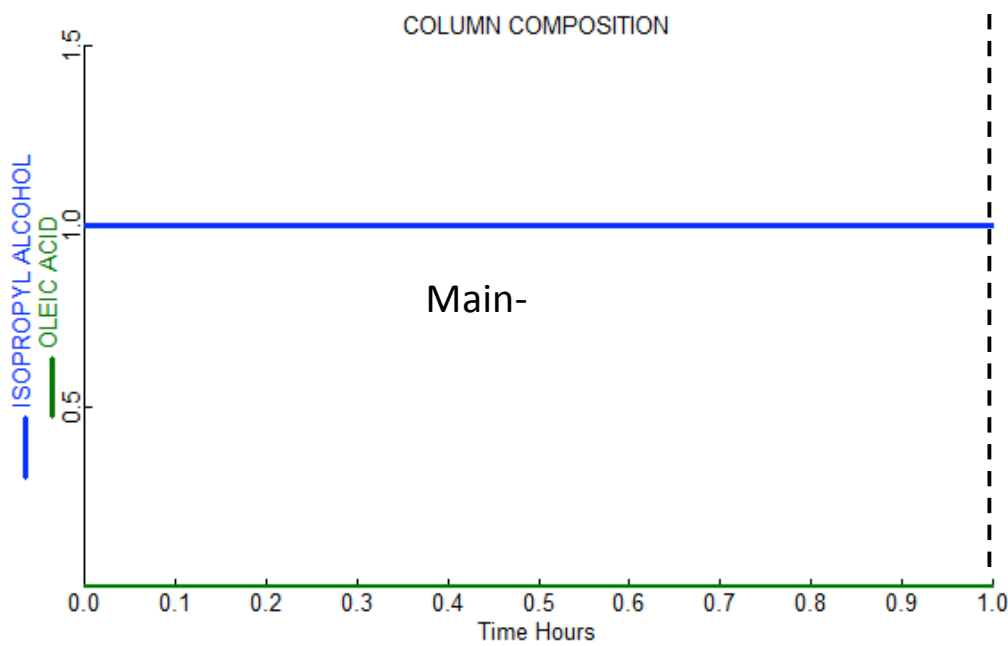


Fig. 5.11: Column Composition for Batch 2 distillation. Only IPA is boiled up through the column, making recovery extremely easy.

Equipment List

Unit	Description
ACC-201	Reflux Accumulator
COL-201	Tower
HX-201	Jacket Heater
HX-202	Condenser
P-201	Pump
P-202	Pump
P-203	Reflux Pump
P-204	Pump
P-205	Pump
P-206	Pump
POT-201	Batch Pot
R-201	Receiver
R-202	Receiver
R-203	Holding Tank
R-204	Storage Tank
R-205	Storage Tank
R-206	Storage Tank

Table 5.12 Equipment list for the batch process

Unit Descriptions

All equipment is constructed from stainless steel unless otherwise specified. Unit sizing and costing for the column, reboiler, and condenser are calculated from *Batch Distillation: Design and Principles* by I.M. Mujtaba. All other unit costs are calculated from Warren Seider's spreadsheet *Capital Cost Estimation* and relevant sizing and costing factors are calculated from *Process and Product Design Principles* by Seider, et al. Reported costs are in 2011-2012 fiscal cycle values, and these will be used in the economic analysis section.

Batch Distillation Column

COL-201 – Specification sheet on page 79

COL-201 is a stainless steel batch distillation column containing 11 sieve trays. It processes 4600 gallon batches of co-solvent mixture every 12 hours (47.6% IPA, 37.4% NPB, 7.5% oleic acid, and 7.5% water).

The purpose of the column is to send the IPA and water out the top as distillate, leaving the NPB and oleic acid behind in the column and pot. The column operates at 17 psia. The height is 28 ft and the diameter is 1.84 ft.

The column operates at a reflux ratio of 1 for an hour, when most of the IPA and water is taken off the top and transferred to R-201. Then the reflux ratio ramps up to 2 for the remainder of the first six-hour shift. The second batch separates NPB from the oleic acid left over from the first batch. This separation takes place in COL-201 as well. See Gantt Chart (Fig 5.2). The purchase cost of the unit is \$50,700, and the bare module cost is \$210,800.

Column Pot

POT-201 – Specification sheet on page 80

POT-201 is a vertical stainless steel vessel located at the bottom of the COL-201. It is 10 ft in height and 10 ft in diameter and was designed to contain the entire volume of a co-solvent batch. The pot is surrounded by a steam-heated jacket and maintains pot contents at an average temperature of 181°F. The purchase cost of the unit is \$93,900, and the bare module cost is \$390,800.

Pot Jacket

HX-201 – Specification sheet on page 81

HX-201 is a carbon-steel jacket that surrounds POT-201. Its purpose is to maintain pot contents at sufficient boiling temperatures by circulating high-pressure steam. The jacket circulates 5,841 lb steam/hr at 150 psig, 366°F. It was modeled as a shell-and-tube heat exchanger, with a total heat transfer area of 422 ft². The average heating duty is 5 MM But/hr. The purchase cost of the unit is \$12,000, and the bare module cost is \$47,800.

Column Condenser

HX-202 – Specification sheet on page 82

HX-202 is a shell-and-tube carbon-steel heat exchanger that utilizes cooling water at 90°F to totally condense the vapor distillate from COL-201. The exiting cooling water temperature is 120°F. The inlet and outlet temperatures of the distillate are 184.4°F and 177.7°F, respectively. The heat transfer area totals 761 ft². Cooling water is pumped at 89,200 lb/hr. The average cooling duty is 2.7 MM BTU/hr.

The purchase cost of the unit is \$22,800 and the bare module cost is \$91,300.

Reflux Drum

ACC-201 – Specification sheet on page 101

ACC-201 is a stainless steel, horizontal vessel that collects the condensed distillate before sending it back to the column or receivers. It was designed for an aspect ratio of 2, with a diameter of 5.5 ft and length of 11 ft. The total volume is 262 ft³. The purchase cost of the unit is \$43,900, and the bare module cost is \$133,900.

Receiver Tanks

R-201 – Specification sheet on page 79

R-201 is a vertical, open storage tank that receives the first batch's water waste. The tank is filled by the distillate stream between hours 1 and 2 and is transferred by the reflux pump P-203. The receiver is sized to contain 4 weeks' worth of material, with each batch generating 44 lbmol of water waste (83.9% water, 15.7% IPA, 0.4% NPB, and 0% oleic acid). The receiver is

held at ambient temperature and 14.7 psia. This vessel has a length of 10 ft, diameter of 7.15 ft, and total volume of 3000 gallons. The purchase cost is \$5,700, and the bare module cost is \$5,700.

R-202 – Specification sheet on page 84

R-202 is a vertical, closed storage tank that receives the IPA/NPB co-solvent product. The tank is filled by the distillate stream between hours 2-7 and 9-10, and is transferred by the reflux pump P-203. The receiver is sized to contain 457.7 lbmol of each batch's final products contents (54.4% IPA, 44.8% NPB, 0.8% water, and 0% oleic acid). The receiver is held at ambient temperature and 14.7 psia. This vessel has a length of 15.2 ft, diameter of 7.5 ft, and total volume of 5000 gallons. The purchase cost is \$10,000, and the bare module cost is \$10,000.

R-203 – Specification sheet on page 85

R-203 is a vertical, closed storage tank that temporarily stores the IPA/oleic acid pot contents between batches 1 and 2. Pump P-201 drains the pot and sends the contents to R-203 between hour 7:00 and 7:10. After the column's other contents have been drained, the contents of R-203 are pumped back into the still between 7:50 and 8:00 by pump P-205. The receiver is sized to contain 129.7 lbmol of each batch's final products contents (68.1% IPA, 31.9% oleic acid, 0% NPB, and 0% water). The receiver is held at ambient temperature and 14.7 psia. This vessel has a height of 11.4 ft, diameter of 5.5 ft, and total volume of 2,000 gallons. The purchase cost is \$5,000, and the bare module cost is \$5,000.

R-204 – Specification sheet on page 86

R-204 is a vertical, closed storage tank that holds the final oleic acid waste product. The tank is filled with the final pot contents at hour 10:20, after the second batch is completed. The contents are pumped to R-204 using pump P-201. The receiver is sized to contain four weeks' worth of oleic product waste (89.0% oleic acid, 11.0% IPA, 0.8% NPB, and 0% water). The receiver is held at ambient temperature and 14.7 psia. This vessel has a diameter of 10.6 ft, height of 15 ft, and total volume of 10,000 gallons. The purchase cost is \$20,000, and the bare module cost is \$20,000.

R-205 – Specification sheet on page 86

R-205 is a vertical, closed storage tank that holds the final product contents before truck pickup. The tank is filled with the final pot contents at hour 10:30, after the second batch is completed. The contents are pumped to R-205 using pump P-204. The receiver is sized to two batches' worth of final IPA/NPB product solvent (54.4% IPA, 44.8% NPB, 0.8% water, and 0% oleic acid). The receiver is held at ambient temperature and 14.7 psia. This vessel has a diameter of 10.6 ft, height of 15 ft, and total volume of 10,000 gallons. The purchase cost is \$20,000, and the bare module cost is \$20,000.

R-206 – Specification sheet on page 87

R-206 is a vertical, closed storage tank that holds the feed mixture before the Batch 1 begins. The tank is filled whenever the delivery trucks arrive and are sized to hold 2 batches' worth of starting material. The contents are pumped to R-206 using the truck's pump, and are pumped out of R-206 using pump P-206. The receiver is sized to two batches' worth of starting feed mixture (47.6% IPA, 37.4% NPB, 7.5% water, and 7.5% oleic acid). The receiver is held at ambient temperature and 14.7 psia. This vessel has a diameter of 10.6 ft, height of 15 ft, and total volume of 10,000 gallons. The purchase cost is \$20,000, and the bare module cost is \$20,000.

Pumps**P-201** – Specification sheet on page 88

P-201 is used after Batch 1, to pump the pot contents to a temporary holding receiver at time 7:00. It is also used after Batch 2, to pump the final pot contents to REC-204 at time 10:20. It is designed to handle 171 gpm and generates 38 ft of pump head. It is a centrifugal pump composed of cast steel and requires 75 HP to operate. P-201 needs 3,180 BTU/min of electricity during operation, costing \$273/yr. The purchase cost is \$3,100, and the bare module cost is \$10,300.

P-202 – Specification sheet on page 89

P-202 is used to pump cooling water through the column condenser, HX-202 from time 0:00 to 09:10 during the batch process. P-202 is a centrifugal pump composed of cast steel and

requires 75 HP to operate. P-202 needs 190,800 BTU/hr of electricity during operation, costing \$7,400/yr. The purchase cost is \$3,100, and the bare module cost is \$10,200.

P-203 – Specification sheet on page 90

P-203 is used during distillation to pump the overhead reflux back into the distillation column, and also to pump the distillate stream to the appropriate receivers. It is a gear pump designed to handle 25 gpm and requires 75 HP to operate. P-203 needs 2,200 BTU/hr of electricity during operation, costing \$83/yr. The purchase cost is \$5,600, and the bare module cost is \$18,600.

P-204 – Specification sheet on page 91

P-204 is used after Batch 2, to pump the contents from receiver R-202 to final product holding tank R-205. The transfer takes 10 minutes and occurs at time 10:30. P-204 is a centrifugal pump designed to handle 482 gpm and generates 58 ft of pump head. It is composed of cast steel and requires 75 HP to operate. P-204 needs 3,180 BTU/min of electricity during operation, costing \$136/yr. The purchase cost is \$3,900, and the bare module cost is \$12,900.

P-205 – Specification sheet on page 92

P-205 is a centrifugal pump used after Batch 1, to pump the contents from temporary holding receiver R-203 back into the pot before the start of Batch 2. It is designed to handle 85.4 gpm and generates 58 ft of pump head. It is composed of cast steel and requires 75 HP to operate. P-205 needs 3,180 BTU/min of electricity during operation, costing \$273/yr. The purchase cost is \$3,000, and the bare module cost is \$9,800.

P-206 – Specification sheet on page 93

P-206 is used to pump the feed from the feed holding tank to the pot. It is designed to handle 70 gpm and generates 50 ft of pump head. It is composed of cast steel and requires 75 HP to operate. P-206 needs 190,800 BTU/hr of electricity during operation, costing \$820/yr. The purchase cost is \$2,900, and the bare module cost is \$9,600.

Utilities Summary

The annual cost of utilities for the batch process is a significant contribution to the overall process costs. This is due partly to the fact that heat is constantly being supplied to the heat jacket surrounding batch pot to keep it at a constant temperature of 350°F during the entire process. Since the batch process handles all of the initial 4,600 gallons of co-solvent at one time, the flow rates through the condenser and into the reflux drum are a lot greater than what was seen in the continuous process. This increases the cooling duty of the condenser, increasing the amount of cooling water utility needed. These larger volumes also require larger pumps, increasing the cost of electricity.

The batch process requires high pressure steam, cooling water, and electricity. As stated in the utilities summary for the continuous process, the prices for the utilities were taken from the cost sheet outline in Table 23.1 of *Product and Process Design Principles* (Seider *et al*, pg. 604). Since the table provides utility prices from 1995, the current prices had to be estimated using the CEPCIs for 1995 and 2011, which are 381 and 564, respectively (*Business News*). Table 5.13 below is a summary of the prices used for each utility.

Utility	1995 Prices	2012 Prices
High Pressure Steam (per 1000 lb)	\$4.80	\$7.11
Cooling Water (per 1000 lb)	\$0.0094	\$0.014
Electricity (per 1000 BTU)	\$0.018	\$0.026

Table 5.13 Market utility prices for high pressure steam (150 psig, 366°F), cooling water (90°F), and electricity in 1995 and 2011. The CEPCI indexes for 1995 and 2011 are 381 and 564, respectively.

The greatest contribution to the batch utility costs comes from the high pressure steam, which is the heating utility used to keep the jacket surrounding the pot at a constant temperature of 350°F. Less expensive, low pressure steam does not provide the necessary amount energy to heat the jacket because its temperature, 298 °F, is below the jacket requirements. Therefore, high pressure steam at 150 psig and 366°F is used. The second greatest contribution comes from cooling water at 90°F, which is used as the cooling utility for the overhead condenser. The lowest contributor to utility costs is electricity. Table 5.14 summarizes the utility requirements for each process unit in the batch scheme.

UTILITY COSTS				
Utility	Unit	Quantity	Price	Annual Cost (\$/yr)
High Pressure Steam	HX-201	(lb/batch) 52,600	(\$/1000lb) \$7.11	\$61,600
Cooling Water	HX-202	(lb/batch) 802,800	(\$/1000lb) \$0.014	\$1,840
Electricity		(MBTU/batch)	(\$/1000BTU)	
	P-201	63.6	\$0.026	\$270
	P-202	1,720	\$0.026	\$7,380
	P-203	19.4	\$0.026	\$90
	P-204	31.8	\$0.026	\$140
	P-205	63.6	\$0.026	\$270
	P-206	190.8	\$0.026	\$820.00
			Total	\$72,410

Table 5.14 Per-unit utility requirements for the batch facility.

The batch process requires a total of about 52,600 lb of high pressure steam, 802,800 lb of cooling water, and 2.1 MM BTU of electricity per batch. The annual utility costs are approximately \$61,600/year for high pressure steam, \$1,840/year for cooling water, and \$8,970/year for electricity, totaling to an annual utilities cost of approximately \$72,410. Table 5.15 below summarizes the consumption of each utility per pound of reclaimed co-solvent mixture, which is produced at approximately 39,500 lb/batch.

Utility	Total Amount	Per lb Product
High Pressure Steam (lb/batch)	52,600	1.33
Cooling Water (lb/batch)	802,800	20.30
Electricity (MBTU/batch)	2090	52.80

Table 5.15 Hourly and per-pound-of-product utility consumption for the batch process.

Equipment Specification Sheets

BATCH DISTILLATION COLUMN				
Identification:	<i>Vertical, Trayed Distillation Column</i>		<i>April, 2012</i>	
Item No.	COL-201	JW/ CS/ HD/ AM		
No. required	1			
Cost of Bare Module:	\$344,700			
Function:	Separate H ₂ O and oleic acid from n-propyl bromide and isopropyl alcohol mixture through a batch distillation process.			
Operation:	Batch			
Materials Handled:	<i>Initial Charge</i>	<i>Receiver 1 Final</i>	<i>Receiver 2 Final</i>	<i>Pot Final</i>
Quantity (lb/batch):	52,977	1,101	40,030	11,937
Molar Composition:				
IPA	0.374	0.157	0.544	0.110
NPB	0.476	0.004	0.448	0.000
H ₂ O	0.075	0.839	0.008	0.000
Oleic Acid	0.075	0.000	0.000	0.890
Time Collected (hr):	9			7
Design Data:			Molar Reflux Ratio:	1 & 2 (see Gantt chart)
Number of Trays:	11		Tray Spacing:	2 ft
Tray Type:	Sieve			
Pressure (psig):	5			
Functional Height (ft):	28			
Material:	Stainless Steel			
Inside Diameter (in):	1.84			
Tray Efficiency:	60%			
No. of Direct Receivers:	3			
Batch Lifetime (hr):	12			
REFLUX ACCUMULATOR				
Type:	horizontal pressure vessel			
Aspect Ratio	2			
Volume (ft ³):	262			
Diameter (ft):	5.5			
Length (ft):	11			
Material:	Stainless Steel			
Utilities:				
Controls:				
Tolerances:				
Comments and Drawings:				

POT VESSEL		
Identification:	<i>Vertical Pressure Vessel</i>	
Item No.	POT-201	<i>April, 2012</i>
No. required	1	JW/ CS/ HD/ AM
Cost of Bare Module:	\$390,800	
Function:	Collects liquid at the bottom of distillation column and provides continuous jacket heating required for distillation.	
Operation:		
Materials Handled:	<i>Initial Charge</i>	<i>Final Contents</i>
Molar Composition:		
IPA	0.374	0.110
NPB	0.476	0.000
H ₂ O	0.075	0.000
Oleic Acid	0.075	0.890
Temperature (°F):	71.7	96.2
Design Data:	Type:	Vertical pressure vessel
	Average Temperature (°F):	175
	Operating Pressure (psi):	18.5
	Aspect Ratio:	1
	Length (ft):	10
	Inner Diameter (ft):	10
	Volume (ft ³):	1047
	Average Heat Duty (BTU/hr):	5,000,000
	Material:	Stainless
		Steel
Utilities	Steam (150psig, 366°F) at 5841 lb/hr provides jacket heating for pot	
Controls:		
Comments and Drawings:		

POT HEATER

Identification:	<i>Shell and Tube Heat Exchanger</i>	<i>April, 2012</i>
Item No.	HX-201	JW/ CS/ HD/ AM
No. required	1	

Cost of Bare Module:	\$47,800
Function:	Maintain heat jacket surrounding pot at a constant temperature of 350°F.
Operation:	Continuous

Design Data:

Jacket Temperature (°F):	350
Average Heat Duty (MMBTU/hr):	5
Heat Transfer Coefficient (BTU/°F-ft ² - hr):	120
Heat Transfer Area (ft ²):	422
Heating Material:	150 psig steam at 366°F
Shell Material:	Stainless Steel
Tube Material:	Stainless Steel

Utilities:	Steam (150 psig, 366°F) at 5841 lb/hr
Comments & Drawings:	Operates 9h 10 min for every batch

CONDENSER

Identification:		<i>Shell and Tube Heat Exchanger</i>	<i>April, 2012</i>
	Item No.	HX-202	JW/ CS/ HD/ AM
	No. required	1	

Cost of Bare Module:	\$91,300
Function:	Total condensation of vapor distillate stream of column COL-201.
Operation:	Continuous

Design Data:		Inlet Temperature (°F):	184.4
		Outlet Temperature (°F):	177.7
		Pressure (psi):	17
		Net Heat Duty (MMBTU/hr):	2.7
		Heat Transfer Coefficient (BTU/°F-ft ² - hr):	120
		Heat Transfer Area (ft ²):	761
		Heating Material:	Cooling water (90-120°F)
		Shell Material:	Stainless Steel
		Tube Material:	Stainless Steel

Utilities:	Cooling water (90°F - 120°F) at 89,200 lb/hr
Comments & Drawings:	Runs continuously from hour 0:00 to hour 9:10

RECEIVER		
Identification:	<i>Vertical, open storage tank</i>	<i>April, 2012</i>
Item No.	REC-201	JW/ CS/ HD/ AM
No. required	1	
Cost of Bare Module:	\$5,738	
Function:	Receiver collects water and IPA waste from column distillate.	
Materials Handled:		
Quantity (lb/ batch):	1,334	
Molar Composition:		
<i>IPA</i>	0.157	
<i>NPB</i>	0.004	
<i>H₂O</i>	0.839	
<i>Oleic Acid</i>	0.000	
Collection Time (hr):	1:00-2:00	
Design Data:	Type:	Open, vertical storage tank
	Temperature (°F):	70
	Pressure (psi):	14.7
	Volume (gal):	3000
	Length (ft):	10
	Diameter (ft):	7.15
	Material:	Carbon
		Steel
Utilities:		
Controls:		
Tolerances:		
Comments and Drawings:	Must be emptied every 4 weeks.	

RECEIVER

Identification: *Vertical, closed storage tank* *April, 2012*
 Item No. REC-202 JW/ CS/ HD/ AM
 No. required 1

Cost of Bare Module: \$10,000

Function: Collects co-solvent product from column distillate and pot.

Materials Handled: *Final Contents*

Quantity (lb/batch):	39,504
Molar Composition:	
<i>IPA</i>	0.544
<i>NPB</i>	0.448
<i>H₂O</i>	0.008
<i>Oleic Acid</i>	0.000

Design Data:

Type:	Closed, vertical storage tank
Volume (gal):	5000
Temperature (°F):	70
Pressure (psi):	14.7
Length (ft):	15.2
Diameter (ft):	7.5
Material:	Carbon Steel

Utilities:

Controls:

Tolerances:

Comments and Drawings:

STORAGE TANK

Identification: *Vertical, closed storage tank* *April, 2012*
Item No. REC-203 JW/ CS/ HD/ AM
No. required 1

Cost of Bare Module: \$5,000
Function: Temporarily stores pot contents (IPA and oleic acid) during batch cycle.

Operation:
Materials Handled: *Tank Contents*
Quantity (lb/batch): 12,229
Molar Composition:
IPA 0.319
NPB 0.000
H₂O 0.000
Oleic Acid 0.681

Design Data:
Type: Closed, vertical storage tank
Volume (gal): 2,000
Temperature (°F): 70
Pressure (psi): 14.7
Height (ft): 11.4
Diameter (ft): 5.5
Material: Carbon Steel

Utilities:
Controls:
Tolerances:
Comments and Drawings:

STORAGE TANK

Identification: *Vertical, closed storage tank* *April, 2012*
 Item No. REC-204,205 JW/ CS/ HD/ AM
 No. required 2

Cost of Bare Module: \$20,000
Function: REC-204 collects the final pot contents, which is mostly oleic acid, and REC-205 collects final product from receiver 2.

Materials Handled:	<i>Oleic Acid Storage</i>	<i>Product Storage</i>
Quantity (lb/batch):		
Molar Composition:		
<i>IPA</i>	0.110	0.544
<i>NPB</i>	0.000	0.448
<i>H₂O</i>	0.000	0.008
<i>Oleic Acid</i>	0.890	0.000
Collection Times (hr):	10:20	10:30

Design Data:

Type:	Closed, vertical storage tank
Volume (gal):	10,000
Temperature (°F):	<100
Pressure (psi):	14.7
Height (ft):	15
Diameter (ft):	10.6
Material:	Carbon Steel

Utilities:
Controls:
Tolerances:
Comments and Drawings: Oil storage tank must be emptied every 4 weeks.

STORAGE TANK

Identification: *Vertical, closed storage tank* *April, 2012*
Item No. REC-206 JW/ CS/ HD/ AM
No. required 1

Cost of Bare Module: \$25,000

Function: REC-206 stores feed mixture so that multiple shipments of co-solvent can be stored while a batch is running.

Design Data:

Type:	Closed, vertical storage tank
Volume (gal):	10,000
Temperature (°F):	<100
Pressure (psi):	14.7
Height (ft):	21.9
Diameter (ft):	10.8
Material:	Carbon Steel

Utilities:

Controls:

Tolerances:

Comments and Drawings:

PUMP

Identification: *Centrifugal pump* *April, 2012*
 Item No. P-201 JW/ CS/ HD/ AM
 No. required 1

Cost of Bare Module: \$10,300

Function: To pump pot contents from pot to temporary holding receiver, REC-203 at hour 7:00 during batch and to pump final pot contents to REC-204 at hour 10:20.

Operation: Discrete

Design Data:

Volumetric Flow Rate (gpm): 171
 Head Developed (ft): 38
 Single Stage: Yes
 Material: Cast Steel
 Work Required (HP): 75

Utilities: Electricity; 3180 BTU/min

Cost of Utilities: \$273/ yr

Comments & Drawings: Pump runs for 10 minutes each time; 1st time is to pump IPA/oleic acid mixture from pot into temporary storage tank REC-203 at hour 7:00, 2nd time is to pump oleic acid from pot to storage tank REC-204 at hour 10:20.

PUMP

Identification: *Centrifugal pump* *April, 2012*
 Item No. P-202 JW/ CS/ HD/ AM
 No. required 1

Cost of Bare Module: \$10,200
Function: To pump cooling water through distillation column condenser.
Operation: Continuous

Design Data:

Volumetric Flow Rate (gpm): 178
 Head Developed (ft): 42
 Single Stage: Yes
 Material: Cast Steel
 Work Required (HP): 75

Utilities: Electricity; 190,800 BTU/hr
Cost of Utilities: \$7380/ year
Comments & Drawings: Pump runs continuously from hour 0:00 to hour 9:10.

REFLUX PUMP

Identification: *External Gear Pump* *April, 2012*
 Item No. P-203 JW/ CS/ HD/ AM
 No. required 1

Cost of Bare Module: \$18,600
Function: To pump the overhead reflux back into distillation column and distillate stream to receivers.
Operation: Continuous

Materials Handled: *Maximum Flow*
 Inlet Stream ID:
 Quantity (lb/h): 96812
 Temperature (°F): 146
 Time (hr): 1.6

Design Data:
 Volumetric Flow Rate (gpm): 25
 Single Stage: Yes
 Material: Cast Steel
 Efficiency
 Work Required (HP): 6
 Pressure Change (psi):

Utilities: Electricity; 2200 BTU/h
Cost of Utilities: \$83/ yr
Comments & Drawings: Pump runs continuously from hour 0:00 to hour 9:10.

PUMP

Identification: *Centrifugal pump* *April, 2012*
 Item No. P-204 JW/ CS/ HD/ AM
 No. required 1

Cost of Bare Module: \$14,300

Function: To pump product from receiver REC-202 to product holding tank REC-205.

Operation: Discrete

Design Data:

Volumetric Flow Rate (gpm): 482

Head Developed (ft): 58

Single Stage: Yes

Material: Cast Steel

Efficiency

Work Required (HP): 75

Pressure Change:

Utilities: Electricity; 3180 BTU/min

Cost of Utilities: \$136/ yr

Comments & Drawings: Pump runs for 10 minutes at hour 10:30.

PUMP

Identification: *Centrifugal pump* *April, 2012*
 Item No. P-205 JW/ CS/ HD/ AM
 No. required 1

Cost of Bare Module: \$12,800

Function: To pump oil and IPA mixture from temporary holding tank, REC-203 back into pot for 2nd phase of batch.

Operation: Discrete

Design Data:

Volumetric Flow Rate (gpm): 85.4
 Head Developed (ft): 58
 Single Stage: Yes
 Material: Cast Steel
 Work Required (HP): 75

Utilities: Electricity; 3180 BTU/min

Cost of Utilities: \$273/ yr

Comments & Drawings: Pump runs for 20 minutes per batch at hour 7:50.

PUMP

Identification: *Centrifugal pump* *April, 2012*
 Item No. P-206 JW/ CS/ HD/ AM
 No. required 1

Cost of Bare Module: \$9,649
Function: To pump feed from feed holding tank, REC-206 to pot.
Operation: Discrete

Design Data:

Volumetric Flow Rate (gpm): 70
 Head Developed (ft): 50
 Single Stage: Yes
 Material: Cast Steel
 Work Required (HP): 75

Utilities: Electricity; 190,800 BTU/h
Cost of Utilities: \$820/ yr
Comments & Drawings: Pump runs for 1 hour from hour 10:30 to hour 11:30 of the batch process

ECONOMIC SUMMARY

Economic Introduction

The economic profitability of both the continuous process and the batch process depends greatly on the resale price of the reclaimed co-solvent product. For a product mass composition of roughly 63% NPB and 37% IPA, the cost of purchasing fresh co-solvent in these proportions is valued at \$1.57/lb. This was calculated based on the market prices of IPA and NPB, which are approximately \$0.68/lb and \$2.10/lb, respectively. In order for our processes to be desirable to potential clients, our selling price should be less than that for fresh co-solvent and should also be comparable to the existing market prices for reclaimed co-solvent. Sensitivity analyses were performed to observe the effect that product selling price has on an important profitability measure, the internal rate of return (IRR). These analyses are displayed in Figure 6.1 below.

