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Process Design for the Production of N-Butanol from Ethanol

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Abstract
This project aims to produce n-butanol from ethanol using a catalyst and pressurized hydrogen. Our process converts 100MM gallons of ethanol to 71.4 MM gallons of 95% pure butanol per year. The fixed-bed catalytic reactor contains spherical pellets of Ru(acac)3 with a void fraction of 0.391, and operates at 374 °F and 725 psi. Following the reaction, the hydrogen is removed from the product stream using two flash separation units before being recycled to the reactor. The butanol product is then taken from the bottoms of a distillation tower. The remaining ethanol and water are separated using two distillation units and ethylene glycol as an entrainer. The plant will be located in Iowa, U.S.A. where an adjoining ethanol plant uses corn as a feedstock for its process.

Since this project assumes a future market for butanol biofuel, and our process uses ethanol as a feedstock, the price of butanol is assumed to be some multiple of the ethanol price. At the current ethanol price, assuming that butanol is 1.5 times the price of ethanol, our process is not profitable. It was found that in order to have a positive Net Present Value after 15 years, the price of butanol would need to be 2.225 times the price of ethanol, which would currently be $6.54 per gallon of butanol. Therefore, while profitability is not achievable in the current market, this process should be seriously considered in the future due to the high volatility of biofuel prices and policies.

Disciplines
Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering

Process Design for the Production of N-Butanol from Ethanol

Design Project By:

Shawna Downing
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Presented To:

Professor Leonard Fabiano
Dr. Robert Riggleman

April 15, 2014
Department of Chemical and Biomolecular Engineering
University of Pennsylvania
School of Engineering and Applied Science

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Professor Leonard Fabiano
Dr. Robert Riggleman
University of Pennsylvania
School of Engineering and Applied Science
Department of Chemical and Biomolecular Engineering

Dear Professor Fabiano and Dr. Riggleman,

We are pleased to present our completion of the *Ethanol to Butanol* project proposed by Mr. Bruce Vrana. Our plant, located in Iowa, is designed to produce 71.4 MM gallons of butanol (95% pure) per year from 100MM gallons of ethanol produced in an adjoining plant. The conversion is achieved using the Guerbet reaction path which requires a $Ru(acac)_3$ catalyst and pressurized hydrogen. The reaction will take place in a packed bed reactor with spherical catalytic pellets at 725 psi and 374 °F. The products leaving the reactor are separated using flash vessels, distillation units, and ethylene glycol as an entrainer. The ethanol and hydrogen are recycled to ensure maximum conversion.

This method of butanol production would compete with two current methods of production, namely the reaction from propylene and the direct fermentation from biomaterials. It is expected to supply butanol as a biofuel addition to gasoline and diesel engines, much as ethanol is used today. This market for butanol has yet to develop, and the profitability of our process is highly dependent on its relative price to ethanol.

We have determined that at current prices of raw materials and products, the process would not be profitable. It was found that in order to have a positive Net Present Value after 15 years, the price of butanol would need to be 2.225 times the price of ethanol, which would currently be $6.54 per gallon of butanol. However, provided that the market outlook is positive in the future, this plant has potential to achieve a strong hold on this emerging market.

Sincerely,

Shawna Downing	Catharine Haak	Nader Jouzy	Kyle Sarnataro

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Section I

Abstract

Abstract

This project aims to produce n-butanol from ethanol using a catalyst and pressurized hydrogen. Our process converts 100MM gallons of ethanol to 71.4 MM gallons of 95% pure butanol per year. The fixed-bed catalytic reactor contains spherical pellets of $Ru(acac)_3$ with a void fraction of 0.391, and operates at 374 °F and 725 psi. Following the reaction, the hydrogen is removed from the product stream using two flash separation units before being recycled to the reactor. The butanol product is then taken from the bottoms of a distillation tower. The remaining ethanol and water are separated using two distillation units and ethylene glycol as an entrainer. The plant will be located in Iowa, U.S.A. where an adjoining ethanol plant uses corn as a feedstock for its process.

Since this project assumes a future market for butanol biofuel, and our process uses ethanol as a feedstock, the price of butanol is assumed to be some multiple of the ethanol price. At the current ethanol price, assuming that butanol is 1.5 times the price of ethanol, our process is not profitable. It was found that in order to have a positive Net Present Value after 15 years, the price of butanol would need to be 2.225 times the price of ethanol, which would currently be $6.54 per gallon of butanol. Therefore, while profitability is not achievable in the current market, this process should be seriously considered in the future due to the high volatility of biofuel prices and policies.

Section II

Introduction

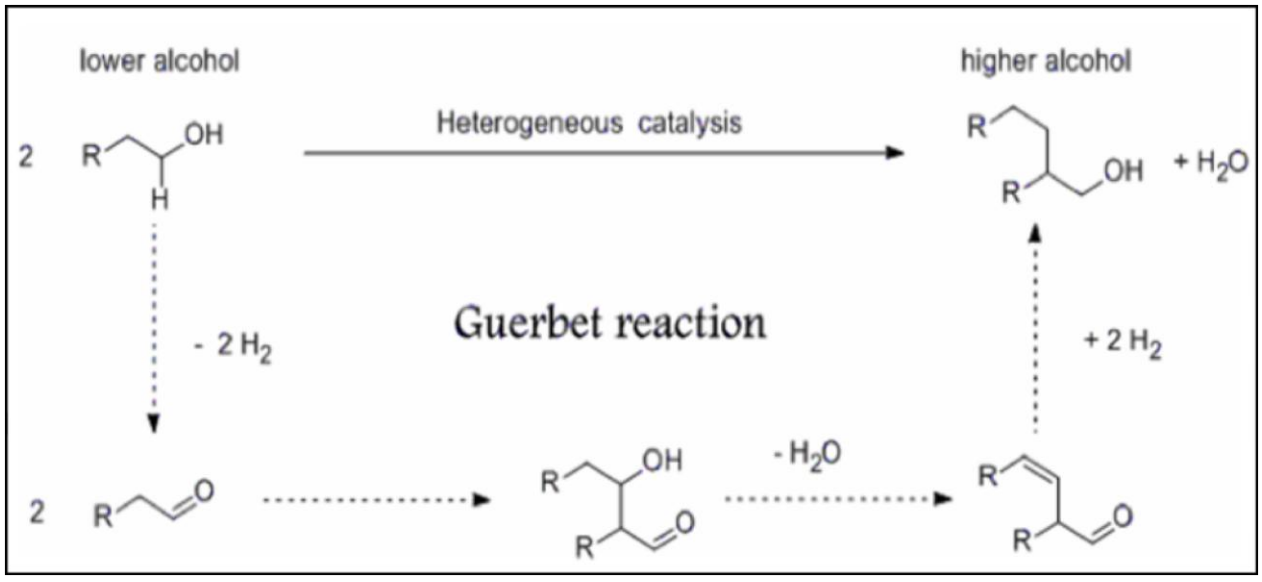
Introduction

This process focuses on using ethanol to produce n-butanol via the Guerbet reactions as an alternative to fermentation. Our goal is to use 100 MM gallons per year of ethanol to produce 71.4 MM gallons per year of butanol. U.S. Patent 8,318,990 (Tanaka and Utsunomiya) has been used as the basis for the design of this process and plant, with several assumptions and optimizations to the process. The net reaction of ethanol to produce n-butanol is shown here.

$$2CH_3CH_2OH \xrightarrow{H_2} H_2O + CH_3(CH_2)_3OH$$

The overall reaction is more extensive, and has the possibility of producing several side products that are part of our overall final product. The full mechanism, assuming ethanol is the starting lower alcohol, is shown in Figure 2.1.

Figure 2.1. Guerbet reaction mechanism.



From the patent, we determined the most efficient catalyst to be $Ru(acac)_3$. This catalyst will be present in the form of spherical packing in a packed bed reactor. The reaction is exothermic and has a selectivity of butanol of approximately 90%, and a single pass yield of approximately 20%, depending on the partial pressure of hydrogen gas in the reactor. Major side products of this reaction include 2-ethylbutanol, 2-ethylhexanol, n-hexanol, and n-octanol.

The goal of our project is to use this reaction to produce butanol for fuel and build a plant that meets safety and environmental regulations at the local, state, and federal levels for the chosen location. The ethanol for this process will be provided by an adjunct ethanol-producing plant. One hundred percent of the plant's ethanol production will go directly to the butanol plant. In order to optimize cost and productivity, there were four possible choices for location: rural Brazil, industrial Brazil, rural United States, or industrial United States. Each of these locations provided us with different opportunities and challenges that will be addressed in the coming report.

Section III

Project Charter

Project Charter

Project Name: Process Design for the Production of N-Butanol from Ethanol

Project Champions: Mr. Bruce Vrana, Professor Leonard Fabiano, Dr. Robert Riggleman

Team Members: Catharine Haak, Kyle Sarnataro, Nader Jouzy, Shawna Downing

Specific Goal:

To produce a profitable process for the production of butanol by converting it from ethanol through Guerbet reactions with the aid of a catalyst.

Considerations: Use the entire 100MM gal/yr of ethanol from an existing plant
To choose the ideal location to build a plant and carry out this process
- Rural or industrial area
- United States or Brazil

Project Scope: *In Scope*
- Butanol for addition to gasoline
- Use 100MM gal/yr ethanol

Out of Scope
- Production of ethanol
- Manufacture of the catalyst
- Determination of butanol market

Deliverables: Process feasibility assessment
Economic assessment
Technical assessment

Timeline: Completion of project in April 2014

Section IV

Concept Assessment

Background

Butanol is mainly used as an intermediate in industrial chemical manufacturing processes. Its downstream applications include the production of butyl acetate, butyl acrylate, glycol ethers, resins and plasticizers. (Research and Markets) It is also used directly as a solvent for industrial applications such as paint thinners, coatings, textiles, and hydraulic fluids.

In 1916, industrial production of butanol began as a side product in the manufacture of acetone for use in WWI. The process used direct fermentation, using the bacteria strain *clostridium acetobutylicum*, to convert biomass to acetone, butanol, and ethanol. The process was named ABE after these main products. At first, the butanol was ignored until it was realized that adding nitrocellulose created a quick-drying lacquer. Soon, its many other useful properties were discovered and production increased dramatically due to its use in synthetic rubber during WWII. (Biobutanol)

Until the 1950s, the ABE process was still the major method of production, using mainly corn and molasses as feedstocks. Since that time, oil has been cheaper than sugar in the US, so the fermentation route gave way to another process that uses propylene as the reactant. This process reacts propylene with syngas to produce n-butyraldehyde in a low-pressure, catalytic reactor. This intermediate is then hydrogenated to n-butanol. Currently, this is the main method of industrial butanol production. However, companies have recently been reexamining the direct fermentation route using different bacteria and improved process efficiencies.

Market Analyses

The global butanol demand is increasing, especially due to growing demand in Asia-Pacific. In 2012, China consumed 34.8% of the global n-butanol. (Research and Markets) Butanol is mainly produced and exported from Europe and North America, and is used for the industrial products and manufacturing purposes mentioned above.

Our project aims to produce butanol for another end use altogether. Butanol has the potential to take over a substantial portion of the biofuel market from ethanol due to its many advantages as a fuel additive to gasoline. Butanol is not currently used for this purpose since the existing techniques of butanol production have not made its adoption economically feasible. Some companies have focused on direct fermentation of butanol from biomass sources, however this route of production has many challenges. Our project will use an existing supply of ethanol from an adjoining plant, and convert it to butanol using an catalyst to achieve the Guerbet dimerization process.

Ethanol is regularly added to gasoline in Brazil and the United States, but butanol has not been adopted for this purpose. Since this market has yet to develop, it is necessary to look at the global ethanol market for economic projections. In our project statement, it was suggested to assume the price per gallon of butanol to be 1.3 to 1.5 times the price of ethanol. In 2012, the U.S. produced 13.3 billion gallons of ethanol for fuel, and consumed 12.95 billion gallons. (EIA) Together, the U.S. and Brazil produced 87.1% of global ethanol fuel in 2011 (RFA) In the U.S., ethanol is almost entirely produced from corn, whereas it is produced from sugarcane in Brazil. The price of ethanol in the U.S. fluctuates around $2 per gallon.

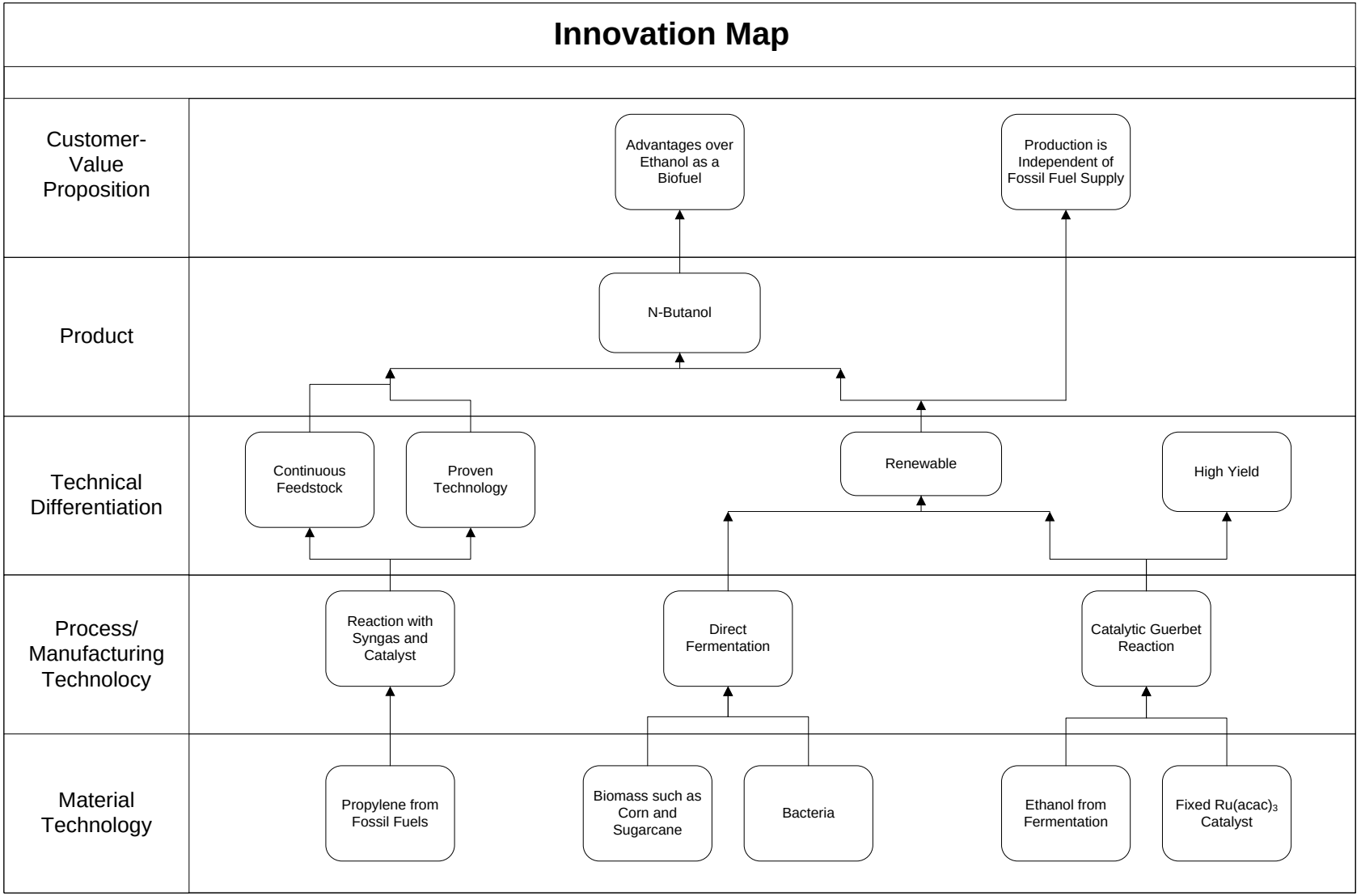
Butanol has significant advantages over ethanol that make this process worthwhile from the standpoints of economics, efficiency, and social benefit. Butanol has higher energy content than ethanol, at 110,000 BTU per gallon and 84,000 BTU per gallon, respectively. By comparison, gasoline has an energy content of 115,000 BTU per gallon. Currently, most ethanol-gasoline mixtures contain only 10% ethanol because engine modifications are required at higher ethanol concentrations (up to 85% ethanol). Butanol, however, can replace gasoline entirely with no modifications necessary to an existing gasoline engine. This concept was proven in 2005 when an unmodified 1992 Buick was driven across the United States fueled 100% by butanol. (Holan)

Butanol is also a cleaner fuel than gasoline. Per kilogram of butanol, only 2.03 kg of CO_2 are produced, compared to 3.3 kg of CO_2 per kg of gasoline. Lower CO_2 emissions are critical in addressing environmental concerns over greenhouse gases and climate change. In addition, butanol does not produce sulfur or nitrogen oxides during combustion. This is a major ecological and human health benefit. Lastly, butanol can be transported through existing gasoline pipelines, where ethanol cannot. This means that its implementation would require lower costs of infrastructure modification. (Biobutanol)

It is important to consider that biofuel prices are highly dependent on government policy. Biofuels are considered more renewable than fossil fuels from a sustainability standpoint, as they will not run out with continued use. This is a major advantage for our process going forward. However, there are growing concerns over using corn and sugarcane for biofuels because it can raise the price of food. This is a significant social concern, and will need to be addressed in the future. One solution is to produce ethanol, and subsequently butanol, from non-food sources such as wood and switchgrass.

Innovation Map

Figure 4.1. Innovation Map for Butanol Production



Customer Requirements

The main customers for our product are fuel companies and distributors. The Innovation Map in Figure 4.1 shows that several paths for the production of n-butanol already exist, and that the fuel produced from all of them has significant advantages over ethanol. Customers will be interested in knowing that our product is safe, secure and efficient. Unlike the process that makes butanol from propylene, our process is not reliant on the limited availability of fossil fuels. In addition, our process has higher yields and more reliable control than the direct fermentation routes currently in development. Both the supply of sugarcane in Brazil and corn in the US are renewable resources, and concerns over competition with food are being addressed by looking into non-food sources of biomaterial.

Our final product will be 95.3 mol% n-butanol with small amounts of heavier hydrocarbon side products. These include n-hexanol, n-octanol, 2-ethylhexanol and 2-ethylbutanol, all on the order of about 1.2 mol% each. Lastly, about 0.1 mol % ethanol exists in the final product. This composition would be suitable for direct injection into gasoline engines with little to no modifications necessary.

Assembly of Database

The economic analysis for this report was based on parameters given in the problem statement, correlations provided by faculty and industrial consultants, and market reports. The price per gallon of butanol was specified in the problem statement as 1.3 to 1.5 times the price of ethanol. This is necessary for our cost projections since a fuel market for butanol has yet to develop. The feed of ethanol to our process was also specified in the project statement as 100MM gallons per year from an adjoining ethanol plant.

The location-dependent cost of hydrogen feed to our process was given in the problem statement. For a rural site in either the U.S. or Brazil, hydrogen would cost $0.75/lb to purchase. At an industrial site, hydrogen would cost $0.50/lb in the U.S. and $0.60/lb in Brazil to transport by pipeline. In addition, a rural site assumes no transport costs for ethanol feed, but $0.05/gal cost for butanol freight to the market. This assumption is reversed for an industrial site, with a negligible cost of butanol transport and $0.05/gal for the freight costs of ethanol to the site. The catalyst used in the reactors is $Ru(acac)_3$ costs approximately $31/lb and must be replaced four times a year.

The process simulation was completed using the ASPEN PLUS program. In order to model the thermodynamic and physical interactions of our materials, the NRTL property method was specified, and hydrogen was listed as a Henry's Law component. Lastly, the reaction kinetic data was taken directly from U.S. Patent 8,318,990 examples 1 to 6. Here, the reaction ran at 180°C (356°F) and a hydrogen gas pressure of 3.0 MPa. This produced a 20% yield of n-butanol, with a 92% selectivity of ethanol to n-butanol.

Section V

Process Flow Diagram and Material Balances

Section 100

Figure 5.1. Flow Diagram of Section 100.