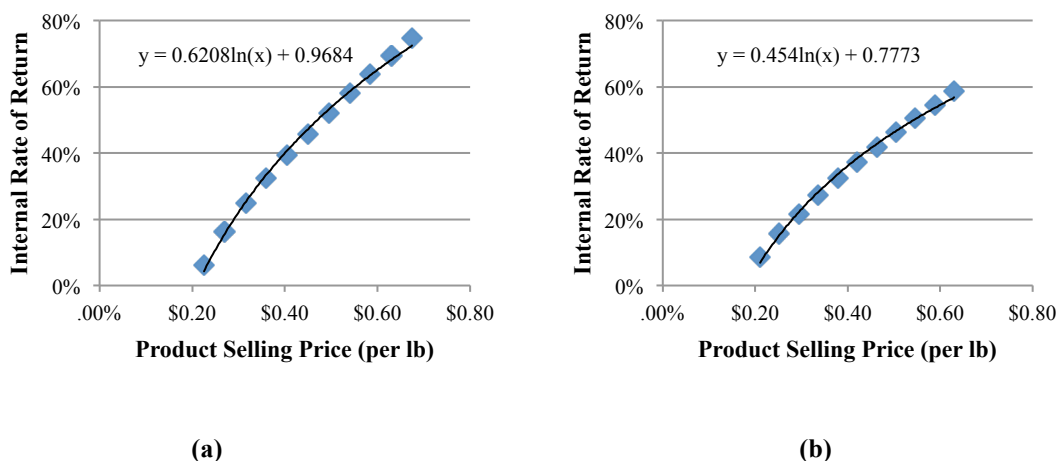


Figure 6.1 Sensitivity Analyses to measure internal rate of return against reclaimed co-solvent selling price for (a) the continuous process and (b) the batch process. The reclaimed co-solvent product is a 37/63 (by mass) mixture of IPA and NPB.

Even through extensive market research and requests for quotes, it is difficult to find information on typical prices for the resale of such co-solvents. However, for this preliminary design proposition, we feel it most important to keep the selling price consistent between continuous and batch for comparison purposes, assuming the selling price will later be changed based on further research and investigation.

In order to keep the selling price consistent between continuous and batch, we must take into account the differences in their final product compositions. The batch co-solvent product is about 0.8% water by mole, whereas the continuous product is only 0.5% water by mole.

Therefore, the reclaimed co-solvent produced by the continuous process is of greater value to our customer than that produced by batch for the fact that it can be used 4.8% longer before reaching its 7.5% water saturation capacity. From this we conclude that the continuous product should be worth approximately 4.8% more than the batch product in order to reflect their relative values. These calculations can be found in Appendix C.

An important consideration in choosing a selling price is that it should provide an IRR above 12%, which is the annualized rate of return for S&P 500. In other words, the process economics should foresee greater returns than what is possible through stock market investments. The product selling prices that produce this minimum allowable IRR are \$0.25/lb for the continuous process and \$0.23/lb for the batch process, and we recommend that our product is priced above these values. We feel that an acceptable price should produce an IRR between 25% and 50% and also be significantly less than the market price of fresh co-solvent, \$1.57/lb.

The remainder of this analysis is based on resale prices of \$0.45/lb for the continuous process and \$0.42/lb for the batch process, producing internal rates of return of 44.9% and 36.8%, respectively.

This market is somewhat unpredictable due to the possibility of future NPB regulation due to environmental concerns. It can also be considered a niche market due to its customer specificity. Because of these considerations and the small size of each facility, we assume a production lifetime of ten years, reaching maximum production capacity one year after start-up.

Equipment Costs

The installation costs of the process equipment are a major contributor to the overall capital investment for the continuous process. Equipment sizes are calculated using the methods and correlations given by *Product and Process Design Principles* (Seider *et al*, Ch.19). Equipment purchase costs are computed by the *Capital Cost Estimation* spreadsheet provided by Professor Seider. The distillation column for the batch process is sized and priced using the methods described in *Batch Distillation, Design and Operation* (Mujtaba, Chapter 7). Low-flow pumps are priced based on size, material, and typical market prices for small, gear pumps, and the correlation used can be found in Appendixes B & D. Bare module factors, specific to each unit, are provided by the *Product and Process Design Principles* and are used to calculate equipment bare module costs. Sizing calculations and per-unit costing spreadsheets for the continuous process can be found in Appendix B and those for the batch process can be found in Appendix D.

The total equipment bare module cost for the batch process totals \$1,026,800. This is over twice the equipment bare module cost for the continuous process, which totals \$450,800. This significant difference is due to the fact that the batch equipment is larger in size because it processes greater volumes. The batch process must handle the initial 6,240 gallon feed all at once, whereas the continuous process ‘continuously’ handles the feed over a two-day period.

Continuous

Table 6.2 below summarizes the f.o.b purchase costs and the bare module costs for each piece of equipment in the continuous process. The equipment f.o.b purchase costs total to \$173,300, and the total bare module costs to \$446,900. The greatest contributors to the equipment bare module cost are the distillation tower, COL-at \$183,300, the decanter, D-101 at \$54,000, and the reflux accumulator, ACC-101 at \$47,800.

Process Equipment Costs			
Unit	Unit Description	F.o.b. Purchase Cost	Bare Module Cost
ACC-101	Reflux Accumulator	\$15,700	\$47,800
COL-101	Tower	\$44,100	\$183,300
D-101	Decanter	\$17,700	\$54,000
F-101	Flash Vessel	\$4,700	\$19,500
HX-101	Double Pipe Heat Exchanger	\$900	\$3,400
HX-102	Double Pipe Heat Exchanger	\$1,500	\$5,900
HX-103	Double Pipe Heat Exchanger	\$1,200	\$4,500
HX-104	Double Pipe Heat Exchanger	\$1,500	\$5,500
HX-105	Condenser	\$2,700	\$10,300
HX-106	Kettle Reboiler	\$2,000	\$8,200
HX-107	Rising Film Evaporator	\$1,900	\$7,300
HX-108	Double Pipe Heat Exchanger	\$1,600	\$6,000
P-101	Pump	\$700	\$2,100
P-102	Reflux Pump	\$700	\$2,300
P-103	Reboiler Pump	\$600	\$2,100
P-104	Pump	\$400	\$1,300
P-105	Pump	\$600	\$1,900
P-106	Pump	\$600	\$1,800
P-107	Pump	\$600	\$1,900
P-108	Pump	\$400	\$1,300
P-109	Pump	\$700	\$2,300
P-110	Pump	\$800	\$2,500
R-101	Storage Tank	\$25,000	\$25,000
R-102	Storage Tank	\$5,700	\$5,700
R-103	Storage Tank	\$20,000	\$20,000
R-104	Storage Tank	\$20,000	\$20,000
R-105	Collecting Tank	\$1,000	\$1,000
		Total	\$446,900

Table 6.2 F.o.b. purchase costs and bare module costs for each piece of equipment in the continuous process.

Batch

Equipment installation costs are a major contributor to the overall capital investment for the batch process. Although fewer pieces of equipment are needed, they make up for it in size and purchase costs due to the larger feed volume that is processed in each batch. The total equipment f.o.b purchase costs total to \$325,600, and the total bare module costs to \$1,026,800. Table 6.3 below summarizes equipment f.o.b purchase costs and bare module costs for the batch process. The greatest contributors to the equipment bare module cost are the pot, POT-201 at

\$390,800, the distillation column, COL-201 at \$210,800, and the reflux accumulator at \$133,900.

Process Equipment Costs			
Unit	Unit Description	F.o.b. Purchase Cost	Bare Module Cost
ACC-201	Reflux Accumulator	\$43,900	\$133,900
COL-201	Tower	\$50,700	\$210,800
HX-201	Jacket Heater	\$12,000	\$47,800
HX-202	Condenser	\$22,800	\$91,300
P-201	Pump	\$3,100	\$10,300
P-202	Pump	\$3,100	\$10,300
P-203	Reflux Pump	\$5,600	\$18,600
P-204	Pump	\$3,900	\$12,900
P-205	Pump	\$3,000	\$9,800
P-206	Pump	\$2,900	\$9,600
POT-201	Batch Pot	\$93,900	\$390,800
R-201	Receiver	\$5,700	\$5,700
R-202	Receiver	\$10,000	\$10,000
R-203	Holding Tank	\$10,000	\$10,000
R-204	Storage Tank	\$10,000	\$10,000
R-205	Storage Tank	\$20,000	\$20,000
R-206	Storage Tank	\$25,000	\$25,000
		Total	\$1,026,800

Table 6.3 F.o.b. purchase costs and bare module costs for each piece of equipment in the batch process

Capital Investment Summary

The total capital investment is an important parameter because it summarizes the overall investment required to build and start up the projected facility. Incorporated into the total capital investment are the total bare module costs, costs of site preparations and service facilities, contingency and contractor fees, costs of land and plant start-up, and working capital. The total capital investment is calculated using the *Profitability Analysis* spreadsheet provided by Professor Seider. Input summaries can be found in Appendix C for the continuous process and Appendix E for the batch process. Overall results from the profitability spreadsheet can be found at the end of this economic analysis.

Continuous

The equipment bare module costs for the continuous process, listed in Table 6.2, total \$446,900. The total bare module costs (C_{TBM}) also include a 7,000-gallon truck and spare pumps for each of the pumps listed. Based on market prices, the truck was estimated to have a purchase cost of approximately \$200,000 and an assumed bare module factor of 1.5 to account for \$100,000 worth of maintenance over the facility's lifetime. The total bare module cost for this process totals \$1,244,400.

The direct permanent investment (C_{DPI}) is calculated as the sum of the C_{TBM} and the costs of site preparations and service facilities, estimated to be 10% of the C_{TBM} . Adding in costs of site preparations and service facilities, the C_{DPI} becomes \$1,368,900. The total depreciable capital (C_{TDC}) is the sum of the C_{TPI} and a contingency fee of 15% of the direct permanent investment. The C_{TDC} for the process has a value of \$1,615,300.

Total permanent investment (C_{TPI}) is computed by adding the costs of land and start-up to the total depreciable capital. The cost of land is estimated to be 2% of the C_{TDC} , and the cost of start-up is estimated to be 10% of the C_{TDC} . The New Jersey facility has an assumed site factor coefficient of 1.00, and the resulting total permanent investment takes on a value of \$1,809,100.

The working capital is the final contributor to the total capital investment, C_{TCI} . Working capital, defined below, is the monetary sum of the accounts receivable, cash reserves, product inventory, and raw materials minus accounts payable.

$$C_{WC} = \text{accounts receivable} + \text{cash reserves} + \text{inventory} + \text{raw materials} - \text{accounts payable}$$

Funds are provided to cover accounts receivable and cash reserves for 30 days, raw materials for 2 days, and product inventory for 4 days. The working capital calculated for the first two years of production totals to approximately \$213,600 for the first year and \$91,500 for the second. At an interest rate of 15%, the net present value of the working capital for the first three years of production is approximately \$253,300.

The total capital investment C_{TCI} is the sum of the total permanent investment and the net present value of the total working capital. The total capital investment for the continuous process is valued at \$2,062,400.

Batch

The equipment bare module costs for the batch process, listed above in Table 6.3, total \$1,026,800. As in the continuous process, the total bare module costs (C_{TBM}) also include a 7,000-gallon truck with a purchase cost of \$200,000 and spare pumps for each of the pumps listed. We assumed the truck to have a bare module factor of 1.5 to account for \$100,000 worth of maintenance over the facility's lifetime. The total bare module costs of the batch process totals \$1,810,800.

The direct permanent investment (C_{DPI}) of the batch process, calculated by summing the C_{TBM} and the costs of site preparations and service facilities (10% of the C_{TBM}), has a value of \$1,991,900. Adding on a contingency fee of 15% of the direct permanent investment, the total depreciable capital (C_{TDC}) totals \$2,350,500. The total permanent investment (C_{TPI}) of the process takes into account the costs of land and start-up, which are estimated to be 2% and 10% of the C_{TDC} , respectively. Assuming a site factor coefficient of 1.00, the total permanent investment becomes \$2,632,500.

The working capital for the batch process was calculated by assuming that funds are needed to cover accounts receivable and cash reserves for 30 days, raw materials for 2 days, and product inventory for 4 days. The working capital calculated for the first two years of production, which is the time it takes to reach maximum production capacity, is \$185,100 for the first year and \$79,300 for the second. At a compounded interest rate of 15%, the net present value of the working capital during the first two years of production is approximately \$225,400.

The total capital investment (C_{TCI}) for the batch process, calculated as the sum of the total permanent investment and the net present value of the working capital, has a value of \$2,857,900.

Total Variable Cost

The variable costs can be broken up into four main categories: general expenses, raw materials, byproducts, and utilities. Figure 6.4 below displays the monetary distributions of the total variable cost for both the continuous and batch processes.

General Expenses

General expenses take into account selling and transfer expenses, direct research, allocated research, administrative expense, and management incentive compensation. The total general expenses were calculated using the *Profitability Analysis* spreadsheet provided by Professor Seider and were based on the overall process costs. The general expenses total \$338,800/yr for the continuous process and \$316,200/yr for the batch process.

Raw Materials

The raw materials needed include IPA, NPB, and diesel fuel. In order to resell the IPA/NPB co-solvent product in its original 56/44 composition, we must replace the amount of IPA and NPB that was lost during each separation. From the original co-solvent feed mixture, 962 lb of IPA is lost during the continuous process at a rate of 0.024 lb IPA per lb co-solvent product, and 694 lb of IPA is lost during the batch process at a rate of 0.014 lb IPA per lb co-solvent product. Assuming that IPA is purchased in bulk at a market price of \$0.68/lb, the annual cost of IPA is \$107,921/yr for the continuous process and \$77,800/yr for batch. Similarly, from the original co-solvent feed mixture, 199 lb of NPB is lost during the continuous process at a rate of 0.005 lb NPB per lb co-solvent product, and 28 lb of NPB is lost during the batch process at a rate of 0.00058 lb NPB per lb co-solvent product. Assuming NPB is purchased at \$2.10/lb, a price provided in our project statement, the annual cost of NPB totals \$32,800/yr for the continuous process and \$9,700/yr for the batch process.

Diesel fuel is needed for the co-solvent transportation service provided by our company. The price of diesel fuel is estimated at the current U.S. market price of \$4.15/gal. Based on typical gas-to-mileage ratios for large, semi-trucks, we estimate our truck to run at 7 miles per gallon. Assuming an average travel distance of 180 miles/day, diesel fuel will be consumed at a rate of approximately 0.0013 gallons per pound of reclaimed co-solvent. The annual cost of diesel fuel is approximately \$36,200/yr for both processes.

The total annual cost of raw materials totals \$210,000/yr for the continuous process and \$105,200/yr for the batch process. Raw material calculations can be found in Appendix C for continuous and Appendix E for batch.

Byproducts

The cost of byproducts includes the sales produced by the outlet oleic acid. The project statement assumes that our oleic acid will sell at the current price of crude oil, approximately \$0.48/lb (*Oil Prices*). However, since the outlet oleic acid is outputted in a ratio of about 80% oleic acid and 20% IPA by mass, we felt this assumption unreasonable and estimate \$0.30/lb to be a better oleic acid selling price. The outlet oleic acid is collected at a rate of 0.3 lb per lb co-solvent product for the continuous process and 0.239 lb per lb co-solvent product for the batch process, generating annual revenues of \$586,600/yr and \$467,400/yr, respectively. Byproduct calculations can be found in Appendix C for the continuous process and Appendix E for batch.

Utilities

The breakdown of the annual utilities costs for batch and continuous is summarized in their respective utilities sections. Total utility costs for the continuous process, totaling \$16,700/yr, only contribute 2.9% of the total variable costs. The utility costs for the batch process, totaling \$72,400/yr, are more significant, contributing 14.7% to the total variable costs.

Utilities needed for the continuous process include low-pressure steam, water, and electricity. Low-pressure steam at 50.3 psig and 298°F is used to heat the column reboiler and HX-107 and is needed at a total flow rate of 416 lb/hr. Steam is purchased at \$4.44/1000lb, and the annual cost of steam for this process is \$14,600/yr. The column condenser, HX-104, and HX-108 require cooling water at 90°F at a total rate of 11,900 lb/hr. Cooling water is purchased at \$0.02/1000lb, and the annual cost of cooling water for this process is \$1,300/yr. Electricity is needed to power small gear pumps, requiring a total of 2,800 BTU/hr. Electricity is priced at \$0.026/1000BTU, and the annual cost of electricity for our process only amounts to about \$500/yr. The total annual cost of utilities for the continuous process totals \$16,700/yr.

Utilities required for the batch process include high-pressure steam, water, and electricity. High-pressure steam at 150 psig and 366°F at 52,600 lb/batch is needed to heat the jacket surrounding the pot to 350°F. High pressure steam is purchased at \$7.11/1000lb, and the annual

cost of steam is \$61,600/yr. The column condenser requires cooling water at 90°F at an amount of 802,800 lb/batch. Cooling water is purchased at \$0.02/1000lb, and the annual cost of cooling water is \$2,500/yr. Electricity is needed at 2.1 MMBTU/batch to power five 75 HP centrifugal pumps and one small gear pump. Electricity costs \$0.026/1000BTU, and the annual expense to provide electricity for the batch process is \$9,000/yr. The total annual utility cost for the batch process totals \$72,400/yr.

Variable Cost Summary

Due to the revenues produced by oleic acid sales, the total variable costs for both the continuous process and the batch process turn out to be annual profits of \$49,800/yr and \$16,600/yr, respectively. Figure 6.4 below shows the breakdown of the annual variable costs for each process, excluding byproduct sales. As can be seen, annual utility costs are more significant for the batch process than for continuous. This is due to the fact that the batch process operates at higher temperatures and greater volumetric flow rates.

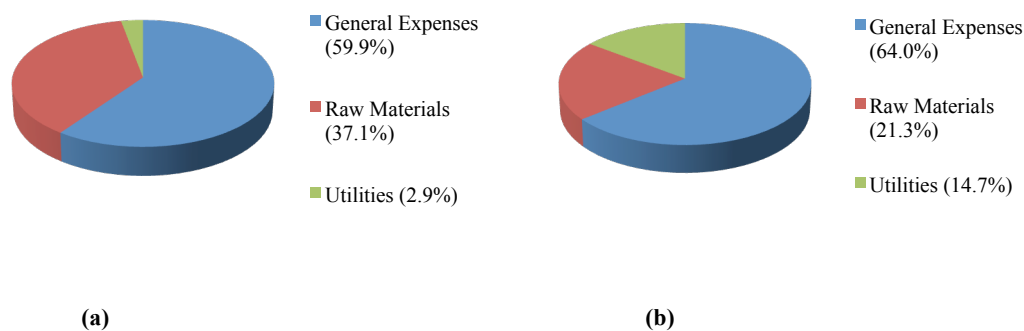


Figure 6.4: Monetary distribution of total variable costs for (a) the continuous process and (b) the batch process

Fixed Costs

Annual fixed costs take into account the cost of operations, maintenance, operating overhead, property taxes and insurance, and other annual expenses. These costs were calculated using the *Profitability Analysis* spreadsheet provided by Professor Sieder. Results can be found at the end of this Economic Summary, and input summaries can be found in Appendix C for the continuous process and Appendix E for the batch process. The annual fixed costs total \$981,400 for the continuous process and \$654,000 for the batch process. Figure 6.5 displays the monetary distribution of the fixed costs for both processes.

Continuous

The annual operations costs for the continuous process incorporate direct wages and benefits, direct salaries and benefits, and operating supplies and services. The direct wages and benefits are calculated by assuming two operators per shift at three shifts per day and one driver at one shift per day for 330 days/yr. An hourly wage of \$35 is used for each operator and driver, resulting in an annual cost of direct wages and benefits of \$508,900/yr. Direct salaries and benefits are calculated at 15% of the total cost of wages, and the cost of operating supplies and services is calculated at 6% of the total cost of wages. The total annual operations cost is approximately \$615,700/yr.

Annual maintenance costs incorporate maintenance wages and benefits, maintenance salaries and benefits, materials and services, and maintenance overhead. Maintenance wages and benefits are calculated at 4.5% of the total depreciable capital. The maintenance salaries and benefits are estimated as 25% of the maintenance wages and benefits, and the cost of materials and services is estimated to be equal to that of maintenance wages and benefits. The cost of maintenance overhead is calculated at 5% of the cost of maintenance wages and benefits. The annual cost for plant maintenance is \$167,200/yr.

The annual operating overhead costs include the costs of general plant overhead, mechanical department services, employee relations department, and business services. These costs are all calculated using the sum of the direct wages, salaries and benefits and the maintenance wages, salaries, and benefits, which has a value of \$676,100/yr. The annual cost of general plant overhead is calculated at 7.1% of this value, mechanical department services at

2.4%, employee relations department at 5.9%, and business services at 7.4%. The total cost of the operating overhead is \$154,100/yr.

Miscellaneous costs include waste and oil pickup services. Tanks R-102 and R-104, that contain non-hazardous water/IPA waste and oleic acid, respectfully, need to be emptied every four weeks. We estimate this service to cost approximately \$500 per emptied tank, totaling to \$1000 per month for two tanks. Assuming twelve pick-up sessions per year, the annual cost of this service is estimated to be \$12,000/yr.

The total annual fixed costs for the continuous process total \$981,400/yr. Figure 6.5a displays the breakdown of the annual fixed costs for the continuous process.

Batch

The direct wages and benefits for the batch process are calculated by assuming two operators and one driver per shift at one shift per day for 330 days/yr. An hourly wage of \$35 is used for each operator and driver, resulting in an annual cost of direct wages and benefits of \$218,400/yr. Direct salaries and benefits are calculated at 15% of the total cost of wages, and cost of operating supplies and services is calculated at 6%, resulting in an annual operations cost of \$264,300/yr.

Maintenance wages and benefits, calculated at 4.5% of the total depreciable capital, total \$105,800/yr. The maintenance salaries and benefits are estimated at 25% of the maintenance wages and benefits, maintenance overhead at 5%, and materials and services at 100%. The annual cost for plant maintenance is \$243,300/yr.

The annual operating overhead costs include the costs of general plant overhead, mechanical department services, employee relations department, and business services. These costs of general plant overhead, mechanical department services, employee relations department, and business services are calculated using the sum of the direct wages, salaries, and benefits and the maintenance wages, salaries, and benefits. This sum totals \$383,400. The annual cost of general plant overhead is calculated at 7.1% of this value, mechanical department services at 2.4%, employee relations department at 5.9%, and business services at 7.4%. The total annual cost of the operating overhead has a value of \$87,400/yr.

Like the continuous process, annual miscellaneous costs for the process include the cost of waste and oil pickup services. Tanks R-201 and R-204 that store non-hazardous water/IPA

waste and oleic acid, respectfully need to be emptied every four weeks. This service, valued at an assumed \$500 per emptied tank, will cost approximately \$12,000/yr.

The total annual fixed costs for the batch process total \$654,000/yr. Figure 6.5b displays the breakdown of annual fixed costs for the batch process.

Fixed Cost Summary

As shown in Figure 6.5 below, the monetary distributions of annual fixed costs for continuous and batch process are significantly different. The continuous process fixed costs are dominated by operations, which account for 64.9% of the total fixed costs, whereas batch operations only account for 40.1% of the total fixed costs. This is due to the fact that operators are needed at the continuous facility twenty-four hours a day at three shifts per day. The batch process only requires one shift per day. Maintenance costs, however, are more significant in the batch process due to the fact that the batch process has a higher total depreciable capital due to more expensive equipment.

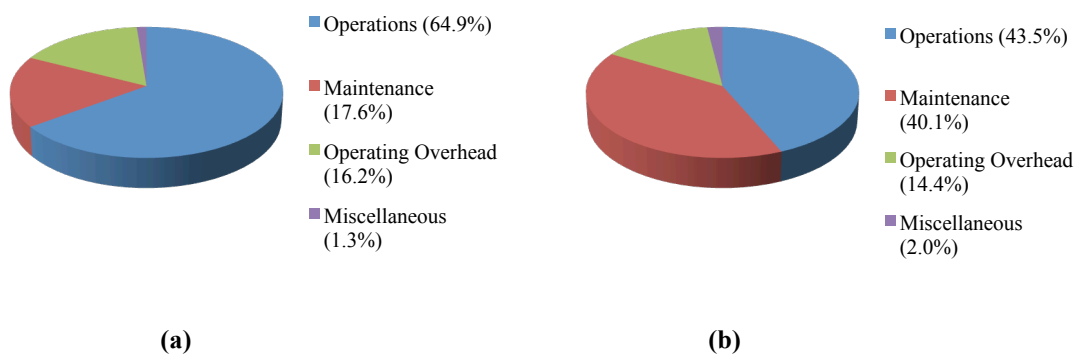


Figure 6.5 Monetary distribution of total annual fixed cost for **(a)** the continuous process and **(b)** the batch process

Cash Flows

A cash flow analysis is performed for each process at their respective co-solvent resale prices (\$0.45/lb for continuous, \$0.42/lb for batch). These analyses can be found at the end of this economic summary section. The 5-year Modified Accelerated Cost Recovery System (MACRS) is utilized to calculate the tax-basis depreciation schedule for our process (see Appendix C & Appendix E). The cash flow summaries display net earnings, cash flows, and cumulative net present values at an interest rate of 15% throughout the ten-year lifetime of the facilities. These analyses were calculated by the *Profitability Analysis* spreadsheet provided by Professor Seider. Input summaries for the spreadsheet can be found in Appendixes C for the continuous process and Appendix E for the batch process. Table 6.6 below provides the internal rate of return (IRR), the cumulative net present value (NPV), and the rate of return on investment (ROI) for both the continuous and batch facilities.

Profitability Measure	Continuous	Batch
IRR	45.8%	37.2%
ROI	43.5%	32.6%
NPV	\$2,657,300	\$2,452,500

Table 6.6 Internal rate of return (IRR), rate of return on investment (ROI) and cumulative net present value (NPV) for the continuous process at a product selling price of \$0.45/lb and for the batch process at a product selling price of \$0.42/lb.

Continuous

Assuming it takes one year to reach maximum production capacity, the sales revenue for the continuous process totals \$1.85 million in 2014 and \$2.64 million at maximum capacity in 2015. Each subsequent year after 2015 also predicts sales revenues of \$2.64 million/yr.

Annual net earnings are calculated by subtracting fixed costs, variable costs, and depreciation capital from annual sales and then multiplying that by 0.6 to account for a 40% income tax. Annual cash flow is then computed by adding the depreciation capital to the net earnings and then subtracting the working capital. The net present value can then be calculated for a compounded interest rate of 15%.

The cumulative net present value after the tenth (final) year of production totals \$2,657,300. Figures 6.7 and 6.8 below show annual cash flows and the cumulative net present values at 15% interest rate during the facility’s lifetime.