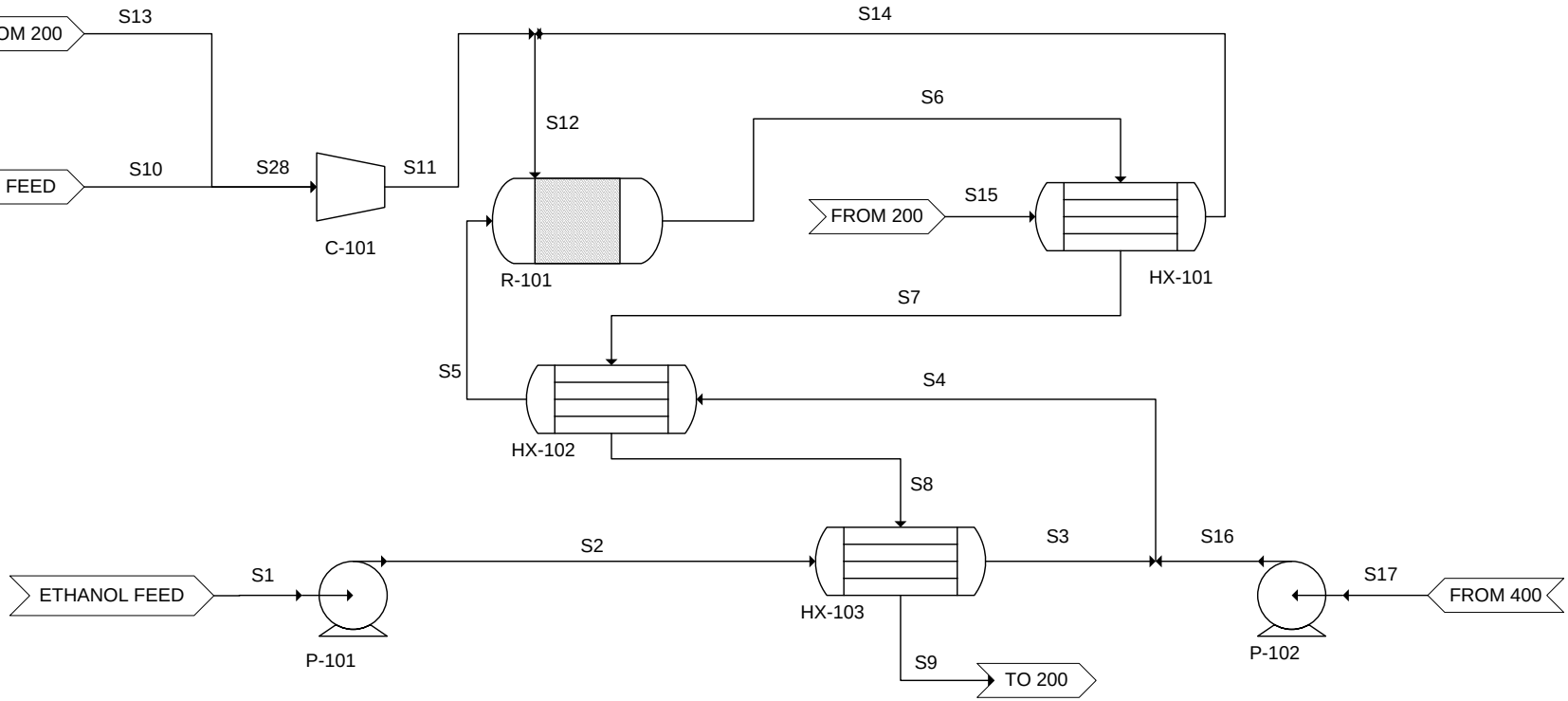


Table 5.1. Section 100 Streams (A)

Stream Summary	S1	S2	S3	S4	S5	S6	S7
Component Mass Flow (lb/hr)							
Water	0	0	0	16	16	16,637	16,637
Ethanol	82,268	82,268	82,268	378,526	378,526	296,553	296,553
Butanol	0	0	0	0	0	60,943	60,943
Hydrogen	0	0	0	0	0	2,222	2,222
2-Ethylbutanol	0	0	0	0	0	1,020	1,020
2-Ethylhexanol	0	0	0	0	0	1,300	1,300
Hexanol	0	0	0	0	0	1,020	1,020
Octanol	0	0	0	0	0	1,300	1,300
Ethylene Glycol	0	0	0	0	0	0	0
Total Mass Flow (lb/hr)	82,268	82,268	82,268	378,542	378,542	380,996	380,996
Temperature (°F)	80.0	86.7	131.0	168.1	356.0	374.0	371.8
Pressure (psi)	15.0	725.2	725.2	725.2	725.2	725.2	725.2
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.21	0.21
Enthalpy (Btu/hr)	-2.13E+08	-2.13E+08	-2.10E+08	-9.57E+08	-8.84E+08	-8.86E+08	-8.88E+08
Density (lb/ft^3)	49.73	49.46	47.62	46.00	35.79	11.16	11.35

Table 5.2. Section 100 Streams (B)

Stream Summary	S8	S9	S10	S11	S12	S13	S14
Component Mass Flow (lb/hr)							
Water	16,637	16,637	0	7	12	7	4
Ethanol	296,553	296,553	0	132	214	132	81
Butanol	60,943	60,943	0	4	6	4	2
Hydrogen	2,222	2,222	1	65	2,222	64	2,157
2-Ethylbutanol	1,020	1,020	0	0	0	0	0
2-Ethylhexanol	1,300	1,300	0	0	0	0	0
Hexanol	1,020	1,020	0	0	0	0	0
Octanol	1,300	1,300	0	0	0	0	0
Ethylene Glycol	0	0	0	0	0	0	0
Total Mass Flow (lb/hr)	380,996	380,996	1	208	2,454	207	2,245
Temperature (°F)	223.7	216.9	86.0	1232.0	339.1	85.8	302.0
Pressure (psi)	725.2	725.2	217.6	725.2	725.2	14.5	725.2
Vapor Fraction	0.12	0.12	1.00	1.00	1.00	1.00	1.00
Enthalpy (Btu/hr)	-9.60E+08	-9.63E+08	3.61E+01	1.54E+04	1.49E+06	-3.35E+05	1.47E+06
Density (lb/ft^3)	19.10	19.34	7.49E-02	2.34E-01	1.87E-01	1.47E-02	1.86E-01

Table 5.3. Section 100 Streams (C)

Stream Summary	S15	S16	S17	S28
Component Mass Flow (lb/hr)				
Water	4	16	16	7
Ethanol	81	296,258	296,258	132
Butanol	2	0	0	4
Hydrogen	2,157	0	0	65
2-Ethylbutanol	0	0	0	0
2-Ethylhexanol	0	0	0	0
Hexanol	0	0	0	0
Octanol	0	0	0	0
Ethylene Glycol	0	0	0	0
Total Mass Flow (lb/hr)	2,245	296,275	296,275	208
Temperature (°F)	86.0	177.9	173.0	85.8
Pressure (psi)	725.2	725.2	14.7	14.5
Vapor Fraction	1.00	0.00	0.00	1.00
Enthalpy (Btu/hr)	-1.41E+05	-7.47E+08	-7.48E+08	-3.35E+05
Density (lb/ft^3)	2.59E-01	45.56	45.79	1.45E-02

Section 200

Figure 5.2. Flow Diagram of Section 200.

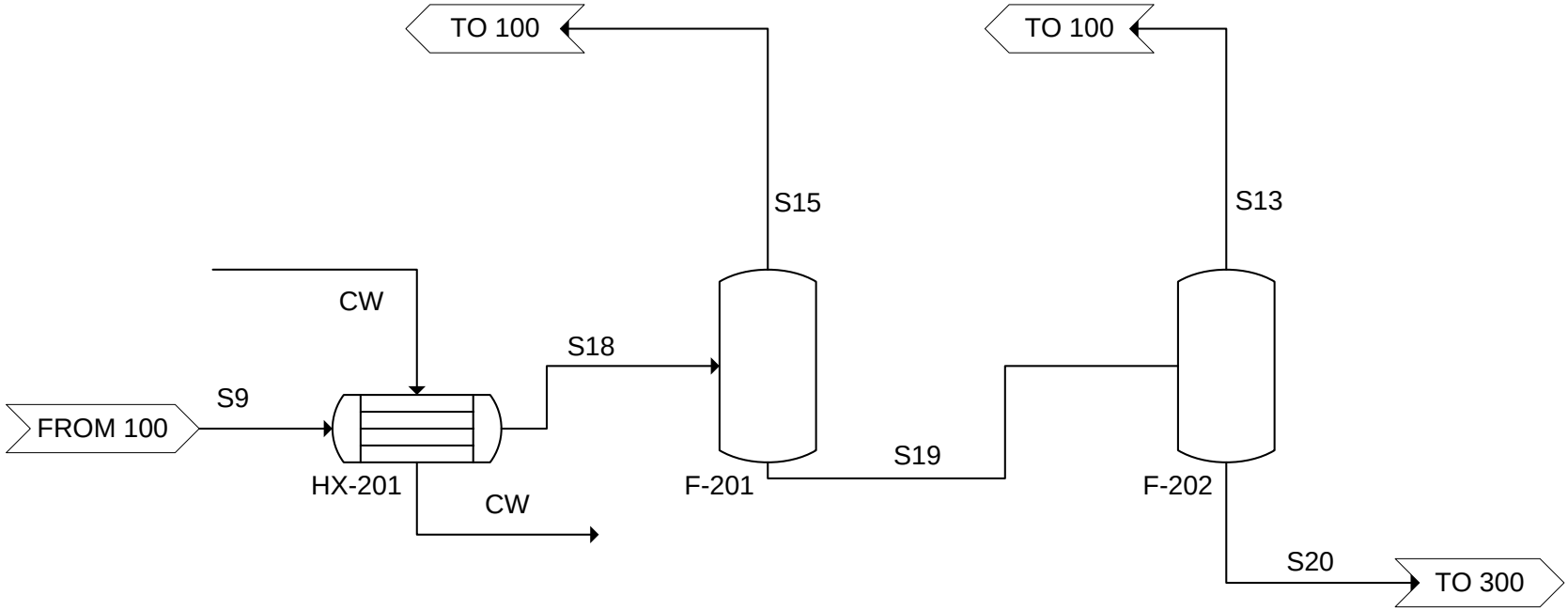


Table 5.4. Section 200 Streams

Stream Summary	S9	S13	S15	S18	S19	S20
Component Mass Flow (lb/hr)						
Water	16,637	7	4	16,637	16,633	16,625
Ethanol	296,553	132	81	296,553	296,472	296,339
Butanol	60,943	4	2	60,943	60,941	60,937
Hydrogen	2,222	64	2,157	2,222	65	0
2-Ethylbutanol	1,020	0	0	1,020	1,020	1,020
2-Ethylhexanol	1,300	0	0	1,300	1,300	1,300
Hexanol	1,020	0	0	1,020	1,020	1,020
Octanol	1,300	0	0	1,300	1,300	1,300
Ethylene Glycol	0	0	0	0	0	0
Total Mass Flow (lb/hr)	380,996	207	2,245	380,996	378,750	378,542
Temperature (°F)	216.9	85.8	86.0	86.0	86.0	85.8
Pressure (psi)	725.2	14.5	725.2	725.2	725.2	14.5
Vapor Fraction	0.12	1.00	1.00	0.11	0.00	0.00
Enthalpy (Btu/hr)	-9.63E+08	-3.35E+05	-1.41E+05	-1.00E+09	-1.00E+09	-1.00E+09
Density (lb/ft^3)	19.34	1.47E-02	2.59E-01	23.50	50.11	50.32

Section 300

Figure 5.3. Flow Diagram of Section 300.

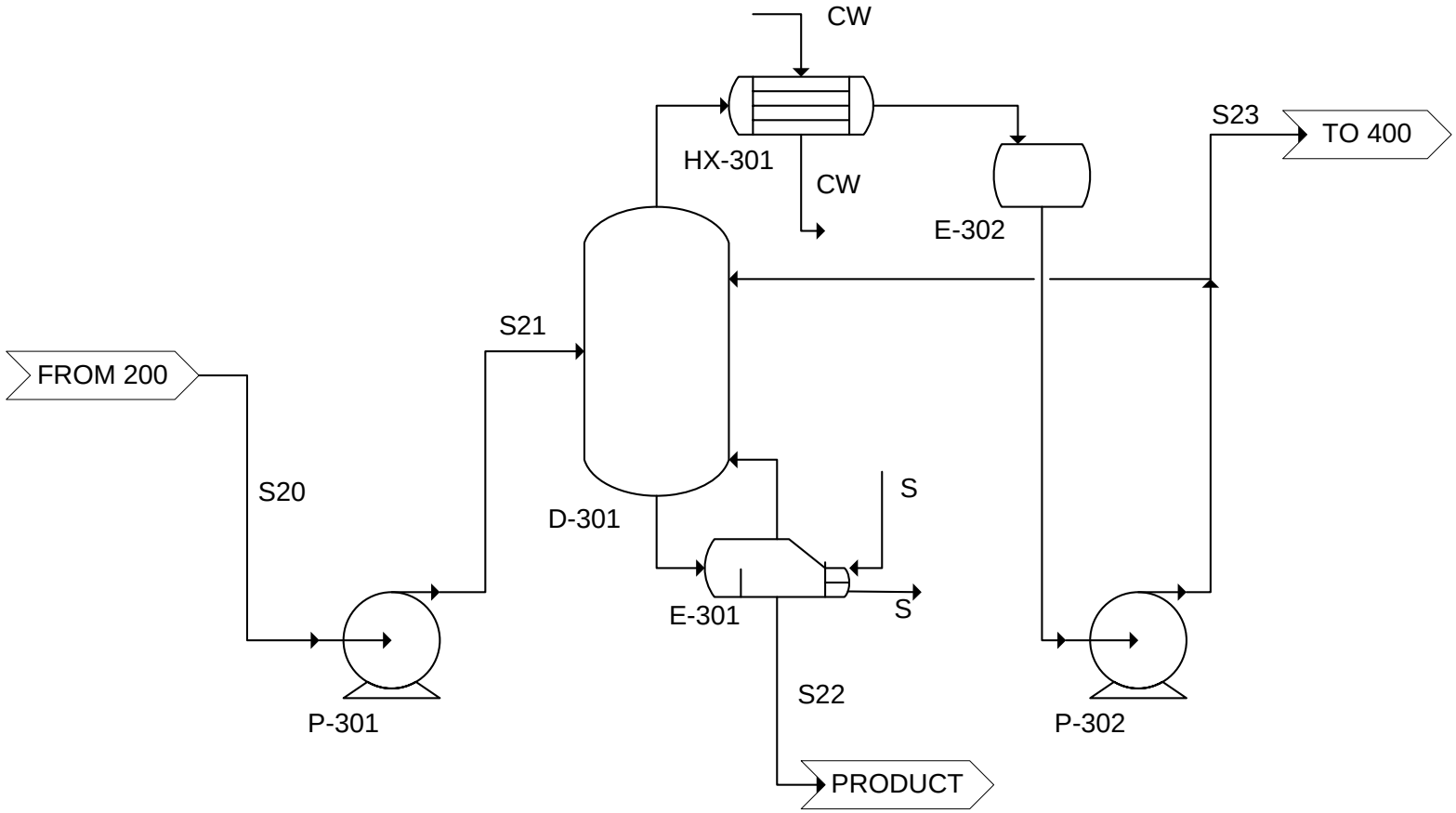


Table 5.5. Section 300 Streams

Stream Summary	S20	S21	S22	S23
Component Mass Flow (lb/hr)				
Water	16,625	16,625	0	16,625
Ethanol	296,339	296,339	20	296,320
Butanol	60,937	60,937	60,907	30
Hydrogen	0	0	0	0
2-Ethylbutanol	1,020	1,020	1,020	0
2-Ethylhexanol	1,300	1,300	1,300	0
Hexanol	1,020	1,020	1,020	0
Octanol	1,300	1,300	1,300	0
Ethylene Glycol	0	0	0	0
Total Mass Flow (lb/hr)	378,542	378,542	65,567	312,975
Temperature (°F)	85.8	85.8	265.3	172.1
Pressure (psi)	14.5	20.3	21.2	14.5
Vapor Fraction	0.00	0.00	0.00	0.00
Enthalpy (Btu/hr)	-1.00E+09	-1.00E+09	-1.14E+08	-8.60E+08
Density (lb/ft^3)	50.32	50.32	43.73	46.41

Section 400

Figure 5.4. Flow Diagram of Section 400.

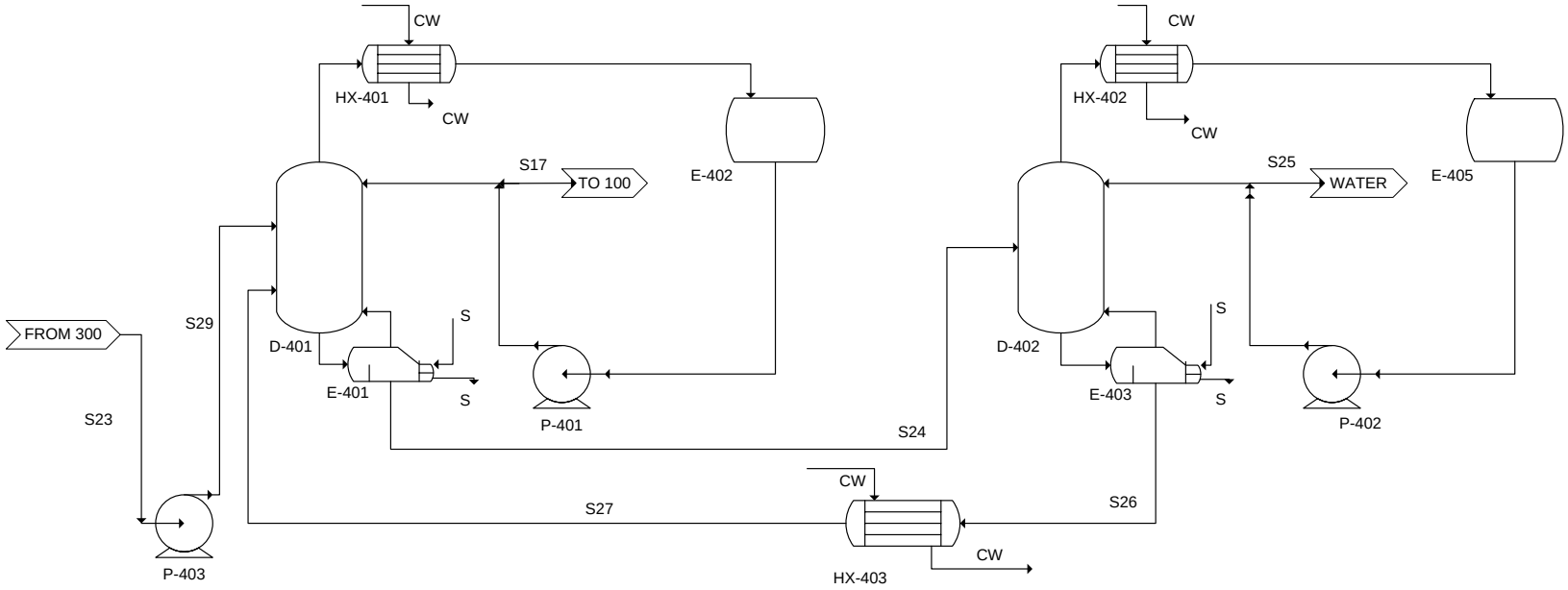


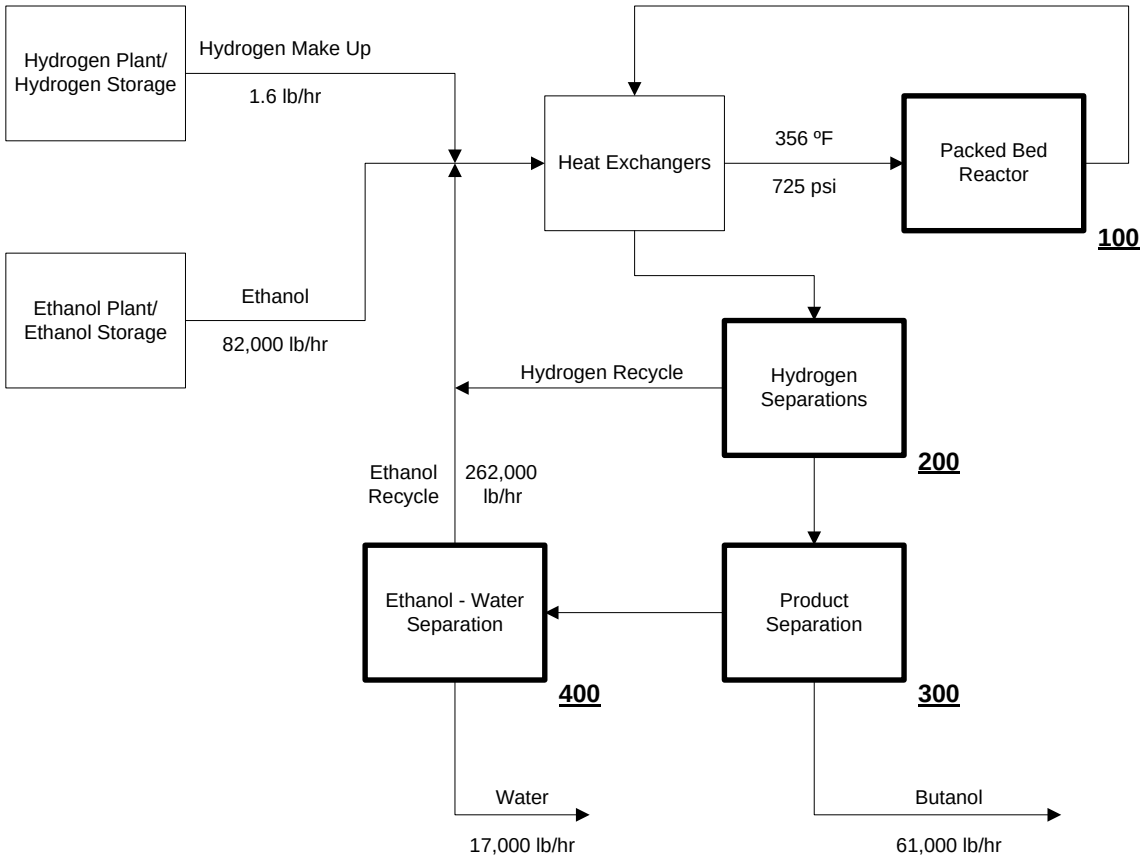
Table 5.6. Section 400 Streams

Stream Summary	S17	S23	S24	S25	S26	S27	S29
Component Mass Flow (lb/hr)							
Water	16	16,625	16,611	16,609	2	2	16,625
Ethanol	296,258	296,320	61	61	0	0	296,320
Butanol	0	30	30	30	0	0	30
Hydrogen	0	0	0	0	0	0	0
2-Ethylbutanol	0	0	0	0	0	0	0
2-Ethylhexanol	0	0	0	0	0	0	0
Hexanol	0	0	0	0	0	0	0
Octanol	0	0	0	0	0	0	0
Ethylene Glycol	0	0	314,726	0	314,726	314,726	0
Total Mass Flow (lb/hr)	296,275	312,975	331,428	16,701	314,728	314,728	312,975
Temperature (°F)	173.0	172.1	335.3	210.5	408.8	140.0	172.1
Pressure (psi)	14.7	14.5	21.9	14.7	20.9	29.4	21.8
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Enthalpy (Btu/hr)	-7.48E+08	-8.60E+08	-1.06E+09	-1.11E+08	-9.32E+08	-9.88E+08	-8.60E+08
Density (lb/ft^3)	45.79	46.41	60.80	57.30	58.35	67.86	46.41

Section VI

Process Description

Figure 6.1. Process Summary.



Overview

The process is divided into four key sections, as shown in the Process Summary diagram in Figure 6.1. The first section (100) includes the reaction portion of the process, in which ethanol from a storage tank and a recycle stream are combined and react in the presence of hydrogen to form butanol and water. In the second section (200), temperature and pressure changes are utilized to remove hydrogen and recycle it back to the reactor. Section three (300) uses a distillation column to separate the product butanol, with small amounts of heavier alcohols, from the unreacted ethanol and the water byproduct. Finally, this primarily water-ethanol system is separated in section four (400) using ethylene glycol as an entrainer in order to purge water and recycle almost pure ethanol to the reactor.

Feed Storage

Ethanol

The ethanol feed for this process will be taken from an adjoining ethanol plant owned by our company. Since this plant is already considered fully operational, it is assumed that the plant already contains adequate storage to prevent any downtime for our butanol plant. If the existing storage is not adequate, new storage must be added to our plant, which would increase costs and affect our profitability.

Hydrogen

Hydrogen will also require an onsite production facility, which is assumed to provide the constant supply of hydrogen makeup necessary for the process. Approximately a two-day supply of hydrogen, however, will be stored on site in the form of liquid hydrogen in two 60-gallon tanks. These tanks will be used to ensure no downtime at our plant in case of unexpected problems with the hydrogen facility.

Reactor

The reactor (R-101, see p. 43), shown in Section 100, is a packed bed reactor containing $Ru(acac)_3$, the necessary catalyst for the reaction. The reactor operates at 374 ^oF and 725 psia based on patent data, so the inlet streams are preheated by the reactor effluent and either pumped or compressed to achieve this pressure. The ethanol feed is first pumped to 725 psi (P-101, see p. 41) and heated to 131 ^oF (HX-103, see p. 44) by the reactor effluent. This feed is then combined with the ethanol recycle which has also been pumped to 725 psi (P-102, p. 41), before this mixed stream is heated to 356 ^oF by the reactor effluent (upstream of HX-103) and supplied to the reactor. The hydrogen feed is combined with the low pressure hydrogen recycle stream and is compressed to 725 psi (C-101, see p. 50). This stream then mixes with the high pressure hydrogen recycle, which has been preheated to 302 ^oF by the reactor effluent (upstream of HX-102, see p. 44), and the mixed stream enters the reactor at 339 ^oF and 725 psi. The reactor effluent is used as the hot stream for multiple heat exchangers in order to recover heat and minimize costs. After these exchanges, the effluent goes to the hydrogen separation at 217 ^oF and 725 psi with a vapor fraction of 0.12.

Separations

Hydrogen

After the reactor section, the products and the unreacted feed materials enter a series of separations to isolate the product and recover raw materials. First, the stream is further cooled to 86 ^{o}F (HX-201, see p. 44) and enters a flash drum also at 725 psi (F-201, see p. 50). At this temperature, 97% (by mass) of the hydrogen is recycled at the reactor pressure, which is important for minimizing the cost of compressing hydrogen. The liquid phase, containing almost all of the water, ethanol, butanol, and side-products from the reactor, then proceeds to another flash drum operating at 14.5 psi (F-202, see p. 50). At this lower pressure, 98% of the remaining hydrogen is recovered and recycled, with small amounts of water, ethanol, and butanol. This two flash system allows for recovery of almost all of the hydrogen and significantly decreases the cost of compression at steady state.

Butanol

Once the hydrogen has been recycled, the rest of the reactor effluent is pumped to a pressure of 20.3 psi (P-301, see p. 41) and enters a 40-stage distillation column (D-301, see p. 47) above stage 20. The purpose of this column is to separate the butanol, and the heavier alcohol products, from ethanol and water. The bottom of the column yields a stream with a total flow rate of 66,000 lb/hr and a composition of 93% butanol and 7% heavier alcohols, with trace amounts of ethanol and essentially no water. Based on our specifications, this is considered pure product and leaves at 265 ^{o}F and 21.2 psi. The top of the column produces a stream with a total flow rate of 313,000 lb/hr leaving at 172 ^{o}F and 14.5 psi. This stream contains 95% ethanol and 5% water, with a trace amount of butanol.

Ethanol and Water

The water-ethanol mixture leaving the first distillation column needs to be separated in order to purge the water and decrease the size of the recycle stream, so an azeotropic distillation is employed. The top stream from the first column is first pumped to 20.3 psi (P-401, see p. 42), and then fed to a 45 stage azeotropic distillation column (D-401, see p. 47) on stage 30. A recycle of the containing 315,000 lb/hr of the entrainer, ethylene glycol, from the recovery column (D-402, see p. 47) is also fed to the azeotropic column on stage 13. The distillate stream from this column contains 296,000 lb/hr of almost pure ethanol, which is recycled the reactor portion of the process. The bottoms stream leaves at 21.9 psi and enters the 35 stage recovery

column on stage 15. The distillate stream from the recovery column leaves at 211 ^{o}F and 14.7 psi, with a total flow rate of 17,000 lb/hr and a composition of 99.45% water, 0.37% ethanol, and 0.18% butanol. The bottoms stream, essentially pure ethylene glycol and a trace amount of water, then gets cooled to 140 ^{o}F (HX-403, see p. 46) before being recycled to the azeotropic separation column as mentioned above.

Product Storage

The butanol product taken from D-301 is fed directly into railroad tank cars for transportation to industrial areas. Based on tanks filled to 30,000 gallons, tanks would have to be switched every 200 minutes. In order to ensure continuous production, a one million gallon tank is included in the plant in order to store approximately 4.5 days of butanol in case of transportation delays.

Section VII

Energy Balance and Utility Requirements

Utility Requirements

The major heating requirements of the plant lie in the heating of the inlet streams to the reactor (HX-101, HX-102, and HX-103, see p. 43 and p. 44) and the kettle reboilers at the base of each of the distillation columns (E-301, E-401 and E-403, see p. 48 and p. 49). Together, these six units account for 553 MM BTU/hr. The pumps and compressor that are present throughout the process contribute to the overall energy requirements of the process as well. Other major energy requirements lie in the cooling heat exchangers that are present in each of the distillation towers as well as in two other locations in the system (HX-201, HX-301, HX-401, HX-402, and HX-403, see p. 44 to p. 46), which use cooling water to reach the desired outlet temperature, and from the non-adiabatic reactor.

The heat exchangers in section 100, namely, HX-101, HX-102, and HX-103, all use reactor effluent to heat ethanol and hydrogen feeds and recycles to the reactor, and therefore do not contribute to the heat duty of the overall process.

Table 7.1 shows a complete list of all necessary utilities. Cooling water, high-pressure steam (400 psig), and other streams are also used to achieve the proper heating and cooling within the process. Also shown are the electrical power requirements of each piece of equipment.

Table 7.1. Utility Requirements

Energy Requirements of the Process			
Equipment	Description	Duty/ Electricity Use	Source
Section 100			
R-101-1	Reactor	-1,727,961.94 BTU/hr	Cooling Water
R-101-2	Reactor	-1,727,961.94 BTU/hr	Cooling Water
P-101	Pump	102.262 kW	Electricity
P-102	Pump	330.67 kW	Electricity
HX-101	Heat Exchanger	1,612,673.79 BTU/hr	Reactor Effluent
HX-102	Heat Exchanger	72,522,737 BTU/hr	Reactor Effluent
HX-103	Heat Exchanger	2,420,010.74 BTU/hr	Reactor Effluent
C-101	Compressor	102.77 kW	Electricity

Table 7.1	Continued		
Section 200			
HX-201	Heat Exchanger	-39,426,380 BTU/hr	Cooling Water
F-201	Flash Drum	0	N/A
F-202	Flash Drum	0	N/A
Section 300			
P-301	Pump	3.09 kW	Electricity
D-301	Distillation Tower	0	N/A
HX-301	Condenser	-182,222,782 BTU/hr	Cooling Water
E-301	Reboiler	210,574,315 BTU/hr	Steam
E-302	Reflux Accumulator	0	N/A
P-302	Pump	220.24 kW	Electricity
Section 400			
D-201	Distillation Tower	0	N/A
HX-401	Condenser	-349,803,269 BTU/hr	Cooling Water
P-401	Pump	274.12 kW	Electricity
E-401	Reboiler	210,594,315 BTU/hr	Steam
E-402	Reflux Accumulator	0	N/A
D-402	Distillation Tower	0	N/A
HX-402	Condenser	-40,650,755.3 BTU/hr	Cooling Water
P-402	Pump	10.91 kW	Electricity
E-403	Reboiler	55,532,817 BTU/hr	Steam
E-405	Reflux Accumulator	0	N/A
HX-403	Heat Exchanger	-56,139,440 BTU/hr	Cooling Water
P-403	Pump	3.502 kW	Electricity
Totals			
		Usage	*Cost per hour*
	Integrated Streams	76,555,422 BTU/hr	$0.00
	Cooling Water	-671,518,550 BTU/hr	$150.25
	Steam @ 400 psi	476,701,447 BTU/hr	$1,735.21
	Electricity	917.794 kW	$42.03
	Total		$1,927.49

Section VIII

Equipment List and Unit Descriptions

Table 8.1. Equipment List

Pumps	
Equipment ID	Type
P-101	Centrifugal Pump
P-102	Centrifugal Pump
P-301	Centrifugal Pump
P-302	Centrifugal Pump
P-401	Centrifugal Pump
P-402	Centrifugal Pump
P-403	Centrifugal Pump
Reactor	
Equipment ID	Type
R-101-1	Fixed Bed Catalytic Reactor
R-101-2	Fixed Bed Catalytic Reactor
Heat Exchangers	
Equipment ID	Type
HX-101	Shell and Tube Heat Exchanger
HX-102	Shell and Tube Heat Exchanger
HX-103	Shell and Tube Heat Exchanger
HX-201	Shell and Tube Heat Exchanger
HX-301	Condenser
HX-401	Condenser
HX-402	Condenser
HX-403	Shell and Tube Heat Exchanger
Flash Drums	
Equipment ID	Type
F-201	Vertical Flash Vessel
F-202	Vertical Flash Vessel

Reboilers	
Equipment ID	Type
E-301	U Tube Kettle Reboiler
E-401	U Tube Kettle Reboiler
E-403	U Tube Kettle Reboiler
Compressor	
Equipment ID	Type
C-101	Centrifugal Compressor
Reflux Accumulators	
Equipment ID	Type
E-302	Horizontal Storage Vessel
E-402	Horizontal Storage Vessel
E-405	Horizontal Storage Vessel

Unit Descriptions

Pumps

P-101 (see p. 58) is a carbon steel centrifugal pump used to pressurize the ethanol feed stream S1, that has a liquid flow rate of 226.88 gpm, from 15 Psi to 725 Psi. The pump has a fluid head of 2,060 ft and an efficiency of 62.3%. The total estimated purchase cost of P-101 is $85,100, while the installation cost estimate is $273,171. The calculated electric requirement is 102.3 kW and the net work required is 137 hp. This pump would have a utility cost of $7.98/hr.

P-102 (see p. 58) is a carbon steel centrifugal pump used to pressurize the ethanol recycle stream S17, that has a liquid flow rate of 887.39 gpm, from 14.7 Psi to 725 Psi. The pump has a fluid head of 2238 ft and an efficiency of 75.4%. The total estimated purchase cost of P-102 is $161,000, while the installation cost estimate is $516,810. The calculated electric requirement is 330.7 kW and the net work required is 443 hp. This pump would have a utility cost of $25.79/hr.

P-301 (see p. 59) is a carbon steel centrifugal pump used to pressurize the liquid stream S20, that has a liquid flow rate of 1,031.6 gpm, from 14.5 Psi to 20.3 Psi. This pump is required to ensure the feed stream S21 is at a higher pressure than the feed stage in the distillation column D-301. The pump has a fluid head of 2238 ft and an efficiency of 76.6%. The total estimated purchase cost of P-301 is $12,200, while the installation cost estimate is $39,162. The calculated electric requirement is 3.1 kW and the net work required is 4.1 hp. This pump would have a utility cost of $0.24/hr.

P-302 (see p. 59) is a carbon steel centrifugal pump used to pressurize the reflux stream from E-302 to D-301 and S23. P-302 pumps the reflux at a flow rate of 1,931.12 gpm. This pump is required to ensure the reflux stream is at a higher pressure than the stage in the distillation column D-301. The pump has an efficiency of 70%. The total estimated purchase cost of P-302

is $25,500, while the installation cost estimate is $81,855. The calculated electric requirement is 220.24kWand would have a utility cost of $17.18/hr.

P-401 (see p. 60) is a carbon steel centrifugal pump used to pressurize the reflux stream from E-402 to D-401 and S17. P-401 pumps the reflux at a flow rate of 2,403.62 gpm. This pump is required to ensure the reflux stream is at a higher pressure than the stage in the distillation column D-401. The pump has an efficiency of 70%. The total estimated purchase cost of P-401 is $38,700, while the installation cost estimate is $124,227. The calculated electric requirement is 274.12kW and would have a utility cost of $21.38/hr.

P-402 (see p. 60) is a carbon steel centrifugal pump used to pressurize the reflux stream from E-405 to D-402 and S25. P-403 pumps the reflux at a flow rate of 95.67 gpm. This pump is required to ensure the reflux stream is at a higher pressure than the stage in the distillation column D-402. The pump has an efficiency of 70%. The total estimated purchase cost of P-402 is $5,700, while the installation cost estimate is $18,297. The calculated electric requirement is 10.91kW and would have a utility cost of $0.85/hr.

P-403 (see p. 61) is a carbon steel centrifugal pump used to pressurize the distillate stream S23 of D-301 from 14.5 Psi to 21.76 Psi with a flow rate of 924.78 gpm. This pump is required to ensure the Feed stream S29is at a higher pressure than the stage in the distillation column D-401. The pump has an efficiency of 76% and a fluid heat of 22.5ft. The total estimated purchase cost of P-403 is $11,000, while the installation cost estimate is $35,310. The calculated electric requirement is 3.5 kW, with 4.7hp of net work required and would have a utility cost of $0.27/hr.

Reactor

R-101 and ***R-102*** (see p. 62 and p. 63) are identical stainless steel fixed bed catalytic reactors that convert ethanol to butanol in the presence of pressurized hydrogen. The reactors are run in parallel to avoid the large purchase and installation costs of one large reactor. The inlet streams S5 and S12 are split evenly and the product streams are mixed into stream S6. Inlet streams S12 feeds the pressurized hydrogen at 725.2 Psi and 374°F while stream S5 is the ethanol feed and the recycled ethanol also at 725.2 Psi and 374°F. The reactants have a combined volumetric flow rate of 17,097 ft^3/hr and a mass flow rate of 380,995 lbs/hr. The catalyst used is Ruthenium(III) Acetylacetonate, $Ru(acac)_3$, has a volume of 6,852 ft^3 and weighs 658,727 lbs. The reactor vessels each have a volume of 8,758.3 ft^3 with a diameter of 7.5ft, length of 26.5 ft and a wall thickness of 1.7 inches. The heat duty for this reactor is -1,727,962 Btu/hr and requires a cooling water flow of 194,188 lbs/hr. The total estimated cost of each reactor is $411,200, while the installation cost estimate is $1,319,952. The catalyst costs $10,516,575 with a lifetime of 90 days, which then accumulates to a yearly cost of $42,066,300. The hourly utility cost of R-101 and R-102 is $0.39/hr each.

Heat Exchangers

HX-101 (see p. 69) is a counter current shell and tube heat exchanger used to heat stream S15 from 86°F to 302°F using the reactor product stream S6 which is at 374°F. Stream S15 is the recovered hydrogen from F-201 that needs to be heated to feed into the reactor. HX-101 is a counter current heat exchanger with inlet stream S6 on the shell side and stream S15 on the tube side. Stream S6 is cooled from 374°F to 371.8°F and stream S15 is heated from 86°F to 302°F simultaneously. The flow rates of stream S6 and S15 are 380,996 lbs/hr and 2,245lbs/hr respectively. HX-101 has 120 tubes, a transfer area of 69.47 ft^2 and an overall heat transfer coefficient of 149.69 Btu/hr*ft^2 *R that allows for 1,612,674 Btu/hr of heat to transfer with no utility costs. The total estimated purchase cost of HX-101 is $10,700, while the installation cost estimate is $34,347.

HX-102 (see p. 70) is a counter current shell and tube heat exchanger used to heat stream S4 from 168°F to 356°F using the slightly cooled reactor product stream S7 which is at 371.8°F. Stream S4 is the ethanol feed and the recovered Ethanol from D-401 that needs to be heated before feeding into the reactor. HX-102 is a counter current heat exchanger with inlet stream S7 on the shell side and stream S4 on the tube side. Stream S7 is cooled from 371.8°F to 223.7°F and stream S4 is heated from 168°F to 356°F simultaneously. The flow rates of stream S7 and S4 are 380,996 lbs/hr and 378,542 lbs/hr respectively. HX-102 has 120 tubes, a transfer area of 15,326 ft^2 and an overall heat transfer coefficient of 149.7 Btu/hr*ft^2 *R that allows for 75,522,737 Btu/hr of heat to transfer with no utility costs. The total estimated purchase cost of HX-102 is $548,000, while the installation cost estimate is $1,759,080.

HX-103 (see p. 71) is a counter current shell and tube heat exchanger used to heat stream S2 from 86.7°F to 131°F using the reactor product stream S8 after it comes out of HX-102 which is as 223.7°F.

Stream S2 is the ethanol feed that has been pumped to 725.19 Psi and needs to be heated before feeding into the reactor. HX-103 is a counter current heat exchanger with inlet stream S8 on the shell side and stream S2 on the tube side. Stream S8 is cooled from 223.7°F to 216.9°F and stream S2 is heated from 86.7°F to 131°F simultaneously. The flow rates of stream S8 and S2 are 380,996 lbs/hr and 82,268 lbs/hr respectively. HX-103 has 120 tubes, a transfer area of 146.47ft^2 and an overall heat transfer coefficient of 149.7 Btu/hr*ft^2 *R that allows for 2,420,010 Btu/hr of heat to transfer with no utility costs. The total estimated purchase cost of HX-103 is $19,300, while the installation cost estimate is $61,953.

HX-201 (see p. 72) is a counter current shell and tube heat exchanger used to cool stream S9 from 216.9°F to 86°F using cooling water at 68°F. Stream S9 is the reactor product coming out of HX-103 and needs to be cooled before feeding into F-201 to ensure efficient use of the flash vessel and high hydrogen recovery. HX-201 is a counter current heat exchanger with cooling water on the shell side and stream S9 on the tube side. Stream S9 is cooled from 216.9°F to 86°F

and the cooling water is heated from 68°F to 78°F simultaneously. The flow rates of stream S9 and the cooling water are 380,996 lbs/hr and 4,392,930 lbs/hr respectively. HX-201 has 120 tubes, a transfer area of 13,046 ft^2 that allows for 39,426,380 Btu/hr of heat to transfer with $8.82 of utility costs. The total estimated purchase cost of HX-201 is $393,300, while the installation cost estimate is $1,262,493.

HX-301 (see p. 73) is a counter current shell and tube heat exchanger used to completely condense the distillate products in D-301 using cooling water at 68°F. The distillate product is in the vapor phase and must be condensed before going into E-302, the reflux accumulator for D-301. HX-301 is a counter current heat exchanger with cooling water on the shell side and the distillate stream of D-301 on the tube side. The distillate stream is completely condensed while the cooling water is heated from 68°F to 78°F simultaneously. The flow rates of the distillate stream and the cooling water are 7,355 lbs/hr and 20,303,460 lbs/hr respectively. HX-301 has 120 tubes, a transfer area of 13,916 ft^2 that allows for 182,222,782 Btu/hr of heat to transfer with $40.76 of utility costs. The total estimated purchase cost of HX-301 is $269,200, while the installation cost estimate is $864,132.

HX-401 (see p. 74) is a counter current shell and tube heat exchanger used to completely condense the distillate products in D-401 using cooling water at 68°F. The distillate product is in the vapor phase and must be condensed before going into E-402, the reflux accumulator for D-401. HX-401 is a counter current heat exchanger with cooling water on the shell side and the distillate stream of D-401 on the tube side. The distillate stream is completely condensed while the cooling water is heated from 68°F to 78°F simultaneously. The flow rates of the distillate stream and the cooling water are 6,432 lbs/hr and 38,975,460 lbs/hr respectively. HX-401 has 120 tubes, a transfer area of 26,542 ft^2 that allows for 349,803,269 Btu/hr of heat to transfer with $78.24 of utility costs. The total estimated purchase cost of HX-401 is $499,800 while the installation cost estimate is $1,604,358.

HX-402 (see p. 75) is a counter current shell and tube heat exchanger used to completely condense the distillate products in D-402 using cooling water at 68°F. The distillate product is in the vapor phase and must be condensed before going into E-405, the reflux accumulator for D-402. HX-402 is a counter current heat exchanger with cooling water on the shell side and the distillate stream of D-402 on the tube side. The distillate stream is completely condensed while the cooling water is heated from 68°F to 78°F simultaneously. The flow rates of the distillate stream and the cooling water are 924 lbs/hr and 4,529,351 lbs/hr respectively. HX-402 has 120 tubes, a transfer area of 1,412 ft^2 that allows for 40,650,755 Btu/hr of heat to transfer with $9.09 of utility costs. The total estimated purchase cost of HX-402 is $34,300 while the installation cost estimate is $110,103.

HX-403 (see p. 76) is a counter current shell and tube heat exchanger used to cool stream S26 from 408.8°F to 140°F using cooling water at 68°F. Stream S26 is the recovered ethylene-glycol in the bottoms product of D-402. This stream needs to be cooled before feeding into D-401 to ensure efficient use of the distillation column to separate ethanol and water. HX-403 is a counter current heat exchanger with cooling water on the shell side and stream S26 on the tube side. Stream S26 is cooled from 408.8°F to 140°F and the cooling water is heated from 68°F to 78°F simultaneously. The flow rates of stream S26 and the cooling water are 314,728 lbs/hr and 6,255,117 lbs/hr respectively. HX-403 has 120 tubes, a transfer area of 4,476 ft^2 that allows for 56,139,440 Btu/hr of heat to transfer with $12.56 of utility costs. The total estimated purchase cost of HX-403 is $86,400, while the installation cost estimate is $277,344.