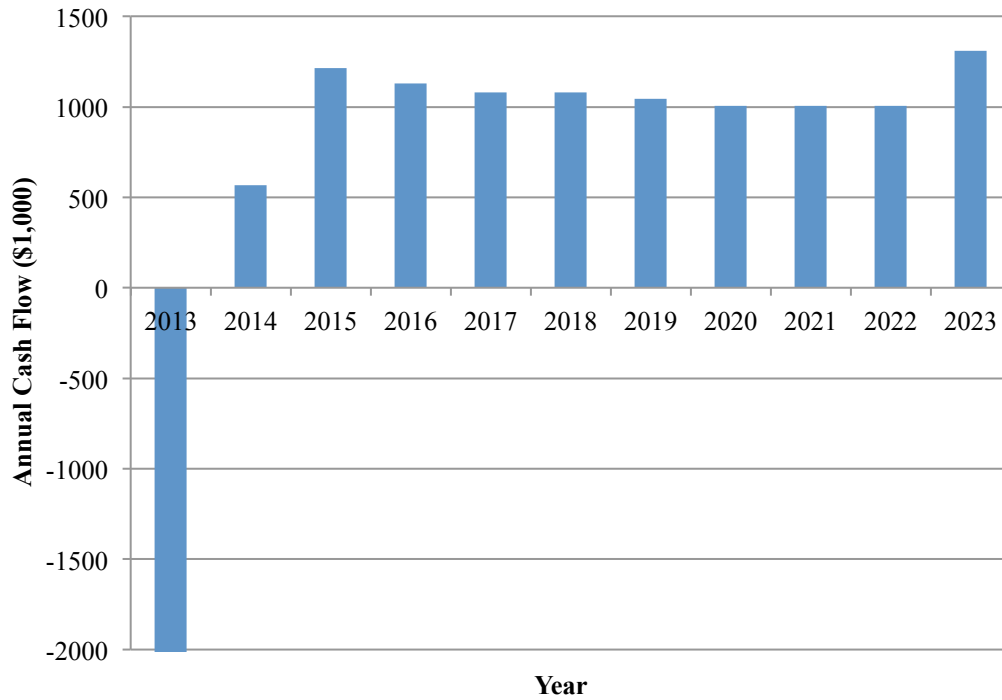


Figure 6.7 Annual cash flows for continuous facility during 10-year production lifetime at a product selling price of \$0.45/lb

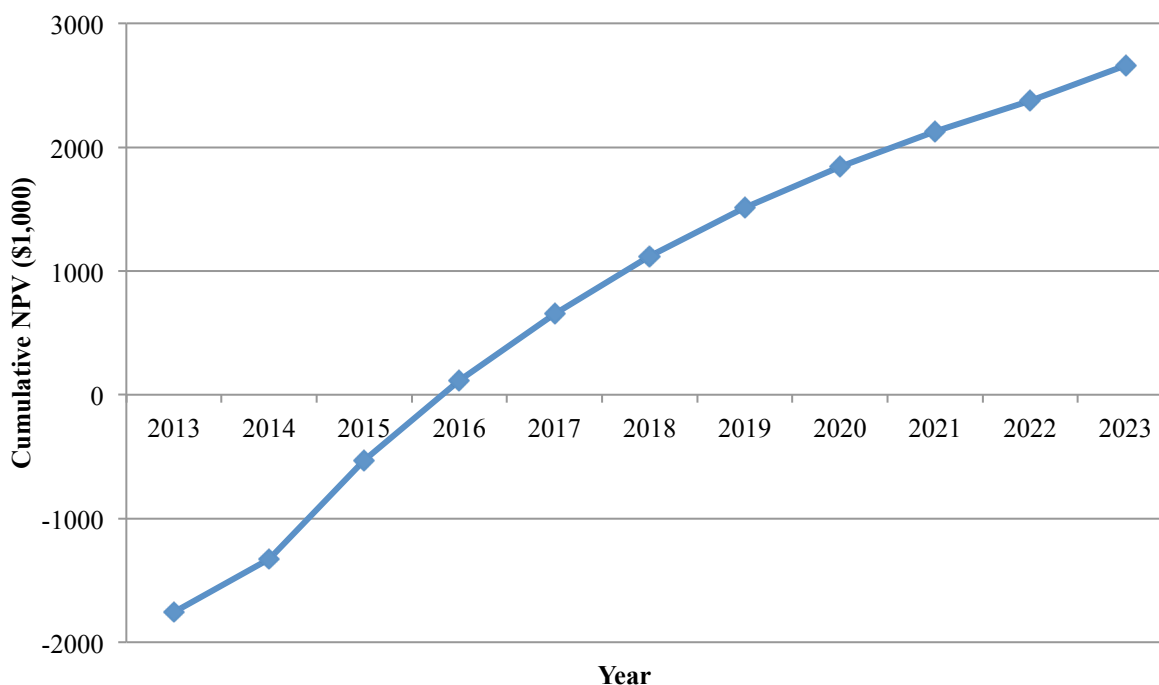


Figure 6.8 Cumulative net present value (NPV) for continuous facility during a 10-year production lifetime at a product selling price of \$0.45/lb and compounded interest rate of 15%

The internal rate of return (IRR) is the interest rate at which the net present value in the tenth year is zero. This value was calculated iteratively by the *Profitability Analysis* spreadsheet, and at a product sales price of \$0.45/lb, it calculates an IRR of 45.6%.

The rate of return on investment (ROI) is the annual interest rate made by the profits on the original investment (Seider 2006) and measures the “economic goodness” of the plant. The plant projects a 43.5% ROI.

Batch

Assuming it takes one year to reach maximum production capacity as in the continuous process, the sales revenue for the batch process totals \$1.72 million in 2014 and \$2.46 million at maximum capacity in 2015. Each subsequent year after 2015 also has sales valued at \$2.46 million.

In the tenth year of production, the cumulative net present value of the batch process is \$2,452,500. Figures 6.9 and 6.10 below show the annual cash flows and the cumulative net present value at 15% interest rate during each year of the facility’s lifetime.

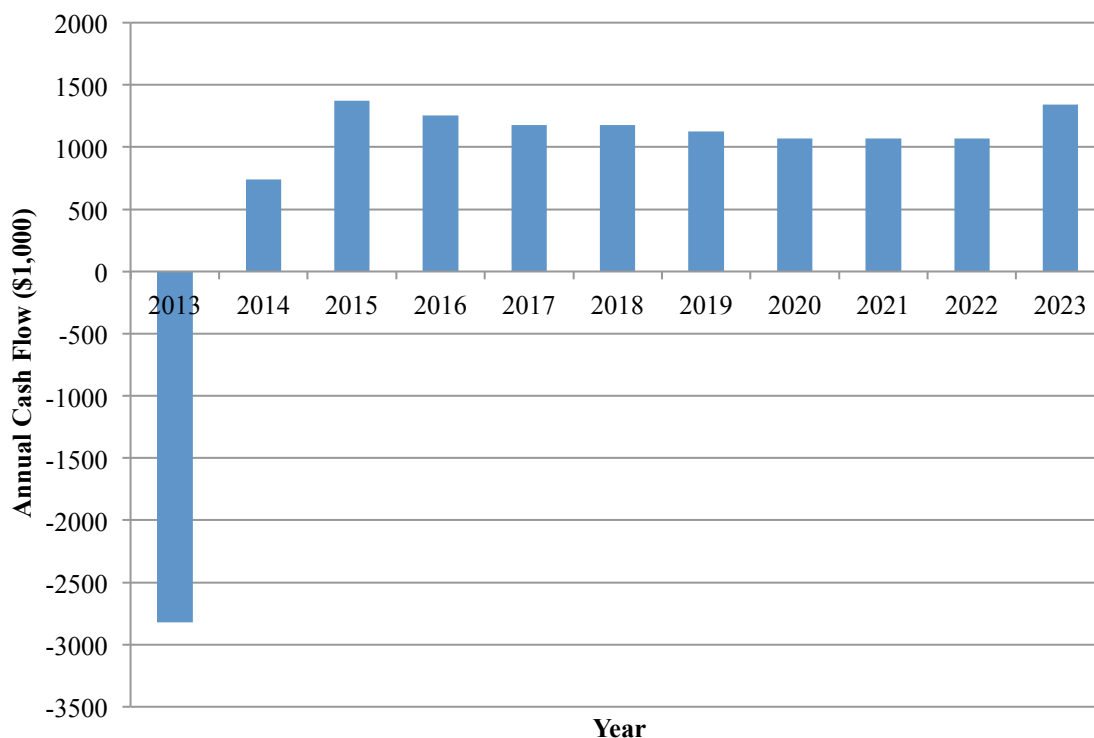


Figure 6.9 Annual cash flows for batch facility during 10-year production lifetime at a product selling price of \$0.42/lb

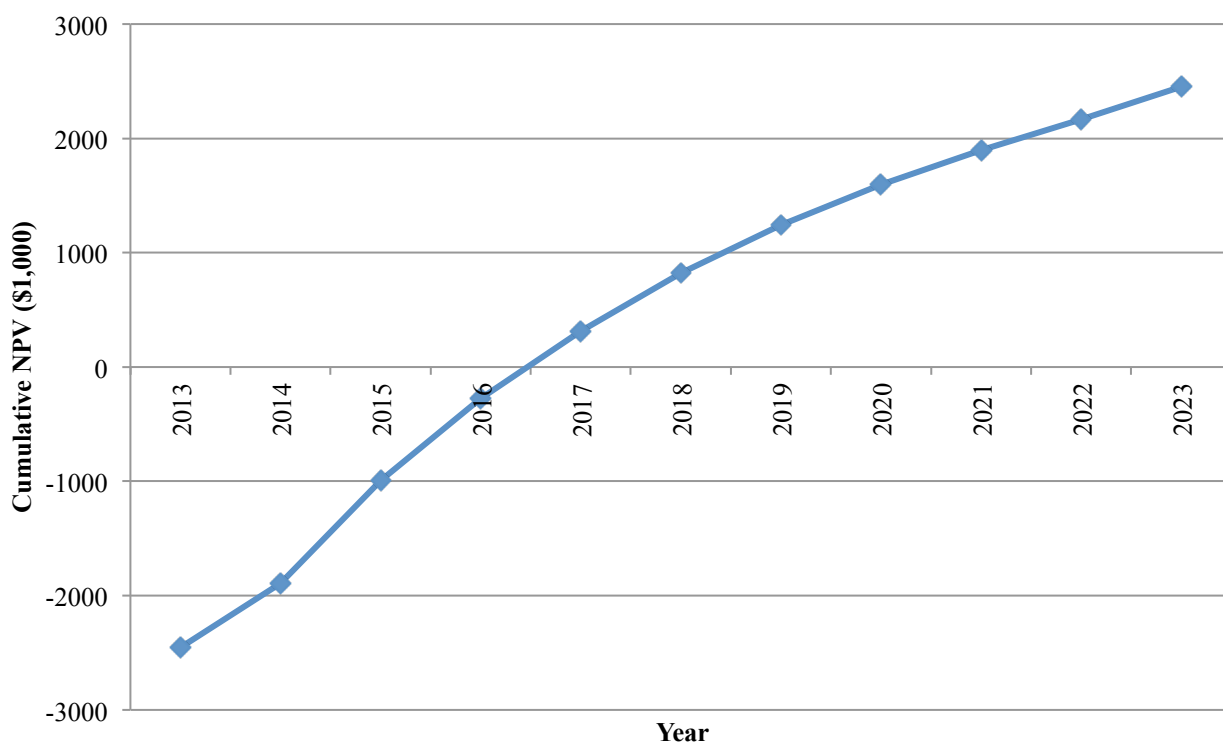


Figure 6.10 Cumulative net present value (NPV) for batch facility during a 10-year production lifetime at a product selling price of \$0.42/lb and compounded interest rate of 15%

The internal rate of return (IRR) for the batch process, calculated by the *Profitability Analysis* spreadsheet, is 37.2% for a product sales price of \$0.42/lb. The ROI for the batch process was calculated to be 32.6%.

Overall Summary

Both the continuous process and the batch process as designed appear to be economically profitable at reclaimed co-solvent resale prices of \$0.45/lb and \$0.42/lb, respectively. Economic analyses over a ten-year production lifetime predict the continuous process to have an internal rate of return of 45.6% and a cumulative net present value of \$2,657,300 suggesting it to be profitable. Similar analyses for the batch process predict an internal rate of return of 37.2% and a cumulative net present value of \$2,452,500, suggesting the batch process to also be profitable. Extensive cash flow summaries using the MACRS 5-year depreciation schedule as well as results summaries from the *Profitability Analysis* spreadsheet can be found at the end of this economic summary for both processes. Input summaries for the spreadsheet can be found in Appendix C (continuous) and Appendix E (batch).

Further Batch Considerations

Our batch cycle is most efficient at a schedule of twelve hours per batch. Sticking to the proposed schedule of one batch per two days for continuous/batch comparison purposes, however, limits the batch cycle's potential because it only runs six hours per day. We therefore feel it necessary to also investigate the economic profitability of two other batch alternatives. The first alternative is to increase the batch production schedule to two batches every two days (one batch per day), and the second alternative is to increase the production schedule to four batches every two days (two batches per day). At these alternative schedules, the batch process is capable of producing up to four-times the amount of product produced by the continuous process. Although the batch process is initially weighed against the continuous process on a two-day schedule, the batch process may be a wise investment from a future production perspective because it allows room for growth.

The economic analyses of the two alternative schedules suggest that they are highly profitable at a co-solvent resale price of \$0.42/lb. The first alternative, at a schedule of 2 batches every 2 days, predicts an IRR of 64.4% and a net present value of \$7,469,000. The second alternative, at a batch schedule of 4 batches every 2 days, predicts an IRR of 129.7% and a net present value of \$22,494,500.

These highly profitable alternatives make the batch case very attractive. For the case of an increase in demand, the batch process is able to handle up to 2 batches per day, which is 4 times as much as the continuous case is designed for. Not only does the batch process allow for potential growth, but it promotes it. This is represented by the large rates of return produced for the two alternative cases at the current selling price of \$0.50. Additionally, if demand were to increase enough to promote one of these alternatives, it could significantly lower prices for our customers.

Continuous Profitability Results*Cash Flow Summary – Continuous*

<u>Year</u>	<u>Percentage of Design Capacity</u>	<u>Product Unit Price</u>	<u>Sales</u>	<u>Capital Costs</u>	<u>Working Capital</u>	<u>Var. Costs</u>	<u>Fixed Costs</u>	<u>Depreciation</u>	<u>Taxable Income</u>	<u>Taxes</u>	<u>Net Earnings</u>	<u>Cash Flow</u>	<u>Cumulative Net Present Value at 15%</u>
2012	0%												
2013	0%			-1,809,100	-2,12,200		-981,400					-2,021,300	-1,757,600
2014	63%	\$0.45	1,847,900		-90,900	13,400	-981,400	-323,100	556,800	-222,700	334,100	566,200	-1,329,500
2015	90%	\$0.45	2,639,900			19,100	-981,400	-516,900	1,160,700	-464,300	696,400	1,213,300	-531,700
2016	90%	\$0.45	2,639,900			19,100	-981,400	-310,100	1,367,500	-547,000	820,500	1,130,600	114,700
2017	90%	\$0.45	2,639,900			19,100	-981,400	-186,100	1,491,500	-596,600	894,900	1,081,000	652,100
2018	90%	\$0.45	2,639,900			19,100	-981,400	-186,100	1,491,500	-596,600	894,900	1,081,000	1,119,500
2019	90%	\$0.45	2,639,900			19,100	-981,400	-93,000	1,584,500	-633,800	950,700	1,043,800	1,511,900
2020	90%	\$0.45	2,639,900			19,100	-981,400		1,677,600	-671,000	1,006,600	1,006,600	1,840,900
2021	90%	\$0.45	2,639,900			19,100	-981,400		1,677,600	-671,000	1,006,600	1,006,600	2,127,000
2022	90%	\$0.45	2,639,900			19,100	-981,400		1,677,600	-671,000	1,006,600	1,006,600	2,375,800
2023	90%	\$0.45	2,639,900		303,100	19,100	-981,400		1,677,600	-671,000	1,006,600	1,309,700	2,657,300

*Variable Cost Summary – Continuous***Variable Costs at 100% Capacity:****General Expenses**

Selling / Transfer Expenses:	\$ 87,995
Direct Research:	\$ 140,792
Allocated Research:	\$ 14,666
Administrative Expense:	\$ 58,663
Management Incentive Compensation:	\$ 36,665

Total General Expenses \$ 338,781

Raw Materials \$0.032215 per lb of Reclaimed Co-Solv \$209,983

Byproducts \$0.090000 per lb of Reclaimed Co-Solv (\$586,634)

Utilities \$0.002555 per lb of Reclaimed Co-Solv \$16,651

Total Variable Costs \$ **(21,219)**

*Fixed Cost Summary – Continuous***Operations**

Direct Wages and Benefits	\$508,872	
Direct Salaries and Benefits	\$76,331	
Operating Supplies and Services	\$30,532	
Technical Assistance to Manufacturing	\$	-
Control Laboratory	\$	-
Total Operations	\$615,735	

Maintenance

Wages and Benefits	\$72,688	
Salaries and Benefits	\$18,172	
Materials and Services	\$72,688	
Maintenance Overhead	\$3,634	
Total Maintenance	\$167,182	

Operating Overhead

General Plant Overhead:	\$48,000	
Mechanical Department Services:	\$16,225	
Employee Relations Department:	\$39,888	
Business Services:	\$50,029	
Total Operating Overhead	\$154,142	

Property Taxes and Insurance

Property Taxes and Insurance:	\$32,306	
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Other Annual Expenses

Rental Fees (Office and Laboratory Space):	\$	-
Licensing Fees:	\$	-
Miscellaneous:	\$12,000	
Total Other Annual Expenses	\$12,000	

<u>Total Fixed Costs</u>	<u>\$981,365</u>	
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Investment Summary – Continuous

<u>Bare Module Costs</u>		
Fabricated Equipment	\$360,554	
Process Machinery	\$	-
Spares	\$6,077	
Storage	\$558,300	
Other Equipment	\$319,509	
Catalysts	\$	-
Computers, Software, Etc.	\$	-
<u>Total Bare Module Costs:</u>		<u>\$1,244,440</u>
<u>Direct Permanent Investment</u>		
Cost of Site Preparations:	\$62,222	
Cost of Service Facilities:	\$62,222	
Allocated Costs for utility plants and related facilities:	\$	-
<u>Direct Permanent Investment</u>		<u>\$1,368,884</u>
<u>Total Depreciable Capital</u>		
Cost of Contingencies & Contractor Fees	\$246,399	
<u>Total Depreciable Capital</u>		<u>\$1,615,283</u>
<u>Total Permanent Investment</u>		
Cost of Land:	\$32,306	
Cost of Royalties:	\$	-
Cost of Plant Start-Up:	\$161,528	
Total Permanent Investment - Unadjusted		\$1,809,117
Site Factor		1
<u>Total Permanent Investment</u>		<u>\$1,809,117</u>

Working Capital and Total Permanent Investment Summary – Continuous

	<u>2013</u>	<u>2014</u>
Accounts Receivable	\$151,882	\$65,092
Cash Reserves	\$51,057	\$21,881
Accounts Payable	(\$11,735)	(\$5,029)
Reclaimed Co-Solvent Mixture Inventory	\$20,251	\$8,679
Raw Materials	\$725	\$311
Total	\$212,179	\$90,934
<i>Present Value at 15%</i>	\$184,504	\$68,759
<u>Total Capital Investment</u>		<u>\$2,062,380</u>

Profitability Summary – Continuous

The Internal Rate of Return (IRR) for this project is 45.79%

The Net Present Value (NPV) of this project in 2012 is \$ 2,657,300

ROI Analysis (Third Production Year)

Annual Sales	2,639,855
Annual Costs	(962,268)
Depreciation	(144,729)
Income Tax	(613,143)
Net Earnings	919,715
Total Capital Investment	<u>2,112,230</u>
ROI	43.54%

Batch Profitability Results**Cash Flow Summary – Batch****Cash Flow Summary**

<u>Year</u>	<u>Percentage of Design Capacity</u>	<u>Product Unit Price</u>	<u>Sales</u>	<u>Capital Costs</u>	<u>Working Capital</u>	<u>Var Costs</u>	<u>Fixed Costs</u>	<u>Depreciation</u>	<u>Taxable Income</u>	<u>Taxes</u>	<u>Net Earnings</u>	<u>Cash Flow</u>	<u>Cumulative Net Present Value at 15%</u>
2012	0%			-2,632,500	-188,800								
2013	0%				-80,900	-16,700	-654,000	-470,100	584,000	-233,600	350,400	-2,821,300	-2,453,300
2014	63%	\$0.42	1,724,700						1,034,000	-413,600	620,400	739,600	-1,894,100
2015	90%	\$0.42	2,463,900			-23,800	-654,000	-752,200	1,334,800	-533,900	800,900	1,372,500	-991,700
2016	90%	\$0.42	2,463,900			-23,800	-654,000	-451,300	1,515,300	-606,100	909,200	1,252,200	-275,700
2017	90%	\$0.42	2,463,900			-23,800	-654,000	-270,800	1,515,300	-606,100	909,200	1,180,000	310,900
2018	90%	\$0.42	2,463,900			-23,800	-654,000	-270,800	1,515,300	-606,100	909,200	1,180,000	821,100
2019	90%	\$0.42	2,463,900			-23,800	-654,000	-135,400	1,650,700	-660,300	990,400	1,125,800	1,244,300
2020	90%	\$0.42	2,463,900			-23,800	-654,000		1,786,100	-714,400	1,071,700	1,071,700	1,594,600
2021	90%	\$0.42	2,463,900			-23,800	-654,000		1,786,100	-714,400	1,071,700	1,071,700	1,899,300
2022	90%	\$0.42	2,463,900			-23,800	-654,000		1,786,100	-714,400	1,071,700	1,071,700	2,164,200
2023	90%	\$0.42	2,463,900		269,700	-23,800	-654,000		1,786,100	-714,400	1,071,700	1,341,400	2,452,500

*Variable Cost Summary – Batch***Variable Costs at 100% Capacity:****General Expenses**

Selling / Transfer Expenses:		\$ 82,129
Direct Research:		\$ 131,406
Allocated Research:		\$ 13,688
Administrative Expense:		\$ 54,753
Total General Expenses		\$ 281,976
<u>Raw Materials</u>	\$0.000000	\$0
<u>Byproducts</u>	\$0.000000	\$0
<u>Utilities</u>	\$0.000000	\$0
<u>Total Variable Costs</u>		<u>\$ 281,976</u>

Fixed Cost Summary – Batch**Operations**

Direct Wages and Benefits	\$218,400	
Direct Salaries and Benefits	\$32,760	
Operating Supplies and Services	\$13,104	
Technical Assistance to Manufacturing	\$	-
Control Laboratory	\$	-

Total Operations **\$264,264**

Maintenance

Wages and Benefits	\$105,771	
Salaries and Benefits	\$26,443	
Materials and Services	\$105,771	
Maintenance Overhead	\$5,289	

Total Maintenance **\$243,274**

Operating Overhead

General Plant Overhead:	\$27,220	
Mechanical Department Services:	\$9,201	
Employee Relations Department:	\$22,619	
Business Services:	\$28,370	

Total Operating Overhead **\$87,409**

Property Taxes and Insurance

Property Taxes and Insurance:	\$47,010	
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Other Annual Expenses

Rental Fees (Office and Laboratory Space):	\$	-
Licensing Fees:	\$	-
Miscellaneous:	\$12,000	

Total Other Annual Expenses **\$12,000**

Total Fixed Costs **\$653,957**

*Investment Summary – Batch***Bare Module Costs**

Fabricated Equipment	\$849,402	
Process Machinery	\$	-
Spares	\$	-
Storage	\$558,300	
Other Equipment	\$403,142	
Catalysts	\$	-
Computers, Software, Etc.	\$	-
<u>Total Bare Module Costs:</u>		<u>\$1,810,844</u>

Direct Permanent Investment

Cost of Site Preparations:	\$90,542	
Cost of Service Facilities:	\$90,542	
Allocated Costs for utility plants and related facilities:	\$	-
<u>Direct Permanent Investment</u>		<u>\$1,991,928</u>

Total Depreciable Capital

Cost of Contingencies & Contractor Fees	\$358,547	
<u>Total Depreciable Capital</u>		<u>\$2,350,476</u>

Total Permanent Investment

Cost of Land:	\$47,010	
Cost of Royalties:	\$	-
Cost of Plant Start-Up:	\$235,048	
Total Permanent Investment - Unadjusted		\$2,632,533
Site Factor		1
<u>Total Permanent Investment</u>		<u>\$2,632,533</u>

Working Capital Summary – Batch

	<u>2013</u>	<u>2014</u>
Accounts Receivable	\$141,757	\$60,753
Cash Reserves	\$36,992	\$15,854
Accounts Payable	(\$9,196)	(\$3,941)
Reclaimed Co-solvent Mixture Inventory	\$18,901	\$8,100
Raw Materials	\$363	\$156
Total	\$188,816	\$80,921
<i>Present Value at 15%</i>	\$164,188	\$61,188
<u>Total Capital Investment</u>		<u>\$2,857,909</u>

Profitability Summary – Batch

The Internal Rate of Return (IRR) for this project is 37.17%

The Net Present Value (NPV) of this project in 2012 is \$ 2,542,500

ROI Analysis (Third Production Year)

Annual Sales	2,463,864
Annual Costs	(677,753)
Depreciation	(210,603)
Income Tax	(630,204)
Net Earnings	<u>945,305</u>
Total Capital Investment	<u>2,902,270</u>
ROI	32.57%

COMPARISON OF CONTINUOUS AND BATCH PROCESSES

Introduction

Management asked our team to compare the potential for both batch and continuous separations processes. Traditionally, batch has performed best in low-volume, high-value markets such as pharmaceuticals and fine chemicals. Certain advantages such as lower initial investment costs, flexibility in scheduling demands, and potential for producing multiple products using the same equipment have given batch an edge in specific industries. It is especially common to see batch used with emerging technologies such as “microelectronics, optical fibers, biotechnology, and high-performance materials” (Doherty 2). However, as these industries mature, they gradually make the shift to continuous processes. Continuous processes generally have the benefits of lower energy consumption, shorter downtime, and lower labor costs. These reasons have made continuous processing predominant in the petrochemical and commodity chemical industries.

Both options have been shown to possess different advantages, economic and otherwise. We will be analyzing the various economics in Part I of our comparison, and then elaborate in Part II on important growth considerations of which management should be aware.

Economic Comparison

The Economic Analysis sections show that both options are economically viable because the rate of return for both options clear the minimum acceptable rate of 12%. This minimum rate is derived from the high estimate for the annualized rate of return in the S&P 500.

To compare the options on a level basis, the amount and frequency of co-solvent collection must be set equivalent - that is, both processes receive one 6,240 gallon batch of material every two days. Additionally, the price and quality of the final solvent product must be standardized between the two process alternatives because the composition of water in the final product differs when utilizing the continuous or batch process. After these parameters are set, it is then possible to gauge the economic viability of the two alternatives using the IRR and NPV parameters. The final product of the batch contains 0.8% water while that for the continuous process only contains 0.5% water, making the product from the continuous process more valuable. Because clients can use their solvents until the water reaches 7.5% on a molar basis, the solvents from the continuous process can be used nearly 4.8% longer on the basis of two weeks. That is why the batch product is sold at \$0.42/lb and the continuous product can be sold at a slightly higher price, \$0.45/lb. Now that the rates of production for both processes have been standardized, the IRR for both processes can be compared. The IRR for the continuous process is 45.6%, which is greater than that for the batch alternative, which is 37.2%.

Growth and Flexibility Comparison

Despite the importance of the profitability and economics of the potential plant, selecting one of these alternatives cannot be strictly based on financial factors alone; other considerations such as operating capacity and process variability must be considered. Currently, the continuous process runs 24 hours a day for 330 days every year. However, the batch process only requires one 6 hour window each day to complete the same separation for a shipment (6,240 gallons every two days). The batch process units (and associated labor, utilities, etc.) are only in use for 12 hours per two days, or 25% of the time, while a proposed continuous plant requires the full 48 hours to produce the purified solvent.

The reason for this time discrepancy is simple: growth potential. The continuous plant must be running at capacity to avoid costly and time-consuming start-up and shut-down procedures. Also, it is designed at the optimal size and operating conditions required to separate the dirty solvent from the client. The designed continuous plant therefore needs to be running at full capacity to accomplish the designed separation. The batch plant is similarly restricted by batch size, but has no such restrictions in operating hours. Because the batch unit only needs two 6-hour windows (one per day, over two days) to process one batch, there is potential for running the batch during idle times. Accordingly, the batch alternative can easily handle spikes in demand that result from seasonal changes, economic trends, the introduction of novel solvents, or the acquisition of new clients from competitors. At a maximum, the batch process can handle up to four truckloads of solvent every two days, while the continuous plant can only process one.

Due to the batch plant's potential for handling an increased demand, an economic analysis was conducted for processing one truck-load a day and two truck-loads per day. Accounting for this increased demand increases variable costs because extra work shifts are needed and an additional transportation truck must be purchased. Nevertheless, the profitability of our process improves immensely, and the IRR increases to 64.4% for one truck-load per day and 129.7% for two truck-loads per day at a selling price of \$0.42/lb. With such high internal rates of return, the company can then afford to lower its product price, making it much more competitive.

Another factor, process flexibility, also clearly favors the batch alternative. This project asks for a final product of IPA/NPB co-solvent in a 56/44 ratio, while specifying very clearly that the initial solution to be cleaned consists of this NPB and IPA as well as 15% of equal parts

of water and oleic acid. While this assumption was valuable for solving the problem, it is unlikely that truckloads of used solvent delivered to the plant will have this exact composition. Realistically, it is probable that different clients will use NPB and IPA to clean differing amounts of oil and water, as each customer may have different standards for how much water and oleic acid can build up on machinery. Preliminary simulation data demonstrates that the batch process has the potential to handle a feed with up to 15% water by mole but this sacrifices IPA recovery. Additionally, clients may use different ratios of their co-solvents or even use a different co-solvent mixture altogether; the batch process may still be able to effectively separate a new solvent because undesirable waste portions can be discarded. Operating conditions can easily be adjusted from batch to batch, whereas manipulating conditions for a distribution of compositions in the continuous process would be considerably more challenging. From this discussion, it is clear the batch process has a significant process flexibility advantage.