Distillation Columns

D-301 (see p. 66) is a carbon steel, sieve tray distillation column used to separate the product, mostly butanol with some ethyl butanol, ethyl hexanol, hexanol, and octanol, from the water and unreacted ethanol. The tower has 40 stages, with a pressure drop of 0.12 psi per stage, and the tray efficiency was determined to be 73% for a total of 55 trays. The column has 24-inch tray spacing, with a total height of 122 feet and a diameter of 23 feet. The column operates at 265 °F and a molar reflux ratio of 0.448, and the overhead pressure in 14.5 psi. The feed stream, S21, enters the column on tray 28 at a flow rate of 379,000 lb/hr and a temperature of 86 °F. The distillate, S23, leaves the column at 172 °F and a flow rate of 313,000 lb/hr, while the bottoms, S22, leaves at 265 °F and a flow rate of 66,000 lb/hr. The total estimated purchase cost of D-301 is $1,673,400, while the installation cost estimate is $5,371,614.

D-401 (see p. 67) is a carbon steel, sieve tray distillation column used to separate the ethanol from water, using ethylene glycol as an entrainer, in order to recycle ethanol to the reactor. The tower has 45 stages, with a pressure drop of 0.12 psi per stage, and the tray efficiency was determined to be 73% for a total of 62 trays. The column has 24-inch tray spacing, with a total height of 136 feet and a diameter of 25 feet. The column operates at 335 °F and a molar reflux ratio of 2.2, and the overhead pressure is 14.7 psi. The feed stream from D-301, S29, enters the column on tray 42 at a flow rate of 313,000 lb/hr and a temperature of 172 °F. The second feed stream recycled from D-402, S27, enters the column on tray 18 at a flow rate of 315,000 lb/hr and a temperature of 140 °F. The distillate, S23, leaves the column at 173 °F and a flow rate of 296,000 lb/hr, while the bottoms, S22, leaves at 335 °F and a flow rate of 331,000 lb/hr. The total estimated purchase cost of D-401 is $1,991,100, while the installation cost estimate is $6,391,431.

D-402 (see p. 68) is a carbon steel, sieve tray distillation column used to separate ethylene glycol from water, in order to purge water from the system and recycle ethylene glycol to the azeotropic distillation column, D-401. The tower has 35 stages, with a pressure drop of 0.12 psi per stage,

and the tray efficiency was determined to be 73% for a total of 48 trays. The column has 24-inch tray spacing, with a total height of 108 feet and a diameter of 12.5 feet. The column operates at 409 °F and a molar reflux ratio of 1.5, and the overhead pressure is 14.7 psi. The feed stream from D-401, S24, enters the column on tray 21 at a flow rate of 331,000 lb/hr and a temperature of 334 °F. The distillate, S25, leaves the column at 211 °F and a flow rate of 16,700 lb/hr, while the bottoms, S22, leaves at 409 °F and a flow rate of 315,000 lb/hr. The total estimated purchase cost of D-402 is $592,700, while the installation cost estimate is $1,902,567.

Other Equipment

E-301 (see p. 79) is a counter current U tube kettle reboiler made from carbon steel that reboils the bottoms product of column D-301. Most of the bottoms product of D-301 must be vaporized and returned to the column while the final product will leave E-301 from stream S22. E-301 is a counter current heat exchanger with the bottoms product on the shell side and the steam on the tube side. The bottoms product is vaporized using steam at 448°F and 400 Psi. The flow rates of the bottoms product and steam are 862 lbs/hr and 284,904 lbs/hr respectively. E-301 has 120 tubes, a transfer area of 24,738 ft^2 that allows for 210,594,315 Btu/hr with $3,336 of utility costs. The total estimated purchase cost of E-301 is $641,400, while the installation cost estimate is $2,058,894.

E-401 (see p. 80) is a counter current U tube kettle reboiler made from carbon steel that reboils the bottoms product of column D-401. Most of the bottoms product of D-401 must be vaporized and returned to the column while the bottoms product will leave E-401 from stream S24 and feed to D-402. E-401 is a counter current heat exchanger with the bottoms product on the shell side and the steam on the tube side. The bottoms product is vaporized using steam at 448°F and 400 Psi. The flow rates of the bottoms product and steam are 5,994 lbs/hr and 529,965 lbs/hr respectively. E-401 has 120 tubes, a transfer area of 61,939 ft^2 that allows for 391,737,157 Btu/hr with $6,206 of utility costs. The total estimated purchase cost of E-401 isIn$1,658,600, while the installation cost estimate is $5,324,106.

E-403 (see p. 81) is a counter current U tube kettle reboiler made from carbon steel that reboils the bottoms product of column D-403. Most of the bottoms product of D-403 must be vaporized and returned to the column while the ethylene-glycol bottoms product will leave E-403 from stream S26 and feed to HX-403 before recycled into column D-401. E-403 is a counter current heat exchanger with the bottoms product on the shell side and the steam on the tube side. The bottoms product is vaporized using steam at 448°F and 400 Psi. The flow rates of the bottoms product and steam are 5,071 lbs/hr and 75,128 lbs/hr respectively. E-403 has 120 tubes, a transfer area of 14,468 ft^2 that allows for 55,532,817 Btu/hr with $880 of utility costs. The total estimated purchase cost of E-403 is $496,200, while the installation cost estimate is $1,592,802.

E-302 (see p. 82) is a carbon steel horizontal vessel that is used as a reflux accumulator for D-301 that accumulates the overhead products before returning the reflux to the column or leaving in the distillate stream S23. E-302 is operating at 172°F and 14.5 Psi with a height of 27 ft and a diameter of 8.5ft that allows for a storage volume of 11,462 gallons. The total estimated purchase cost of E-302 is $50,800, while the installation cost estimate is $163,068.

E-402 (see p. 83) is a carbon steel horizontal vessel that is used as a reflux accumulator for D-401 that accumulates the overhead products before returning the reflux to the column or leaving in the distillate stream S17, which is the ethanol recycle. E-402 is operating at 173°F and 14.7 Psi with a height of 29 ft and a diameter of 9ft that allows for a storage volume of 13,802 gallons. The total estimated purchase cost of E-402 is $41,100, while the installation cost estimate is $131,931.

E-405 (see p. 83) is a carbon steel horizontal vessel that is used as a reflux accumulator for D-402 that accumulates the overhead products before returning the reflux to the column or leaving in the distillate stream S25 which is the water stream. E-405 is operating at 210.6°F and 14.7 Psi with a height of 10 ft and a diameter of 3.5 ft that allows for a storage volume of 720 gallons. The total estimated purchase cost of E-405 is $14,100, while the installation cost estimate is $45,261.

Flash Vessels

F-201 (see p. 77) is vertical, carbon steel drum used to separate hydrogen from the rest of the components stream S18, in order to recycle it at the reactor pressure. The feed flows into the drum at 381,000 lb/hr, where it separates into a vapor stream, which leaves at 2,250 lb/hr, and a liquid stream, which leaves at 379,000 lb/hr. The drum has a diameter of 7.5 feet, a height of 23 feet, and a volume of 7600 gallons, and it operates at 86 °F and 725 psi. The total estimated purchase cost of F-201 is $120,300, while the installation cost estimate is $386,163.

F-202 (see p. 78) is vertical, carbon steel drum used to separate the remaining hydrogen from the rest of the components stream S19, in order to recover more and minimize costs. The feed flows into the drum at 379,000 lb/hr, where it separates into a vapor stream, which leaves at 210 lb/hr, and a liquid stream, which leaves at 379,000 lb/hr. The drum has a diameter of 7.5 feet, a height of 23 feet, and a volume of 7600 gallons, and it operates at 86 °F and 14.5 psi. The total estimated purchase cost of F-202 is $120,300, while the installation cost estimate is $386,163.

Compressor

C-101 (see p. 82) is a carbon steel, centrifugal compressor, used to raise the pressure of the low pressure hydrogen recycle and the hydrogen makeup to reactor pressure. The inlet stream, S28, enters at 420 gallons per minute and is compressed from 14.5 psi to 725 psi. The pump has a head of 944,000 feet lb_f/lb_m and has electricity and work requirements of 103 kW and 138 hp respectively. The total estimated purchase cost is $1,741,700, the installation cost estimate is $5,590,857, and the utility cost estimate is $7.96/hr.

Section IX

Location

Location

Our problem statement (Appendix D) limited the possible locations for our process to the United States and Brazil since these countries currently produce large amounts of ethanol for use as a fuel additive. The problem statement further distinguished between locating the plant at a rural or industrial site, as this affects the transportation costs of our material. The profitability of our project will largely depend on the choice of location. This section will outline the major factors that went into our final decision to locate in rural United States.

Ethanol Price

The price of ethanol is perhaps the most critical factor in determining the profitability of our process. It is possible that producing butanol could actually lose money when compared to just selling the product from the ethanol plant. The price of butanol is assumed to be 1.3 to 1.5 times the price of ethanol in either country. Therefore, if the price of ethanol were substantially larger in one country, it would easily make that country the more profitable choice. However, the ethanol prices in the U.S. and Brazil are roughly the same, hovering around $2-3/gallon. In addition, the prices of biofuels are highly dependent on government policy and subsides, making this analysis difficult to base wholly on predictions of future prices.

Ethanol Supply

The continuous supply of ethanol in the United States makes it highly suitable for our process. In the U.S., ethanol is almost entirely produced from corn. Corn can be harvested year-round, which translates to an uninterrupted, continuous supply of ethanol. In Brazil, ethanol is produced from sugarcane, which can only be harvested nine months of the year. Locating in Brazil would lead to two possible ways to run our process. Either run at a higher rate of production for nine months out of the year, or run at the same level of production year-round while utilizing enormous ethanol storage tanks. Both of these options would result in higher capital and utility costs, and the first option would lead to problems with employing workers for only nine months out of the year. Therefore, the continuous supply of ethanol is a major reason for locating our plant in the U.S.

Transportation

The costs of transportation mainly influence the decision to locate our process in a rural rather than an industrial site. It is assumed that the ethanol plant is located in a rural environment, and that the butanol must be transported to an industrial environment. Therefore it is advantageous to locate in the area with the lowest costs of transportation. Our problem statement states that it costs $0.05/gallon to transport ethanol to an industrial site, which equates to $5.0 million per year for our feed of 100 MM gallons. There are no costs of butanol transportation from an industrial site. The problem statement also states that it costs $0.05/gallon to transport butanol from a rural site, which comes to $3.3 million per year for our production of 71.4 MM gallons. There are no costs of ethanol transportation to a rural site. Solely based on the costs of ethanol and butanol transportation, choosing to locate at a rural site saves $1.7 million per year.

The other cost data given in the problem statement relates to the purchase/transportation costs of hydrogen. It costs more to use hydrogen in a rural setting, at $0.75/lb in both the U.S. and Brazil. This leads to an annual cost of approximately $10,000 for a hydrogen requirement of 12,800 lb/year. In an industrial setting, hydrogen costs $0.50/lb in the U.S. and $0.60/lb in Brazil. This translates to approximately $8,000/year and $6,500/year respectively. Clearly the several thousand dollars in savings on hydrogen cost achieved by locating at an industrial site are overshadowed by the $1.7 million in savings mentioned above. For this reason, and the other reasons outlined in this section, our plant will be located at a rural site in the United States.

Section X

Important Considerations

Safety

Butanol and ethanol are both flammable materials, and both will be stored and transported in substantial quantities in around the plant. Precautions must be taken to ensure that they are kept at the correct temperature and pressure, and with the proper sensors and control systems to detect leaks. The auto-ignition point of butanol is 649 °F, and the auto-ignition point of ethanol is 685 °F. The highest temperature that either of these species experience is at the process is the exit from the reactor (S6) at 374 °F. This temperature is safely below the auto-ignition point, meaning that there is no risk of auto-ignition.

Care must be taken to ensure that the ethanol and butanol storage tanks are in cool, well-ventilated areas without risk of electrical sparks. Butanol must not be allowed to reach its flammability limit of 1.4% in air, as this would pose a serious safety hazard. Similarly, ethanol must not be allowed to reach its flammability limit of 3.3% in air.

The side products of the reaction are hexanol, octanol, 2-ethylhexanol, and 2-ethylbutanol. These are all flammable hydrocarbons, but are at such low concentrations throughout the process that they do not pose a hazard from a safety standpoint. The process is charged with ethylene glycol, which is flammable with an auto-ignition point of 748 °F. It reaches a temperature of 409 °F at almost pure ethylene glycol (S26). This is well below the auto-ignition temperature. Lastly, the pressurized hydrogen recycle stream (S11) reaches a temperature of 1232 °F, which could increase the risk of ignition. However, the flow rate of this stream is low at only 208 lb/hr and the hazard can be controlled with the proper equipment.

Environmental

Our process will strictly adhere to regional and federal regulations to ensure that the transportation, storage, and discharge of our materials are done in an environmentally friendly manner. The ethanol and butanol storage tanks and transportation vehicles pose a potential environmental hazard in the event of an accidental release of material. Employee training and education is essential to preventing such an accident.

The water stream (S25) leaving distillation unit D-402 is 99.6 mol% water, with 0.1 mol% butanol and 0.3% ethanol. The EPA regulates discharge water very tightly in order to

protect groundwater and drinking water. The proper permits must be obtained in order to begin discharging this water into the environment.

Pilot Plant

This process is based on several assumptions that will need to be tested at pilot plant scale prior to the implementation of the full-scale plant. In particular, the reaction data obtained from U.S. Patent 8,318,990 was for a small batch reaction, not for the large continuous reaction proposed in this report. The conversion and selectivity to butanol may be different what was listed in the patent, and these differences must be quantified through further research.

The packed bed reactor design may need to be modified to compensate for these differences. The residence time in the reactor, hydrogen partial pressure, reactor temperature, and ethanol recycle rate are some of the factors that might be adjusted when more research is done. The separation sequences, however, would probably not be affected except to accommodate higher or lower flow rates of material. A pilot plant will be able to answer these questions and determine whether the development of the full-scale plant is feasible.

Section XI

Specification Sheets

Pumps

P-101					
Block Type:	Pump			*Inlet Stream:*	S1
		Type:	Centrifugal	*Outlet Stream:*	S2
Function:	To raise the pressure of stream S1 to 725 psia				
Design:		*Casing Material:*	Carbon Steel	*Inlet Pressure:*	15 psia
		Liquid Flow Rate:	226.88 gpm	*Outlet Pressure:*	725.19 psia
		Fluid Head:	2059.5 ft	*Electricity:*	102.262 kW
		Pump Efficiency:	62.31 %	*Net Work Required:*	137.136 hp
		Total Weight:	16,582 lb		
Cost:		*Purchase Cost:*	*Bare Module Cost:*	*Utility (USD/hr):*	
		$85,100.00	$273,171.00	$7.98	
Remarks:					

P-102					
Block Type:	Pump			*Inlet Stream:*	S18
		Type:	Centrifugal	*Outlet Stream:*	S19
Function:	To raise the pressure of stream S18 to 725 psi				
Design:		*Casing Material:*	Carbon Steel	*Inlet Pressure:*	14.7 psia
		Liquid Flow Rate:	815.09 gpm	*Outlet Pressure:*	725.19 psia
		Fluid Head:	2055.39 ft	*Electricity:*	306.531 kW
		Pump Efficiency:	74.71%	*Net Work Required:*	411.064 hp
		Total Weight:	31,536 lb		
Cost:		*Purchase Cost:*	*Bare Module Cost:*	*Utility (USD/hr):*	
		$155,700.00	$499,797.00	$23.91	
Remarks:					

P-301					
Block Type:	Pump			*Inlet Stream:*	S23
		Type:	Centrifugal	*Outlet Stream:*	S24
Function:	To raise the pressure of stream S23 to 23.3 psia				
Design:		*Casing Material:*	Carbon Steel	*Inlet Pressure:*	14.5 psia
		Liquid Flow Rate:	1031.62 gpm	*Outlet Pressure:*	23.3 psia
		Fluid Head:	16.625 ft	*Electricity:*	3.09 kW
		Pump Efficiency:	76.57%	*Net Work Required:*	4.14 hp
		Total Weight:	10767 lb		
Cost:		*Purchase Cost:*	*Bare Module Cost:*	*Utility (USD/hr):*	
		$12,200.00	$39,162.00	$0.24	
Remarks:					

P-302					
Block Type:	Reflux Pump for D-301			*Inlet Stream:*	Reflux
		Type:	Centrifugal	*Outlet Stream:*	Reflux
Function:	To enable the reflux flow to reach the top of the column				
Design:		*Casing Material:*	Carbon Steel	*Electricity:*	220.24 kW
		Liquid Flow Rate:	1931.21 gpm		
		Pump Efficiency:	70%		
		Total Weight:	19, 721 lb		
Cost:		*Purchase Cost:*	*Bare Module Cost:*	*Utility (USD/hr):*	
		$25,500.00	$81,855.00	$17.18	
Remarks:					

P-401					
Block Type:	Pump			*Inlet Stream:*	Reflux
		Type:	Centrifugal	*Outlet Stream:*	Reflux
Function:	To enable the reflux flow to reach the top of the column				
Design:		*Casing Material:*	Carbon Steel	*Electricity:*	274.12 kW
		Liquid Flow Rate:	2403.62 gpm		
		Pump Efficiency:	70%		
		Total Weight:	22,439 lb		
Cost:		*Purchase Cost:*	*Bare Module Cost:*	*Utility (USD/hr):*	
		$38,700.00	$124,227.00	$21.38	
Remarks:					

P-402					
Block Type:	Pump			*Inlet Stream:*	Reflux
		Type:	Centrifugal	*Outlet Stream:*	Reflux
Function:	To enable the reflux flow to reach the top of the column				
Design:		*Casing Material:*	Carbon Steel	*Electricity:*	10.91 kW
		Liquid Flow Rate:	95.67 gpm		
		Pump Efficiency:	70%		
		Total Weight:	4629 lb		
Cost:		*Purchase Cost:*	*Bare Module Cost:*	*Utility (USD/hr):*	
		$5,700.00	$18,297.00	$0.85	
Remarks:					

P-403					
Block Type:	Pump			*Inlet Stream:*	S23
		Type:	Centrifugal	*Outlet Stream:*	S29
Function:	To raise the pressure of stream S23 to 27.75 psi				
Design:		*Casing Material:*	Carbon Steel	*Inlet Pressure:*	14.5 psi
		Liquid Flow Rate:	420.38 gpm	*Outlet Pressure:*	21.76 psi
		Fluid Head:	22.5 ft	*Electricity:*	3.502 kW
		Pump Efficiency:	75%	*Net Work Required:*	4.70 hp
		Total Weight:	10,561 lb		
Cost:		*Purchase Cost:*	*Bare Module Cost:*	*Utility (USD/hr):*	
		$11,000.00	$35,310.00	$0.27	
Remarks:					

Reactors

R-101-1				
Block Type:	Fixed Bed Catalytic Reactor			
Function:	To convert ethanol to butanol			
	Main Reaction: 2 Ethanol--> 1 Butanol + 1 Water			
	Secondary Reaction: 14 Ethanol--> 10 Water+ 4 Side Products			
Materials:		*Inlet*	*Outlet*	
	Stream	S5, S13	- - -	
	Mass Flow (lb/hr)	380995	380995	
	Volumetric Flow (ft3/hr)	17097	- - - - -	
Breakdown	(lb/hr):			
	Water	28	8333	
	Ethanol	378740	337646	
	Butanol	6	30475	
	Hydrogen	2222	2222	
	2-Ethyl Hexanol	Trace	510	
	2-Ethyl Butanol	Trace	650	
	n-Hexanol	Trace	510	
	n-Octanol	Trace	650	
	Ethylene Glycol	Trace	Trace	
Operating Conditions:		*Inlet*	*Outlet*	
	Temperature (F)	374	374	
	Pressure (psia)	725.19	725.14	
Design Data:				
	Contruction Material	Stainless Steel	Catalyst	Ru(acac)3
	Vessel Weight (lb)	109400	Residence Time (hr)	0.76
	Volume (gal)	8758.3	Catalyst Volume (ft3)	6851.81
	Diameter (ft)	7.5	Catalyst Weight (lb)	658726.9
	Length (ft)	26.5	Catalyst Cost	$10,516,574.96
	Wall Thickness (in)	1.7	Catalyst Life	90

R-101-1 Continued				
	Heat Duty (btu/hr)	-1727961.94	Cooling Water Flow (lb/hr)	194187.5
Costs:				
	Purchase Cost:	Bare Module Cost:	Annual Catalyst Cost:	Hourly Utility Cost:
	$411,200.00	$1,319,952.00	$42,066,299.83	$0.39
Remarks:	First of 2 reactors. Reactors are in parallel.			

R-101-2				
Block Type:	Fixed Bed Catalytic Reactor			
Function:	To convert ethanol to butanol			
	Main Reaction: 2 Ethanol--> 1 Butanol + 1 Water			
	Secondary Reaction: 14 Ethanol--> 10 Water+ 4 Side Products			
Materials:		*Inlet*	*Outlet*	
	Stream	- - -	S6	
	Mass Flow (lb/hr)	380985	380985	
	Volumetric Flow (ft3/hr)	- - - - -	34139.34	
	Breakdown (lb/hr):			
	Water	8333	16637	
	Ethanol	337646	296553	
	Butanol	30475	60943	
	Hydrogen	2222	2222	
	2-Ethyl Hexanol	510	1020	
	2-Ethyl Butanol	650	1300	
	n-Hexanol	510	1020	
	n-Octanol	650	1300	
	Ethylene Glycol	Trace	Trace	
Operating Conditions:		*Inlet*	*Outlet*	
	Temperature (F)	374	374	
	Pressure (psia)	725.14	725.08	
Design Data:				
	Contruction Material	Stainless Steel	Catalyst	Ru(acac)3
	Vessel Weight (lb)	109400	Residence Time (hr)	0.76

R-101-2 Continued				
	Volume (gal)	8758.3	Catalyst Volume (ft3)	6851.81
	Diameter (ft)	7.5	Catalyst Weight (lb)	658726.9
	Length (ft)	26.5	Catalyst Cost	$10,516,574.96
	Wall Thickness (in)	1.7	Catalyst Life	90
	Heat Duty (btu/hr)	-1727961.94	Cooling Water Flow (lb/hr)	194187.5
Costs:				
	Purchase Cost:	Bare Module Cost:	Annual Catalyst Cost:	Hourly Utility Cost:
	$411,200.00	$1,319,952.00	$42,066,299.83	$0.39
Remarks:	Second of 2 reactors. Reactors are in parallel.			

Distillation Columns

D-301				
Block Type:	Sieve Tray Distillation Tower			
Function:	To remove ethanol and water from the butanol and heavy alcohols that make up the product			
Materials:		*Feed*	*Distillate*	*Bottoms*
	Stream	S21	S23	S22
	Temperature (F)	86	172	265
	Pressure (psi)	20	15	21
	Mass Flow (lb/hr)	378542	312975	65567
Breakdown (lb/hr)				
	Water	16625	16625	Trace
	Ethanol	296339	296320	20
	Butanol	60937	30	60907
	Hydrogen	0	0	0
	2-Ethyl Hexanol	1020	Trace	1020
	2-Ethyl Butanol	1300	Trace	1300
	n-Hexanol	1020	Trace	1020
	n-Octanol	1300	Trace	1300
	Ethylene Glycol	Trace	Trace	Trace
Design Data:				
	Number of Stages:	40	Tray Type:	Sieve
	Height (ft):	122	Feed Stage:	20
	Diameter (ft):	23	Molar Reflux Ratio:	0.448
	Weight (lb):	930,078	Stage Pressure Drop (psi):	0.12
	Material:	Carbon Steel	Overhead Pressure (psi):	14.5
	Tray Spacing (ft):	2	Operating Temperature (F):	265
	Number of Trays:	55		
Costs:				
	Purchase Cost:	$1,673,400.00	Bare Module Cost:	$5,371,614.00
Remarks:				

D-401				
Block Type:	Sieve Tray Distillation Tower			
Function:	To separate ethanol for the purpose of recycling it back to the reactor			
Materials:		*Feed*	*Distillate*	*Bottoms*
	Stream	S29, S27	S17	S24
	Temperature (F)	156	173	335
	Pressure (psi)	21.8	14.7	21.9
	Mass Flow (lb/hr)	627703	296275	331428
Breakdown (lb/hr)				
	Water	16627	16	16611
	Ethanol	296320	296258	61
	Butanol	30	Trace	30
	Hydrogen	0	0	0
	2-Ethyl Hexanol	0	0	0
	2-Ethyl Butanol	0	0	0
	n-Hexanol	0	0	0
	n-Octanol	0	0	0
	Ethylene Glycol	314726	Trace	314726
Design Data:				
	Number of Stages:	45	Tray Type:	Sieve
	Height (ft):	136	Feed Stages:	13, 30
	Diameter (ft):	25	Molar Reflux Ratio:	2.2
	Weight (lb):	1,100,000	Stage Pressure Drop (psi):	0.12
	Material:	Carbon Steel	Overhead Pressure (psi):	14.7
	Tray Spacing (ft):	2	Operating Temperature (F):	335
	Number of Trays:	62		
Costs:				
	Purchase Cost:		Bare Module Cost:	
		$816,900.00		$2,622,249.00
Remarks:				

D-402				
Block Type:	Sieve Tray Distillation Tower			
Function:	To remove water from the system			
Materials:		*Feed*	*Distillate*	*Bottoms*
	Stream	S24	S25	S26
	Temperature (F)	335	211	409
	Pressure (psi)	21.9	14.7	20.9
	Mass Flow (lb/hr)	331428	16700	314728
Breakdown (lb/hr)				
	Water	16611	16609	2
	Ethanol	61	61	0
	Butanol	30	30	0
	Hydrogen	0	0	0
	2-Ethyl Hexanol	0	0	0
	2-Ethyl Butanol	0	0	0
	n-Hexanol	0	0	0
	n-Octanol	0	0	0
	Ethylene Glycol	314726	0	314726
Design Data:				
	Number of Stages:	35	Tray Type:	Sieve
	Height (ft):	108	Feed Stage:	15
	Diameter (ft):	12.5	Molar Reflux Ratio:	1.5
	Weight (lb):	314,036	Stage Pressure Drop (psi):	0.12
	Material:	Carbon Steel	Overhead Pressure (psi):	14.7
	Tray Spacing (ft):	2	Operating Temperature (F):	409
	Number of Trays:	48		
Costs:				
	Purchase Cost:		Bare Module Cost:	
		$592,700.00		$1,902,567.00
Remarks:				

Heat Exchangers

HX-101			
Block Type: Shell and Tube Heat Exchanger			
Function: To heat stream S15 to 302 F			
		Inlet	*Outlet*
Shell			
	Stream	S6	S7
	Temperature (F)	374	371.8
	Pressure (psi)	725.19	725.19
	Flow Rate (lb/hr)	380996	380996
Tube			
	Stream	S15	S14
	Temperature (F)	86	302
	Pressure (psi)	725.19	725.19
	Flow Rate (lb/hr)	2245.33	2245.33
Design Data:	Weight (lb)	10904	
	Construction Material	Carbon Steel	
	Flow Direction	Counter Current	
	Number of Tubes	120	
	Number of Tube Passes	1	
	Number of Shell Passes	1	
	Transfer Area (ft2)	69.47	
	Overall Heat Transfer Coefficient (BTU/(hr*ft2*R)	149.69	
	Heat Transferred (BTU/hr)	1612673.79	
Costs:			
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:
	$11,000.00	$35,310.00	$0.00
Remarks:			

HX-102			
Block Type: Shell and Tube Heat Exchanger			
Function: To heat stream S4 to 356 F			
		Inlet	*Outlet*
Shell			
	Stream	S7	S8
	Temperature (F)	371.8	223.7
	Pressure (psi)	725.19	725.19
	Flow Rate (lb/hr)	380996	380996
Tube			
	Stream	S4	S5
	Temperature (F)	168.1	356
	Pressure (psi)	725.19	725.19
	Flow Rate (lb/hr)	378542	378542
Design Data:	Weight (lb)	260512	
	Construction Material	Carbon Steel	
	Flow Direction	Counter Current	
	Number of Tubes	120	
	Number of Tube Passes	1	
	Number of Shell Passes	1	
	Transfer Area (ft2)	16811.12	
	Overall Heat Transfer Coefficient (BTU/(hr*ft2*R)	149.7	
	Heat Transferred (BTU/hr)	72,522,737	
Costs:			
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:
	$548,000.00	$1,759,080.00	$0.00
Remarks:			

HX-103				
Block Type: Shell and Tube Heat Exchanger				
Function: To heat stream S2 to 131 F				
		Inlet	*Outlet*	
Shell				
	Stream	S8	S9	
	Temperature (F)	223.7	216.9	
	Pressure (psi)	725.19	725.19	
	Flow Rate (lb/hr)	380996	380996	
Tube				
	Stream	S2	S3	
	Temperature (F)	86.7	131	
	Pressure (psi)	725.19	725.19	
	Flow Rate (lb/hr)	82267.53	82267.53	
Design Data:	Weight (lb)	16450		
	Construction Material	Carbon Steel		
	Flow Direction	Counter Current		
	Number of Tubes	120		
	Number of Tube Passes	1		
	Number of Shell Passes	1		
	Transfer Area (ft2)	146.47		
	Overall Heat Transfer Coefficient (BTU/(hr*ft2*R)	149.69		
	Heat Transferred (BTU/hr)	2420010.74		
Costs:				
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:	
	$19,300.00	$61,953.00	$0.00	
Remarks:				

HX-201			
Block Type:	Shell and Tube Heat Exchanger		
Function:	To cool stream S9 to 86 F		
		Inlet	*Outlet*
Shell			
	Stream	CW	CW
	Temperature (F)	68	78
	Pressure (psi)	14.7	14.7
	Flow Rate (lb/hr)	4392930.15	4392930.15
Tube			
	Stream	S9	S18
	Temperature (F)	216.9	86
	Pressure (psi)	725.19	725.19
	Flow Rate (lb/hr)	380996	380996
Design Data:	Weight (lb)	83040	
	Construction Material	Carbon Steel	
	Flow Direction	Counter Current	
	Number of Tubes	120	
	Number of Tube Passes	1	
	Number of Shell Passes	1	
	Heat Transferred (BTU/hr)	-39,426,380	
Costs:			
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:
	$162,600.00	$521,946.00	$8.82
Remarks:			

HX-301			
Block Type:	Condenser for D-301		
Function:	To completely condense the distillate phase of column D-301		
		Inlet	*Outlet*
Shell			
	Stream	CW	CW
	Temperature (F)	68	78
	Pressure (psi)	14.7	14.7
	Flow Rate (lb/hr)	20303460.5	20303460.5
Tube			
	Stream	Reflux	Reflux
	Temperature (F)	172.1	172.1
	Pressure (psi)	14.5	14.5
	Flow Rate (lbmol/hr)	7355.3285	7355.3285
Design Data:	Weight (lb)	130,218	
	Construction Material	Carbon Steel	
	Flow Direction	Counter Current	
	Number of Tubes	120	
	Number of Tube Passes	1	
	Number of Shell Passes	1	
	Heat Transferred (BTU/hr)	-182,222,782	
Costs:			
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:
	$269,200.00	$864,132.00	$40.76
Remarks:			

HX-401			
Block Type:	Condenser for D-401		
Function:	To completely condense distillate for D-401		
		Inlet	*Outlet*
Shell			
	Stream	CW	CW
	Temperature (F)	68	78
	Pressure (psi)	14.7	14.7
	Flow Rate (lb/hr)	38975460.5	38975460.5
Tube			
	Stream	Reflux	Reflux
	Temperature (F)	173	173
	Pressure (psi)	14.7	14.7
	Flow Rate (lbmol/hr)	6431.7	6431.7
Design Data:	Weight (lb)	234518	
	Construction Material	Carbon Steel	
	Flow Direction	Counter Current	
	Number of Tubes	120	
	Number of Tube Passes	1	
	Number of Shell Passes	1	
	Heat Transferred (BTU/hr)	-349803269	
Costs:			
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:
	$499,800.00	$1,604,358.00	$78.24
Remarks:			

HX-402			
Block Type:	Condenser for D-402		
Function:	To completely condense distillate for D-402		
		Inlet	*Outlet*
Shell			
	Stream	CW	CW
	Temperature (F)	68	78
	Pressure (psi)	14.7	14.7
	Flow Rate (lb/hr)	4529351.35	4529351.35
Tube			
	Stream	Reflux	Reflux
	Temperature (F)	210.5	210.5
	Pressure (psi)	14.7	14.7
	Flow Rate (lbmol/hr)	923.7	923.7
Design Data:	Weight (lb)	27318	
	Construction Material	Carbon Steel	
	Flow Direction	Counter Current	
	Number of Tubes	120	
	Number of Tube Passes	1	
	Number of Shell Passes	1	
	Heat Transferred (BTU/hr)	-40650755.3	
Costs:			
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:
	$34,300.00	$110,103.00	$9.09
Remarks:			

HX-403			
Block Type:	Shell and Tube Heat Exchanger		
Function:	To cool stream S26 to 140 F		
		Inlet	*Outlet*
Shell			
	Stream	CW	CW
	Temperature (F)	68	78
	Pressure (psi)	14.7	14.7
	Flow Rate (lb/hr)	6255117.45	6255117.45
Tube			
	Stream	S26	S27
	Temperature (F)	408.8	140
	Pressure (psi)	20.9	29.4
	Flow Rate (lb/hr)	314728	314728
Design Data:	Weight (lb)	54944	
	Construction Material	Carbon Steel	
	Flow Direction	Counter Current	
	Number of Tubes	120	
	Number of Tube Passes	1	
	Number of Shell Passes	1	
	Heat Transferred (BTU/hr)	-56139440	
Costs:			
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:
	$86,400.00	$277,344.00	$12.56
Remarks:			

Flash Vessels

F-201				
Block Type:	Flash Drum			
Function:	To separate hydrogen from the product			
Materials:		*Feed*	*Vapor*	*Liquid*
	Stream	S18	S15	S19
	Phase	MIX	VAP	LIQ
	Mass Flow Rate (lb/hr)	380996	2245.329	378750
Breakdown	(lb/hr)			
	Water	16637.06	4.427597	16632.63
	Ethanol	296553	81.42814	296472
	Butanol	60943.37	2.310741	60941.06
	Hydrogen	2222.127	2157.151	64.97619
	2-Ethyl hexanol	1020.024	0.00622906	1020.018
	2-Ethyl butanol	1300.065	0.000740605	1300.064
	n-Hexanol	1020.019	0.00401007	1020.015
	n-Octanol	1300.065	0.000657462	1300.064
	Ethylene Glycol	Trace	Trace	Trace
Operating Conditions:				
	Temperature (F)	86		
	Pressure (psi)	725.2		
Design Data:				
	Construction Material	Carbon Steel	Diameter (ft)	7.5
	Weight (lb)	84492	Height (ft)	23
	Volume (gal)	7601.5		
Costs:				
	Purchase Cost:		Bare Module Cost:	
		$120,300.00		$386,163.00
Remarks:				

F-202				
Block Type:	Flash Drum			
Function:	To separate hydrogen from the product			
Materials:		*Feed*	*Vapor*	*Liquid*
	Stream	S19	S13	S20
	Phase	MIX	VAP	LIQ
	Mass Flow Rate (lb/hr)	378750	207.0603	378543
Breakdown	(lb/hr)			
	Water	16632.63	7.217157	16625.41
	Ethanol	296472	132.272	296339
	Butanol	60941.06	3.750573	60937.31
	Hydrogen	64.97619	63.8017	1.174487
	2-Ethyl hexanol	1020.018	0.010088	1020.008
	2-Ethyl butanol	1300.064	0.00119456	1300.063
	n-Hexanol	1020.015	0.00649329	1020.008
	n-Octanol	1300.064	0.00106354	1300.063
	Ethylene Glycol	Trace	Trace	Trace
Operating Conditions:				
	Temperature (F)	85.8		
	Pressure (psi)	14.5		
Design Data:				
	Construction Material	Carbon Steel	Diameter (ft)	7.5
	Weight (lb)	84492	Height (ft)	23
	Volume (gal)	7601.5		
Costs:				
	Purchase Cost:		Bare Module Cost:	
		$120,300.00		$386,163.00
Remarks:				

Reboilers

E-301			
Block Type:	U Tube Kettle Reboiler		
Function:	To reboil bottoms stream in column D-301		
		Inlet	*Outlet*
Shell			
	Stream	Bottoms	Bottoms
	Temperature (F)	265.3	265.3
	Pressure (psi)	21.2	21.2
	Flow Rate (lbmol/hr)	862.1	862.1
Tube			
	Stream	S	S
	Temperature (F)	448	448
	Pressure (psi)	400	400
	Flow Rate (lb/hr)	284904.1	284904.1
Design Data:	Weight (lb)	255151	
	Construction Material	Carbon Steel	
	Flow Direction	Counter Current	
	Number of Tubes	120	
	Number of Tube Passes	1	
	Heat Transfer Area (ft2)	24,738	
	Heat Transferred (BTU/hr)	210,594,315	
Costs:			
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:
	$641,400.00	$2,058,894.00	$3,336.23
Remarks:			

E-401			
Block Type:	U Tube Kettle Reboiler		
Function:	To reboil bottoms stream in column D-401		
		Inlet	*Outlet*
Shell			
	Stream	Bottoms	Bottoms
	Temperature (F)	335.3	335.3
	Pressure (psi)	21.9	21.9
	Flow Rate (lbmol/hr)	5994.4	5994.4
Tube			
	Stream	S	S
	Temperature (F)	448	448
	Pressure (psi)	400	400
	Flow Rate (lb/hr)	529964.6	529964.6
Design Data:	Weight (lb)	605053	
	Construction Material	Carbon Steel	
	Flow Direction	Counter Current	
	Number of Tubes	120	
	Number of Tube Passes	1	
	Heat Transfer Area (ft2)	61,939	
	Heat Transferred (BTU/hr)	391,737,157.00	
Costs:			
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:
	$1,658,600.00	$5,324,106.00	$6,205.88
Remarks:			

E-403			
Block Type:	U Tube Kettle Reboiler		
Function:	To reboil bottoms stream in column D-403		
		Inlet	*Outlet*
Shell			
	Stream	Bottoms	Bottoms
	Temperature (F)	408.76	408.76
	Pressure (psi)	20.9	20.9
	Flow Rate (lbmol/hr)	5070.7	5070.7
Tube			
	Stream	S	S
	Temperature (F)	448	448
	Pressure (psi)	400	400
	Flow Rate (lb/hr)	75128.0	75128.0
Design Data:	Weight (lb)	187188	
	Construction Material	Carbon Steel	
	Flow Direction	Counter Current	
	Number of Tubes	120	
	Number of Tube Passes	1	
	Heat Transfer Area (ft2)	14,468	
	Heat Transferred (BTU/hr)	55,532,817	
Costs:			
	Purchase Cost:	Bare Module Cost:	Utilities Cost per hour:
	$496,200.00	$1,592,802.00	$879.75
Remarks:			

Compressor

C-101				
Block Type:	Compressor		*Inlet Stream:*	S28
	Type:	Centrifugal	*Outlet Stream:*	S11
Function:	To raise the pressure of stream S28 to 725.19 psi			
Design:	*Casing Material:*	Carbon Steel	*Inlet Pressure:*	14.5 psi
	Inlet Volumetric Flow Rate:	420.38 gpm	*Outlet Pressure:*	725.19 psi
	Head:	943528 ft lbf/lbm	*Electricity:*	102.77 kW
	Total Weight:	38,279 lb	*Net Work Required:*	137.82 hp
Cost:	*Purchase Cost:*	*Bare Module Cost:*	*Utility (USD/hr):*	
	$1,741,700.00	$5,590,857.00	$7.96	

Reflux Accumulators

E-302				
Block Type:	Reflux Accumulator for D-301		*Inlet Stream:*	Reflux
	Type:	Horizontal Vessel	*Outlet Stream*	Reflux
Function:	To accumulate reflux and distillate before it returns to the column D-301 or ir leaves in distillate stream S23			
Design Data:				
	Construction Material	Carbon Steel	*Temperature:*	172.08 F
	Storage Volume:	11462 gal	*Pressure:*	14.5 psi
	Diameter:	8.5 ft	*Weight:*	48,390 lb
	Height:	27 ft		
Costs:				
	Purchase Cost:		Bare Module Cost:	
		$50,800.00		$163,068.00

E-402				
Block Type:	Reflux Accumulator for D-401		*Inlet Stream:*	Reflux
	Type:	Horizontal Vessel	*Outlet Stream*	Reflux
Function:	To accumulate reflux and distillate before it returns to the column D-401 or ir leaves in distillate stream S17			
Design Data:				
	Construction Material	Carbon Steel	*Temperature:*	172.96 F
	Storage Volume:	13802 gal	*Pressure:*	14.7 psi
	Diameter:	9 ft	*Weight:*	44,782 lb
	Height:	29 ft		
Costs:				
	Purchase Cost:		Bare Module Cost:	
		$41,100.00		$131,931.00

E-405				
Block Type:	Reflux Accumulator for D-402		*Inlet Stream:*	Reflux
	Type:	Horizontal Vessel	*Outlet Stream*	Reflux
Function:	To accumulate reflux and distillate before it returns to the column D-402 or ir leaves in distillate stream S25			
Design Data:				
	Construction Material	Carbon Steel	*Temperature:*	210.55 F
	Storage Volume:	719.8 gal	*Pressure:*	14.7 psi
	Diameter:	3.5 ft	*Weight:*	12,494 lb
	Height:	10 ft		
Costs:				
	Purchase Cost:		Bare Module Cost:	
		$14,100.00		$45,261.00

Section XII

Cost Summaries

Table 12.1. General Input Summary

General Information

Process Title:	**Ethanol to Butanol**
Product:	**Butanol**
Plant Site Location:	**United States**
Site Factor:	**1.00**
Operating Hours per Year:	**7920**
Operating Days Per Year:	**330**
Operating Factor:	**0.9041**

Product Information

This Process will Yield

	9,026	gal of Butanol per hour
	216,624	gal of Butanol per day
	71,485,920	gal of Butanol per year
Price	**$4.41**	**/gal**

Chronology

Year	Action	Distribution of Permanent Investment	Production Capacity	Depreciation 5 year MACRS	Product Price
2014	Design		0.0%		
2015	Construction	100%	0.0%		
2016	Production	0%	45.0%	20.00%	$4.41
2017	Production	0%	67.5%	32.00%	$4.41
2018	Production	0%	90.0%	19.20%	$4.41
2019	Production		90.0%	11.52%	$4.41
2020	Production		90.0%	11.52%	$4.41
2021	Production		90.0%	5.76%	$4.41
2022	Production		90.0%		$4.41
2023	Production		90.0%		$4.41
2024	Production		90.0%		$4.41
2025	Production		90.0%		$4.41
2026	Production		90.0%		$4.41
2027	Production		90.0%		$4.41
2028	Production		90.0%		$4.41
2029	Production		90.0%		$4.41
2030	Production		90.0%		$4.41

Table 12.2. Equipment Cost Input Summary

Equipment Costs		
Equipment Description		**Bare Module Cost**
R-01	Fabricated Equipment	$1,319,952
R-02	Fabricated Equipment	$1,319,952
C-101	Process Machinery	$6,131,100
HX-101	Fabricated Equipment	$35,310
HX-102	Fabricated Equipment	$1,759,080
HX-103	Fabricated Equipment	$61,953
P-101	Process Machinery	$273,171
P-102	Process Machinery	$499,797
HX-201	Fabricated Equipment	$1,259,925
F-201	Fabricated Equipment	$386,163
F-202	Fabricated Equipment	$386,163
D-301	Fabricated Equipment	$5,473,371
E-301	Fabricated Equipment	$1,498,107
HX-301	Fabricated Equipment	$860,601
E-302	Fabricated Equipment	$162,105
P-302	Process Machinery	$124,227
D-401	Fabricated Equipment	$6,391,431
HX-401	Fabricated Equipment	$1,605,000
E-401	Fabricated Equipment	$5,304,846
E-402	Storage	$131,931
P-401	Process Machinery	$124,227
D-402	Fabricated Equipment	$1,902,567
HX-402	Fabricated Equipment	$110,424
E-403	Fabricated Equipment	$1,593,765
E-404	Storage	$45,261
P-402	Process Machinery	$18,297
HX-403	Fabricated Equipment	$277,344
Ru(acac)3	Catalysts	$1,288,109
Ethylene Glycol	Catalysts	$496,322
ST-01	Storage	$6,940,341
ST-02	Storage	$7,441,743
ST-03	Storage	$56,496
P-301	Process Machinery	$39,162
Total		***$55,318,243***