Comparison Summary

Considering all of the factors discussed above, we recommend pursuing the batch process. That is not to say the continuous process is not feasible – it certainly is; in fact, it has a higher IRR than the batch process does as currently designed. However, the growth potential and processing flexibility advantages of the batch process are too compelling to ignore, especially given that our company can still make a hefty base-line profit without expanding batch operations. Ultimately, if we can secure a large-enough clientele and reach max operating capacity, our batch process has an IRR of 130%, which greatly exceeds the IRR of the continuous process of 45.6%.

SEPARATION ALTERNATIVES

When first attempting to solve the client's problem, our project team considered several different separation methods. One of the most logical ideas was to use drying agents to adsorb water from the dirty solvent mixture. Common drying agents are anhydrous inorganic salts, such as calcium chloride (CaCl_2), sodium sulfate (Na_2SO_4), and magnesium sulfate (MgSO_4), and these are commonly used in small-scale operations to remove water from solvents. However, in addition to water, drying agents often adsorb other polar compounds to lesser degrees, so IPA and NPB could potentially get adsorbed if one were to be introduced.

After preliminary research, our group was not able to find a water-targeting desiccant that also explicitly did not adsorb either of the desired co-solvents. This alone was not a barrier to using drying agents, but after conducting more research about the drying efficiency of some common agents (usually less than 30% mass adsorbed per mass of drying agent), it became clear that a large quantity of adsorbent was required. Taken collectively, this means that a process using an adsorption unit to remove water would not only require large quantities of drying agent (and the need to remove and regenerate it), but could also potentially remove a portion of our desired product, and so our team chose not to pursue this option. However, drying agents are not completely without value; using desiccants in either of the processes could augment the water removal. This would be especially useful if our clients required a better separation than what our process can currently attain, or if the batch column had to process a co-solvent feed with a different composition.

Catalytic chemistry was discussed briefly but never seriously considered for this design project. In addition to having to account for side reactions and catalyst regeneration needs, we did not wish to introduce additional reaction complexity into the process when it became clear that a non-reactive separation process was possible. Therefore, although we have not discounted the potential for chemical removal of either water or oleic acid, it is not the focus of this project.

POTENTIAL CO-SOLVENT ALTERNATIVES

Isopropyl alcohol has historically been accepted as a cleaning and water removal agent and is not currently regulated or forecasted to be regulated in the near future. Thus, this discussion for potential new solvents will be restricted to solvents for mineral and vegetable oils that need to be removed from the machines. As described in the problem statement, historically, effective solvents for these oils have been outlawed completely or are being increasingly regulated due to environmental concerns and health hazards. The vegetable oil (oleic acid) cleaning solvent in this process, n-propyl bromide, is currently unregulated but has shown preliminary carcinogenic and flammable effects, necessitating the identification of new solvents.

Vegetable oils are composed of fatty acids, and are insoluble in water and aqueous solutions. In organic solutions, solubility increases dramatically, but the presence of a carboxyl group necessitates hydrogen-bonding and polar interaction capability in the solvent as well. The chemical used in this process, NPB, is a solvent that successfully meets all of these solubility requirements. The Hansen solubility parameters quantitatively describe the solubility for a chemical, and values for constituent groups are found from Hansen Solubility Parameters: A User's Handbook by Hansen. Using Pro-Pred program, NPB's nonpolar parameter value (δ_D) is high, as expected at 16.52; however the hydrogen-bonding parameter (δ_H) and the polar parameter (δ_P) also contribute significantly at 4.36 and 5.12, respectively. If the solvent is designed with only the purpose of cleaning mineral oil in mind, it does not require δ_H or δ_D to be above zero since mineral oils are straight chain or cyclic hydrocarbons (It should be noted that solvents for vegetable oils will likely dissolve mineral oils as long as the nonpolar solubility parameter is sufficiently high). Any potential new solvent must therefore display similar solubility behavior and have roughly the same or improved solubility parameters as those of NPB.

Additionally, any proposed solvent must be nontoxic, nonflammable, and environmentally benign. NPB is the current cleaning oil solvent of choice after TCA, CFC-113 and many other CFCs have been banned because of toxicity and ozone depletion concerns. However, NPB may not be the long-term solution and has demonstrated preliminary carcinogenic properties (but safe ozone depletion levels). Toxicity and the environmental impact of a chemical are easily quantified by the lethal concentration factor (LC50) and the bioconcentration factor (BCF). In theory, the LC50 of a substance describes the concentration required to kill half of an exposed population; in practice the LC50 is typically scaled to the mass

of living cells killed when exposed to a standardized quantity of the substance. The LC50 of NPB as calculated by Pro-Pred is 5.129×10^{-4} . Likewise, the BCF is also an important determinant in toxicity and environmental safety and is the concentration of chemical in an organism per concentration of chemical in the environment. The BCF of NPB as calculated by Pro-Pred is 23.23. In order to be accepted as a viable solvent in the case that NPB is regulated, any potential new solvent must display less toxicity and potential environmental danger than NPB. Table 9.1 summarizes the current relevant property requirements for NPB and the necessary properties that a new solvent should have.

Property	NPB Value	New Solvent Requirement
Nonpolar solubility parameter δ_D	16.52	>15
Hydrogen-bonding solubility parameter δ_H	4.36	>0 for mineral oils >3 for vegetable oils
Polar solubility parameter δ_P	5.12	>0 for mineral oils >3 for vegetable oils
Bioconcentration factor	23.23	<23.23
Lethal toxicity concentration factor	0.0005129	<0.0005129

Table 9.1: Current Properties of NPB and required properties of new co-solvent

Hydrofluoroethers (HFEs) were recommended to be analyzed according to the solubility requirements because they are environmentally friendly. When using Pro-CAMD to identify potential HFEs, the program generated over 200 matches (for a maximum of 8 functional groups) for a suitable solvent using the parameters in table 9.1 above. One reason for the high quantity of these matches is that Pro-CAMD does not consider the dangers of combustibility, ozone layer degradation, or greenhouse gas accumulation. Thus, while Pro-CAMD is a useful preliminary screener of the desired solubility and toxicity parameters, it is not specific enough to provide all the necessary information about the potential solvent. Extensive research and development on the potential of the solvents identified by Pro-CAMD is needed to test their efficacy, safety, and other properties. Recently, 3M Company has made considerable advances

in HFEs and is now selling them as cleaning solvents. Some of their marketed cleaning HFEs are HFE-7100 (methyl-nonafluorobutyl-ether), HFE-7200 (ethyl-nonafluorobutyl-ether), and HFE-7500 (2-trifluoromethyl-3-ethoxydodecafluorohexane), and these are able to clean oils that accumulate on machines.

Summarizing, alternative oil-cleaning solvents to NPB certainly appear to exist, including ones that are more environmentally and health friendly. The Pro-Pred software is able to provide a preliminary estimate of the solubility and toxicology requirements of NPB, which are then input into the Pro-CAMD software to identify possible solvents. However, this is just the first step, and significant research must be done to arrive at a final substitute solvent product. One of these outcomes, HFEs, has already been developed by 3M and looks to be a promising cleaning solvent in the future.

OTHER CONSIDERATIONS

Environmental and Safety Considerations

Neither the continuous process nor the batch process as designed poses unusual safety or environmental hazards. The only chemical waste produced by our facilities is a diluted mixture of approximately 80% water and 20% isopropyl alcohol. This non-hazardous waste is only produced at a rate of about 2,200 gallons every four weeks, which amounts to less than 0.1% of volume of product produced at the facilities. Another important consideration to note is that both processes are significantly more environmentally-safe than the alternative solution of purchasing fresh co-solvent and discarding dirty co-solvent as waste. This alternative would produce 6,241 gallons of waste every two weeks. Such waste would also need to be handled and discarded as hazardous waste because it contains flammable chemicals such as IPA and NPB in significant proportions.

Both processes are relatively safe from an operational standpoint. They both operate at pressures ranging from atmospheric to 5 psig. The highest temperature in the continuous process is 264°F and the batch reaches 350°F. Batch does use high pressure steam at 150 psig and 366°F. Measures were taken to ensure that all outlet streams leave the process at temperatures below 100°F. All tanks containing combustibles such as oleic acid use a nitrogen blanket, and a nitrogen purge is performed for each process prior to start-up to ensure safe operating conditions.

Approach to Design

After our project team read the customer's product needs in the problem statement, the precise specifications and requirements for the reclaimed co-solvent were spelled out. However, despite knowing the exact product requirements, we still encountered many challenges in designing both the continuous and batch separation schemes. The very first obstacle was deciding on a 'type' of separation process. As stated earlier in section eight, sorption using drying agents for removing water was considered and catalytic chemistry was also briefly considered as a separation option. We struggled to find enough relevant sources on these possible separations using IPA, NPB, oleic acid, and water, and so our team, with the help of some consultant advice, ultimately chose to use distillation as the basis for our process design.

After selecting distillation as the separation method, we had to undertake a four component, non-ideal separation. Numerous attempts were made to first separate out one of IPA, NPB, oleic acid, or water, but the only separable chemical was oleic acid, which required boiling up the rest of the mixture. As stated in section three, our project team pursued this alternative, as other separation avenues were closed until we were able to understand the non-ideal behavior of our system via ternary diagrams. Four component quaternary equilibrium diagrams were not readily available for the IPA, NPB, oleic acid, and water system, so we had no way of reading such a diagram and determining what temperature and pressure conditions could isolate a specific composition of IPA, NPB, oleic acid, or water. Thus, the major challenge of our project finding different pathways to produce the desired solvent ratios without knowing what process machinery or operating conditions were needed to arrive at the final compositions.

Trial and error for input specifications for the continuous distillation column ensued, and we noticed that the column had a tendency to move almost all of the water into the distillate stream. After varying the reflux ratios and distillate flow rates, we observed similar water behavior every time, and so we aimed to identify the scientific reason behind this separation that we had discovered haphazardly. To do this, our team broke down the four component system into discrete three component systems such as IPA, NPB, and oleic acid; IPA, NPB, and water; and NPB, oleic acid, and water. Distillation of these three component systems was simulated using Aspen, and it quickly became apparent that the separation behavior of the four component

mixture was very similar to the behavior of only a three-component system of IPA, NPB, and water. This made sense because of the comparatively high boiling point of oleic acid compared to the other three chemicals, such that the oleic acid behaved as essentially a very “heavy” bottoms liquid.

Knowing that water’s behavior in the distillation column was caused by equilibrium interactions between IPA, NPB, and water, our team moved to understand the ternary equilibrium map of the system, in order to figure out how to best optimize water removal in the distillate stream. First, oleic acid was “removed” from the composition of the mixture, such that the total compositions were 47.6% IPA, 37.4% NPB, and 7.5% water, but only out of 92.5% of total material (7.5% of oleic acid was disregarded). Scaling for a three component system, the compositions came to be 51.5% IPA, 40.4% NPB, and 8.1% water by mole. On the ternary diagram (at 14.7 psia), this feed can be distilled up to an azeotropic line, which signifies a range of potential distillate product compositions. The distillate boundary line has the added advantage of lying in the two liquid phase region, so liquid-liquid-equilibrium can be taken advantage of for the distillate product. The two phase envelope splits into an organic phase of no more than 5% water and an aqueous phase of no less than about 80% water at the azeotropic boundary, so it became clear that utilizing a distillation followed by liquid-liquid-separation would satisfy our client’s water removal needs. The realization that the water removal specification would be satisfied without having to cross the distillation boundary was very helpful; the final aqueous phase composition in the two-liquid region was similar regardless of the starting location (see tie lines in Figure 10.1). Therefore, we did not have to include any azeotropic distillation methods such as pressure swing distillation, separating agent introduction, etc.

Our team capitalized on this information and optimized the operating conditions for the distillation column, specifying that the maximum quantity of water be removed into the distillate product. Next, it was only a matter of including a liquid-liquid separation vessel, a decanter, to separate the two liquid streams. After successfully running a simulation with these process units for the three-component IPA, NPB, and water system, we incorporated oleic acid into the fold and ran the simulation at identical conditions. This resulted in product compositions very similar to that of the three-component system, and this would become our base case operating conditions to remove water from the initial co-solvent feed. Figure 10.1 below illustrates the previous

discussion, and is very helpful in understanding how the bottoms and distillate compositions result.

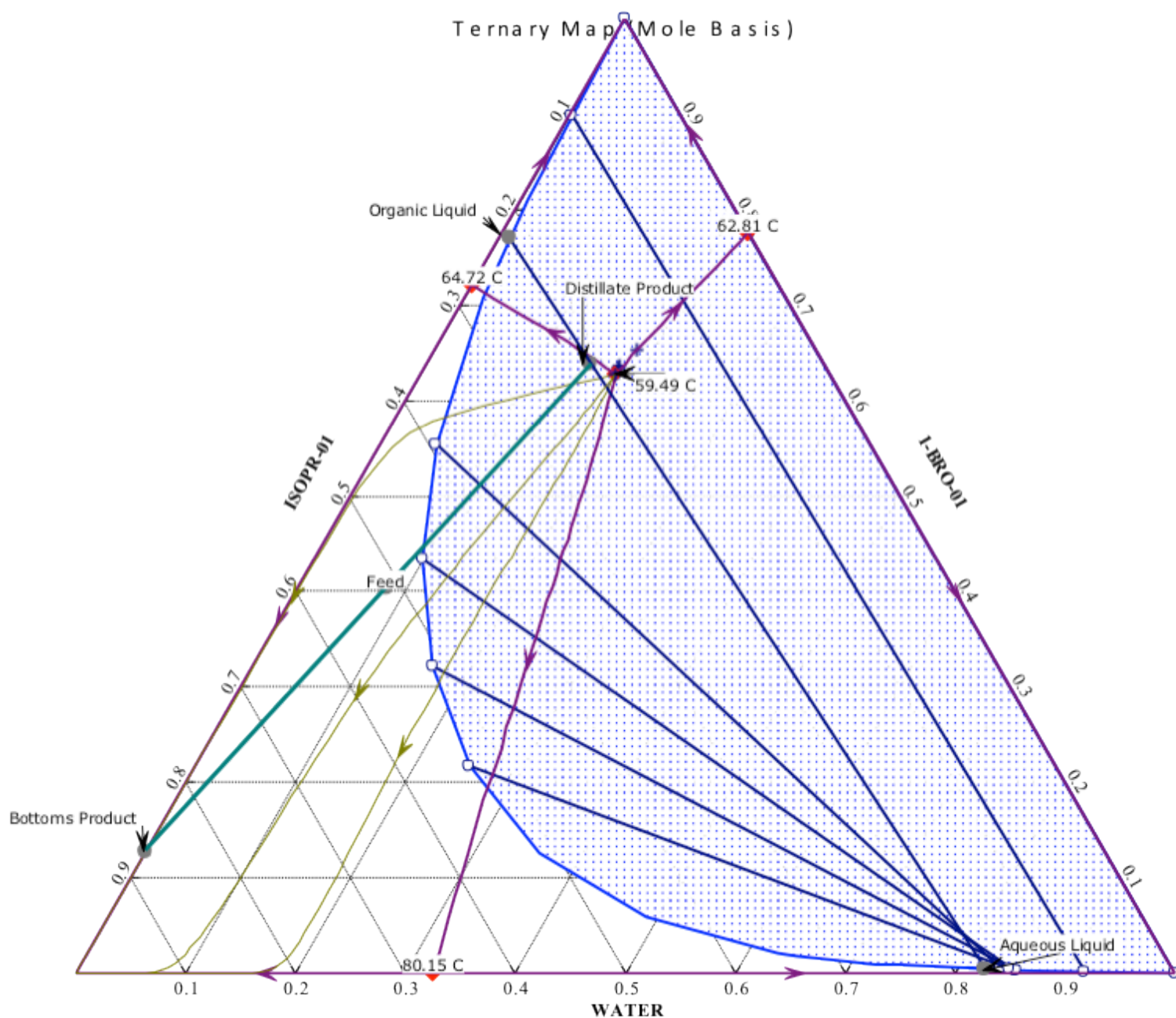


Figure 10.1: Ternary diagram for an IPA, NPB, and water system at 14.7 psia. Oleic acid is removed from consideration when analyzing the system. The feed lies outside the two liquid envelope so extraction or decantation cannot be considered immediately. During distillation, the feed, distillate product, and bottoms product all lie on a distillation line as expected, and the distillate composition is limited by an azeotropic boundary. The distillate lies inside the two phase region, and the tie lines indicate what the aqueous and organic compositions are.

Since water was absent in the bottoms liquid from the column, it was only necessary to separate oleic acid from the remaining IPA and NPB in that stream. We already knew this could be done via heating, so we simply added more heat to this mixture and took advantage of the properties of a rising film evaporator to do this. One interesting note: our selected process (distillation followed by decanter to remove water from distillate product and further heating to remove oleic acid from bottoms product) should theoretically separate the initial mixture to the same degree as the process discussed in section three (heating to remove oleic acid followed by distillation and decanter to remove water), but we could not get the same quality of separation in the latter case. The utilities of the discarded alternative were also higher so the continuous process described above appeared more advantageous, but it would be interesting to see if the discarded alternative can be optimized to separate at a cleaner output composition.

With a sound process foundation for a continuous separation scheme, our focus shifted to devising a batch alternative, and we were able to use the information from the ternary diagram to our advantage. Approaching the separation in a similar manner, we initially tried operating at conditions that would remove water, which we removed as the first off-cut or waste product. Next, a main cut was collected as IPA and NPB boiled off. Finally the oleic acid and any remaining IPA and NPB were separated after more intensive heating, and only oleic acid was left in the pot. Figures 5.10 and 5.11 and their accompanying discussion illustrate this process well, and a more detailed description of optimizing the batch process operating conditions is in the process description part of section five. The batch distillation column behaves similarly to the entire continuous separation process: the initial off cut is analogous to the water removed in the decanter, the next main cut is analogous to the organic product from the decanter, and the final IPA cut (and preceding heating) is very similar to the product from the vertical separation vessel following the rising film evaporator.

CONCLUSIONS AND RECCOMENDATIONS

This proposal describes the science and highlights the promising economic potential of two separation pathways for the co-solvents NPB and IPA from an incoming co-solvent mixture containing water and oleic acid waste. Both continuous and batch process solutions were pursued and analyzed closely, from which the continuous IRR and NPV are 49.5% and \$3,254,700, and the batch IRR and NPV are 41.4% and \$3,210,200. Because these economic factors are relatively even, other factors need to be considered to make the correct decision to maximize profitability. The batch process has the ability to absorb an increase in demand, and greatly increase its IRR and NPV. Additionally, the batch process has much more flexibility, allowing it to handle different compositions and solvents.

The market for the service is already saturated based on our cursory market research. That is why it is imperative to sell the cleaned co-solvent at the lowest price possible without sacrificing the project's profitability. It also requires the differentiation of our service, which should include pick-up and drop-off to the client using our owned transport trucks. Additionally, our proposed batch plant has the added processing capability of separating different compositions of co-solvents and it can potentially separate different co-solvents. This is an important advantage owing to the possibility of new co-solvent introduction should NPB become regulated in the future.

Finally, before implementing this recommended batch plant, more market research is necessary. Since the batch process does not run at maximum capacity, in-depth market research showing limited growth potential would allow scaling down of the batch equipment. This would in turn lower fixed and variable costs, and would further increase the IRR and NPV. This proposal is the most favorable scenario for our company because we could increase profitability with either a larger or smaller client base.

Acknowledgements

We would like to thank Professors Holleran and Fabiano for their ongoing patience, input, and guidance to this project. Especially valuable was Professor Fabiano's industry-related advice, which often allowed us to make assumptions and solve problems when presented with a dilemma. Additionally, we extend special thanks to Mr. Steve Tieri, Mr. Adam Brostow, Mr. Dave Kolesar, and Mr. Bruce Vrana for the time and energy they extended to our group, and for the multitude of ideas that their consultations spawned. We are also grateful for the help of fellow classmate Greg Cameron in using the Pro-Pred and Pro-CAMD software. Finally, none of this would be possible without our chemical engineering education up to date, and we are indeed indebted to all of the chemical and biomolecular engineering faculty at Penn.

References

- "1-Bromopropane." *ChemSpider: The Free Chemical Database*. RCS. Web. 10 Jan. 2012.
<<http://www.chemspider.com/Chemical-Structure.7552.html>>.
- "1-Bromopropane MSDS." *Sciencelab*. Web. 2 Apr. 2012.
<<http://www.sciencelab.com/msds.php?msdsId=9923169>>.
- "Business News: Economic Indicators." *Chemical Engineering Essentials for the Global Chemical Processing Industries*. Chemical Engineering, Apr. 2011. Web. 26 Mar. 2012.
<<http://www.che.com>>.
- "Bioconcentration." *Toxic Substances Hydrology Program*. USGS, 10 Aug. 2011. Web. 1 Apr. 2012.
<<http://toxics.usgs.gov/definitions/bioconcentration.html>>.
- "Carbon Steel Tanks - For Sale." *Used Carbon Steel Tanks*. Bid-on Equipment. Web. 17 Mar. 2012.
<<http://www.bid-on-equipment.com/7550.htm?gclid=CMSCheyhl68CFQjd4AodbHxxxA>>.
- "Crude Oil Price: Oil, Energy, Petroleum." *CRUDE OIL PRICE: Oil*. Oil-Price.net. Web. 26 Mar. 2012.
<<http://www.oil-price.net>>.
- Diwekar, Urmila M. *Batch Distillation: Simulation, Optimal Design and Control*. Bristol: Taylor & Francis, 1996. Print.
- Doherty, M. F., and M. F. Malone. *Conceptual Design of Distillation Systems*. Boston: McGraw-Hill, 2001. Print.
- Hansen, Charles M. Hansen Solubility Parameters: a User's Handbook. CRC Press (2000): Boca Raton, FL.
- "IPA, Isopropyl Alcohol, (CAS No. 67-63-0), South Korea, Good Manufacturer Products, Buy IPA, Isopropyl Alcohol, (CAS No. 67-63-0), South Korea, Good Manufacturer Products from Alibaba.com." *Alibaba*. Alibaba Group. Web. 09 Apr. 2012. <http://www.alibaba.com/product-tp/121366453/IPA_Isopropyl_Alcohol_CAS_No_67.html>.
- "Isopropyl Alcohol MSDS." *Sciencelab*. Web. 2 Apr. 2012.
<<http://www.sciencelab.com/msds.php?msdsId=9924412>>.
- Kehren, Jason. "A Comparison of Hydrofluoroether and Other Alternative Solvent Cleaning Systems." *Data Tech*. 3M. Web. 26 Mar. 2012.
<http://multimedia.3m.com/mws/mediawebserver?mwsId=SSSSSu7zK1fslxtU4x2vNx_Gev7qe17zHvTSevTSeSSSSSS-->>.
- Morgan, D. L. "Toxicology and Carcinogenesis Studies of 1-Bromopropane (CAS No. 106-94-5) in F344/N Rats and B6C3F1 Mice (Inhalation Studies)." *National Center for Biotechnology Information*. U.S. National Library of Medicine, Aug. 2011. Web. 2 Mar. 2012.
<[http://www.ncbi.nlm.nih.gov/pubmed?term=NTP Toxicology and Carcinogenesis Studies of 1-Bromopropane](http://www.ncbi.nlm.nih.gov/pubmed?term=NTP+Toxicology+and+Carcinogenesis+Studies+of+1-Bromopropane)>.
- Mujtaba, I. M. *Batch Distillation: Design and Operation*. Vol. 3. London: Imperial College, 2004. Print.
- Nemhauser, J. B. "Neurologic Illness Associated with Occupational Exposure to the Solvent 1-Bromopropane." *Centers for Disease Control and Prevention*. Centers for Disease Control and

Prevention, 5 Dec. 2008. Web. 02 Mar. 2012.

<<http://www.cdc.gov/mmwr/preview/mmwrhtml/mm5748a2.htm>>.

"Oleic Acid." *ChemSpider: The Free Chemical Database*. RCS. Web. 10 Jan. 2012.

<<http://www.chemspider.com/Chemical-Structure.393217.html?rid=32f987bb-c9c2-4456-ba9c-7cd8f9dc7d5d>>.

"Oleic acid MSDS." *Sciencelab*. Web. 2 Apr. 2012.

<<http://www.sciencelab.com/msds.php?msdsId=9927682>>.

"Oleic Acid - PubChem." *PubChem Compound*. NCBI. Web. 10 Jan. 2012.

<<http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=445639>>.

"Pumps - Gear Pumps." *Cole-Parmer*. Cole-Palmer, 2011. Web. 10 Feb. 2012.

<<http://www.coleparmer.com/Home.aspx>>.

"Q and A: 2007 Final and Proposed Regulations for N-Propyl Bromide (nPB) | Alternatives / SNAP | US EPA." *EPA*. US Environmental Protection Agency, 19 Aug. 2012. Web. 02 Apr. 2012.

<<http://www.epa.gov/ozone/snap/solvents/2007nPBRegsQA.html>>.

Seider, Warren D., J. D. Seader, Daniel R. Lewin, and Soemantri Widagdo. *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*. 3rd ed. Hoboken, NJ: John Wiley & Sons, 2009. Print.

"Techtride - NPB (n-propyl Bromide)." *Parts Cleaning Technologies*. PCT, 2010. Web. 1 Apr. 2012.

<<http://www.partscleaningbgky.com/Chemicals/TechtrideNPB/tabid/88/Default.aspx>>.

Appendix A

Project Description

12. New Environmentally Acceptable Co-solvent for the Reclamation of Co-Solvents (recommended by Leonard A. Fabiano, U. Penn)

The CBE Department recently obtained a powerful software package that CBE students were introduced to in CBE 400. ProCAMD in ICAS 14 is a property-prediction software developed at the Denmark Technical University. Government oversight has ruled out the use of several solvents to be used as cleaning co-solvents. One co-solvent is described below as the currently allowable one. There are always concerns that a regulation could disallow its use, requiring that other solvents be found. These must not be carcinogenic, not be toxic to the environment, and not form azeotropes with the cleaning fluids to avoid difficult separation problems. In this problem, one or more solvents will be found for this application using ProCAMD.

This problem presents the opportunity to make a difference in the future of this process and business, while learning more about molecular structure design and the principles of batch distillation.

Your company, Creative Trollers of America, has been asked to study and prepare proposals to recover co-solvents and reject the removed oil-water mixture from spent metal-working cleansing fluids. Also, the oil used in machining must impart its lubricating properties so that friction between the moving parts and the contact surface of any cutting tool is reduced (Forbes, 1943). From an OSHA perspective, a high percentage of water in the emulsion prevents the oil from misting into the atmosphere, exposing operators to potentially hazardous materials. As a result, the part being machined has a working surface that contains an inorganic contaminant, water, and an organic contaminant, oil. The overall cleansing strategy is to use an alcohol to remove the water and an organic solvent to remove the oil. Examples of the machined metal parts are those cut to a specific geometry

- bearings, drawn tubes, or coils for heat-exchange equipment. The aircraft and rocket production industries also utilize large baths to clean oil and water from the parts' surfaces.

Mineral and vegetable oils are used in machining emulsions. The most commonly used mineral oils are refined paraffinic (C_nH_{n+2}) or naphthenic (C_nH_n) oils (Natchman and Kalpakjian, 1985), which are characterized by API gravity, viscosity, and flash point. Vegetable oils, on the other hand, consist of fatty acids and are used for their profound effect on the surface tension of water. Oleic acid or 9-octadecenoic acid ($C_{18}H_{34}O_2$) is a good example of a vegetable oil used in machining and will be used in this project.

In recent years, environmental concerns and laws have changed the choices of solvents. As a result, TCA and CFC-113 are now banned substances and have since been replaced by regulated solvents such as perchloroethylene (PCE), trichloroethylene (TCE), HCFCs, and volatile methyl siloxanes and terpenes in aerosol form. However, with ever growing legislation, cleaning manufacturers and their customers often find managing regulated solvents like PCE and TCE a difficult task riddled with headaches. Thus, there has been recent interest in the use of non-regulated and/or more environmentally-friendly solvents like n-propyl bromide (NPB) and inseparable isomers of methoxy-nonafluoro-butane ($C_4F_9OCH_3$) or hydrofluoroethers (HFEs). NPB is a non-regulated solvent with cleaning capabilities similar to TCE and PCE. However, it is not clear how long NPB will remain a non-regulated substance. HFEs, on the other hand, are a class of compounds marketed by the 3M Company (1996 – reference not available) more as rinsing agents than as solvents since they are often mixed with trans-1,2-dichloroethylene and

sold in a variety of non- azeotropic and azeotropic co-solvent cleaners. Isopropyl alcohol (IPA) has long been an accepted cleaning reagent in the medical industry and for water removal.