Table 12.3. Costs of Raw Materials and Utilities Input Summary

Raw Materials

	Raw Material:	Unit:	Required Ratio:		Cost of Raw Material:	
1	Ethanol	gal	1.39	gal per gal of Butanol	$2.940	per gal
2	Hydrogen	lb	0.000192	lb per gal of Butanol	$0.05	per lb
3	Ru(acac)3	lb	0.0368	lb per gal of Butanol	$31.93	per lb
	Total Weighted Average:				$5.262	per gal of Butanol

Utilities

	Utility:	Unit:	Ratio to Product		Utility Cost	
1	Steam @ 100 psi	lb	0.003450792	lb per gal of Butanol	$8.140E-03	per lb
2	Steam @ 165 psi	lb	0.006729597	lb per gal of Butanol	$9.760E-03	per lb
3		lb	0.001045121	lb per gal of Butanol	$9.760E-03	per lb
4	Cooling Water	lb	0.060542231	lb per gal of Butanol	$1.200E-04	per lb
5	Electricity	kWh	0.0000174	kWh per gal of Butanol	$0.078	per kWh
	Total Weighted Average:				$1.126E-04	per gal of Butanol

Table 12.4. Variable Costs, Working Capital and Total Permanent Investment Input Summary

Variable Costs			
General Expenses:			
Selling / Transfer Expenses:		**3.00 %**	**of Sales**
Direct Research:		**4.80 %**	**of Sales**
Allocated Research:		**0.50 %**	**of Sales**
Administrative Expense:		**2.00 %**	**of Sales**
Management Incentive Compensation:		**1.25 %**	**of Sales**
Working Capital			
Accounts Receivable	a	**30**	**Days**
Cash Reserves (excluding Raw Materials)	a	**30**	**Days**
Accounts Payable	a	**30**	**Days**
Butanol Inventory	a	**4**	**Days**
Raw Materials	a	**2**	**Days**
Total Permanent Investment			
Cost of Site Preparations:		**5.00 %**	**of Total Bare Module Costs**
Cost of Service Facilities:		**5.00 %**	**of Total Bare Module Costs**
Allocated Costs for utility plants and related facilities:		**$0**	
Cost of Contingencies and Contractor Fees:		**18.00 %**	**of Direct Permanent Investment**
Cost of Land:		**2.00 %**	**of Total Depreciable Capital**
Cost of Royalties:		**$0**	
Cost of Plant Start-Up:		**10.00 %**	**of Total Depreciable Capital**

Table 12.5. Fixed Costs Input Summary

Operations			
	Operators per Shift:	**1**	**(assuming 5 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:	**$0.0 0**	**per year, for each Operator per Shift**
	Control Laboratory:	**$0.0 0**	**per year, for each Operator per Shift**
Maintenance			
	Wages and Benefits:	**4.50 %**	**of Total Depreciable Capital**
	Salaries and Benefits:	**25%**	**of Maintenance Wages and Benefits**
	Materials and Services:	**100 %**	**of Maintenance Wages and Benefits**
	Maintenance Overhead:	**5%**	**of Maintenance Wages and Benefits**
Operating Overhead			
	General Plant Overhead:	**7.10 %**	**of Maintenance and Operations Wages and Benefits**
	Mechanical Department Services:	**2.40 %**	**of Maintenance and Operations Wages and Benefits**
	Employee Relations Department:	**5.90 %**	**of Maintenance and Operations Wages and Benefits**
	Business Services:	**7.40 %**	**of Maintenance and Operations Wages and Benefits**
Property Taxes and Insurance			
	Property Taxes and Insurance:	**2%**	**of Total Depreciable Capital**
Straight Line Depreciation			
Direct Plant:	8.00 %	**of Total Depreciable Capital, less 1.18 times the Allocated Costs for Utility Plants and Related Facilities**	
Allocated Plant:	6.00 %	**of 1.18 times the Allocated Costs for Utility Plants and Related Facilities**	
Other Annual Expenses			
	Rental Fees (Office and Laboratory Space):	**$0**	
	Licensing Fees:	**$0**	
	Miscellaneous:	**$0**	
Depletion Allowance			
	Annual Depletion Allowance:	**$0**	

Table 12.6. Variable Cost Summary

Variable Cost Summary			
Variable Costs at 100% Capacity:			
General Expenses			
Selling / Transfer Expenses:			$9,457,587
Direct Research:			$15,132,140
Allocated Research:			$1,576,265
Administrative Expense:			$6,305,058
Management Incentive Compensation:			$3,940,661
Total General Expenses			$36,411,711
Raw Materials	$5.261634	per gal of Butanol	$376,132,719
Byproducts	$0.000113	per gal of Butanol	($8,049)
Utilities	$0.000000	per gal of Butanol	$0
Total Variable Costs			**$412,536,381**

Table 12.7. Fixed Cost Summary

Fixed Cost Summary		
Operations		
	Direct Wages and Benefits	$364,000
	Direct Salaries and Benefits	$54,600
	Operating Supplies and Services	$21,840
	Technical Assistance to Manufacturing	$-
	Control Laboratory	$-
	Total Operations	**$440,440**
Maintenance		
	Wages and Benefits	$3,231,139
	Salaries and Benefits	$807,785
	Materials and Services	$3,231,139
	Maintenance Overhead	$161,557
	Total Maintenance	**$7,431,619**
Operating Overhead		
	General Plant Overhead:	$316,484
	Mechanical Department Services:	$106,981
	Employee Relations Department:	$262,994
	Business Services:	$329,857
	Total Operating Overhead	**$1,016,315**
Property Taxes and Insurance		
	Property Taxes and Insurance:	$1,436,062
Other Annual Expenses		
	Rental Fees (Office and Laboratory Space):	$-
	Licensing Fees:	$-
	Miscellaneous:	$-
	Total Other Annual Expenses	**$-**
Total Fixed Costs		**$10,324,436**

Table 12.8. Investment Summary

Investment Summary		
Bare Module Costs		
Fabricated Equipment	$31,708,059	
Process Machinery	$7,209,981	
Spares	$-	
Storage	$14,615,772	
Other Equipment	$-	
Catalysts	$1,784,431	
Computers, Software, Etc.	$-	
Total Bare Module Costs:		**$55,318,243**
Direct Permanent Investment		
Cost of Site Preparations:	$2,765,912	
Cost of Service Facilities:	$2,765,912	
Allocated Costs for utility plants and related facilities:	$-	
Direct Permanent Investment		**$60,850,067**
Total Depreciable Capital		
Cost of Contingencies & Contractor Fees	$10,953,012	
Total Depreciable Capital		**$71,803,079**
Total Permanent Investment		
Cost of Land:	$1,436,062	
Cost of Royalties:	$-	
Cost of Plant Start-Up:	$7,180,308	
Total Permanent Investment - Unadjusted		$80,419,449
Site Factor		1.00
Total Permanent Investment		**$80,419,449**

Table 12.9. Working Capital

Working Capital

	2015	2016	2017
Accounts Receivable	$11,660,039	$5,830,020	$5,830,020
Cash Reserves	$381,863	$190,931	$190,931
Accounts Payable	$(13,911,758)	$(6,955,879)	$(6,955,879)
Butanol Inventory	$1,554,672	$777,336	$777,336
Raw Materials	$927,451	$463,725	$463,725
Total	**$612,266**	**$306,133**	**$306,133**
Present Value at 15%	*$532,405*	*$231,481*	*$201,287*

Total Capital Investment **$81,384,622**

Table 12.10. Cash Flow Summary (A)

Year	Percentage of Design Capacity	Product Unit Price	Sales	Capital Costs	Working Capital	Var Costs	Fixed Costs
2014	0.00		0.00	0.00	0.00	0.00	0.00
2015	0.00		0.00	(80419400.00)	(612266.05)	0.00	0.00
2016	0.45	4.41	141863808.24	0.00	(306133.02)	(185641371.26)	(10324435.60)
2017	0.68	4.41	212795712.36	0.00	(306133.02)	(278462056.88)	(10324435.60)
2018	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2019	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2020	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2021	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2022	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2023	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2024	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2025	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2026	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2027	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2028	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2029	0.90	4.41	283727616.48	0.00	0.00	(371282742.51)	(10324435.60)
2030	0.90	4.41	283727616.48	0.00	1224532.09	(371282742.51)	(10324435.60)

Table 12.11. Cash Flow Summary (B)

Year	Depreciation	Depletion Allowance	Taxible Income	Taxes	Net Earnings	Cash Flow	Cumulative Net Present Value
2014	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2015	0.00	0.00	0.00	0.00	0.00	(81031700.00)	(70462360.86)
2016	(14360600.00)	0.00	(68462600.00)	25331200.00	(43131447.13)	(29077000.00)	(92448723.26)
2017	(22977000.00)	0.00	(98967800.00)	36618100.00	(62349692.29)	(39678800.00)	(118538204.58)
2018	(13786200.00)	0.00	(111665800.00)	41316300.00	(70349424.31)	(56563200.00)	(150878416.67)
2019	(8271700.00)	0.00	(106151300.00)	39276000.00	(66875304.12)	(58603600.00)	(180014757.91)
2020	(8271700.00)	0.00	(106151300.00)	39276000.00	(66875304.12)	(58603600.00)	(205350706.81)
2021	(4135900.00)	0.00	(102015400.00)	37745700.00	(64269713.97)	(60133900.00)	(227957250.86)
2022	0.00	0.00	(97879600.00)	36215400.00	(61664123.83)	(61664100.00)	(248115362.32)
2023	0.00	0.00	(97879600.00)	36215400.00	(61664123.83)	(61664100.00)	(265644154.90)
2024	0.00	0.00	(97879600.00)	36215400.00	(61664123.83)	(61664100.00)	(280886583.23)
2025	0.00	0.00	(97879600.00)	36215400.00	(61664123.83)	(61664100.00)	(294140868.73)
2026	0.00	0.00	(97879600.00)	36215400.00	(61664123.83)	(61664100.00)	(305666334.38)
2027	0.00	0.00	(97879600.00)	36215400.00	(61664123.83)	(61664100.00)	(315688478.43)
2028	0.00	0.00	(97879600.00)	36215400.00	(61664123.83)	(61664100.00)	(324403386.29)
2029	0.00	0.00	(97879600.00)	36215400.00	(61664123.83)	(61664100.00)	(331981567.05)
2030	0.00	0.00	(97879600.00)	36215400.00	(61664123.83)	(60439600.00)	(338440430.10)

Section XIII

Economic Analysis

Economic Analysis

The major purpose and one of the most pressing difficulties with this project is the viability and profitability of changing ethanol into butanol. At current market prices, the price per gallon of ethanol changes daily, depending on demand and time of year. For the purposes of this report, we used $2.94 per gallon of ethanol as the starting point. In order to estimate the viability of our project, we included the price of ethanol as part of the raw material costs for our project. In our initial analyses, we estimated the price of butanol to be approximately 1.5 times the price of ethanol. This is based on specifications given to us in the problem statement. As can be seen in the cost summary, the Net Present Value of the venture loses value at this ratio of butanol and ethanol prices. This is the result of a negative Internal Rate of Return, as can be seen in Table 13.1.

Table 13.1. Profitability Measures and Sensitivity Analysis on IRR

Profitability Measures

The Internal Rate of Return (IRR) for this project is	Negative IRR
The Net Present Value (NPV) of this project in 2014 is	$ (338,440,400)

ROI Analysis (Third Production Year)

Annual Sales	**283,727,616**	
Annual Costs	**(381,607,178)**	
Depreciation	**(6,433,556)**	
Income Tax	**38,595,853**	
Net Earnings	**(65,717,264)**	
Total Capital Investment		**81,643,981**
ROI	**-80.49%**	

Sensitivity Analyses

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

Table 13.2. IRR Analysis

Product Price \ Variable Costs	$206,268,190	$247,521,828	$288,775,466	$330,029,104	$371,282,743	***$412,536,381***	$453,790,019	$495,043,657	$536,297,295	$577,550,933	$618,804,571
$2.21	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$2.65	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.09	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.53	24.38%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.97	41.70%	17.05%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$4.41	56.18%	35.72%	8.64%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$4.85	69.19%	50.59%	29.65%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$5.29	81.20%	63.77%	45.05%	23.38%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$5.73	92.46%	75.87%	58.43%	39.51%	16.74%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$6.17	103.12%	87.18%	70.64%	53.17%	33.96%	9.37%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$6.62	113.28%	97.86%	82.00%	65.50%	47.96%	28.33%	0.38%	Negative IRR	Negative IRR	Negative IRR	Negative IRR

In order to produce a product where the Internal Rate of Return is not negative, it is necessary that the price of butanol be much greater. Our initial explorations showed that in order to reach a positive IRR, the price of butanol must be at least 2.124 times the price of ethanol, or $6.25 per gallon of butanol. At this ratio between the prices of butanol and ethanol, however, the net present value of the venture is still negative after 15 years of production, as can be seen in Table 13.3.

Table 13.3. Cumulative Net Present Value

Year	Cumulative Net Present Value at 15%
2014	-
2015	(75,244,100)
2016	(74,436,000)
2017	(69,889,600)
2018	(64,614,000)
2019	(61,041,000)
2020	(57,934,000)
2021	(55,807,500)
2022	(54,458,700)
2023	(53,285,800)
2024	(52,265,900)
2025	(51,379,000)
2026	(50,607,800)
2027	(49,937,200)
2028	(49,354,000)
2029	(48,846,900)
2030	(47,099,800)

After some experimentation, it was found that in order to have a positive Net Present Value after 15 years, the price of butanol must be at least 2.225 times the cost of ethanol, or $6.54 per gallon.

Section XIV

Conclusions and Recommendations

Conclusions and Recommendations

After extensive analysis, we have determined that at current prices of raw materials and products, the process would not be profitable. A significant drop in ethanol prices or increase in butanol prices would be necessary to ensure a positive Internal Rate of Return and Net Present Value. The market for butanol, however, is not fully established, and as such, the price of butanol may be subject to changes of this magnitude. Butanol offers a number of benefits over ethanol for use as a fuel source, and we expect butanol to develop a stronger market position in the near future. As butanol surpasses ethanol, the relative price should rise to a level that would make this process profitable.

In the mean time, a number of other factors will also affect the profitability of the process. Large changes in transportation costs or utilities cost would have a significant impact on the total variable costs, and may affect the choice of location for this plant. Additionally, the catalyst represents one of the largest costs associated with the process, so a decrease in the price or an increase in the life cycle of the catalyst could lead to positive returns. This is an important factor because limited experimental data is available for modeling the reactor with this catalyst.

Before committing to developing this process, it would also be necessary to perform more experimentation to analyze the effectiveness of operating the reactor continuously and determine kinetic data. Provided that these experiments are successful and the market outlook is positive, this plant has potential to achieve a strong hold on this emerging market.

Section XV

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Section XVI

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Section XVII

Appendix

Appendix Table of Contents

Appendix A. Sample Calculations

Ethanol Feed Calculations

Known: We wish to use 100 million gallons of ethanol per year

We will operate for 330 days per year

The density of ethanol is 8.33 lb/gal

Therefore the mass flow rate of ethanol is as follows:

$$m_{ethanol} = \left(\frac{100\ million\ gallons\ ethanol}{year}\right)\left(\frac{8.33\ lb\ ethanol}{gallon\ ethanol}\right)\left(\frac{1\ year}{330\ days}\right)\left(\frac{1\ day}{24\ hours}\right)$$

$$m_{ethanol} = 105{,}176.77\ {}^{lb}/_{hr}$$

Reactor Pressure Drop Calculations

Ergun Equation

$$\Delta p = \frac{150\mu(1-\epsilon)^2 V_s L}{\epsilon^3 D_p^2} + \frac{1.75(1-\epsilon)\rho V_s^2 L}{\epsilon^3 D_p}$$

Void Fraction (Ɛ)	0.391			
Vesel Diameter	21.5	ft	6.55319979	m
Vessel Height	157.5	ft	48.00599846	m
Packing Height (L)	156.5	ft	47.70119847	m
Mass Flow Rate	168266	kg/hr		
Density	0.00447707	g/mL		
Volume Flow rate	15233.3	L/min	913.998	m^3/hr
Vessel Area	33.72847448	m^2		
Vs	0.00752741822	m/s		
Dp	0.01	m		
mu	0.000102689	Pa/s		
delta P	364.7330373	Pa		

Total Pressure drop in the reactor=0.0529 psi

Heat Exchanger Calculation (HX-201)

The purpose of HX-201 is to cool stream S9 to 86 °F using cooling water. In addition, the heat transferred is 39,426,380 BTU/hr. The following inlet and outlet temperatures were obtained from the Aspen Plus simulation:

$T_{h,in}$= 216.9 °F

$T_{h,out}$=86 °F

$T_{c,in}$=68 °F

$T_{c,out}$=78 °F

The ΔT_{lm} calculation is completed below.

$$\Delta T_{lm} = \frac{\Delta T_1 - \Delta T_2}{ln(\Delta T_1/\Delta T_2)} = 59.16\ °\text{F}$$

The heat exchanger transfer area is calculated by assuming a heat transfer coefficient of

U= 50 BTU/ft^2-hr-°F.

$$A = \frac{Q}{U\Delta T_{lm}} = \frac{39{,}426{,}380\ BTU/hr}{50\ BTU/(ft^2 hr °\text{F}) * 59.16\ °\text{F}} = 13{,}328\ ft^2$$

This is very close to the transfer area calculated by Aspen Plus, at 13,046 ft^2. This results shows that Aspen Plus was using a heat transfer coefficient of U= 51.1 BTU/ft^2-hr-°F.

Appendix B. Sample Aspen Plus Simulation Results

Convergence

```
                                PROBLEM STATUS SECTION

BLOCK STATUS
------------

*****************************************************************************
*                                                                           *
* Calculations were completed normally                                      *
*                                                                           *
* All Unit Operation blocks were completed normally                         *
*                                                                           *
* All streams were flashed normally                                         *
*                                                                           *
* All Convergence blocks were completed normally                            *
*                                                                           *
*****************************************************************************
```

Distillation Tower D-401

```
BLOCK:  D-401    MODEL: RADFRAC
------------------------------
   INLETS   - S27      STAGE  13
              S29      STAGE  30
   OUTLETS  - S17      STAGE   1
              S24      STAGE  45
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                    ***  MASS AND ENERGY BALANCE  ***
                                    IN                OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)              12426.1           12426.1          0.00000
      MASS(LB/HR   )              627703.           627703.        -0.297890E-08
      ENTHALPY(BTU/HR  )       -0.184787E+10     -0.180593E+10    -0.226931E-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                                          45
 ALGORITHM OPTION                                         NEWTON
 INITIALIZATION OPTION                                    AZEOTROPIC
 HYDRAULIC PARAMETER CALCULATIONS                         NO
 DESIGN SPECIFICATION METHOD                              SIMULT
 MAXIMUM NO. OF NEWTON ITERATIONS                          200
 MAXIMUM NUMBER OF FLASH ITERATIONS                         30
 FLASH TOLERANCE                                            0.000100000
 COLUMN EQUATIONS CONVERGENCE TOLERANCE                     0.100000-06

****    COL-SPECS    ****

 MOLAR VAPOR DIST / TOTAL DIST                              0.0
 MOLAR REFLUX RATIO                                         2.20000
 MOLAR DISTILLATE RATE          LBMOL/HR                6,431.66

****     PROFILES    ****

 P-SPEC           STAGE    1  PRES, PSIA                    14.6959
                           2                               17.6351

                      ********************
                      ****  RESULTS  ****
                      ********************


***    COMPONENT SPLIT FRACTIONS    ***

                          OUTLET STREAMS
                          --------------
                 S17           S24
 COMPONENT:
 WATER        .98679E-03    .99901
 ETHANOL      .99979        .20660E-03
 BUTANOL     0.0000        1.0000
 ETHYLGLY     .27739E-14    1.0000


***     SUMMARY OF KEY RESULTS     ***

 TOP STAGE TEMPERATURE          F                          172.958
 BOTTOM STAGE TEMPERATURE       F                          335.333
 TOP STAGE LIQUID FLOW          LBMOL/HR                14,149.6
 BOTTOM STAGE LIQUID FLOW       LBMOL/HR                 5,994.40
 TOP STAGE VAPOR FLOW           LBMOL/HR                    0.0
 BOILUP VAPOR FLOW              LBMOL/HR                18,678.3
 MOLAR REFLUX RATIO                                         2.20000
 MOLAR BOILUP RATIO                                         3.11595
 CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                     -0.349803+09
 REBOILER DUTY                  BTU/HR                      0.391737+09

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

 DEW POINT                      0.58006E-10  STAGE= 42
 BUBBLE POINT                   0.58006E-10  STAGE= 42
 COMPONENT MASS BALANCE         0.11115E-04  STAGE= 13 COMP=WATER
 ENERGY BALANCE                 0.14553E-08  STAGE= 13


****     PROFILES    ****

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

                                          ENTHALPY
STAGE TEMPERATURE    PRESSURE             BTU/LBMOL          HEAT DUTY
```

	F	PSIA	LIQUID	VAPOR	BTU/HR
1	172.96	14.696	-0.11626E+06	-99418.	-.34980+09
2	181.43	17.635	-0.11596E+06	-99268.	
10	183.53	18.435	-0.11589E+06	-99231.	
11	183.81	18.535	-0.11592E+06	-99227.	
12	184.33	18.635	-0.11646E+06	-99239.	
13	189.91	18.735	-0.13832E+06	-99415.	
14	190.14	18.835	-0.13829E+06	-99412.	
29	193.90	20.335	-0.13767E+06	-99488.	
30	193.12	20.435	-0.13201E+06	-99525.	
31	193.34	20.535	-0.13199E+06	-99522.	
40	196.12	21.435	-0.13192E+06	-99776.	
41	197.87	21.535	-0.13237E+06	-0.10006E+06	
42	204.00	21.635	-0.13364E+06	-0.10070E+06	
44	255.24	21.835	-0.14629E+06	-0.10338E+06	
45	335.33	21.935	-0.17652E+06	-0.11561E+06	.39174+09