Nowadays the cleansing systems are vapor-phase degreasing processes. That is, the contents of the degreasing equipment are maintained at typically 180°F, depending on the co-solvent, in this project case. The degreasing equipment ranges from 4 to 80 feet long, with the smallest unit holding 100 gal of co-solvent and the largest unit containing four 4,600 gal truck loads. The vapor rises to envelop the metal parts and remove the oil from the metal surfaces. The effluent vapor rises to chillers for condensation, with the liquid recycled. The metal parts are cleansed while moving through the process at an elevated temperature, emerging completely dry. The design and operation of the degreasing equipment to minimize or eliminate fugitive emissions is the responsibility of the cleaning system operations organization. Note: the reclamation company does not operate the onsite cleansing equipment. Their only goal is to clean up and resell the solvents.

The co-solvent mixture is initially at 56 mol% IPA and 44 mol% NPB, as this mixture has been determined to have superior characteristics/properties. During processing, after the co-solvent composition is reduced to 85 mol%, with 7.5 mole% oil and 7.5 mole% water, the resulting mixture is ready to be processed. Note that the initial clean co-solvent is always at a fixed purity. It is expected that the paraffinic oil, oleic acid, can be removed completely. Your company must decide the extent to which the water content can be lowered – to keep the equipment and operating costs reasonable. However, the water composition should not exceed 2.5 mol%.

Design a process to recover the co-solvent, NPB/IPA, from a degreasing system that requires one tank truck (4,600 gal) of fresh co-solvent. Typically a batch of co-solvent can be used for two weeks before the threshold of 15 mol% oil/water is reached. Note that the return mixture will contain 15 mole% oil/water. Your management requests that you consider a batch process, a continuous process, and a combination of the two. Determine the processing capacities at which the batch and continuous processes are economical. Does the combined process offer economic advantages? Is there a capacity below which only batch processing should be considered?

The Parts Cleaning Technology Company in Cinimminson, NJ, should be of interest. Its facility provides fresh co-solvent to customers. It collects and sends the recycled mixture to its complex in Charlotte, NC, for recovery. It also has a facility in Bowling Green, KY, that manufactures cleaning equipment. Its website provides much general information: <http://www.partscleaning.net/equipment.htm>.

Given this collection point in Cinimminson, NJ, it seems clear that many local users need their co-solvent to be reclaimed. Suggest a good location for our proposed tolling operation. Steam, electricity, and cooling water utilities are needed. A location in the vicinity of a steam generation plant for the purchase of steam “over the fence” would be preferable to buying a steam-generation facility. It should be possible to make the other utilities available on site, along with process air and nitrogen (purchased).

Parts Cleaning Technologies sells NPB at \$2.10/lb. IPA prices in bulk need to be found. At this point, we anticipated that the oil recovered will be incinerated. It likely contains some solid residues. You can assume fuel value for the oil.

References

Forbes W. G., *Lubricants and Cutting Oils for Machine Tools*, Wiley, 1943.

Natchman, E. S., and S. Kalpakjian, *Lubricants and Lubrication in Metalworking Operations*, Marcel Dekker, New York (1985)

Appendix B

Continuous Simulation/Sizing/Costing

Tower Diameter (COL-101) - Method of Seider Chpt. 19

$$D_T \left[\frac{4G}{(f u_f) \pi \left(1 - \frac{A_i}{A_T}\right) \rho_G} \right]^{\frac{1}{2}}$$

$$u_f = C \left(\frac{\rho_L - \rho_G}{\rho_G} \right)^{\frac{1}{2}} \quad C = C_{SB} F_{ST} F_F F_{HA}$$

$$F_{ST} = \left(\frac{\sigma}{20} \right)^{.20} \quad \sigma = 71.815 (1 - T_r)^{1.2362}$$

(C_{SB} is found using F_{LG} in Figure 19.4 of Seider)

$$F_{LG} = \left(\frac{L}{G} \right) \left(\frac{\rho_G}{\rho_L} \right)^{\frac{1}{2}}$$

$$\underline{\text{Tower Height} = H = (\text{No. Trays} - 1) (\text{Tray Spacing}) + 10' + 4'}$$

* Calculations are completed using parameters from top tray

```

OUTLETS - C-12      STAGE 1
          C-20      STAGE 8
PROPERTY OPTION SET:  NRTL      RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***
                                IN          OUT          RELATIVE DIFF.
TOTAL BALANCE
MOLE(LBMOL/HR)                11.3400        11.3400          0.00000
MASS(LB/HR )                   1101.58        1101.58        -0.273283E-12
ENTHALPY(BTU/HR )              -0.133691E+07  -0.131873E+07  -0.135933E-01
    
```

```

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E              0.00000        LB/HR
PRODUCT STREAMS CO2E           0.00000        LB/HR
NET STREAMS CO2E PRODUCTION    0.00000        LB/HR
UTILITIES CO2E PRODUCTION      0.00000        LB/HR
TOTAL CO2E PRODUCTION          0.00000        LB/HR
    
```

 **** INPUT DATA ****

**** INPUT PARAMETERS ****

```

NUMBER OF STAGES                8
ALGORITHM OPTION                STANDARD
ABSORBER OPTION                 NO
INITIALIZATION OPTION          STANDARD
HYDRAULIC PARAMETER CALCULATIONS NO
INSIDE LOOP CONVERGENCE METHOD  BROYDEN
DESIGN SPECIFICATION METHOD     NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS 200
MAXIMUM NO. OF INSIDE LOOP ITERATIONS  10
MAXIMUM NUMBER OF FLASH ITERATIONS    30
FLASH TOLERANCE                 0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE  0.000100000
    
```

**** COL-SPECS ****

```

MOLAR VAPOR DIST / TOTAL DIST  0.0
MOLAR REFLUX RATIO              2.00000
MOLAR DISTILLATE RATE           LBMOL/HR  5.67000
    
```

**** PROFILES ****

```

P-SPEC      STAGE 1  PRES, PSIA      14.7000
    
```

 **** RESULTS ****

*** COMPONENT SPLIT FRACTIONS ***

```

                                OUTLET STREAMS
                                -----
                                C-12      C-20
COMPONENT:
WATER                .99903      .96504E-03
OLEIC-01             .36676E-14  1.0000
1-BRO-01             .85451      .14549
ISOPR-01             .22161      .77839
    
```

*** SUMMARY OF KEY RESULTS ***

```

TOP STAGE TEMPERATURE          F          125.070
BOTTOM STAGE TEMPERATURE       F          179.392
    
```

Reclamation of Isopropyl Alcohol and N-Propyl Bromide

Wessels, Schwait, Mu, Deng

TOP STAGE LIQUID FLOW	LBMOL/HR	11.3400
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	5.67000
TOP STAGE VAPOR FLOW	LBMOL/HR	0.0
BOILUP VAPOR FLOW	LBMOL/HR	16.3824
MOLAR REFLUX RATIO		2.00000
MOLAR BOILUP RATIO		2.88932
CONDENSER DUTY (W/O SUBCOOL)	BTU/HR	-258,780.
REBOILER DUTY	BTU/HR	276,954.

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.14032E-04	STAGE=	6
BUBBLE POINT	0.96619E-04	STAGE=	2
COMPONENT MASS BALANCE	0.75232E-06	STAGE=	3 COMP=OLEIC-01
ENERGY BALANCE	0.14889E-03	STAGE=	8

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL		HEAT DUTY BTU/HR
			LIQUID	VAPOR	
1	125.07	14.700	-78568.	-65939.	-.25878+06
2	141.95	14.914	-77310.	-63354.	
3	149.78	15.129	-95170.	-62856.	
4	152.86	15.343	-95522.	-62290.	
5	154.57	15.557	-98284.	-62962.	
6	157.22	15.771	-0.10673E+06	-66149.	
7	164.15	15.986	-0.12099E+06	-75782.	
8	179.39	16.200	-0.15401E+06	-92652.	.27695+06

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	17.01	0.000				5.6700	
2	11.74	17.01					
3	24.24	17.41	11.3400				
4	24.36	18.57					
5	24.12	18.69					
6	23.28	18.45					
7	22.05	17.61					
8	5.670	16.38				5.6700	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	1599.	0.000				532.9330	
2	1187.	1599.					
3	2454.	1720.	1101.5793				
4	2468.	1885.					
5	2398.	1899.					
6	2178.	1830.					
7	1841.	1610.					
8	568.6	1272.				568.6462	

**** MOLE-X-PROFILE ****

STAGE	WATER	OLEIC-01		1-BRO-01		ISOPR-01	
1	0.14986	0.55014E-15	0.63917	0.21097			
2	0.19199E-01	0.71742E-08	0.66538	0.31542			
3	0.12746E-01	0.35090E-01	0.53872	0.41344			
4	0.32146E-02	0.34912E-01	0.53391	0.42797			
5	0.91951E-03	0.35260E-01	0.50143	0.46239			
6	0.38220E-03	0.36531E-01	0.40312	0.55997			
7	0.24044E-03	0.38567E-01	0.23534	0.72585			

8	0.14476E-03	0.15000	0.10883	0.74103
**** MOLE-Y-PROFILE ****				
STAGE	WATER	OLEIC-01	1-BRO-01	ISOPR-01
1	0.35725	0.11196E-22	0.57822	0.64530E-01
2	0.14986	0.55014E-15	0.63917	0.21097
3	0.61749E-01	0.48378E-08	0.65684	0.28141
4	0.16594E-01	0.58901E-08	0.67000	0.31341
5	0.41459E-02	0.67898E-08	0.66285	0.33300
6	0.11576E-02	0.93347E-08	0.62208	0.37676
7	0.45864E-03	0.19844E-07	0.49786	0.50168
8	0.27355E-03	0.18599E-06	0.27913	0.72060
**** K-VALUES ****				
STAGE	WATER	OLEIC-01	1-BRO-01	ISOPR-01
1	2.3836	0.20351E-07	0.90468	0.30586
2	7.8131	0.76685E-07	0.96042	0.66910
3	4.8481	0.13784E-06	1.2191	0.68079
4	5.1657	0.16867E-06	1.2547	0.73246
5	4.5122	0.19248E-06	1.3217	0.72030
6	3.0301	0.25542E-06	1.5430	0.67288
7	1.9079	0.51436E-06	2.1154	0.69117
8	1.8899	0.12398E-05	2.5648	0.97245
**** MASS-X-PROFILE ****				
STAGE	WATER	OLEIC-01	1-BRO-01	ISOPR-01
1	0.28723E-01	0.16533E-14	0.83639	0.13489
2	0.34198E-02	0.20037E-07	0.80916	0.18742
3	0.22680E-02	0.97897E-01	0.65443	0.24540
4	0.57167E-03	0.97345E-01	0.64820	0.25388
5	0.16659E-03	0.10016	0.62022	0.27945
6	0.73595E-04	0.11029	0.52994	0.35969
7	0.51897E-04	0.13052	0.34680	0.52263
8	0.26003E-04	0.42247	0.13346	0.44404
**** MASS-Y-PROFILE ****				
STAGE	WATER	OLEIC-01	1-BRO-01	ISOPR-01
1	0.79035E-01	0.38836E-22	0.87334	0.47623E-01
2	0.28723E-01	0.16533E-14	0.83639	0.13489
3	0.11258E-01	0.13830E-07	0.81759	0.17115
4	0.29442E-02	0.16385E-07	0.81156	0.18549
5	0.73504E-03	0.18874E-07	0.80232	0.19694
6	0.21028E-03	0.26587E-07	0.77148	0.22831
7	0.90409E-04	0.61334E-07	0.67002	0.32989
8	0.63474E-04	0.67666E-06	0.44217	0.55777

COL-101

	Symbol	Magnitude	Units
Tray Spacing		1	ft
# Trays		15	---
Tower Height	H	28.0	ft
Reflux Ratio	RR	2.0	---
Distillate Rate	D	532.9	lb/hr
Liquid Rate	L	1065.8	lb/hr
Top Tray Temp.	T	125.0	F
Liquid Density	p _L	72.1	lb/ft ³
Vapor Density	p _G	0.19	lb/ft ³
Vapor Rate	G	1599.0	lb/hr

Flow Ratio Parameter	F_{LG}	0.034	---
Sieve Plate Parameter	C_{SB}	0.160	ft/s
Reduced Temperature	T_R	0.503	---
Surface Tension	σ	30.287	
Surface Tension Factor	F_{ST}	1.087	---
Foaming Factor	F_F	1	---
Hole-Area Factor	F_{HA}	1	---
Capacity Parameter	C	0.174	---
Flooding Velocity	U_f	3.38	ft/s
Area Ratio	A_d/A_T	0.10	---
Fraction of Velocity	f	0.85	---
<u>Inside Tower Diamter</u>	D_T	1.07	ft

COL-101

VESSEL SIZING			
Vessel Type	Tower	Vessel Material (Cost)	Stainless Steel 304
		Material Factor	1.7
Height/Length (ft)	28		
Diameter (ft)	1.07	Vessel Cost - Eq. (22.57)	\$ 32,195.95
		Platforms & Ladders Cost - Eq. (22.58)	\$ 4,540.29
Operating Pressure (psig)	0	Tray/Packing?	Tray
Design Pressure (psig)	0		
Material (Stress)	Carbon Steel (SA-285 Grade C)	Tray Type	Sieve
Design Temperature (F)	-20 to 650	Tray Type Factor	1
Maximum Allowable Stress (psig)	13750		
		Tray Material	Carbon Steel
		Material Factor	1
		Number of Trays	8
Minimum Wall Thickness		Tray Number Factor	13.0
Inside Diameter Range	Up to 4 ft		
Minimum Thickness (in.)	0.25	Tray Cost - Eq. (22.67)	\$ 7,334.80
Weld Efficiency		Total f.o.b. Purchase Cost	\$ 44,071.04
Wall Thickness Range	Up to 1.25 in.		
Efficiency	0.85	Bare-Module Factor	4.16
Estimated Wall Thickness (in.)	0.1689	Total Bare-Module Cost	\$ 183,335.52
Corrosion Allowance (in.)	0.125		
Vessel Wall Thickness (in) - Eq. (22.60/22.62)	0.375		Clear
Enter Round Thickness (in.)			
Vessel Weight (lbs) - Eq. (22.59)	1529		

Vessel Sizing: ACC-101, D-101, F-101

Q - volumetric flow rate

L - liquid mass flow rate

ρ_L - liquid density

τ - residence time

$$Q = \frac{L}{\rho_L}$$

$$\text{Holdup} = Q\tau$$

$$\text{Volume} = 2^* \text{Holdup}$$

ACC-101 & D-101

$$\text{Aspect Ratio} = 2$$

$$D = \sqrt[3]{\frac{2V}{\pi}}$$

$$L = 2D$$

F-101

$$\text{Aspect Ratio} = 4$$

$$D = \sqrt[3]{\frac{V}{\pi}}$$

$$L = 4D$$

ACC-101

Residence Time	τ	0.083	hr
Liquid Rate	L	1599.0	lb/hr
Density of Liquid Mix	ρ_L	72.1	lb/ft ³
Volumetric Flow Rate	Q	22.2	ft ³ /hr
Holdup		1.85	ft ³
Volume	V	3.70	ft ³
Diameter	D	1.33	ft
Length	L	2.66	ft

ACC-101

VESSEL SIZING			
Vessel Type	Horizontal	Vessel Material (Cost)	Stainless Steel 304
Height/Length (ft)	2.66	Material Factor	1.7
Diameter (ft)	1.33	Vessel Cost - Eq. (22.53)	\$ 13,551.24
Operating Pressure (psig)	0	Platforms & Ladders Cost - Eq. (22.55)	\$ 2,124.46
Design Pressure (psig)	0	Tray/Packing?	Neither
Material (Stress)	Carbon Steel (SA-285 Grade C)		
Design Temperature (F)	-20 to 650		
Maximum Allowable Stress (psig)	13750		
Minimum Wall Thickness			
Inside Diameter Range	Up to 4 ft		
Minimum Thickness (in.)	0.25		
Weld Efficiency			
Wall Thickness Range	Up to 1.25 in.	Total f.o.b. Purchase Cost	\$ 15,675.70
Efficiency	0.85	Bare-Module Factor	3.05
Estimated Wall Thickness (in.)	0.0000		
Corrosion Allowance (in.)	0.125	Total Bare-Module Cost	\$ 47,810.88
Vessel Wall Thickness (in) - Eq. (22.60)	0.375		Clear
Enter Round Thickness (in.)			
Vessel Weight (lbs) - Eq. (22.59)	244		

BLOCK: D-101 MODEL: DECANTER

 INLET STREAM: C-12
 FIRST LIQUID OUTLET: C-13
 SECOND LIQUID OUTLET: C-15
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

	***	MASS AND ENERGY BALANCE	***	
		IN	OUT	RELATIVE DIFF.
TOTAL BALANCE				
MOLE(LBMOL/HR)		5.67000	5.67000	0.00000
MASS(LB/HR)		532.933	532.933	0.668088E-07
ENTHALPY(BTU/HR)		-445482.	-446041.	0.125386E-02

	***	CO2 EQUIVALENT SUMMARY	***
FEED STREAMS CO2E		0.00000	LB/HR
PRODUCT STREAMS CO2E		0.00000	LB/HR
NET STREAMS CO2E PRODUCTION		0.00000	LB/HR
UTILITIES CO2E PRODUCTION		0.00000	LB/HR
TOTAL CO2E PRODUCTION		0.00000	LB/HR

*** INPUT DATA ***

LIQUID-LIQUID SPLIT, TP SPECIFICATION
 SPECIFIED TEMPERATURE F 125.000
 SPECIFIED PRESSURE PSIA 14.7000
 CONVERGENCE TOLERANCE ON EQUILIBRIUM 0.10000E-03
 MAXIMUM NO ITERATIONS ON EQUILIBRIUM 30
 EQUILIBRIUM METHOD EQUATION-SOLVING
 KLL COEFFICIENTS FROM OPTION SET OR EOS
 KLL BASIS MOLE
 KEY COMPONENT(S): WATER

*** RESULTS ***

OUTLET TEMPERATURE F 125.00
 OUTLET PRESSURE PSIA 14.700
 CALCULATED HEAT DUTY BTU/HR -559.27
 MOLAR RATIO 1ST LIQUID / TOTAL LIQUID 0.81974

L1-L2 PHASE EQUILIBRIUM :

COMP	F	X1	X2	K
WATER	0.14986	0.0088801	0.79095	89.0699
1-BRO-01	0.63917	0.77807	0.0075031	0.0096432
ISOPR-01	0.21097	0.21305	0.20154	0.94602

D-101

Residence Time	τ	0.5	hr
Liquid Rate	L	532.9	lb/hr
Density of Liquid Mix	ρ_L	67.4	lb/ft ³
Volumetric Flow Rate	Q	7.91	ft ³ /hr
Holdup		3.96	ft ³
Volume	V	7.91	ft ³
Diameter	D	1.71	ft
Length	L	3.43	ft

D-101

VESSEL SIZING			
Vessel Type	Horizontal	Vessel Material (Cost)	Stainless Steel 304
		Material Factor	1.7
Height/Length (ft)	3.43	Vessel Cost - Eq. (22.53)	\$ 15,469.40
Diameter (ft)	1.71	Platforms & Ladders Cost - Eq. (22.55)	\$ 2,235.62
Operating Pressure (psig)	0	Tray/Packing?	Neither
Design Pressure (psig)	0		
Material (Stress)	Carbon Steel (SA-285 Grade C)		
Design Temperature (F)	-20 to 650		
Maximum Allowable Stress (psig)	13750		
Minimum Wall Thickness			
Inside Diameter Range	Up to 4 ft		
Minimum Thickness (in.)	0.25		
Weld Efficiency		Total f.o.b. Purchase Cost	\$ 17,705.02
Wall Thickness Range	Up to 1.25 in.		
Efficiency	0.85	Bare-Module Factor	3.05
Estimated Wall Thickness (in.)	0.0000		
Corrosion Allowance (in.)	0.125	Total Bare-Module Cost	\$ 54,000.31
Vessel Wall Thickness (in) - Eq. (22.60)	0.375		Clear
Enter Round Thickness (in.)			
Vessel Weight (lbs) - Eq. (22.59)	402		

BLOCK: F-101 MODEL: FLASH2

 INLET STREAM: C-22
 OUTLET VAPOR STREAM: C-23
 OUTLET LIQUID STREAM: C-29
 PROPERTY OPTION SET: NRTL

RENON (NRTL) / IDEAL GAS

		*** MASS AND ENERGY BALANCE ***	***	RELATIVE DIFF.
TOTAL BALANCE		IN	OUT	
MOLE(LBMOL/HR)		5.67000	5.67000	0.00000
MASS(LB/HR)		568.646	568.646	0.510625E-10
ENTHALPY(BTU/HR)		-771139.	-774152.	0.389161E-02

		*** CO2 EQUIVALENT SUMMARY ***	***
FEED STREAMS CO2E		0.00000	LB/HR
PRODUCT STREAMS CO2E		0.00000	LB/HR
NET STREAMS CO2E PRODUCTION		0.00000	LB/HR
UTILITIES CO2E PRODUCTION		0.00000	LB/HR
TOTAL CO2E PRODUCTION		0.00000	LB/HR

		*** INPUT DATA ***	
TWO PHASE TP FLASH			
SPECIFIED TEMPERATURE F			264.000
PRESSURE DROP PSI			0.0
MAXIMUM NO. ITERATIONS			30
CONVERGENCE TOLERANCE			0.000100000

		*** RESULTS ***	
OUTLET TEMPERATURE F			264.00
OUTLET PRESSURE PSIA			14.700
HEAT DUTY BTU/HR			-3012.7
VAPOR FRACTION			0.82269

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
WATER	0.14476E-03	0.14334E-04	0.17287E-03	12.057
OLEIC-01	0.15000	0.84571	0.52128E-04	0.61638E-
1-BRO-01	0.10883	0.26209E-01	0.12663	4.8318
ISOPR-01	0.74103	0.12806	0.87314	6.8177

F-101

Residence Time	τ	0.083	hr
Liquid Rate	L	251.0	lb/hr
Density of Liquid Mix	ρ_L	50.0	lb/ft ³
Bottoms Volume Flow	Q	5.02	ft ³ /hr
Holdup		0.42	ft ³
Volume	V	0.84	ft ³
Diameter	D	0.64	ft
Length	L	2.57	ft

F-101

VESSEL SIZING			
Vessel Type	Vertical	Vessel Material (Cost)	Carbon Steel
		Material Factor	1
Height/Length (ft)	2.57		
Diameter (ft)	0.64	Vessel Cost - Eq. (22.54)	\$ 4,184.40
		Platforms & Ladders Cost - Eq. (22.56)	\$ 506.85
Operating Pressure (psig)	0	Tray/Packing?	Neither
Design Pressure (psig)	0		
Material (Stress)	Carbon Steel (SA-285 Grade C)		
Design Temperature (F)	-20 to 650		
Maximum Allowable Stress (psig)	13750		
Minimum Wall Thickness			
Inside Diameter Range	Up to 4 ft		
Minimum Thickness (in.)	0.25		
Weld Efficiency		Total f.o.b. Purchase Cost	\$ 4,691.25
Wall Thickness Range	Up to 1.25 in.		
Efficiency	0.85	Bare-Module Factor	4.16
Estimated Wall Thickness (in.)	0.0033	Total Bare-Module Cost	\$ 19,515.59
Corrosion Allowance (in.)	0.125		
Vessel Wall Thickness (in) - Eq. (22.60/22.62)	0.375		Clear
Enter Round Thickness (in.)			
Vessel Weight (lbs) - Eq. (22.59)	100		

Heat Exchanger Calculations (HX-101 to HX-108)

$$A = \frac{Q}{\Delta T_{lm} U}$$

$$\Delta T_{lm} = \frac{\Delta T_A - \Delta T_B}{\ln \left(\frac{\Delta T_A}{\Delta T_B} \right)}$$

Reclamation of Isopropyl Alcohol and N-Propyl Bromide

Wessels, Schwait, Mu, Deng

BLOCK: HX-101 MODEL: HEATX

HOT SIDE:

INLET STREAM: C-16
 OUTLET STREAM: C-17
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
 COLD SIDE:

INLET STREAM: C-3
 OUTLET STREAM: C-4
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	12.3621	12.3621	0.00000
MASS(LB/HR)	1129.47	1129.47	0.00000
ENTHALPY(BTU/HR)	-0.149235E+07	-0.149235E+07	-0.156016E-15

*** CO2 EQUIVALENT SUMMARY ***		
FEED STREAMS CO2E	0.00000	LB/HR
PRODUCT STREAMS CO2E	0.00000	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

*** INPUT DATA ***

FLASH SPECS FOR HOT SIDE:

TWO PHASE FLASH
 MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

FLASH SPECS FOR COLD SIDE:

TWO PHASE FLASH
 MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

FLOW DIRECTION AND SPECIFICATION:

COUNTERCURRENT HEAT EXCHANGER
 SPECIFIED HOT OUTLET TEMP
 SPECIFIED VALUE F 100.0000
 LMTD CORRECTION FACTOR 1.00000

PRESSURE SPECIFICATION:

HOT SIDE PRESSURE DROP PSI 6.0000
 COLD SIDE PRESSURE DROP PSI 6.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:

HOT LIQUID	COLD LIQUID	BTU/HR-SQFT-R	149.6937
HOT 2-PHASE	COLD LIQUID	BTU/HR-SQFT-R	149.6937
HOT VAPOR	COLD LIQUID	BTU/HR-SQFT-R	149.6937
HOT LIQUID	COLD 2-PHASE	BTU/HR-SQFT-R	149.6937
HOT 2-PHASE	COLD 2-PHASE	BTU/HR-SQFT-R	149.6937
HOT VAPOR	COLD 2-PHASE	BTU/HR-SQFT-R	149.6937
HOT LIQUID	COLD VAPOR	BTU/HR-SQFT-R	149.6937
HOT 2-PHASE	COLD VAPOR	BTU/HR-SQFT-R	149.6937
HOT VAPOR	COLD VAPOR	BTU/HR-SQFT-R	149.6937

*** OVERALL RESULTS ***

STREAMS:

----->		
C-16	HOT	C-17
T= 1.2508D+02		T= 1.0000D+02
P= 2.0700D+01		P= 1.4700D+01
V= 0.0000D+00		V= 0.0000D+00

Reclamation of Isopropyl Alcohol and N-Propyl Bromide

Wessels, Schwait, Mu, Deng

C-4	<-----	COLD	<-----	C-3
T=	7.1686D+01			T= 7.0454D+01
P=	2.8200D+01			P= 3.4200D+01
V=	0.0000D+00			V= 0.0000D+00

DUTY AND AREA:

CALCULATED HEAT DUTY	BTU/HR	625.4300
CALCULATED (REQUIRED) AREA	SQFT	0.1037
ACTUAL EXCHANGER AREA	SQFT	0.1037
PER CENT OVER-DESIGN		0.0000

HEAT TRANSFER COEFFICIENT:

AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	149.6937
UA (DIRTY)	BTU/HR-R	15.5197

LOG-MEAN TEMPERATURE DIFFERENCE:

LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	F	40.2991
NUMBER OF SHELLS IN SERIES		1

PRESSURE DROP:

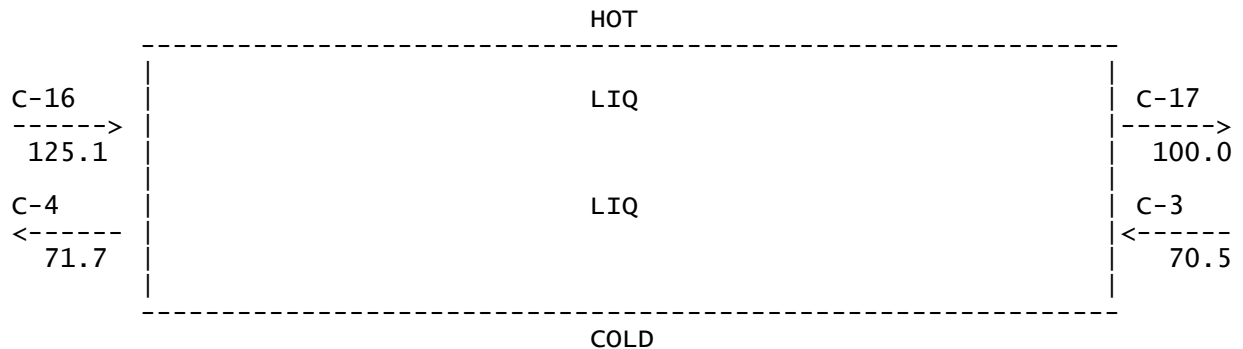
HOT SIDE, TOTAL	PSI	6.0000
COLDSIDE, TOTAL	PSI	6.0000

PRESSURE DROP PARAMETER:

HOT SIDE:	0.29609E+13
COLD SIDE:	0.20075E+10

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:



ZONE HEAT TRANSFER AND AREA:

ZONE	HEAT DUTY BTU/HR	AREA SQFT	LMTD F	AVERAGE U BTU/HR-SQFT-R	UA BTU/HR-R
1	625.430	0.1037	40.2991	149.6937	15.5197

HX-101

EQUIPMENT COSTING	
Equipment Category	Heat Exchangers
Subtype 1	Double Pipe
Subtype 2	
Inner/Outer Pipe Material	Stainless Steel/Stainless Steel
Pressure	Select to use Pressure Factor
Bare-Module Type	Use Bare-Module Factor
Outer Surface Area of Inner Pipe, A, ft²	0.104
Pressure, psig	6
Applicable Range	,
Equipment Base f.o.b. Cost	\$ 883.47
Material Factor	3.00
Pressure Factor	1.00
Bare-Module Factor	1.8
CE Index	500
Equipment Bare-Module Cost	\$ 3,357.20

BLOCK: HX-102 MODEL: HEATX

HOT SIDE:

INLET STREAM: C-27
 OUTLET STREAM: C-28
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
 COLD SIDE:

INLET STREAM: C-4
 OUTLET STREAM: C-5
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	20.6526	20.6526	0.00000
MASS(LB/HR)	1924.12	1924.12	0.00000
ENTHALPY(BTU/HR)	-0.225308E+07	-0.225308E+07	0.00000

*** CO2 EQUIVALENT SUMMARY ***		
FEED STREAMS CO2E	0.00000	LB/HR
PRODUCT STREAMS CO2E	0.00000	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

*** INPUT DATA ***

FLASH SPECS FOR HOT SIDE:

TWO PHASE FLASH
 MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

FLASH SPECS FOR COLD SIDE:

TWO PHASE FLASH
 MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

FLOW DIRECTION AND SPECIFICATION:

COUNTERCURRENT HEAT EXCHANGER
 SPECIFIED HOT OUTLET TEMP
 SPECIFIED VALUE F 100.0000
 LMTD CORRECTION FACTOR 1.00000

PRESSURE SPECIFICATION:

HOT SIDE PRESSURE DROP PSI 6.0000
 COLD SIDE PRESSURE DROP PSI 6.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:

HOT LIQUID	COLD LIQUID	BTU/HR-SQFT-R	149.6937
HOT 2-PHASE	COLD LIQUID	BTU/HR-SQFT-R	149.6937
HOT VAPOR	COLD LIQUID	BTU/HR-SQFT-R	149.6937
HOT LIQUID	COLD 2-PHASE	BTU/HR-SQFT-R	149.6937
HOT 2-PHASE	COLD 2-PHASE	BTU/HR-SQFT-R	149.6937
HOT VAPOR	COLD 2-PHASE	BTU/HR-SQFT-R	149.6937
HOT LIQUID	COLD VAPOR	BTU/HR-SQFT-R	149.6937
HOT 2-PHASE	COLD VAPOR	BTU/HR-SQFT-R	149.6937
HOT VAPOR	COLD VAPOR	BTU/HR-SQFT-R	149.6937

*** OVERALL RESULTS ***

STREAMS:

C-27		HOT	C-28	
T=	1.4529D+02		T=	1.0000D+02
P=	2.0700D+01		P=	1.4700D+01
V=	0.0000D+00		V=	0.0000D+00

Reclamation of Isopropyl Alcohol and N-Propyl Bromide

Wessels, Schwait, Mu, Deng

C-5	<-----	COLD	<-----	C-4
T=	1.0561D+02			T= 7.1686D+01
P=	2.2200D+01			P= 2.8200D+01
V=	0.0000D+00			V= 0.0000D+00

DUTY AND AREA:

CALCULATED HEAT DUTY	BTU/HR	17489.5981
CALCULATED (REQUIRED) AREA	SQFT	3.4692
ACTUAL EXCHANGER AREA	SQFT	3.4692
PER CENT OVER-DESIGN		0.0000

HEAT TRANSFER COEFFICIENT:

AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	149.6937
UA (DIRTY)	BTU/HR-R	519.3098

LOG-MEAN TEMPERATURE DIFFERENCE:

LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	F	33.6785
NUMBER OF SHELLS IN SERIES		1

PRESSURE DROP:

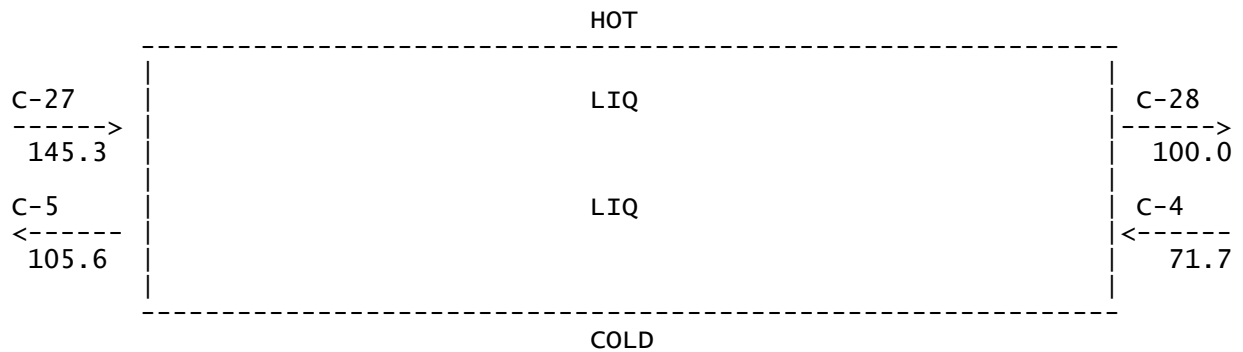
HOTSIDE, TOTAL	PSI	6.0000
COLDSIDE, TOTAL	PSI	6.0000

PRESSURE DROP PARAMETER:

HOT SIDE:	0.37090E+10
COLD SIDE:	0.19846E+10

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:



ZONE HEAT TRANSFER AND AREA:

ZONE	HEAT DUTY BTU/HR	AREA SQFT	LMTD F	AVERAGE U BTU/HR-SQFT-R	UA BTU/HR-R
1	17489.598	3.4692	33.6785	149.6937	519.3098

HX-102

EQUIPMENT COSTING	
Equipment Category	Heat Exchangers
Subtype 1	Double Pipe
Subtype 2	
Inner/Outer Pipe Material	Stainless Steel/Stainless Steel
Pressure	Select to use Pressure Factor
Bare-Module Type	Use Bare-Module Factor
Outer Surface Area of Inner Pipe,	3.47
Pressure, psig	6
Applicable Range	0 - 3,000 psig
Equipment Base f.o.b. Cost	\$ 1,548.54
Material Factor	3.00
Pressure Factor	1.00
Bare-Module Factor	1.8
CE Index	500
Equipment Bare-Module Cost	\$ 5,884.43

BLOCK: HX-103 MODEL: HEATX

HOT SIDE:

INLET STREAM: C-30
OUTLET STREAM: C-31
PROPERTY OPTION SET: NRTL
COLD SIDE:

RENON (NRTL) / IDEAL GAS

 INLET STREAM: C-5
 OUTLET STREAM: C-6
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	12.3454	12.3454	0.00000
MASS(LB/HR)	1352.73	1352.73	0.00000
ENTHALPY(BTU/HR)	-0.164309E+07	-0.164309E+07	-0.141703E-15

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	LB/HR
PRODUCT STREAMS CO2E	0.00000	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

*** INPUT DATA ***

FLASH SPECS FOR HOT SIDE:
 TWO PHASE FLASH
 MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

FLASH SPECS FOR COLD SIDE:
 TWO PHASE FLASH
 MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

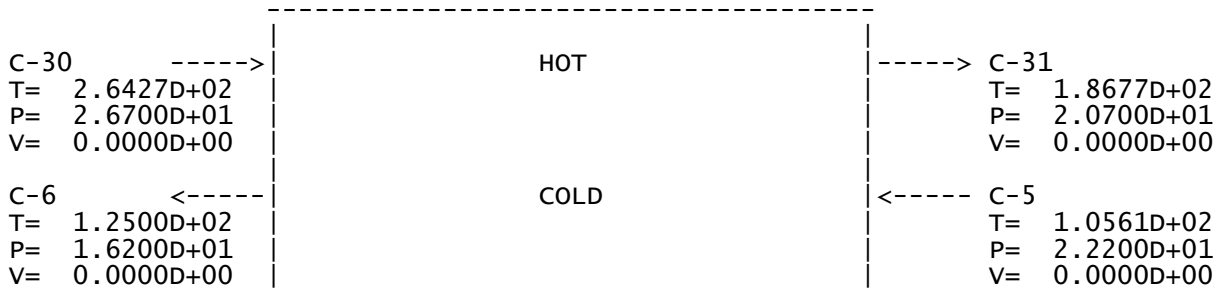
FLOW DIRECTION AND SPECIFICATION:
 COUNTERCURRENT HEAT EXCHANGER
 SPECIFIED COLD OUTLET TEMP
 SPECIFIED VALUE F 125.0000
 LMTD CORRECTION FACTOR 1.00000

PRESSURE SPECIFICATION:
 HOT SIDE PRESSURE DROP PSI 6.0000
 COLD SIDE PRESSURE DROP PSI 6.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:
 HOT LIQUID COLD LIQUID BTU/HR-SQFT-R 149.6937
 HOT 2-PHASE COLD LIQUID BTU/HR-SQFT-R 149.6937
 HOT VAPOR COLD LIQUID BTU/HR-SQFT-R 149.6937
 HOT LIQUID COLD 2-PHASE BTU/HR-SQFT-R 149.6937
 HOT 2-PHASE COLD 2-PHASE BTU/HR-SQFT-R 149.6937
 HOT VAPOR COLD 2-PHASE BTU/HR-SQFT-R 149.6937
 HOT LIQUID COLD VAPOR BTU/HR-SQFT-R 149.6937
 HOT 2-PHASE COLD VAPOR BTU/HR-SQFT-R 149.6937
 HOT VAPOR COLD VAPOR BTU/HR-SQFT-R 149.6937

*** OVERALL RESULTS ***

STREAMS:



DUTY AND AREA:
 CALCULATED HEAT DUTY BTU/HR 10267.2822

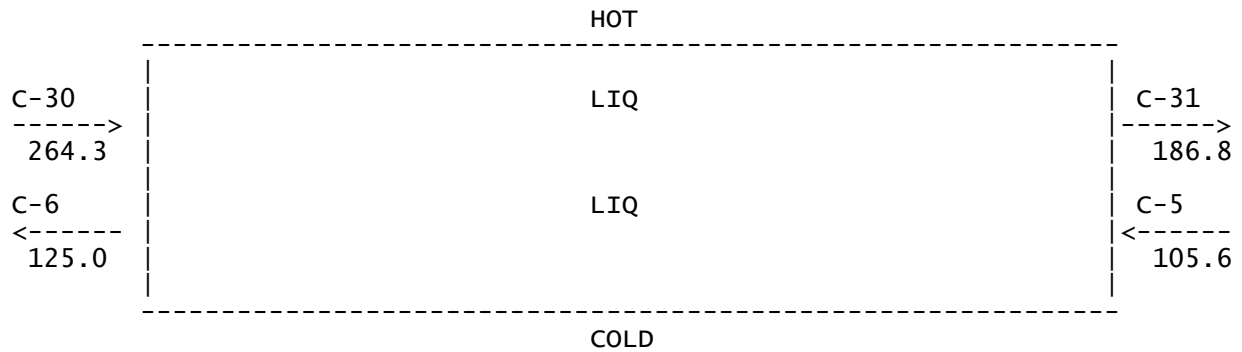
Reclamation of Isopropyl Alcohol and N-Propyl Bromide

Wessels, Schwait, Mu, Deng

CALCULATED (REQUIRED) AREA	SQFT	0.6373
ACTUAL EXCHANGER AREA	SQFT	0.6373
PER CENT OVER-DESIGN		0.0000
HEAT TRANSFER COEFFICIENT:		
AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	149.6937
UA (DIRTY)	BTU/HR-R	95.4068
LOG-MEAN TEMPERATURE DIFFERENCE:		
LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	F	107.6158
NUMBER OF SHELLS IN SERIES		1
PRESSURE DROP:		
HOTSIDE, TOTAL	PSI	6.0000
COLDSIDE, TOTAL	PSI	6.0000
PRESSURE DROP PARAMETER:		
HOT SIDE:		0.33554E+11
COLD SIDE:		0.19500E+10

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:



ZONE HEAT TRANSFER AND AREA:

ZONE	HEAT DUTY BTU/HR	AREA SQFT	LMTD F	AVERAGE U BTU/HR-SQFT-R	UA BTU/HR-R
1	10267.282	0.6373	107.6158	149.6937	95.4068

HX-103

EQUIPMENT COSTING	
Equipment Category	Heat Exchangers
Subtype 1	Double Pipe
Subtype 2	
Inner/Outer Pipe Material	Stainless Steel/Stainless Steel
Pressure	Select to use Pressure Factor
Bare-Module Type	Use Bare-Module Factor
Outer Surface Area of Inner Pipe,	0.637
Pressure, psig	6
Applicable Range	0 - 3,000 psig
Equipment Base f.o.b. Cost	\$ 1,180.68
Material Factor	3.00
Pressure Factor	1.00
Bare-Module Factor	1.8
CE Index	500
Equipment Bare-Module Cost	\$ 4,486.57

Reclamation of Isopropyl Alcohol and N-Propyl Bromide

Wessels, Schwait, Mu, Deng

BLOCK: HX-104 MODEL: HEATER

 INLET STREAM: C-31
 OUTLET STREAM: C-32
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	1.00537	1.00537	0.00000
MASS(LB/HR)	251.148	251.148	0.00000
ENTHALPY(BTU/HR)	-306180.	-316569.	0.328186E-01

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	LB/HR
PRODUCT STREAMS CO2E	0.00000	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

*** INPUT DATA ***

TWO PHASE TP FLASH		
SPECIFIED TEMPERATURE	F	100.000
SPECIFIED PRESSURE	PSIA	14.7000
MAXIMUM NO. ITERATIONS		30
CONVERGENCE TOLERANCE		0.000100000

*** RESULTS ***

OUTLET TEMPERATURE	F	100.00
OUTLET PRESSURE	PSIA	14.700
HEAT DUTY	BTU/HR	-10389.
OUTLET VAPOR FRACTION		0.0000
PRESSURE-DROP CORRELATION PARAMETER		0.34853E+11

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
WATER	0.14334E-04	0.14334E-04	0.18906E-03	0.37779
OLEIC-01	0.84571	0.84571	0.16879E-06	0.57168E-08
1-BRO-01	0.26209E-01	0.26209E-01	0.26001	0.28417
ISOPR-01	0.12806	0.12806	0.73980	0.16547

HX-104

Condenser Duty	Q	10390	BTU/hr
Cold In	$T_{C,i}$	90	F
Cold Out	$T_{C,o}$	120	F
Hot In	$T_{H,i}$	186.7	F
Hot Out	$T_{H,o}$	100	
Log Mean T Difference	T_{LM}	29.9	F
Heat Transfer Coeff.	U	150	BTU/hr ft ² F
Area	A	2.32	ft ²

HX-104

EQUIPMENT COSTING	
Equipment Category	Heat Exchangers
Subtype 1	Double Pipe
Subtype 2	
Inner/Outer Pipe Material	Stainless Steel/Stainless Steel
Pressure	Select to use Pressure Factor
Bare-Module Type	Use Bare-Module Factor
Outer Surface Area of Inner Pipe,	2.32
Pressure, psig	6
Applicable Range	0 - 3,000 psig
Equipment Base f.o.b. Cost	\$ 1,451.93
Material Factor	3.00
Pressure Factor	1.00
Bare-Module Factor	1.8
CE Index	500
Equipment Bare-Module Cost	\$ 5,517.34

HX-105

To see ASPEN output for HX-105, please refer to the condenser in COL-101.

Condenser Duty	Q	258780	BTU/hr
Cooling Water In	$T_{CW,i}$	90	F
Cooling Water Out	$T_{CW,o}$	120	F
Top Stage Temp	T	125	F
Log Mean T Difference	T_{LM}	15.42	F
Heat Transfer Coeff.	U	150	BTU/hr ft ³ F
Area	A	111.90	ft ²

HX-105

EQUIPMENT COSTING	
Equipment Category	Heat Exchangers
Subtype 1	Double Pipe
Subtype 2	
Inner/Outer Pipe Material	Stainless Steel/Stainless Steel
Pressure	Select to use Pressure Factor
Bare-Module Type	Use Bare-Module Factor
Outer Surface Area of Inner Pipe,	111.9
Pressure, psig	6
Applicable Range	0 - 3,000 psig
Equipment Base f.o.b. Cost	\$ 2,699.49
Material Factor	3.00
Pressure Factor	1.00
Bare-Module Factor	1.8
CE Index	500
Equipment Bare-Module Cost	\$ 10,258.05

HX-106

To see ASPEN output for HX-106, please refer to the reboiler in COL-101.

Reboiler Duty	Q	276954	BTU/hr
Steam Temp	T _s	292	F
Bottoms Temp	T _b	179.4	F
ΔT		112.6	F
Heat Transfer Coeff.	U	150	BTU/hr ft ³ F
Area	A	16.40	ft ²

HX-106

EQUIPMENT COSTING	
Equipment Category	Heat Exchangers
Subtype 1	Double Pipe
Subtype 2	
Inner/Outer Pipe Material	Stainless Steel/Stainless Steel
Pressure	Select to use Pressure Factor
Bare-Module Type	Use Bare-Module Factor
Outer Surface Area of Inner Pipe,	16.4
Pressure, psig	6
Applicable Range	0 - 3,000 psig
Equipment Base f.o.b. Cost	\$ 1,985.38
Material Factor	3.00
Pressure Factor	1.00
Bare-Module Factor	1.8
CE Index	500
Equipment Bare-Module Cost	\$ 7,544.44

BLOCK: HX-107 MODEL: HEATER

 INLET STREAM: C-21
 OUTLET STREAM: C-22
 PROPERTY OPTION SET: NRTL

RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	5.67000	5.67000	0.00000
MASS(LB/HR)	568.646	568.646	0.00000
ENTHALPY(BTU/HR)	-873218.	-771139.	-0.116900

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	LB/HR
PRODUCT STREAMS CO2E	0.00000	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

*** INPUT DATA ***

TWO PHASE TP FLASH		
SPECIFIED TEMPERATURE	F	274.000
SPECIFIED PRESSURE	PSIA	14.7000
MAXIMUM NO. ITERATIONS		30
CONVERGENCE TOLERANCE		0.000100000

*** RESULTS ***

OUTLET TEMPERATURE	F	274.00
OUTLET PRESSURE	PSIA	14.700
HEAT DUTY	BTU/HR	0.10208E+06
OUTLET VAPOR FRACTION		0.82716
PRESSURE-DROP CORRELATION PARAMETER		0.58058E+08

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
WATER	0.14476E-03	0.12035E-04	0.17249E-03	14.330
OLEIC-01	0.15000	0.86748	0.80130E-04	0.92372E-04
1-BRO-01	0.10883	0.23490E-01	0.12666	5.3921
ISOPR-01	0.74103	0.10902	0.87309	8.0084

HX-107

Condenser Duty	Q	102079	BTU/hr
Cold In	$T_{C,i}$	180	F
Cold Out	$T_{C,o}$	274	F
Hot In	$T_{H,i}$	292	F
Hot Out	$T_{H,o}$	292	
Log Mean T Difference	T_{LM}	51.42	F
Heat Transfer Coeff.	U	150	BTU/hr ft ² F
Area	A	13.23	ft ²

HX-107

EQUIPMENT COSTING	
Equipment Category	Heat Exchangers
Subtype 1	Double Pipe
Subtype 2	
Inner/Outer Pipe Material	Stainless Steel/Stainless Steel
Pressure	Select to use Pressure Factor
Bare-Module Type	Use Bare-Module Factor
Outer Surface Area of Inner Pipe,	13.23
Pressure, psig	6
Applicable Range	0 - 3,000 psig
Equipment Base f.o.b. Cost	\$ 1,918.31
Material Factor	3.00
Pressure Factor	1.00
Bare-Module Factor	1.8
CE Index	500
Equipment Bare-Module Cost	\$ 7,289.56

BLOCK: HX-108 MODEL: HEATER

 INLET STREAM: C-23
 OUTLET STREAM: C-24
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	4.66463	4.66463	0.00000
MASS(LB/HR)	317.498	317.498	0.00000
ENTHALPY(BTU/HR)	-478201.	-569500.	0.160313

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	LB/HR
PRODUCT STREAMS CO2E	0.00000	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

*** INPUT DATA ***

TWO PHASE PV FLASH		
SPECIFIED PRESSURE	PSIA	14.7000
VAPOR FRACTION		0.0
MAXIMUM NO. ITERATIONS		30
CONVERGENCE TOLERANCE		0.000100000

*** RESULTS ***

OUTLET TEMPERATURE	F	164.98
OUTLET PRESSURE	PSIA	14.700
HEAT DUTY	BTU/HR	-91298.
OUTLET VAPOR FRACTION		0.0000
PRESSURE-DROP CORRELATION PARAMETER		0.0000

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
WATER	0.17287E-03	0.17287E-03	0.26049E-03	1.5069
OLEIC-01	0.52128E-04	0.52128E-04	0.43174E-10	0.82808E-06
1-BRO-01	0.12663	0.12663	0.36857	2.9105
ISOPR-01	0.87314	0.87314	0.63117	0.72287

HX-108

Condenser Duty	Q	91298	BTU/hr
Cold In	$T_{C,i}$	90	F
Cold Out	$T_{C,o}$	120	F
Hot In	$T_{H,i}$	264	F
Hot Out	$T_{H,o}$	264	
Log Mean T Difference	T_{LM}	158.53	F
Heat Transfer Coeff.	U	150	BTU/hr ft ² F
Area	A	3.84	ft ²

HX-108

EQUIPMENT COSTING	
Equipment Category	Heat Exchangers
Subtype 1	Double Pipe
Subtype 2	
Inner/Outer Pipe Material	Stainless Steel/Stainless Steel
Pressure	Select to use Pressure Factor
Bare-Module Type	Use Bare-Module Factor
Outer Surface Area of Inner Pipe,	3.84
Pressure, psig	6
Applicable Range	0 - 3,000 psig
Equipment Base f.o.b. Cost	\$ 1,573.84
Material Factor	3.00
Pressure Factor	1.00
Bare-Module Factor	1.8
CE Index	500
Equipment Bare-Module Cost	\$ 5,980.60

Appendix C

Continuous Economic Input Summary

Raw Materials: NPB & IPARAW MATERIAL: NPB

(continuous)

Initial amount of NPB: 25,038.3 lb
(per client/batch/truckload)

final NPB in co-solvent product: 24,839.5 lb

We lose: 198.8 lb (~ 4.14 lb NPB/hr)

* * per lb co-solvent product:

must add:

0.005 lb NPB / lb co-solvent product

NPB costs \$ 2.10/lb.

annual price of NPB as a raw material = \$ 32,800/yr

RAW MATERIAL: IPA

initial amount of IPA: 15,570 lb
(per client/batch/truckload)

final IPA outputted: 14,608 lb

We lose = 962 lb (~ 20.04 lb IPA/hr)

must add: 0.024 lb IPA / lb co-solvent prod

annual price =

\$ 107,927/yr

Raw Materials: Diesel Fuel for Transportation

Treat diesel fuel as raw material

8 hrs. of driving/day

1 shift/day, 1 driver/shift

assume truck gets 7 miles/gal ← Based on typical semi truck

assume drives ~ 180 miles/day (@ 8 hrs/day)

$$\frac{180 \text{ miles}}{\text{day}} \cdot \frac{\text{gal}}{7 \text{ miles}} \approx \boxed{25.7 \text{ gal/day}}$$

$$\sim 1.1 \text{ gal/hr}$$

↑
if normalized over a 24 hr
pd. (to compare w/
continuous process)

Price of Diesel fuel:

$$\$4.15/\text{gal} \quad (\text{as of } 3/26/12)$$

$$\$4.15/\text{gal} \cdot 1.1 \text{ gal/hr} = \$4.57/\text{hr} \quad \sim \boxed{\$36,155/\text{yr}} \quad \text{Basis of } 330 \text{ days/yr}$$

$$\text{Per lb of co-solvent product} = \boxed{0.0013 \text{ gal diesel fuel/lb product}}$$

Byproduct: Oleic Acid

$$\text{outlet flow rate} = 240.17 \text{ lb/hr}$$

$$\text{per lb of co-solvent product} = \frac{240.17 \text{ lb/hr}}{\text{hr}} \times \frac{\text{hr}}{823 \text{ lb prod}} = \boxed{0.30 \text{ lb oleic/lb prod}}$$

$$\frac{\text{ANNUAL COST}}{\text{REVENUE}} = 240.17 \text{ lb/hr} \times \frac{24 \text{ hr}}{\text{day}} \times \frac{330 \text{ day}}{\text{yr productm}} \times \frac{\$0.30}{\text{lb oleic acid}}$$

$$= \boxed{\$570,644/\text{yr}}$$

Product Selling Price Comparison: Batch vs. ContinuousProduct compositions - mole % of H_2O

continuous: 0.5%

Batch: 0.8%

our clients: 2 wks of cleaning until 7.5% water limit reached14 days for 7.5% H_2O ↳ water collected by IPA/NPB mixture at 0.5357% per day (by mole)For reclaimed IPA/NPB mixture from:

① Continuous:

0.5% water → 7.0% available

$$7\% \times \frac{\text{day}}{0.5357\%} = 13.1 \text{ days of collection}$$

② Batch:

0.8% water → 6.7% available

$$6.7\% \times \frac{\text{day}}{0.5357\%} = 12.5 \text{ days of collection}$$

Analysis

$$\frac{13.1 - 12.5}{12.5} \times 100 = 4.8\%$$

Conclusion:

The continuous process' product can be used 4.8% longer than the Batch product.