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.2058E+05	0.000				6431.6558	
2	0.1440E+05	0.2058E+05					
10	0.1442E+05	0.2085E+05					
11	0.1440E+05	0.2085E+05					
12	0.1416E+05	0.2084E+05					
13	0.1865E+05	0.2060E+05	5070.7242				
14	0.1866E+05	0.2001E+05					
29	0.1902E+05	0.2030E+05					
30	0.2627E+05	0.2038E+05	7355.3285				
31	0.2628E+05	0.2027E+05					
40	0.2668E+05	0.2058E+05					
41	0.2672E+05	0.2069E+05					
42	0.2646E+05	0.2073E+05					
44	0.2467E+05	0.2057E+05					
45	5994.	0.1868E+05				5994.3969	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.9481E+06	0.000				.29627+06	
2	0.6633E+06	0.9481E+06					
10	0.6642E+06	0.9604E+06					
11	0.6636E+06	0.9604E+06					
12	0.6540E+06	0.9599E+06					
13	0.9416E+06	0.9502E+06	.31473+06				
14	0.9420E+06	0.9232E+06					
29	0.9265E+06	0.9134E+06					
30	0.1234E+07	0.9081E+06	.31298+06				
31	0.1235E+07	0.9031E+06					
40	0.1165E+07	0.8697E+06					
41	0.1087E+07	0.8335E+06					
42	0.9105E+06	0.7554E+06					
44	0.8574E+06	0.4265E+06					
45	0.3314E+06	0.5260E+06				.33143+06	

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

STAGE	WATER	ETHANOL	BUTANOL	ETHYLGLY
1	0.14160E-03	0.99986	0.14399E-19	0.21869E-14
2	0.12553E-03	0.99987	0.63968E-19	0.43108E-13
10	0.10039E-03	0.99986	0.56090E-15	0.38940E-04
11	0.10032E-03	0.99941	0.17074E-14	0.49437E-03
12	0.10221E-03	0.99343	0.51941E-14	0.64704E-02
13	0.16895E-03	0.72316	0.13499E-13	0.27667

14	0.29297E-03	0.72317	0.47519E-13	0.27654
29	0.60235E-01	0.66932	0.56605E-05	0.27044
30	0.78566E-01	0.72556	0.19729E-04	0.19585
31	0.78703E-01	0.72552	0.19727E-04	0.19576
40	0.19894	0.60565	0.33943E-02	0.19201
41	0.31298	0.48426	0.11298E-01	0.19147
42	0.54475	0.24230	0.18317E-01	0.19463
44	0.61880	0.43463E-02	0.10735E-02	0.37578
45	0.15381	0.22168E-03	0.68574E-04	0.84590

**** MOLE-Y-PROFILE ****

STAGE	WATER	ETHANOL	BUTANOL	ETHYLGLY
1	0.15911E-03	0.99984	0.31309E-20	0.84584E-16
2	0.14160E-03	0.99986	0.14399E-19	0.21869E-14
10	0.11334E-03	0.99988	0.12730E-15	0.21102E-05
11	0.11310E-03	0.99986	0.38787E-15	0.26928E-04
12	0.11306E-03	0.99955	0.11803E-14	0.34177E-03
13	0.11451E-03	0.99544	0.35721E-14	0.44499E-02
14	0.19837E-03	0.99534	0.12581E-13	0.44586E-02
29	0.40412E-01	0.95536	0.16167E-05	0.42251E-02
30	0.56254E-01	0.94012	0.52826E-05	0.36249E-02
31	0.56315E-01	0.94005	0.52855E-05	0.36329E-02
40	0.13845	0.85748	0.10665E-02	0.30021E-02
41	0.21202	0.78106	0.43578E-02	0.25613E-02
42	0.35901	0.62423	0.14545E-01	0.22146E-02
44	0.91991	0.56047E-01	0.74065E-02	0.16634E-01
45	0.76803	0.56700E-02	0.13960E-02	0.22491

**** K-VALUES ****

STAGE	WATER	ETHANOL	BUTANOL	ETHYLGLY
1	1.1237	0.99998	0.21745	0.38677E-01
2	1.1280	0.99998	0.22509	0.50730E-01
10	1.1290	1.0000	0.22696	0.54190E-01
11	1.1275	1.0005	0.22718	0.54468E-01
12	1.1061	1.0062	0.22724	0.52820E-01
13	0.67779	1.3765	0.26461	0.16084E-01
14	0.67711	1.3764	0.26476	0.16123E-01
29	0.67090	1.4274	0.28561	0.15623E-01
30	0.71601	1.2957	0.26776	0.18509E-01
31	0.71554	1.2957	0.26793	0.18558E-01
40	0.69591	1.4158	0.31420	0.15635E-01
41	0.67742	1.6129	0.38572	0.13377E-01
42	0.65904	2.5763	0.79408	0.11378E-01
44	1.4866	12.895	6.8996	0.44266E-01
45	4.9932	25.577	20.357	0.26588

**** MASS-X-PROFILE ****

STAGE	WATER	ETHANOL	BUTANOL	ETHYLGLY
1	0.55379E-04	0.99994	0.23169E-19	0.29467E-14
2	0.49093E-04	0.99995	0.10293E-18	0.58084E-13
10	0.39259E-04	0.99991	0.90250E-15	0.52466E-04
11	0.39225E-04	0.99929	0.27467E-14	0.66599E-03
12	0.39884E-04	0.99126	0.83388E-14	0.86986E-02
13	0.60283E-04	0.65983	0.19818E-13	0.34011
14	0.10454E-03	0.65991	0.69768E-13	0.33998
29	0.22280E-01	0.63308	0.86144E-05	0.34463
30	0.30115E-01	0.71121	0.31115E-04	0.25865
31	0.30171E-01	0.71124	0.31116E-04	0.25856
40	0.82099E-01	0.63914	0.57632E-02	0.27300
41	0.13864	0.54856	0.20591E-01	0.29221
42	0.28516	0.32435	0.39452E-01	0.35103
44	0.32078	0.57617E-02	0.22896E-02	0.67116
45	0.50118E-01	0.18471E-03	0.91932E-04	0.94961

**** MASS-Y-PROFILE ****

STAGE	WATER	ETHANOL	BUTANOL	ETHYLGLY

1	0.62227E-04	0.99994	0.50380E-20	0.11397E-15
2	0.55379E-04	0.99994	0.23169E-19	0.29467E-14
10	0.44324E-04	0.99995	0.20484E-15	0.28432E-05
11	0.44232E-04	0.99992	0.62410E-15	0.36281E-04
12	0.44210E-04	0.99950	0.18990E-14	0.46044E-03
13	0.44715E-04	0.99397	0.57389E-14	0.59865E-02
14	0.77462E-04	0.99392	0.20214E-13	0.59985E-02
29	0.16177E-01	0.97799	0.26629E-05	0.58273E-02
30	0.22749E-01	0.97219	0.87895E-05	0.50505E-02
31	0.22774E-01	0.97216	0.87946E-05	0.50618E-02
40	0.59015E-01	0.93471	0.18704E-02	0.44089E-02
41	0.94816E-01	0.89322	0.80183E-02	0.39464E-02
42	0.17748	0.78916	0.29586E-01	0.37721E-02
44	0.79921	0.12452	0.26475E-01	0.49792E-01
45	0.49133	0.92757E-02	0.36744E-02	0.49572

Heat Exchanger HX-102

```
BLOCK:  HX-102   MODEL: HEATX
------------------------------
  HOT SIDE:
  ---------
  INLET STREAM:              S7
  OUTLET STREAM:             S8
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  COLD SIDE:
  ----------
  INLET STREAM:              S4
  OUTLET STREAM:             S5
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                    ***  MASS AND ENERGY BALANCE  ***
                                    IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            17542.5          17542.5          0.00000
```

```
    MASS(LB/HR    )            759538.          759538.          0.00000
    ENTHALPY(BTU/HR  )      -0.184464E+10    -0.184464E+10    -0.129249E-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                      356.0000
  LMTD CORRECTION FACTOR                                  1.00000

PRESSURE SPECIFICATION:
  HOT  SIDE PRESSURE DROP        PSI                      0.0000
  COLD SIDE PRESSURE DROP        PSI                      0.0000

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:
                 ---------------------------------------
                 |                                     |
S7         ----->|                HOT                  |-----> S8
T=  3.7180D+02   |                                     |       T=  2.2369D+02
P=  7.2519D+02   |                                     |       P=  7.2519D+02
V=  2.1013D-01   |                                     |       V=  1.2125D-01
                 |                                     |
S5         <-----|                COLD                 |<----- S4
T=  3.5600D+02   |                                     |       T=  1.6815D+02
P=  7.2519D+02   |                                     |       P=  7.2519D+02
V=  0.0000D+00   |                                     |       V=  0.0000D+00
                 ---------------------------------------

DUTY AND AREA:
  CALCULATED HEAT DUTY           BTU/HR          72522737.1288
  CALCULATED (REQUIRED) AREA     SQFT               15325.9271
  ACTUAL EXCHANGER AREA          SQFT               15325.9271
  PER CENT OVER-DESIGN                                  0.0000

HEAT TRANSFER COEFFICIENT:
```

```
  AVERAGE COEFFICIENT (DIRTY)     BTU/HR-SQFT-R          149.6937
  UA (DIRTY)                      BTU/HR-R           2294194.0602

LOG-MEAN TEMPERATURE DIFFERENCE:
  LMTD CORRECTION FACTOR                                  1.0000
  LMTD (CORRECTED)                F                      31.6114
  NUMBER OF SHELLS IN SERIES                              1

PRESSURE DROP:
  HOTSIDE, TOTAL                  PSI                     0.0000
  COLDSIDE, TOTAL                 PSI                     0.0000

                    ***  ZONE RESULTS  ***

TEMPERATURE LEAVING EACH ZONE:

                                  HOT
        ------------------------------------------------------------
        |                                                          |
HOT IN  |                          COND                            | HOT OUT
------> |                                                          |------>
 371.8  |                                                          |  223.7
        |                                                          |
COLDOUT |                          LIQ                             | COLDIN
<------ |                                                          |<------
 356.0  |                                                          |  168.1
        |                                                          |
        ------------------------------------------------------------
                                  COLD

  ZONE HEAT TRANSFER AND AREA:

  ZONE       HEAT DUTY        AREA        LMTD       AVERAGE U        UA
             BTU/HR           SQFT         F         BTU/HR-SQFT-R   BTU/HR-R
    1   72522737.129     15325.9271      31.6114    149.6937     2294194.0602
```

Pump P-301

```
BLOCK:  P-301    MODEL: PUMP
------------------------------

  INLET STREAM:          S20
  OUTLET STREAM:         S21
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                   ***  MASS AND ENERGY BALANCE  ***
                                    IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            8217.40          8217.40          0.00000
      MASS(LB/HR    )            378542.          378542.          0.00000
      ENTHALPY(BTU/HR  )      -0.100176E+10    -0.100175E+10    -0.105280E-04

                   ***  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  ***
   OUTLET PRESSURE  PSIA                                  20.3053
   DRIVER EFFICIENCY                                       1.00000

   FLASH SPECIFICATIONS:
   LIQUID PHASE CALCULATION
   NO FLASH PERFORMED
   MAXIMUM NUMBER OF ITERATIONS                           30
   TOLERANCE                                              0.000100000

                         ***  RESULTS  ***
   VOLUMETRIC FLOW RATE  CUFT/HR                      7,522.18
   PRESSURE CHANGE  PSI                                   5.80151
   NPSH AVAILABLE   FT-LBF/LB                            37.5591
   FLUID POWER  HP                                        3.17382
   BRAKE POWER  HP                                        4.14492
   ELECTRICITY  KW                                        3.09087
   PUMP EFFICIENCY USED                                   0.76571
   NET WORK REQUIRED  HP                                  4.14492
   HEAD DEVELOPED FT-LBF/LB                              16.6010
```

Appendix C. MSDS Reports

2-Ethylbutanol

ACROS ORGANICS

Material Safety Data Sheet
2-Ethyl-1-Butanol, 98%

MSDS# 49370

Section 1 - Chemical Product and Company Identification

MSDS Name:	2-Ethyl-1-Butanol, 98%
Catalog Numbers:	AC118170000, AC118170050, AC118171000, AC118175000
Synonyms:	2-Ethylbutyl Alcohol
Company Identification:	Acros Organics BVBA Janssen Pharmaceuticalaan 3a 2440 Geel, Belgium
Company Identification: (USA)	Acros Organics One Reagent Lane Fair Lawn, NJ 07410
For information in the US, call:	800-ACROS-01
For information in Europe, call:	+32 14 57 52 11
Emergency Number, Europe:	+32 14 57 52 99
Emergency Number US:	201-796-7100
CHEMTREC Phone Number, US:	800-424-9300
CHEMTREC Phone Number, Europe:	703-527-3887

Section 2 - Composition, Information on Ingredients

CAS#:	97-95-0
Chemical Name:	2-Ethyl-1-Butanol
%:	98
EINECS#:	202-621-4

Hazard Symbols: XN

Risk Phrases: 10 21/22

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Warning! Flammable liquid and vapor. May be harmful if absorbed through the skin. May be harmful if swallowed. Causes eye and skin irritation. Causes digestive and respiratory tract irritation. Target Organs: None.

Potential Health Effects

Eye:	Causes severe eye irritation.
Skin:	Causes skin irritation. May be harmful if absorbed through the skin.
Ingestion:	Causes gastrointestinal irritation with nausea, vomiting and diarrhea. May be harmful if swallowed.
Inhalation:	May cause respiratory tract irritation. Vapors may cause dizziness or suffocation.
Chronic:	

Section 4 - First Aid Measures

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

Section 5 - Fire Fighting Measures

General Information:	As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Vapors may form an explosive mixture with air. Vapors can travel to a source of ignition and flash back. Will burn if involved in a fire. Use water spray to keep fire-exposed containers cool. Containers may explode in the heat of a fire. Flammable liquid and vapor. Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas.
Extinguishing Media:	For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam. For large fires, use water spray, fog, or alcohol-resistant foam. Use water spray to cool fire-exposed containers. Water may be ineffective. Do NOT use straight streams of water.
Autoignition Temperature:	315 deg C (599.00 deg F)
Flash Point:	57 deg C (134.60 deg F)
Explosion Limits: Lower:	Not available
Explosion Limits: Upper:	Not available
NFPA Rating:	3 - health, 2 - flammability, 0 - instability

Section 6 - Accidental Release Measures

General Information:	Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks:	Absorb spill with inert material (e.g. vermiculite, sand or earth), then place in suitable container. Remove all sources of ignition. Use a spark-proof tool. Provide ventilation. A vapor suppressing foam may be used to reduce vapors.

Section 7 - Handling and Storage

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

Section 8 - Exposure Controls, Personal Protection

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
2-Ethyl-1-Butanol	none listed	none listed	none listed

OSHA Vacated PELs: 2-Ethyl-1-Butanol: None listed

Engineering Controls:

Use adequate ventilation to keep airborne concentrations low.

Exposure Limits

Personal Protective Equipment

Eyes:	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin:	Wear appropriate protective gloves to prevent skin exposure.

Clothing: Wear appropriate protective clothing to prevent skin exposure.

Respirators: Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Section 9 - Physical and Chemical Properties

Physical State: Liquid
Color: colorless
Odor: None reported.
pH: Not available
Vapor Pressure: 1.7 hPa @ 20 C
Vapor Density: 3.4
Evaporation Rate: Not available
Viscosity: 7.6 MPA 20.00 deg C
Boiling Point: 146 deg C @ 760.00mm Hg (294.80°F)
Freezing/Melting Point: -15 deg C (5.00°F)
Decomposition Temperature: Not available
Solubility in water: Slightly soluble
Specific Gravity/Density: .8300g/cm3
Molecular Formula: C6H14O
Molecular Weight: 102.18

Section 10 - Stability and Reactivity

Chemical Stability: Stable under normal temperatures and pressures.
Conditions to Avoid: Incompatible materials, ignition sources, excess heat, strong oxidants.
Incompatibilities with Other Materials: Strong oxidizing agents, acids.
Hazardous Decomposition Products: Carbon monoxide, carbon monoxide, carbon dioxide.
Hazardous Polymerization: Has not been reported.

Section 11 - Toxicological Information

RTECS#: CAS# 97-95-0: EL3850000

RTECS:

CAS# 97-95-0: Oral, rabbit: LD50 = 1200 mg/kg;

LD50/LC50: Oral, rat: LD50 = 1850 mg/kg;
Skin, rabbit: LD50 = 1260 uL/kg;
.

Carcinogenicity: 2-Ethyl-1-Butanol - Not listed as a carcinogen by ACGIH, IARC, NTP, or CA Prop 65.

Other: See actual entry in RTECS for complete information.

Section 12 - Ecological Information

Not available

Section 13 - Disposal Considerations

Dispose of in a manner consistent with federal, state, and local regulations.

Section 14 - Transport Information

US DOT
Shipping Name: 2-ETHYLBUTANOL
Hazard Class: 3
UN Number: UN2275
Packing Group: III
Canada TDG
Shipping Name: Not available
Hazard Class:
UN Number:
Packing Group:

Section 15 - Regulatory Information

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols: XN

Risk Phrases:

R 10 Flammable.

R 21/22 Harmful in contact with skin and if swallowed.

Safety Phrases:

S 9 Keep container in a well-ventilated place.

S 16 Keep away from sources of ignition - No smoking.

S 33 Take precautionary measures against static discharges.

WGK (Water Danger/Protection)

CAS# 97-95-0: 1

Canada

CAS# 97-95-0 is listed on Canada's DSL List

Canadian WHMIS Classifications: Not available

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

CAS# 97-95-0 is listed on Canada's Ingredient Disclosure List

US Federal

TSCA

CAS# 97-95-0 is listed on the TSCA Inventory.

Section 16 - Other Information

MSDS Creation Date: 5/01/1998
Revision #5 Date 7/20/2009

[redacted] Reviewed
2012.11.06
11:05:11 -05'00'

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

2-Ethylhexanol

SAFETY DATA SHEET

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier
Product name: Eastman(TM) 2-Ethylhexanol

Product No.: EAN 903608. 00175-00, P0017500, P0017501, P0017503, P0017504, P0017505, P001750A, P001750B, E00175E1, E00175E2, E00175E3, E0017504, P0017506, P0017508

Synonyms, Trade Names: 2EH, 00175-00

Additional identification
Chemical name: 2-ethylhexanol
CAS-No.: 104-76-7

1.2 Relevant identified uses of the substance or mixture and uses advised against
Identified uses: Solvent
Uses advised against: None known.

1.3 Details of the supplier of the safety data sheet
Manufacturer / Supplier
Eastman Chemical Company
200 South Wilcox Drive
Kingsport, TN 37660-5280 US
+14232292000

Visit our website at www.EASTMAN.com or email emnmsds@eastman.com

1.4 Emergency telephone number:
For emergency health, safety, and environmental information, call 1-423-229-4511 or 1-423-229-2000.

For emergency transportation information, in the United States: call CHEMTREC at 800-424-9300 or call 423-229-2000.

SECTION 2: Hazards identification

WARNING!
COMBUSTIBLE LIQUID AND VAPOR
HARMFUL IF INHALED
CAUSES SKIN AND EYE IRRITATION
AT ELEVATED TEMPERATURES, VAPOR MAY CAUSE IRRITATION OF EYES AND RESPIRATORY TRACT

SECTION 3: Composition/information on ingredients

3.1 / 3.2 Substances / Mixtures

General information:

EASTMAN
SDSUS / EN / 12
Version: 3.2
Revision date: 05/22/2012
Initiator: 0001
150000000124

Chemical name	Concentration	Additional identification	Notes
2-ethylhexanol	100%	CAS-No.: 104-76-7 EC No.: 203-234-3	

* All concentrations are percent by weight unless ingredient is a gas. Gas concentrations are in percent by volume.
# This substance has workplace exposure limit(s).
PBT: persistent, bioaccumulative and toxic substance.
vPvB: very persistent and very bioaccumulative substance.

SECTION 4: First aid measures

4.1 Description of first aid measures

Inhalation: Move to fresh air. If breathing is difficult, give oxygen. If breathing stops, provide artificial respiration. Get medical attention immediately.

Eye contact: Immediately flush with plenty of water for at least 15 minutes. If easy to do, remove contact lenses. Get medical attention. In case of irritation from airborne exposure, move to fresh air. Get medical attention if symptoms persist.

Skin contact: Immediately flush with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Get medical attention. Wash contaminated clothing before reuse. Destroy or thoroughly clean contaminated shoes.

Ingestion: Seek medical advice.

4.2 Most important symptoms and effects, both acute and delayed: No data available.

4.3 Indication of any immediate medical attention and special treatment needed

Hazards: None known.

Treatment: Treat symptomatically.

SECTION 5: Firefighting measures

General fire hazards: Combustible liquid and vapor. USE WATER WITH CAUTION. Material will float and may ignite on surface of water.

5.1 Extinguishing media

Suitable extinguishing media: Water spray. Dry chemical. Carbon Dioxide. Foam.

Unsuitable extinguishing media: None known.

5.2 Special hazards arising from the substance or mixture: None known.

5.3 Advice for firefighters

Special Fire Fighting Procedures:	Use water spray to keep fire-exposed containers cool.
Special protective equipment for fire-fighters:	Self-contained breathing apparatus and full protective clothing must be worn in case of fire.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures:	Wear appropriate personal protective equipment.
6.2 Environmental precautions:	Avoid release to the environment.
6.3 Methods and material for containment and cleaning up:	Eliminate sources of ignition. Absorb spill with vermiculite or other inert material, then place in a container for chemical waste. Large Spillages: Flush spill area with water spray. Prevent runoff from entering drains, sewers, or streams. Dike for later disposal.
Notification Procedures:	In the event of a spill or accidental release, notify relevant authorities in accordance with all applicable regulations.

SECTION 7: Handling and storage:

7.1 Precautions for safe handling:	Avoid breathing vapor. Avoid contact with eyes, skin, and clothing. Use only with adequate ventilation. Wash thoroughly after handling.
7.2 Conditions for safe storage, including any incompatibilities:	Keep container closed.
7.3 Specific end use(s):	Solvent

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limits

If exposure limits have not been established, maintain airborne levels to an acceptable level.

8.2 Exposure controls

Appropriate engineering controls:	Good general ventilation (typically 10 air changes per hour) should be used. Ventilation rates should be matched to conditions. If applicable, use process enclosures, local exhaust ventilation, or other engineering controls to maintain airborne levels below recommended exposure limits. If exposure limits have not been established, maintain airborne levels to an acceptable level.