Profitability Input Summary – Continuous

Process Title: **Continuous Process - Senior Design Project #12**

Product: **Reclaimed Co-Solvent Mixture**

Plant Site Location:

Timeline:

Number of Years for Design	1
Number of Years for Construction	1
Number of Years for Production	10
Total Number of Years for Project	12
Start Year	2012
Site Factor	1.00

Continuous Operation:

Days per Year	330
OR	
Hours per Year	0
OR	
Operating Factor	0.0000

Discrete Operation:

Hours per Day	0
AND	
Days per Year	0
	0

Production Capacity	90% of Design Capacity
Start production at	60% of Production Capacity
Years to achieve full capacity	2

Number of Shifts	3
------------------	---

Depreciation Schedule	5 year
-----------------------	--------

Income Tax Rate	40%
Cost of Capital (for the NPV Calculation)	15% (discount rate)
General Inflation Rate	0%
Product Inflation Rate	0%
Variable Cost Inflation Rate	0%
Fixed Cost Inflation Rate	0%

Product Information:

Enter Product Units	<i>lb</i>
(i.e. lb, gram, gal, etc)	

Reclamation of Isopropyl Alcohol and N-Propyl Bromide

Wessels, Schwait, Mu, Deng

Raw Materials

Raw Material Unit:	Required Ratio:	Cost of Raw Material:
1 IPA lb	0.033 lb per lb of Reclaimed Co-Solvent Mixture	\$0.68 per lb
2 Diesel fuel gal	0.0013 gal per lb of Reclaimed Co-Solvent Mixture	\$4.15 per gal
<i>Total Weighted Average:</i>		\$0.03 per lb of Reclaimed Co-Solvent Mixture

Byproducts

Byproduct: Unit:	Ratio to Product	Byproduct Selling Price
1 Oleic Acid lb	0.3 lb per lb of Reclaimed Co-Solvent Mixture	\$0.30 per lb
<i>Total Weighted Average:</i>		\$0.09 per lb of Reclaimed Co-Solvent Mixture

Utilities

Utility: Unit:	Required Ratio	Utility Cost
1 High Pressure lb	lb per lb of Reclaimed Co-Solvent Mixture	per lb
2 Low Pressure lb	0.51 lb per lb of Reclaimed Co-Solvent Mixture	4.44E-03 per lb
3 Process Water gal	gal per lb of Reclaimed Co-Solvent Mixture	per gal
4 Cooling Water lb	14.6 lb per lb of Reclaimed Co-Solvent Mixture	1.40E-05 per lb
5 Electricity btu	3.30E+00 btu per lb of Reclaimed Co-Solvent Mixture	2.60E-05 per btu
<i>Total Weighted Average:</i>		2.56E-03 per lb of Reclaimed Co-Solvent Mixture

Other 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	↔	30 Days
Cash Reserves (excluding Raw Materials)	↔	30 Days
Accounts Payable	↔	30 Days
Reclaimed Co-Solvent Mixture Inventory	↔	4 Days
Raw Materials	↔	2 Days

Total Permanent Investment

	% of Total Permanent Investment
<u>Year:</u> 2013	100%
2014	0%
2015	0%
2016	0%

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

Equipment Costs

<u>Equipment Description</u>	<u>Type</u>	<u>Purchase Cost</u>	<u>Bare Module Factor</u>	<u>Bare Module Cost</u>
<u>Name</u>				
COL-101, Trayed Column	Fabricated Equipment	\$44,071	4.16	\$183,335
HX-106, Column Reboiler	Fabricated Equipment	\$2,057	4.00	\$8,228
P-103, Reboiler Pump	Other Equipment	\$627	3.30	\$2,069
Reflux Drum, ACC-101	Fabricated Equipment	\$15,676	3.05	\$47,812
Column Condenser, HX-105	Fabricated Equipment	\$2,798	4.00	\$11,192
HX-101	Fabricated Equipment	\$916	4.00	\$3,664
HX-102	Fabricated Equipment	\$1,604	4.00	\$6,416
D-101, Overhead Decanter	Fabricated Equipment	\$17,705	3.05	\$54,000
F-101, Flash Vessel	Fabricated Equipment	\$4,691	4.16	\$19,515
P-104	Other Equipment	\$413	3.20	\$1,322
P-102, Reflux Pump	Other Equipment	\$704	3.20	\$2,253
R-101, Feed Storage	Storage	\$25,000	1.00	\$25,000
P-101	Other Equipment	\$659	3.20	\$2,109
R-105, Condensate Collectio	Fabricated Equipment	\$1,000	1.00	\$1,000
R-104, Oil Storage	Storage	\$20,000	1.00	\$20,000
P-105	Other Equipment	\$599	3.20	\$1,917
P-107	Other Equipment	\$580	3.20	\$1,856
P-106	Other Equipment	\$571	3.20	\$1,827
P-110	Other Equipment	\$793	3.20	\$2,538
P-109	Other Equipment	\$722	3.20	\$2,310
P-108	Other Equipment	\$409	3.20	\$1,309
HX-103	Fabricated Equipment	\$1,225	4.00	\$4,900
R-102, Open Waste Tank	Storage	\$5,738	1.00	\$5,738
R-103, Product Storage	Storage	\$20,000	1.00	\$20,000
Spare Pumps (b.m. = 1)	Spares	\$6,077	1.00	\$6,077
HX-104	Fabricated Equipment	\$1,505	4.00	\$6,020
HX-107	Fabricated Equipment	\$1,987	4.00	\$7,948
HX-108	Fabricated Equipment	\$1,631	4.00	\$6,524
Truck	Other Equipment	\$200,000	1.50	\$300,000
Total				<u>756,878</u>

Fixed Costs

Operations

Operators per Shift:	2.33 (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:	4.50% of Total Depreciable Capital
Salaries and Benefits:	25.00% of Maintenance Wages and Benefits
Materials and Services:	100.00% of Maintenance Wages and Benefits
Maintenance Overhead:	5.00% 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:	2.00% 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 Plan	6.00% of	1.18 times the Allocated Costs for Utility Plants and Related Facilities

Other Annual Expenses

ental Fees (Office and Laboratory Space):	\$0
Licensing Fees:	\$0
Miscellaneous:	\$12,000

Depletion Allowance

Annual Depletion Allowance:	\$0
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Appendix D

Batch Sizing/Costing

Column/Reboiler/Condenser Sizing (per Mujtaba correlations) – Batch Process

DESIGN AND OPERATION OPTIMIZATION

- MUJTABA, CH.7

SAMPLE ITERATION CALCULATION FOR $N_T = 11$

CAPACITY FACTOR

$$CAP = \frac{\sum_{j=1}^{N_c} P_{rj}}{t_F + 0.5}$$

MW
 H₂O: 18.01
 NPB: 121.97
 OLE: 282.26
 IPA: 60.06

AT ROOM TEMP ρ [lb/ft³]
 H₂O: 62.428
 NPB: 84.465
 OLE: 55.973
 IPA: 49.068

$$CAP = \left(\frac{1}{6h + 0.5} \right) \left[\underset{REC 1}{32.4 \text{ lbmol}} + \underset{REC 2}{275.8 \text{ lbmol}} \right] = 47.415 \text{ lbmol/h}$$

$$V' = \frac{VF}{CAP} = \text{COLUMN VAPOR FLOWRATE}$$

$$= \left(\frac{153.537 \text{ lbmol}}{h} \right) \left(\frac{40.37 \text{ lbmol}}{h} \right) \left(\frac{h}{47.415 \text{ lbmol}} \right) = 130.724 \text{ lbmol/h}$$

$$DIA = \text{DIAMETER} = 2 \left(\frac{M_w V'}{\rho_v \pi V_m} \right)^{1/2}$$

$V_m = \text{MAXIMUM ALLOWABLE SUPERFICIAL VELOCITY, ft/s}$

$$V_m = K_v \left(\frac{P_c - P_v}{P_v} \right)^{1/2} = \left(\frac{0.3 \text{ ft}}{s} \right) \left[\frac{45.4501 \text{ lb/ft}^3 - 0.1893 \text{ lb/ft}^3}{0.1893 \text{ lb/ft}^3} \right]^{1/2} = 4.639 \text{ ft/s}$$

$$DIA = 2 \left[\left(\frac{69.420 \text{ lb}}{\text{lbmol}} \right) \left(\frac{130.724 \text{ lbmol}}{h} \right) \left(\frac{\text{ft}^3}{0.1893 \text{ lb}} \right) \left(\frac{1}{\pi} \right) \left(\frac{s}{4.639 \text{ ft}} \right) \left(\frac{1 \text{ h}}{3600 \text{ s}} \right) \right]^{1/2}$$

$$= \text{1.842 ft}$$

$$Q_{HEAT, MAX} = 7.28845 \text{ MM Btu/h}$$

$$Q_{COND, MAX} = -6.8808 \text{ MM Btu/h}$$

STEAM FLOWRATE = w

$$w_{max} = Q' / H_v = \left(\frac{7.28845 \times 10^6 \text{ Btu}}{915.5 \text{ Btu/lb}} \right) = 7961 \text{ lb/h}$$

steam heat
of vaporisation

$$A_{HEAT} = 422.325 \text{ ft}^2 \text{ PER ASPEN HEAT SUMMARY}$$

$$A_{CW} = \frac{Q_{CON}}{U \Delta T_{LM}} = \frac{6.8808 \text{ MM Btu/h}}{(120 \text{ Btu/h/ft}^2\text{F}) \Delta T_{LM}}$$

Column/Reboiler/Condenser Sizing (per Mujtaba correlations) – Batch Process

$$\Delta T_{LM, CW} = \frac{\Delta T_1 - \Delta T_2}{\ln(T_1/T_2)}$$

$$= \frac{(184.393 - 120) - (177.557 - 90)}{\ln\left[\frac{184.393 - 120}{177.557 - 90}\right]} = 75.383$$

$$A_{CW} = 760.65 \text{ ft}^2$$

CONDENSER/REBOILER EQUIPMENT COST

$$C = 10^3 (0.73 + 0.064 A^{0.65}) F_{EX}$$

↖ 3.00

CONDENSER COST (PURCHASE)

$$= \$16,514$$

REBOILER COST

$$= \$11,961$$

COLUMN COST

$$C_t = C_b F_M + N_T C_{bt} F_{TM} F_{TT} F_{NT} + C_{P1}$$

C_{bt} = COST OF TRAYS AS A FUNCTION OF DIAMETER

$$= 278.38 \exp(0.1739(\text{DIA})) = 383.36$$

C_{P1} = PLATFORM AND LADDER COST AS A FUNCTION OF DIAMETER

$$C_{P1} = 182.50 (\text{DIA})^{0.73960} L^{0.70684} = 3020.17$$

F_{NT} = COST FACTOR FOR NUMBER OF TRAYS

FOR $N_T < 20$

$$F_{NT} = \frac{2.25}{1.0414^{N_T}} = 1.440$$

$$F_{TT} = 1.0 \text{ SIEVE}$$

$$F_{TM}, F_M = 3.0$$

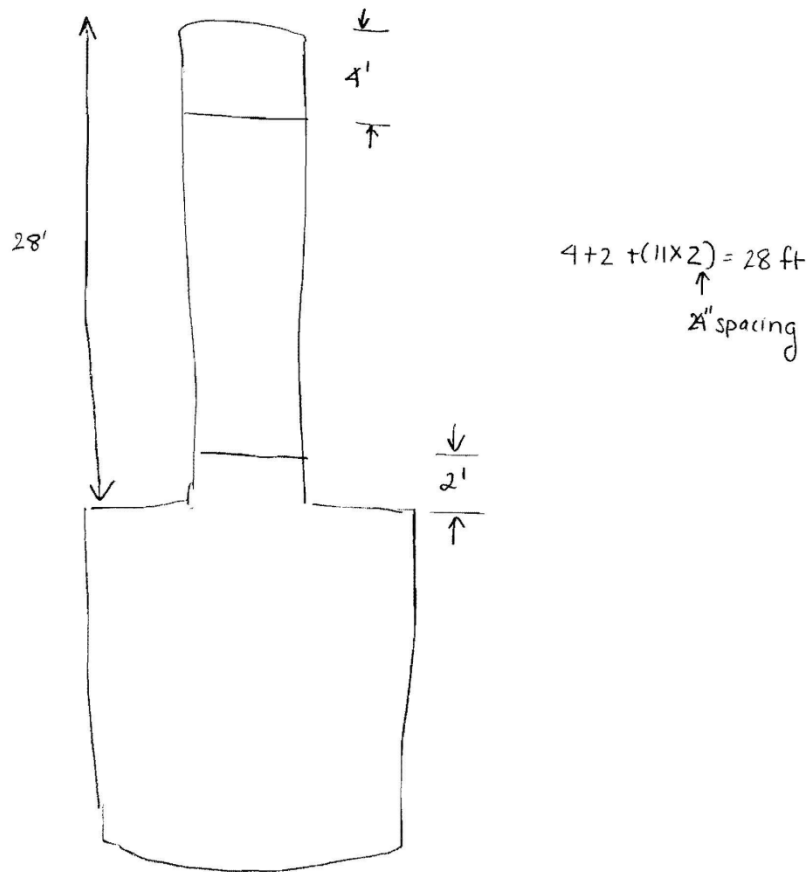
Column/Reboiler/Condenser Sizing (per Mujtaba correlations) – Batch Process

$$C_b = \exp[6.329 + 0.18255(\ln W_s) + 0.0229(\ln W_s)^2]$$

Where W_s = shell weight = 2653 lbs (per Seider's worksheet)

$$C_b = \exp[6.329 + 0.18255(2653) + 0.0229(2653)^2] = 9811.68$$

$$C_t = \textcircled{50,672}$$



Receiver Tanks Sizing/Costing – Batch ProcessCOSTING FOR CLOSED, CARBON STEEL TANKS

(B.M. factor = 1)

- 10,000 gal - \$20,000
- 5,000 gal - \$10,000
- 2,500 gal - \$5,000

* closed tanks not available in
capital cost estimation spreadsheet
* Based prices on market values

* Based on prices for used carbon tanks:

- \$ for used, 10,000 gallon tanks ranged from \$4,000 - \$10,000
- to be on the safe side, assumed we would purchase new carbon steel tanks at twice the maximum asking price for used tanks
- scaled down for ~~\$5,000 gal~~ & ~~\$2,500 gal~~

↑
5,000 gal range: \$2,000 - \$4,000

source

cited: www.bid-on-equipment.com ← to find market prices

Receiver Tanks Sizing/Costing – Batch Process

EQUIPMENT COSTING	
Equipment Category	Storage Tanks
Subtype 1	Open
Subtype 2	
Volume, V, gal	5000
Applicable Range	1,000 - 30,000 gal
Equipment Base f.o.b. Cost	\$ 8,289.55
Bare-Module Factor	1
CE Index	500
Equipment Bare-Module Cost	\$ 8,289.55
Notes/Base Case	See Page 588: Fiberglass

Receiver Tanks Sizing/Costing – Batch Process

VESSEL SIZING		
Vessel Type		Vessel Material (Cost)
Height/Length (ft)		Material Factor
Diameter (ft)		Vessel Cost -
Operating Pressure (psig)		Platforms & Ladders Cost -
Design Pressure (psig)	0	Tray/Packing?
Material (Stress)		
Design Temperature (F)		
Maximum Allowable Stress (psig)		
Minimum Wall Thickness		
Inside Diameter Range	Up to 4 ft	
Minimum Thickness (in.)	0.25	
Weld Efficiency		Total f.o.b. Purchase Cost
Wall Thickness Range		Bare-Module Factor
Efficiency		4.16
Estimated Wall Thickness (in.)		Total Bare-Module Cost
Corrosion Allowance (in.)	0.125	
Vessel Wall Thickness (in) -		
Enter Round Thickness (in.)		
Vessel Weight (lbs) - Eq. (22.59)		

Pot Sizing/Costing – Batch Process

EQUIPMENT COSTING	
Equipment Category	Storage Tanks
Subtype 1	Open
Subtype 2	
Volume, V, gal	
Applicable Range	1,000 - 30,000 gal
Equipment Base f.o.b. Cost	\$ -
Bare-Module Factor	1
CE Index	500
Equipment Bare-Module Cost	\$ -
Notes/Base Case	See Page 588: Fiberglass

Pot Sizing/Costing – Batch Process

VESSEL SIZING			
Vessel Type	Vertical	Vessel Material (Cost)	Stainless Steel 304
Height/Length (ft)	10	Material Factor	1.7
Diameter (ft)	10	Vessel Cost - Eq. (22.54)	\$ 83,831.25
Operating Pressure (psig)	1	Platforms & Ladders Cost - Eq. (22.56)	\$ 10,113.66
Design Pressure (psig)	10	Tray/Packing?	Neither
Material (Stress)	Carbon Steel (SA-285 Grade C)		
Design Temperature (F)	-20 to 650		
Maximum Allowable Stress (psig)	13750		
Minimum Wall Thickness			
Inside Diameter Range	8 - 10 ft		
Minimum Thickness (in.)	0.4375		
Weld Efficiency			
Wall Thickness Range	Up to 1.25 in.	Total f.o.b. Purchase Cost	\$ 93,944.91
Efficiency	0.85	Bare-Module Factor	4.16
Estimated Wall Thickness (in.)	0.0525		
Corrosion Allowance (in.)	0.125	Total Bare-Module Cost	\$ 390,810.84
Vessel Wall Thickness (in) - Eq. (22.60/22.62)	0.563		
Enter Round Thickness (in.)			
Vessel Weight (lbs) - Eq. (22.59)	13049		

Reflux Drum Sizing/Costing – Batch ProcessReflux Accumulator Sizing – Batch

largest flow rate through reflux drum = 96,812 lb/hr @ time = 1.56 hr

$$\dot{V} = 96,812 \frac{\text{lb}}{\text{hr}} \cdot \left[\frac{0.315}{(0.79)(62.4 \text{ lb/ft}^3)} + \frac{0.42}{(1.353)(62.4 \text{ lb/ft}^3)} + \frac{0.264}{(0.89)(62.4 \text{ lb/ft}^3)} + \frac{7.5 \times 10^{-4}}{62.4 \text{ lb/ft}^3} \right] \cdot \frac{7.48 \text{ gal}}{60 \text{ min}} \cdot \text{hr}$$

$$\dot{V} = 196 \text{ gpm} = 26.2 \text{ ft}^3/\text{min}$$

* Size reflux drum to hold twice the volume needed during a 5 min period

$$V(5 \text{ min}) = 131 \text{ ft}^3$$

reflux drum must hold 262 ft³

Heuristic: L/D ≈ 2

See Capital Cost Estimation Sheet + inputs →

L = 11 ft
D = 5.5 ft

Reflux Drum Sizing/Costing – Batch Process

EQUIPMENT COSTING	
Equipment Category	
Subtype 1	
Subtype 2	
Equipment Base f.o.b. Cost	
Bare-Module Factor	1
CE Index	500
Equipment Bare-Module Cost	
Notes/Base Case	

Reflux Drum Sizing/Costing – Batch Process

VESSEL SIZING			
Vessel Type	Horizontal	Vessel Material (Cost)	Stainless Steel 304
Height/Length (ft)	11	Material Factor	1.7
Diameter (ft)	5.512527188	Vessel Cost - Eq. (22.53)	\$ 41,107.71
Operating Pressure (psig)	0	Platforms & Ladders Cost - Eq. (22.55)	\$ 2,835.07
Design Pressure (psig)	0	Tray/Packing?	Neither
Material (Stress)	Carbon Steel (SA-285 Grade C)		
Design Temperature (F)	-20 to 650		
Maximum Allowable Stress (psig)	13750		
Minimum Wall Thickness			
Inside Diameter Range	4 - 6 ft		
Minimum Thickness (in.)	0.3125		
Weld Efficiency			
Wall Thickness Range	Up to 1.25 in.	Total f.o.b. Purchase Cost	\$ 43,942.78
Efficiency	0.85	Bare-Module Factor	3.05
Estimated Wall Thickness (in.)	0.0000		
Corrosion Allowance (in.)	0.125	Total Bare-Module Cost	\$ 134,025.48
Vessel Wall Thickness (in) - Eq. (22.60)	0.438		
Enter Round Thickness (in.)			
Vessel Weight (lbs) - Eq. (22.59)	4799		

Pump P-201 Sizing/Costing – Batch Process

EQUIPMENT COSTING	
Equipment Category	Pumps
Subtype 1	Centrifugal Pumps
Subtype 2	
Construction Material	Stainless Steel
Pump Type	3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 Hp
Bare-Module Type	Use Bare-Module Factor
Flow Rate, Q, gpm	171
Head, H, ft	38
Equipment Base f.o.b. Cost	\$ 3,108.98
Material Factor	2.00
Pump Type Factor	1.00
Bare-Module Factor	3.3
CE Index	500
Equipment Bare-Module Cost	\$ 13,368.62
Notes/Base Case	See Page 559: Includes base plate and driver coupling, but not electric motor

Pump P-201 Sizing/Costing – Batch Process

VESSEL SIZING		
Vessel Type		Vessel Material (Cost) Material Factor
Height/Length (ft) Diameter (ft)		Vessel Cost - Platforms & Ladders Cost -
Operating Pressure (psig) Design Pressure (psig)	0	Tray/Packing?
Material (Stress) Design Temperature (F) Maximum Allowable Stress (psig)		
Minimum Wall Thickness Inside Diameter Range Minimum Thickness (in.)	Up to 4 ft 0.25	
Weld Efficiency Wall Thickness Range Efficiency		Total f.o.b. Purchase Cost
Estimated Wall Thickness (in.) Corrosion Allowance (in.)	0.125	Bare-Module Factor Total Bare-Module Cost
Vessel Wall Thickness (in) - Enter Round Thickness (in.)		
Vessel Weight (lbs) - Eq. (22.59)		

4.16

Pump P-202 Sizing/Costing – Batch Process

EQUIPMENT COSTING	
Equipment Category	Pumps
Subtype 1	Centrifugal Pumps
Subtype 2	
Construction Material	Stainless Steel
Pump Type	3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 Hp
Bare-Module Type	Use Bare-Module Factor
Flow Rate, Q, gpm	178
Head, H, ft	41.47465438
Equipment Base f.o.b. Cost	\$ 3,141.73
Material Factor	2.00
Pump Type Factor	1.00
Bare-Module Factor	3.3
CE Index	500
Equipment Bare-Module Cost	\$ 13,509.44
Notes/Base Case	See Page 559: Includes base plate and driver coupling, but not electric motor

Pump-202 Sizing/Costing – Batch Process

VESSEL SIZING		
Vessel Type		Vessel Material (Cost) Material Factor
Height/Length (ft) Diameter (ft)		Vessel Cost - Platforms & Ladders Cost -
Operating Pressure (psig) Design Pressure (psig)	0	Tray/Packing?
Material (Stress) Design Temperature (F) Maximum Allowable Stress (psig)		
Minimum Wall Thickness Inside Diameter Range Minimum Thickness (in.)	Up to 4 ft 0.25	
Weld Efficiency Wall Thickness Range Efficiency		Total f.o.b. Purchase Cost
Estimated Wall Thickness (in.) Corrosion Allowance (in.)	0.125	Bare-Module Factor Total Bare-Module Cost
Vessel Wall Thickness (in) - Enter Round Thickness (in.)		4.16
Vessel Weight (lbs) - Eq. (22.59)		

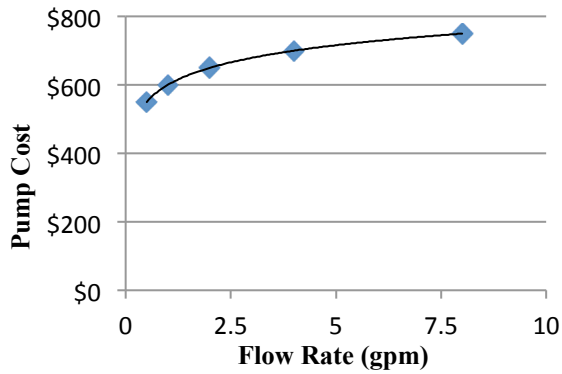
Pump P-203 Sizing/Costing – Batch Process

LOW-FLOW GEAR PUMP COSTING

Flow Rate (gpm)	Estimated Price
8	\$750
4	\$700
2	\$650
1	\$600
0.5	\$550

**Typical market prices for low-flow gear pumps found through Cole Palmer:

http://www.coleparmer.com/Category/Low_Flow_Gear_Pumps/20285



$$\text{\$Price} = 68.2 * \ln(\text{flow rate}) + 601.4$$

Pump P-204 Sizing/Costing - Batch Process

EQUIPMENT COSTING	
Equipment Category	Pumps
Subtype 1	Centrifugal Pumps
Subtype 2	
Construction Material	Cast Steel
Pump Type	3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 Hp
Bare-Module Type	Use Bare-Module Factor
Flow Rate, Q, gpm	482
Head, H, ft	58.33284723
Equipment Base f.o.b. Cost	\$ 3,920.72
Material Factor	1.35
Pump Type Factor	1.00
Bare-Module Factor	3.3
CE Index	500
Equipment Bare-Module Cost	\$ 14,310.63
Notes/Base Case	See Page 559: Includes base plate and driver coupling, but not electric motor

Pump P-204 Sizing/Costing - Batch Process

VESSEL SIZING		
Vessel Type		Vessel Material (Cost)
Height/Length (ft)		Material Factor
Diameter (ft)		Vessel Cost -
Operating Pressure (psig)		Platforms & Ladders Cost -
Design Pressure (psig)	0	Tray/Packing?
Material (Stress)		
Design Temperature (F)		
Maximum Allowable Stress (psig)		
Minimum Wall Thickness		
Inside Diameter Range	Up to 4 ft	
Minimum Thickness (in.)	0.25	
Weld Efficiency		
Wall Thickness Range		Total f.o.b. Purchase Cost
Efficiency		Bare-Module Factor
Estimated Wall Thickness (in.)		4.16
Corrosion Allowance (in.)	0.125	Total Bare-Module Cost
Vessel Wall Thickness (in) -		
Enter Round Thickness (in.)		
Vessel Weight (lbs) - Eq. (22.59)		

Pump P-205 Sizing/Costing – Batch Process

EQUIPMENT COSTING	
Equipment Category	Pumps
Subtype 1	Centrifugal Pumps
Subtype 2	
Construction Material	Stainless Steel
Pump Type	3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 Hp
Bare-Module Type	Use Bare-Module Factor
Flow Rate, Q, gpm	85.4
Head, H, ft	58
Equipment Base f.o.b. Cost	\$ 2,968.81
Material Factor	2.00
Pump Type Factor	1.00
Bare-Module Factor	3.3
CE Index	500
Equipment Bare-Module Cost	\$ 12,765.90
Notes/Base Case	See Page 559: Includes base plate and driver coupling, but not electric motor

Pump P-205 Sizing/Costing – Batch Process

VESSEL SIZING		
Vessel Type		Vessel Material (Cost)
Height/Length (ft)		Material Factor
Diameter (ft)		Vessel Cost -
Operating Pressure (psig)		Platforms & Ladders Cost -
Design Pressure (psig)	0	Tray/Packing?
Material (Stress)		
Design Temperature (F)		
Maximum Allowable Stress (psig)		
Minimum Wall Thickness		
Inside Diameter Range	Up to 4 ft	
Minimum Thickness (in.)	0.25	
Weld Efficiency		
Wall Thickness Range		Total f.o.b. Purchase Cost
Efficiency		Bare-Module Factor
Estimated Wall Thickness (in.)		4.16
Corrosion Allowance (in.)	0.125	Total Bare-Module Cost
Vessel Wall Thickness (in) -		
Enter Round Thickness (in.)		
Vessel Weight (lbs) - Eq. (22.59)		

Pump P-206 Sizing/Costing – Batch Process

EQUIPMENT COSTING	
Equipment Category	Pumps
Subtype 1	Centrifugal Pumps
Subtype 2	
Construction Material	Cast Steel
Pump Type	3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 Hp
Bare-Module Type	Use Bare-Module Factor
Flow Rate, Q, gpm	70
Head, H, ft	50
Equipment Base f.o.b. Cost	\$ 2,923.52
Material Factor	1.35
Pump Type Factor	1.00
Bare-Module Factor	3.3
CE Index	500
Equipment Bare-Module Cost	\$ 10,670.86
Notes/Base Case	See Page 559: Includes base plate and driver coupling, but not electric motor

Pump P-206 Sizing/Costing – Batch Process

VESSEL SIZING		
Vessel Type		Vessel Material (Cost)
Height/Length (ft)		Material Factor
Diameter (ft)		Vessel Cost -
Operating Pressure (psig)		Platforms & Ladders Cost -
Design Pressure (psig)	0	Tray/Packing?
Material (Stress)		
Design Temperature (F)		
Maximum Allowable Stress (psig)		
Minimum Wall Thickness		
Inside Diameter Range	Up to 4 ft	
Minimum Thickness (in.)	0.25	
Weld Efficiency		Total f.o.b. Purchase Cost
Wall Thickness Range		Bare-Module Factor
Efficiency		4.16
Estimated Wall Thickness (in.)		Total Bare-Module Cost
Corrosion Allowance (in.)	0.125	
Vessel Wall Thickness (in) -		
Enter Round Thickness (in.)		
Vessel Weight (lbs) - Eq. (22.59)		

Appendix E

Batch Economic Summary Inputs

Byproduct: Oleic Acid

output amt of oleic acid in R-204 : $(0.89)(46.3 \text{ lbmol}) = 41.21 \text{ lbmol}$

$$41.21 \text{ lbmol} \times \frac{282.3 \text{ lb}}{\text{lbmol}} = 11,633 \text{ lb oleic acid / batch}$$

$$\text{per lb of product} = \frac{11,633 \text{ lb oleic acid / batch}}{\left[0.544 \times \frac{60.1 \text{ lb}}{\text{lbmol}} + 6.448 \times \frac{122 \text{ lb}}{\text{lbmol}} + 0.839 \times \frac{18 \text{ lb}}{\text{lbmol}} \right] \cdot (457.7 \text{ lbmol})}$$

$$= \boxed{0.239 \text{ lb}^{\text{oleic}} / \text{lb product}}$$

$$\text{annual cost} = \frac{11,633 \text{ lb oleic}}{\text{Batch}} \times \frac{4 \text{ Batch}}{2 \text{ days}} \times \frac{330 \text{ prod. days}}{\text{Yr}} \times \frac{\$0.30}{\text{lb oleic acid}}$$

$$= \boxed{\$ 575,800}$$

Raw Materials: IPA & NPB① IPA

$$\text{Initial amt in feed} = 15,658 \text{ lb/Batch}$$

$$\text{final amt in R-202 (product)} = (0.544)(457.7 \text{ lbmal}) \times \frac{60.1 \text{ lb}}{\text{lbmal}} = 14,964 \frac{\text{lb IPA}}{\text{Batch}}$$

$$\text{amt. IPA lost} = 693.8 \text{ lb/batch}$$

$$\begin{aligned} \text{per lb product} &= \frac{693.8 \text{ lb IPA/batch}}{48,602 \text{ lb prod/batch}} \\ &= \boxed{0.014 \text{ lb IPA needed / lb product}} \end{aligned}$$

$$\begin{aligned} \text{annual cost of IPA} &= \frac{693.8 \text{ lb}}{\text{Batch}} \times \frac{1 \text{ Batch}}{2 \text{ days}} \times \frac{330 \text{ production days}}{\text{yr}} \times \frac{\$0.68}{\text{lb IPA}} \\ &= \boxed{\$77,800/\text{yr}} \end{aligned}$$

② NPB

$$\text{Initial amt in feed} = 25,038 \text{ lb/batch}$$

$$\text{NPB final amt in R-202} = (0.448)(457.7 \text{ lbmal}) \times \frac{121.97 \text{ lb NPB}}{\text{lbmal}} = 25,009 \frac{\text{lb NPB}}{\text{Batch}}$$

$$\text{amt lost (needed per Batch)} = 28.05 \text{ lb NPB needed/batch}$$

$$\begin{aligned} \text{per lb product} &= \frac{28.05 \text{ lb NPB/batch}}{48,602 \text{ lb prod/batch}} \\ &= \boxed{5.8 \times 10^{-4} \text{ lb NPB / lb prod}} \end{aligned}$$

$$\text{annual cost of NPB} = \boxed{\$9,700/\text{yr}}$$

Raw Material: Diesel Fuel for Transportation

Treat diesel fuel as raw material

8 hrs. of driving / day

1 shift / day, 1 driver / shift

assume truck gets 7 miles/gal ← Based on typical semi truck

assume drives ~ 180 miles/day (@ 8 hrs/day)

$$\frac{180 \text{ miles}}{\text{day}} \cdot \frac{\text{gal}}{7 \text{ miles}} \approx \boxed{25.7 \text{ gal/day}}$$

$$\sim 1.1 \text{ gal/hr}$$

↑
if normalized over a 24 hr
pd. (to compare w/
continuous process)

Price of Diesel fuel:

$$\$4.15 / \text{gal} \quad (\text{as of } 3/26/12)$$

$$\$4.15 / \text{gal} \cdot 1.1 \text{ gal/hr} = \$4.57 / \text{hr} \quad \sim \boxed{\$36,155 / \text{yr}} \quad \text{Basis of } 330 \text{ days/yr}$$

$$\text{Per lb of co-solvent product} = \boxed{0.0013 \text{ gal diesel fuel/lb product}}$$

Product Selling Price Comparison: Batch vs. ContinuousProduct compositions - mole % of H₂O

continuous: 0.5%

Batch: 0.8%

our clients: 2 wks of cleaning until 7.5% water limit reached14 days for 7.5% H₂O↳ water collected by IPA/NPB mixture at 0.5357% per day (by mole)For reclaimed IPA/NPB mixture from:

① Continuous:

0.5% water → 7.0% available

$$7\% \times \frac{\text{day}}{0.5357\%} = 13.1 \text{ days of collection}$$

② Batch:

0.8% water → 6.7% available

$$6.7\% \times \frac{\text{day}}{0.5357\%} = 12.5 \text{ days of collection}$$

Analysis

$$\frac{13.1 - 12.5}{12.5} \times 100 = 4.8\%$$

Conclusion:

The continuous process' product can be used 4.8% longer than the Batch product.

Profitability Input Summaries – Batch

Process Title: **Batch Process - Senior Design Project #12**

Product: **Reclaimed Co-solvent Mixture**

Plant Site Location: **NJ**

Timeline:

Number of Years for Design	1
Number of Years for Construction	1
Number of Years for Production	10
Total Number of Years for Project	12
Start Year	2012
Site Factor	1.00

Discrete Operation:

Hours per Day	6
AND	
Days per Year	330
	0.2260274

Production Capacity	90% of Design Capacity
Start production at	70% of Production Capacity
Years to achieve full capacity	1
Number of Shifts	1
Depreciation Schedule	5 year

Income Tax Rate	40%
Cost of Capital (for the NPV Calculation)	15%
General Inflation Rate	0%
Product Inflation Rate	0%
Variable Cost Inflation Rate	0%
Fixed Cost Inflation Rate	0%

Product Information:

Enter Product Units	<i>lb</i>
(i.e. lb, gram, gal, etc)	
Price Per Unit	\$0.42 /lb
Number of units per:	
Year	- per Year
OR	
Day	per Day
OR	
Hour	3,292 per Hour

Raw Materials

Raw Material:	Unit:	Required Ratio:	Cost of Raw Material:
1 IPA	lb	0.014 lb per lb of Reclaimed Co-solvent Mixture	\$0.68 per lb
2 Diesel Fuel	gal	0.0013 gal per lb of Reclaimed Co-solvent Mixture	\$4.15 per gal
3 NPB	lb	0.00058 lb per lb of Reclaimed Co-solvent Mixture	\$2.10 per lb
<i>Total Weighted Average:</i>			\$0.02 per lb of Reclaimed Co-solvent Mixture

Byproducts

Byproduct:	Unit:	Ratio to Product	Byproduct Selling Price
1 Oleic Acid	lb	0.239 lb per lb of Reclaimed Co-solvent Mixture	\$0.30 per lb
<i>Total Weighted Average:</i>			\$0.07 per lb of Reclaimed Co-solvent Mixture

Utilities

Utility:	Unit:	Required Ratio	Utility Cost
1 High Pressure Steam	lb	1.33 lb per lb of Reclaimed Co-solvent Mixture	7.11E-03 per lb
2 Low Pressure Steam	lb	lb per lb of Reclaimed Co-solvent Mixture	per lb
3 Process Water	gal	gal per lb of Reclaimed Co-solvent Mixture	per gal
4 Cooling Water	lb	20.3 lb per lb of Reclaimed Co-solvent Mixture	1.40E-05 per lb
5 Electricity	btu	5.28E+01 btu per lb of Reclaimed Co-solvent Mixture	2.60E-05 per btu
<i>Total Weighted Average:</i>			\$0.01 per lb of Reclaimed Co-solvent Mixture

Other 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	⇒	30 Days
Cash Reserves (excluding Raw Materials)	⇒	30 Days
Accounts Payable	⇒	30 Days
Reclaimed Co-solvent Mixture Inventory	⇒	4 Days
Raw Materials	⇒	2 Days

Total Permanent Investment

		% of Total Permanent Investment	
<u>Year:</u>	2013	100%	(default is first year of Construction, otherw
	2014	0%	
	2015	0%	
	2016	0%	

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 Investm
Cost of Land:	2.00% of Total Depreciable Capital
Cost of Royalties:	\$0
Cost of Plant Start-Up:	10.00% of Total Depreciable Capital

Equipment Costs

<u>Equipment Description</u> Name	<u>Type</u> (must be filled-in!)	<u>Purchase Cost</u>	<u>Bare Module Factor</u> (default 3.21 if blank)	<u>Bare Module Cost</u>
Distillation Column, COL-201	Fabricated Equipment	\$50,672	4.16	\$210,796
Pot Heater, HX-201	Fabricated Equipment	\$11,961	4.00	\$47,844
Column Condenser, HX-202	Fabricated Equipment	\$16,514	4.00	\$66,056
Reflux Drum, ACC-201	Fabricated Equipment	\$43,900	3.05	\$133,895
REC-201	Storage	\$5,738	1.00	\$5,738
REC-202	Storage	\$10,000	1.00	\$10,000
REC-204	Storage	\$10,000	1.00	\$10,000
Pump 203	Other Equipment	\$5,637	3.30	\$18,602
Pump 201	Other Equipment	\$3,109	3.30	\$10,260
Pump 202	Other Equipment	\$3,102	3.30	\$10,237
Spare Pumps	Other Equipment	\$21,661	1.00	\$21,661
Pot, POT-201	Fabricated Equipment	\$93,945	4.16	\$390,811
Pump 205	Other Equipment	\$2,969	3.30	\$9,798
REC-205	Storage	\$20,000	1.00	\$20,000
Pump 204	Other Equipment	\$3,920	3.30	\$12,936
REC-203	Other Equipment	\$10,000	1.00	\$10,000
Truck	Other Equipment	\$200,000	1.50	\$300,000
Pump 206	Other Equipment	\$2,924	3.30	\$9,649
REC-206	Storage	\$25,000	1.00	\$25,000
<u>Total</u>				<u>1,323,282</u>

Appendix F

Material Safety Data Sheets

Isopropyl alcohol msds:



Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet

Isopropyl alcohol MSDS

Section 1: Chemical Product and Company Identification

Product Name: Isopropyl alcohol Catalog Codes: SLI1153, SLI1579, SLI1906, SLI1246, SLI1432 CAS#: 67-63-0 RTECS: NT8050000 TSCA: TSCA 8(b) inventory: Isopropyl alcohol CI#: Not available. Synonym: 2-Propanol Chemical Name: isopropanol Chemical Formula: C3-H8-O	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
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Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Isopropyl alcohol	67-63-0	100

Toxicological Data on Ingredients: Isopropyl alcohol: ORAL (LD50): Acute: 5045 mg/kg [Rat]. 3600 mg/kg [Mouse]. 6410 mg/kg [Rabbit]. DERMAL (LD50): Acute: 12800 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:

Hazardous in case of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, sensitizer, permeator).

Potential Chronic Health Effects:

Slightly hazardous in case of skin contact (sensitizer). CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female, Development toxin [POSSIBLE]. The substance may be toxic to kidneys, liver, skin, central nervous system (CNS). 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. Get medical attention.

Skin Contact:

Wash with soap and water. Cover the irritated skin with an emollient. Get medical attention if irritation develops. Cold water may be used.

Serious Skin Contact: Not available.

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. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention if symptoms appear.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 399°C (750.2°F)

Flash Points: CLOSED CUP: 11.667°C (53°F) - 12.778 deg. C (55 deg. F) (TAG)

Flammable Limits: LOWER: 2% UPPER: 12.7%

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. 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. Explosive in presence of open flames and sparks, of heat.

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:

Vapor may travel considerable distance to source of ignition and flash back. CAUTION: MAY BURN WITH NEAR INVISIBLE FLAME. Hydrogen peroxide sharply reduces the autoignition temperature of Isopropyl alcohol. After a delay, Isopropyl alcohol ignites on contact with dioxigenyl tetrafluorborate, chromium trioxide, and potassium tert-butoxide. When heated to decomposition it emits acrid smoke and fumes.

Special Remarks on Explosion Hazards:

Secondary alcohols are readily autooxidized in contact with oxygen or air, forming ketones and hydrogen peroxide. It can become potentially explosive. It reacts with oxygen to form dangerously unstable peroxides which can concentrate and explode during distillation or evaporation. The presence of 2-butanone increases the reaction rate for peroxide formation. Explosive in the form of vapor when exposed to heat or flame. May form explosive mixtures with air. Isopropyl alcohol + phosgene forms isopropyl chloroformate and hydrogen chloride. In the presence of iron salts, thermal decomposition can occur, which in some cases can become explosive. A homogeneous mixture of concentrated peroxides + isopropyl alcohol are capable of detonation by shock or heat. Barium perchlorate + isopropyl alcohol gives the highly explosive alkyl perchlorates.

It forms explosive mixtures with trinitormethane and hydrogen peroxide. It produces a violent explosive reaction when heated with aluminum isopropoxide + crotonaldehyde. Mixtures of isopropyl alcohol + nitroform are explosive.

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. 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 away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Avoid contact with eyes. 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. 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: 983 STEL: 1230 (mg/m3) [Australia] TWA: 200 STEL: 400 (ppm) from ACGIH (TLV) [United States] [1999] TWA: 980 STEL: 1225 (mg/m3) from NIOSH TWA: 400 STEL: 500 (ppm) from NIOSH TWA: 400 STEL: 500 (ppm) [United Kingdom (UK)] TWA: 999 STEL: 1259 (mg/m3) [United Kingdom (UK)] TWA: 400 STEL: 500 (ppm) from OSHA (PEL) [United States] TWA: 980 STEL: 1225 (mg/m3) from OSHA (PEL) [United States] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor:

Pleasant. Odor resembling that of a mixture of ethanol and acetone.

Taste: Bitter. (Slight.)

Molecular Weight: 60.1 g/mole

Color: Colorless.

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

Boiling Point: 82.5°C (180.5°F)

Melting Point: -88.5°C (-127.3°F)

Critical Temperature: 235°C (455°F)

Specific Gravity: 0.78505 (Water = 1)

Vapor Pressure: 4.4 kPa (@ 20°C)

Vapor Density: 2.07 (Air = 1)

Volatility: Not available.

Odor Threshold:

22 ppm (Sittig, 1991) 700 ppm for unadapted panelists (Verschuren, 1983).

Water/Oil Dist. Coeff.: The product is equally soluble in oil and water; log(oil/water) = 0.1

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, methanol, diethyl ether, n-octanol, acetone.

Solubility:

Easily soluble in cold water, hot water, methanol, diethyl ether, n-octanol, acetone. Insoluble in salt solution. Soluble in benzene. Miscible with most organic solvents including alcohol, ethyl alcohol, chloroform.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, Ignition sources, incompatible materials

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

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:

Reacts violently with hydrogen + palladium combination, nitroform, oleum, COCl₂, aluminum triisopropoxide, oxidants
Incompatible with acetaldehyde, chlorine, ethylene oxide, isocyanates, acids, alkaline earth, alkali metals, caustics, amines, crotonaldehyde, phosgene, ammonia. Isopropyl alcohol reacts with metallic aluminum at high temperatures. Isopropyl alcohol attacks some plastics, rubber, and coatings. Vigorous reaction with sodium dichromate + sulfuric acid.

Special Remarks on Corrosivity: May attack some forms of plastic, rubber and coating

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): 3600 mg/kg [Mouse]. Acute dermal toxicity (LD50): 12800 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 16000 8 hours [Rat].

Chronic Effects on Humans:

CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC.
DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female, Development toxin [POSSIBLE]. May cause damage to the following organs: kidneys, liver, skin, central nervous system (CNS).

Other Toxic Effects on Humans:

Hazardous in case of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, sensitizer, permeator).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:

May cause adverse reproductive/teratogenic effects (fertility, fetotoxicity, developmental abnormalities (developmental toxin)) based on animal studies. Detected in maternal milk in human.

Special Remarks on other Toxic Effects on Humans:

Acute Potential Health Effects: Skin: May cause mild skin irritation, and sensitization. Eyes: Can cause eye irritation.
Inhalation: Breathing in small amounts of this material during normal handling is not likely to cause harmful effects. However, breathing large amounts may be harmful and may affect the respiratory system and mucous membranes (irritation), behavior and brain (Central nervous system depression - headache, dizziness, drowsiness, stupor, incoordination, unconsciousness, coma and possible death), peripheral nerve and sensation, blood, urinary system, and liver. Ingestion: Swallowing small amounts during normal handling is not likely to cause harmful effects. Swallowing large amounts may be harmful. Swallowing large amounts may cause gastrointestinal tract irritation with nausea, vomiting and diarrhea, abdominal pain. It also may affect the urinary system, cardiovascular system, sense organs, behavior or central nervous system (somnia, generally depressed activity, irritability, headache, dizziness, drowsiness), liver, and respiratory system (breathing difficulty). Chronic Potential Health Effects: May cause defatting of the skin and dermatitis and allergic reaction. May cause adverse reproductive effects based on animal data (studies).

Section 12: Ecological Information

Ecotoxicity: Ecotoxicity in water (LC50): 100000 mg/l 96 hours [Fathead Minnow]. 64000 mg/l 96 hours [Fathead Minnow].

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 product itself and its products of degradation are not toxic.

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: : Isopropyl Alcohol UNNA: 1219 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information**Federal and State Regulations:**

Connecticut hazardous material survey.: Isopropyl alcohol Illinois toxic substances disclosure to employee act: Isopropyl alcohol Rhode Island RTK hazardous substances: Isopropyl alcohol Pennsylvania RTK: Isopropyl alcohol Florida: Isopropyl alcohol Minnesota: Isopropyl alcohol Massachusetts RTK: Isopropyl alcohol New Jersey: Isopropyl alcohol New Jersey spill list: Isopropyl alcohol Director's list of Hazardous Substances: Isopropyl alcohol Tennessee: Isopropyl alcohol TSCA 8(b) inventory: Isopropyl alcohol TSCA 4(a) final testing order: Isopropyl alcohol TSCA 8(a) IUR: Isopropyl alcohol TSCA 8(d) H

and S data reporting: Isopropyl alcohol: Effective date: 12/15/86 Sunset Date: 12/15/96 TSCA 12(b) one time export: Isopropyl alcohol SARA 313 toxic chemical notification and release reporting: Isopropyl alcohol

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-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):

R11- Highly flammable. R36- Irritating to eyes. S7- Keep container tightly closed. S16- Keep away from sources of ignition - No smoking. S24/25- Avoid contact with skin and eyes. S26- In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

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

Health: 1

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

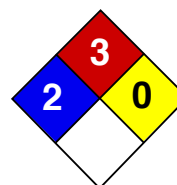
References: Not available.

Other Special Considerations: Not available.

Created: 10/09/2005 05:53 PM

Last Updated: 11/01/2010 12:00 PM

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Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet

1-Bromopropane MSDS

Section 1: Chemical Product and Company Identification

Product Name: 1-Bromopropane	Contact Information:
Catalog Codes: SLB2914	Sciencelab.com, Inc. 14025 Smith Rd. Houston, Texas 77396
CAS#: 106-94-5	US Sales: 1-800-901-7247 International Sales: 1-281-441-4400
RTECS: TX4110000	Order Online: ScienceLab.com
TSCA: TSCA 8(b) inventory: 1-Bromopropane	CHEMTREC (24HR Emergency Telephone), call: 1-800-424-9300
CI#: Not available.	International CHEMTREC, call: 1-703-527-3887
Synonym: n-Propyl bromide; Propyl bromide	For non-emergency assistance, call: 1-281-441-4400
Chemical Name: 1-Bromopropane	
Chemical Formula: C ₃ H ₇ Br	

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{1-}Bromopropane	106-94-5	100

Toxicological Data on Ingredients: 1-Bromopropane: VAPOR (LC50): Acute: 253000 mg/m 0.5 hours [Rat].

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).

Potential Chronic Health Effects:

CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to blood, liver, central nervous system (CNS). 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. Get medical attention.

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. Cold water may be used. 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.

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 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: 490°C (914°F)

Flash Points:

CLOSED CUP: 22°C (71.6°F). - Sigma-Aldrich CLOSED CUP: 25.5 c(78 F) - Chemical Hazard Response Information System (CHRIS)

Flammable Limits: LOWER: 4.6% UPPER: 7.8%

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

Fire Hazards in Presence of Various Substances: Flammable in presence of open flames and sparks.

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. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards: When heated to decomposition it emits highly toxic fumes of Hydrogen Bromide.

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. 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.

Section 7: Handling and Storage**Precautions:**

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.

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: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Not available.

Taste: Not available.

Molecular Weight: 123 g/mole

Color: Colorless. Clear

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

Boiling Point: 71°C (159.8°F) - @ 760 mm Hg

Melting Point: -110°C (-166°F)

Critical Temperature: Not available.

Specific Gravity: 1.353 (Water = 1)

Vapor Pressure: 14.8 kPa (@ 20°C)

Vapor Density: 4.25 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

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:

Soluble in cold water, diethyl ether, acetone. Soluble in Ethanol. Solubility in water: 2.5 g/l @ 20 deg. C

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.
Corrosivity: Non-corrosive in presence of glass.
Special Remarks on Reactivity: Not available.
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 toxicity of the vapor (LC50): 253000 mg/m³ 0.5 hours [Rat].
Chronic Effects on Humans: May cause damage to the following organs: blood, liver, central nervous system (CNS).
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:
Lowest Published Lethal Dose/Conc: LDL [Rat] - Route: Oral; Dose: 4000 mg/kg
Special Remarks on Chronic Effects on Humans: May cause adverse reproductive effects based on animal test data
Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes eye irritation. Eyes: Causes eye irritation. Inhalation: It may cause respiratory tract and mucous membrane irritation and may affect respiration. Vapors may cause dizziness and suffocation. Inhalation of high concentrations may affect behavior/central nervous system (CNS depression) characterized by nausea, headache, dizziness, somnolence, unconsciousness and coma. It may also cause liver and kidney damage, lung injury, weight loss/anorexia, bone marrow changes, and blood abnormalities

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: : Bromopropanes UNNA: 2344 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:

Pennsylvania RTK: 1-Bromopropane Florida: 1-Bromopropane Massachusetts RTK: 1-Bromopropane TSCA 8(b) inventory: 1-Bromopropane

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).

DSCL (EEC):

R10- Flammable. R20- Harmful by inhalation. S9- Keep container in a well-ventilated place. S24- Avoid contact with skin.

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:

Ariel Global View Sigma-Aldrich Registry of Toxic Effects of Chemical Substances (RTECS) Chemical Hazard Response Information System

Other Special Considerations: Not available.

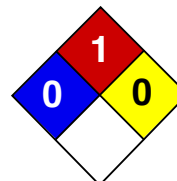
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Oleic acid MSDS:



Health	1
Fire	1
Reactivity	0
Personal Protection	J

Material Safety Data Sheet

Oleic acid MSDS

Section 1: Chemical Product and Company Identification

Product Name: Oleic acid Catalog Codes: SLO1078, SLO1318 CAS#: 112-80-1 RTECS: RG2275000 TSCA: TSCA 8(b) inventory: Oleic acid CI#: Not available. Synonym: 9-Octadecenoic acid Chemical Name: (Z)-9-Octadecenoic Acid Chemical Formula: C18H34O2	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
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Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Oleic acid	112-80-1	100

Toxicological Data on Ingredients: Oleic acid: ORAL (LD50): Acute: 25000 mg/kg [Rat]. 28000 mg/kg [Mouse].

Section 3: Hazards Identification

Potential Acute Health Effects: Slightly hazardous in case of skin contact (irritant, permeator), of eye contact (irritant), of ingestion, of inhalation.

Potential Chronic Health Effects:

CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. Repeated or prolonged exposure is not known to aggravate medical condition.

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. Get medical attention.

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 medical attention.

Inhalation:

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

Serious Inhalation: Not available.

Ingestion:

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 if symptoms appear.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.

Auto-Ignition Temperature: 363°C (685.4°F)

Flash Points: CLOSED CUP: 188.89°C (372°F). OPEN CUP: 198.89°C (390°F) - 218.33 C (425 F).

Flammable Limits: Not available.

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

Fire Hazards in Presence of Various Substances:

Slightly flammable to flammable in presence of heat. 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.

Fire Fighting Media and Instructions:

SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

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

Large Spill:

If the product is in its solid form: Use a shovel to put the material into a convenient waste disposal container. If the product is in its liquid form: Absorb with an inert material and put the spilled material in an appropriate waste disposal. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system.

Section 7: Handling and Storage

Precautions:

Keep away from heat. Keep away from sources of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Wear suitable protective clothing. 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.

Storage:

Keep container tightly closed. Keep container in a cool, well-ventilated area. Sensitive to light. Store in light-resistant containers. Air Sensitive

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. Gloves.

Personal Protection in Case of a Large Spill:

Splash goggles. Full suit. Boots. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Peculiar Lard-Like odor

Taste: Not available.

Molecular Weight: 282.47 g/mole

Color: Colorless to light yellow.

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

Boiling Point: 286.11°C (547°F)

Melting Point: 16.3°C (61.3°F)

Critical Temperature: Not available.

Specific Gravity: 0.895 (Water = 1)

Vapor Pressure: Not available.

Vapor Density: 9.7(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, diethyl ether, acetone.

Solubility:

Soluble in methanol, diethyl ether, acetone. Insoluble in cold water. Soluble in chloroform, most organic solvents, benzene, alcohol, carbon tetrachloride, and fixed and volatile oils.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Excess heat

Incompatibility with various substances: Reactive with oxidizing agents.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:

Air and light sensitive. On exposure to air, especially when impure, it oxidizes and acquires a yellow to brown color and rancid odor. Also incompatible with perchloric acid, and powdered aluminum.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Eye contact.

Toxicity to Animals: Acute oral toxicity (LD50): 25000 mg/kg [Rat].

Chronic Effects on Humans: Not available.

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

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:

Human: passes the placental barrier, detected in maternal milk. May cause cancer based on animal test data. No human data found. May affect genetic material (mutagenic).

Special Remarks on other Toxic Effects on Humans:

Acute Potential Health Effects: Skin: Causes skin irritation. Eyes: May cause eye irritation. Ingestion: May cause digestive tract irritation. It is expected to be a low hazard for usual industrial handling. Inhalation: May cause respiratory tract irritation. It is expected to be a low hazard to usual industrial handling. Note: According the Registry of Toxic Effects of Chemicals, when Oleic acid was administered to rats and mice through intravenous injection, behavior and respiration were affected.

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 product itself and its products of degradation are not toxic.

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: Not a DOT controlled material (United States).

Identification: Not applicable.

Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

Federal and State Regulations:

Rhode Island RTK hazardous substances: Oleic acid Pennsylvania RTK: Oleic acid TSCA 8(b) inventory: Oleic acid

Other Regulations: EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada): Not controlled under WHMIS (Canada).

DSCL (EEC):

R36/38- Irritating to eyes and skin. S24/25- Avoid contact with skin and eyes. S28- After contact with skin, wash immediately with plenty of water. S35- This material and its container must be disposed of in a safe way. S37- Wear suitable gloves.

HMIS (U.S.A.):

Health Hazard: 1

Fire Hazard: 1

Reactivity: 0

Personal Protection: j

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

Health: 0

Flammability: 1

Reactivity: 0

Specific hazard:

Protective Equipment:

Gloves. Lab coat. Not applicable. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/11/2005 01:35 PM

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Appendix G

Equilibrium Data

ASPEN SPLIT ANALYSIS

AZEOTROPE SEARCH REPORT

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

Mixture Investigated For Azeotropes At A Pressure Of 14.7 PSI

Comp 10	Component Name	Classification	Temperature
WATER	WATER	Stable Node	100.03 C
1-BR0-01	1-BROMOPROPANE	Stable Node	70.99 C
ISOPR-'01	ISOPROPYL-ALCOHOL	Stable Node	82.06 C

4 Azeotropes Sorted by Temperature

01	Number Of Components: 2	Temperature 62.81 C		
	Heterogeneous	Classification: Saddle		
		MOLE BASIS	MASS BASIS	
		WATER	0.2247	0.0407
		1-BR0-01	0.7753	0.9593

02	Number Of Components: 3	Temperature 59.49 C		
	Heterogeneous	Classification: Unstable Node		
		MOLE BASIS	MASS BASIS	
		WATER	0.1779	0.0348
		1-BR0-01	0.6289	0.8392
		ISOPR-01	0.1932	0.1260

03	Number Of Components: 2	Temperature 80.15 C		
	Homogeneous	Classification: Saddle		
		MOLE BASIS	MASS BASIS	
		WATER	0.3251	0.1262
		ISOPR-01	0.6749	0.8738

04	Number Of Components: 2	Temperature 64.72 C	
	Homogeneous	Classification: Saddle	
		MOLE BASIS	MASS BASIS
	1-BR0-01	0.7215	0.8413
	ISOPR-01	0.2785	0.1587

ASPEN SPLIT ANALYSIS

AZEOTROPE SEARCH REPORT

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

*Mixture Investigated For Azeotropes At A
Pressure Of 14.7 PSI*

Comp 10	Component Name	Classification	Temperature
OLEIC	OLEIC-ACID	Stable Node	360.05 C
1-BR0-01	1-BROMOPROPANE	Saddle	70.99 C
ISOPR-01	ISOPROPYL-ALCOHOL	Saddle	82.06 C

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01	Number Of Components:2	Temperature 64.72 C	
	Homogeneous	Classification: Unstable Node	
		MOLE BASIS	MASS BASIS
	1-BR0-01	0.7215	0.8413
	ISOPR-01	0.2785	0.1587

ASPEN SPLIT ANALYSIS

AZEOTROPE SEARCH REPORT

PhysicalProperty Model: NRTL-RK Valid
Phase: VAP-LIQ-LIQ

*Mixture Investigated For Azeotropes At A
Pressure Of 14.7 PSI*

Comp 10	Component Name	Classification	Temperature
OLEIC	OLEIC-ACID	Stable Node	360.05 C
1-BR0-01	1.,BROMOPROPANE	Saddle	70.99 C
WATER	WATER	Stable Node	100.03 C

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01	Number Of Components: 2	Temperature 62.81 C	
	Heterogeneous	Classification: Unstable Node	
		MOLE BASIS	MASS BASIS
	1-BR0-01	0.7753	0.9593
	WATER	0.2247	0.0407

ASPEN SPLIT ANALYSIS

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

Mixture Investigated For Azeotropes At A Pressure Of 14.7 PSI

CompID	Component Name	Classification	Temperature
OLEIC	OLEIC-ACID	Stable Node	360.05 C
ISOPR-01	ISOPROPYL-ALCOHOL	Saddle	82.06 C
WATER	WATER	Stable Node	100.03 C

01	Number Of Components: 2	Temperature 80.15 C	
	Homogeneous	Classification: Unstable Node	
		MOLE BASIS	MASS BASIS
		ISOPR-01	0.6749
	WATER	0.3251	0.1262