Individual protection measures, such as personal protective equipment

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General information:	Eye bath. Washing facilities. Safety shower.
Eye/face protection:	Wear safety glasses with side shields (or goggles). Wear a full-face respirator, if needed.
Skin protection	
Hand protection:	Wear chemical-resistant gloves, footwear, and protective clothing appropriate for the risk of exposure. Contact health and safety professional or manufacturer for specific information.
Other:	No data available.
Respiratory Protection:	If engineering controls do not maintain airborne concentrations below recommended exposure limits (where applicable) or to an acceptable level (in countries where exposure limits have not been established), an approved respirator must be worn. In the United States of America, if respirators are used, a program should be instituted to assure compliance with OSHA Standard 63 FR 1152, January 8, 1998. Respirator type: Air-purifying respirator with an appropriate, government approved (where applicable), air-purifying filter, cartridge or canister. Contact health and safety professional or manufacturer for specific information.
Hygiene measures:	Observe good industrial hygiene practices.
Environmental Controls:	No data available.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance	
Physical State:	Liquid
Form:	Liquid
Color:	Colorless
Odor:	musty
Odor Threshold:	0.07 ppm
pH:	No data available.
Freezing Point:	-76 - -70 °C
Boiling Point:	184 °C
Flash Point:	73.3 °C (Tag closed cup)
Evaporation Rate:	No data available.
Flammability (solid, gas):	No data available.
Flammability Limit - Upper (%)–:	No data available.
Flammability Limit - Lower (%)–:	No data available.
Vapor pressure:	No data available.
Vapor density (air=1):	No data available.
Specific Gravity:	0.833 (20 °C)
Solubility(ies)	
Solubility in Water:	0.1 g/l

Solubility (other):	No data available.
Partition coefficient (n-octanol/water):	Pow: 1,260 log Pow: 3.1
Autoignition Temperature:	No data available.
Decomposition Temperature:	(DSC) No exotherm to 500°C
Dynamic Viscosity:	No data available.
Kinematic viscosity:	No data available.
Explosive properties:	No data available.
Oxidizing properties:	No data available.

SECTION 10: Stability and reactivity

10.1 Reactivity:	None known.
10.2 Chemical stability:	Stable
10.3 Possibility of hazardous reactions:	None at ambient temperatures.
10.4 Conditions to avoid:	Heat, sparks, flames.
10.5 Incompatible materials:	Strong oxidizing agents.
10.6 Hazardous decomposition products:	Carbon Dioxide. Carbon Monoxide.

SECTION 11: Toxicological information

Information on likely routes of exposure

Inhalation:	Harmful if inhaled. May cause respiratory irritation.
Ingestion:	None known.
Skin contact:	Causes skin irritation.
Eye contact:	Causes eye irritation.

11.1 Information on toxicological effects

Acute Toxicity

Oral

Product:	No data available.
Specified substance(s) 2-ethylhexanol	Oral LD-50: (Rat): 3,290 mg/kg

Dermal

Product:	No data available.
Specified substance(s) 2-ethylhexanol	Dermal LD-50: (Rat): > 3,000 mg/kg

Inhalation

Product:	No data available.
Specified substance(s) 2-ethylhexanol	LC50 (Rat, 6 h): 1.2 mg/l

Repeated dose toxicity

Product:	No data available.
Specified substance(s) 2-ethylhexanol	No data available.

Skin corrosion/irritation:

Product:	No data available.
Specified substance(s) 2-ethylhexanol	(Rabbit, 24 h): moderate

Serious eye damage/eye irritation:

Product:	No data available.
Specified substance(s) 2-ethylhexanol	(Rabbit): moderate

Respiratory or skin sensitization:

Product:	No data available.
Specified substance(s) 2-ethylhexanol	Skin Sensitization:, (Human) - Not a skin sensitizer.

Germ cell mutagenicity

In vitro

Product:	No data available.
Specified substance(s) 2-ethylhexanol	No data available.

In vivo

Product:	No data available.
Specified substance(s) 2-ethylhexanol	No data available.

Carcinogenicity

Product:	No data available.
Specified substance(s) 2-ethylhexanol	No data available.

Reproductive toxicity

Product:	No data available.
Specified substance(s) 2-ethylhexanol	No data available.

Specific target organ toxicity - single exposure

Product:	No data available.
Specified substance(s)	
2-ethylhexanol	No data available.

Specific target organ toxicity - repeated exposure

Product:	No data available.
Specified substance(s)	
2-ethylhexanol	No data available.

Aspiration hazard

Product:	No data available.
Specified substance(s)	
2-ethylhexanol	No data available.

Other adverse effects: No data available.

SECTION 12: Ecological information

12.1 Toxicity

Acute toxicity

Fish

Product:	No data available.
Specified substance(s)	
2-ethylhexanol	LC-50 (Fathead Minnow, 96 h): 28.2 mg/l

Aquatic invertebrates

Product:	No data available.
Specified substance(s)	
2-ethylhexanol	EC-50 (daphnid, 48 h): 39 mg/l

Chronic Toxicity

Fish

Product:	No data available.
Specified substance(s)	
2-ethylhexanol	No data available.

Aquatic invertebrates

Product:	No data available.
Specified substance(s)	
2-ethylhexanol	No data available.

Toxicity to Aquatic Plants

Product:	No data available.
Specified substance(s)	
2-ethylhexanol	No data available.

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12.2 Persistence and degradability

Biodegradation

Product:	No data available.
Specified substance(s)	
2-ethylhexanol	100 % (14 d)

Biological Oxygen Demand:

Product	No data available.
Specified substance(s)	
2-ethylhexanol	767 mg/g 2,180 mg/g

Chemical Oxygen Demand:

Product	No data available.
Specified substance(s)	
2-ethylhexanol	No data available.

BOD/COD ratio

Product	No data available.
Specified substance(s)	
2-ethylhexanol	No data available.

12.3 Bioaccumulative potential

Product:	No data available.
Specified substance(s)	
2-ethylhexanol	No data available.

12.4 Mobility in soil: No data available.

Known or predicted distribution to environmental compartments

2-ethylhexanol: No data available.

12.5 Results of PBT and vPvB assessment: No data available.

2-ethylhexanol: No data available.

12.6 Other adverse effects: No data available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

General information: No data available.

Disposal Methods: Dispose of waste and residues in accordance with local authority requirements. Incinerate. Since emptied containers retain product residue, follow label warnings even after container is emptied.

SECTION 14: Transport information

Important Note: Shipping descriptions may vary based on mode of transport, quantities, package size, and/or origin and destination. Consult your company's Hazardous Materials/Dangerous Goods expert for information specific to your situation.

DOT

Class combustible liquid, Packing group **III** for quantities of 450 liters (119 gallons) or more; not regulated for smaller quantities

Possible Shipping Description(s):

NA 1993 Combustible liquid, n.o.s. (2-Ethyl Hexanol) combustible liquid **III**

IMDG - International Maritime Dangerous Goods Code

Class not regulated

Possible Shipping Description(s):

not regulated

IATA

Class not regulated

Possible Shipping Description(s):

not regulated

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture:

This product has been classified in accordance with hazard criteria of the Controlled Products Regulations and the MSDS contains all the information required by the Controlled Products Regulations.
WHMIS (Canada) Status: controlled
WHMIS (Canada) Hazard Classification: B/3, D/2/B

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SARA 311-312 Hazard Classification(s):
immediate (acute) health hazard
fire hazard

US EPCRA (SARA Title III) Section 313 - Toxic Chemical List
NONE

OSHA: hazardous

TSCA (US Toxic Substances Control Act): This product is listed on the TSCA inventory. Any impurities present in this product are exempt from listing.

DSL (Canadian Domestic Substances List) and CEPA (Canadian Environmental Protection Act): This product is listed on the DSL. Any impurities present in this product are exempt from listing.

AICS / NICNAS (Australian Inventory of Chemical Substances and National Industrial Chemicals Notification and Assessment Scheme): This product is listed on AICS or otherwise complies with NICNAS.

MITI (Japanese Handbook of Existing and New Chemical Substances): This product is listed in the Handbook or has been approved in Japan by new substance notification.

ECL (Korean Toxic Substances Control Act): This product is listed on the Korean inventory or otherwise complies with the Korean Toxic Substances Control Act.KE-13766

Philippines Inventory (PICCS) : This product is listed on the Philippine Inventory or otherwise complies with PICCS.

Inventory of Existing Chemical Substances in China: All components of this product are listed on the Inventory of Existing Chemical Substances in China (IECSC).

SECTION 16: Other information

HMIS® Hazard Ratings: Health - 2, Flammability - 2, Chemical Reactivity - 0

HMIS® rating involves data interpretations that may vary from company to company. They are intended only for rapid, general identification of the magnitude of the specific hazard. To deal adequately with the safe handling of this material, all the information contained in this MSDS must be considered.

Revision Information: Not relevant.

Key literature references and sources for data: No data available.

Training information: No data available.

Issue Date: 05/22/2012
SDS No:
Disclaimer: This information is provided without warranty. The information is believed to be correct. This information should be used to make an independent determination of the methods to safeguard workers and the environment.

N-Butanol

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Chemicals & Laboratory Equipment

Health	1
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
1-Butanol MSDS

Section 1: Chemical Product and Company Identification

Product Name: 1-Butanol

Catalog Codes: SLB3157, SLB1489

CAS#: 71-36-3

RTECS: EO1400000

TSCA: TSCA 8(b) inventory: 1-Butanol

CI#: Not applicable.

Synonym: Propylcarbinol

Chemical Name: N-Butyl alcohol

Chemical Formula: CH3(CH2)2CH2OH

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{1-}Butanol	71-36-3	100

Toxicological Data on Ingredients: 1-Butanol: ORAL (LD50): Acute: 790 mg/kg [Rat.]. DERMAL (LD50): Acute: 3400 mg/kg [Rabbit.].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant, permeator), of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (sensitizer). Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

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. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Get medical attention immediately.

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

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

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

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

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

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 343°C (649.4°F)

Flash Points: CLOSED CUP: 28.9°C (84°F). OPEN CUP: 36.1°C (97°F) (Cleveland).

Flammable Limits: LOWER: 1.4% UPPER: 11.2%

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. Flammable in presence of heat, of oxidizing materials, of reducing materials, of combustible materials.

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

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards: May form explosive mixtures with air. CAUTION: MAY BURN WITH NEAR INVISIBLE FLAME

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. 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. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, reducing agents.

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:
CEIL: 152 (mg/m3) Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Z)

Odor: Vinous. (Slight.)

Taste: Not available.

Molecular Weight: 74.12g/mole

Color: Colorless.

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

Boiling Point: 117.7°C (243.9°F)

Melting Point: -89.5°C (-129.1°F)

Critical Temperature: Not available.

Specific Gravity: 0.81(Water = 1)

Vapor Pressure: 0.6 kPa (@ 20°C)

Vapor Density: 2.55 (Air = 1)

Volatility: Not available.

Odor Threshold: 1.2 ppm

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

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

Solubility:
Easily soluble in methanol, diethyl ether. Partially soluble in cold water, hot water, n-octanol.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances:
Highly reactive with oxidizing agents, reducing agents. Slightly reactive to reactive with organic materials, acids, alkalis.

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: Dermal contact. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 790 mg/kg [Rat.]. Acute dermal toxicity (LD50): 3400 mg/kg [Rabbit.]. Acute toxicity of the vapor (LC50): 8000 4 hours [Rat.].

Chronic Effects on Humans: Not available.

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

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Can cause gastrointestinal disturbances.

Special Remarks on other Toxic Effects on Humans: Exposure can cause nausea, headache and vomiting.

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 more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Butanol UNNA: UN1120 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: 1-Butanol Massachusetts RTK: 1-Butanol TSCA 8(b) inventory: 1-Butanol

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

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):
R10- Flammable. R22- Harmful if swallowed. R38- Irritating to skin. R41- Risk of serious damage to eyes.

HMIS (U.S.A.):

Health Hazard: 1

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: -Manufacturer's Material Safety Data Sheet.

Other Special Considerations: Not available.

Created: 10/10/2005 08:15 PM

Last Updated: 05/21/2013 12:00 PM

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Ethanol

ScienceLab.com
Chemicals & Laboratory Equipment

Health	2
Fire	3
Reactivity	0
Personal Protection	E

Material Safety Data Sheet
Ethyl alcohol 200 Proof MSDS

Section 1: Chemical Product and Company Identification

Product Name: Ethyl alcohol 200 Proof

Catalog Codes: SLE2248, SLE1357

CAS#: 64-17-5

RTECS: KQ6300000

TSCA: TSCA 8(b) inventory: Ethyl alcohol 200 Proof

CI#: Not applicable.

Synonym: Ethanol; Absolute Ethanol; Alcohol; Ethanol 200 proof; Ethyl Alcohol, Anhydrous; Ethanol, undenatured; Dehydrated Alcohol; Alcohol

Chemical Name: Ethyl Alcohol

Chemical Formula: CH3CH2OH

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Ethyl alcohol 200 Proof	64-17-5	100

Toxicological Data on Ingredients: Ethyl alcohol 200 Proof: ORAL (LD50): Acute: 7060 mg/kg [Rat]. 3450 mg/kg [Mouse]. VAPOR (LC50): Acute: 20000 ppm 8 hours [Rat]. 39000 mg/m 4 hours [Mouse].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant), of inhalation. Slightly hazardous in case of skin contact (permeator), of ingestion.

Potential Chronic Health Effects:
Slightly hazardous in case of skin contact (sensitizer). CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Classified PROVEN for human. DEVELOPMENTAL TOXICITY: Classified Development toxin [PROVEN]. Classified Reproductive system/toxin/female, Reproductive system/toxin/male [POSSIBLE]. The substance is toxic to blood, the reproductive system, liver, upper respiratory tract, 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. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Get medical attention.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. 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 medical attention.

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

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

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. 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: 363°C (685.4°F)

Flash Points: CLOSED CUP: 12.78°C (55°F). OPEN CUP: 17.78°C (64°F) (Cleveland).

Flammable Limits: LOWER: 3.3% UPPER: 19%

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. Slightly flammable to flammable in presence of oxidizing materials.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Slightly explosive in presence of open flames and sparks, of heat, of oxidizing materials, of acids.

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

Special Remarks on Fire Hazards:
Containers should be grounded. CAUTION: MAY BURN WITH NEAR INVISIBLE FLAME Vapor may travel considerable distance to source of ignition and flash back. May form explosive mixtures with air. Contact with Bromine pentafluoride is likely to cause fire or explosion. Ethanol ignites on contact with chromyl chloride. Ethanol ignites on contact with iodine heptafluoride gas. It ignites than explodes upon contact with nitrosyl perchlorate. Additon of platinum black catalyst caused ignition.

Special Remarks on Explosion Hazards:
Ethanol has an explosive reaction with the oxidized coating around potassium metal. Ethanol ignites and then explodes on contact with acetic anhydride + sodium hydrosulfate (ignites and may explode), disulfuric acid + nitric acid, phosphorous(III) oxide platinum, potassium-tert-butoxide+ acids. Ethanol forms explosive products in reaction with the following compound :

ammonia + silver nitrate (forms silver nitride and silver fulminate), iodine + phosphorus (forms ethane iodide), magnesium perchlorate (forms ethyl perchlorate), mercuric nitrate, nitric acid + silver (forms silver fulminate) silver nitrate (forms ethyl nitrate) silver(I) oxide + ammonia or hydrazine (forms silver nitride and silver fulminate), sodium (evolves hydrogen gas). Sodium Hydrazide + alcohol can produce an explosion. Alcohols should not be mixed with mercuric nitrate, as explosive mercuric fulminate may be formed. May form explosive mixture with manganese perchlorate + 2,2-dimethoxypropane. Addition of alcohols to highly concentrate hydrogen peroxide forms powerful explosives. Explodes on contact with calcium hypochlorite

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

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

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves. Use a respirator if the exposure limit is exceeded.

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: 1900 (mg/m3) from OSHA (PEL) [United States] TWA: 1000 (ppm) from OSHA (PEL) [United States] TWA: 1900 (mg/m3) from NIOSH [United States] TWA: 1000 (ppm) from NIOSH [United States] TWA: 1000 (ppm) [United Kingdom (UK)] TWA: 1920 (mg/m3) [United Kingdom (UK)] TWA: 1000 STEL: 1250 (ppm) [Canada]Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Liquid.)

Odor:

Mild to strong, rather pleasant; like wine or whiskey. Alcohol-like; Ethereal, vinous.

Taste: Pungent. Burning.

Molecular Weight: 46.07 g/mole

Color: Colorless. Clear

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

Boiling Point: 78.5°C (173.3°F)

Melting Point: -114.1°C (-173.4°F)

Critical Temperature: 243°C (469.4°F)

Specific Gravity: 0.789 (Water = 1)

Vapor Pressure: 5.7 kPa (@ 20°C)

Vapor Density: 1.59 (Air = 1)

Volatility: Not available.

Odor Threshold: 100 ppm

Water/Oil Dist. Coeff.: The product is more soluble in water; log(oil/water) = -0.3

Ionicity (in Water): Not available.

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

Solubility:
Easily soluble in cold water, hot water. Soluble in methanol, diethyl ether, acetone.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Incompatible materials, heat, sources of ignition.

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

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Ethanol rapidly absorbs moisture from the air. Can react vigorously with oxiders. The following oxidants have been demonstrated to undergo vigorous/explosive reaction with ethanol: barium perchlorate, bromine pentafluoride, calcium hypochlorite, chloryl perchlorate, chromium trioxide, chromyl chloride, dioxygen difluoride, disulfuryl difluoride, fluorine nitrate, hydrogen peroxide, iodine heptafluoride, nitric acid nitrosyl perchlorate, perchloric acid permanganic acid, peroxodisulfuric acid, potassium dioxide, potassium perchlorate, potassium permanganate, ruthenium(VIII) oxide, silver perchlorate, silver peroxide, uranium hexafluoride, uranyl perchlorate. Ethanol reacts violently/expodes with the following compounds: acetyl bromide (evolves hydrogen bromide) acetyl chloride, aluminum, sesquibromide ethylate, ammonium hydroxide & silver oxide, chlorate, chromic anhydride, cyanuric acid + water, dichloromethane + sulfuric acid + nitrate (or) nitrite, hydrogen peroxide + sulfuric acid, iodine + methanol + mercuric oxide, manganese perchlorate + 2,2-dimethoxy propane, perchlorates, permanganates + sulfuric acid, potassium superoxide, potassium tert-butoxide, silver & nitric acid, silver perchlorate, sodium hydrazide, sulfuric acid + sodium dichromate, tetrachlorisilane + water. Ethanol is also incompatible with platinium, and sodium. No really safe conditions exist under which ethyl alcohol and chlorine oxides can be handled. Reacts vigorously with acetyl chloride

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

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

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 3450 mg/kg [Mouse]. Acute toxicity of the vapor (LC50): 39000 mg/m3 4 hours [Mouse].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Classified PROVEN for human. DEVELOPMENTAL TOXICITY: Classified Development toxin [PROVEN]. Classified Reproductive system/toxin/female, Reproductive system/toxin/male [POSSIBLE]. Causes damage to the following organs: blood, the reproductive system, liver, upper respiratory tract, skin, central nervous system (CNS).

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

Special Remarks on Toxicity to Animals:
Lowest Published Dose/Conc: LDL[Human] - Route: Oral; Dose: 1400 mg/kg LDL[Human child] - Route: Oral; Dose: 2000 mg/kg LDL[Rabbit] - Route: Skin; Dose: 20000 mg/kg

Special Remarks on Chronic Effects on Humans:
May affect genetic material (mutagenic) Causes adverse reproductive effects and birth defects (teratogenic) , based on moderate to heavy consumption. May cause cancer based on animal data. Human: passes through the placenta, excreted in maternal milk.

Special Remarks on other Toxic Effects on Humans:
Acute potential health effects: Skin: causes skin irritation Eyes: causes eye irritation Ingestion: May cause gastrointestinal tract irritation with nausea, vomiting, diarrhea, and alterations in gastric secretions. May affect behavior/central nervous system (central nervous system depression - amnesia, headache, muscular incoordination, excitation, mild euphoria, slurred speech, drowsiness, staggaring gait, fatigue, changes in mood/personality, excessive talking, dizziness, ataxia, somnolence, coma/narcosis, hallucinations, distorted perceptions, general anesthetic), peripherial nervous system (spastic paralysis)vision (diplopia). Moderately toxic and narcotic in high concentrations. May also affect metabolism, blood, liver, respiration (dyspnea), and endocrine system. May affect respiratory tract, cardiovascular(cardiac arrhythmias, hypotension), and urinary systems. Inhalation: May cause irritation of the respiratory tract and affect behavior/central nervous system with symptoms similar to ingestion. Chronic Potential Health Effects: Skin: Prolonged or repeated skin contact may casue dermatitis, an allergic reaction. Ingestion: Prolonged or repeated ingestion will have similar effects as acute ingestion. It may also affect the brain.

Section 12: Ecological Information

Ecotoxicity: Ecotoxicity in water (LC50): 14000 mg/l 96 hours [Rainbow trout]. 11200 mg/l 24 hours [fingerling trout].

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: : Ethanol UNNA: 1170 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: Ethyl alcohol 200 Proof (in alcoholic beverages) California prop. 65: This product contains the following ingredients for which the State of California has found to cause birth defects which would require a warning under the statute: Ethyl alcohol 200 Proof (in alcoholic beverages) Connecticut hazardous material survey.: Ethyl alcohol 200 Proof Illinois toxic substances disclosure to employee act: Ethyl alcohol 200 Proof Rhode Island RTK hazardous substances: Ethyl alcohol 200 Proof Pennsylvania RTK: Ethyl alcohol 200 Proof Florida: Ethyl alcohol 200 Proof Minnesota: Ethyl alcohol 200 Proof Massachusetts RTK: Ethyl alcohol 200 Proof Massachusetts spill list: Ethyl alcohol 200 Proof New Jersey: Ethyl alcohol 200 Proof Tennessee: Ethyl alcohol 200 Proof California - Directors List of Hazardous Substances (8 CCR 339): Ethyl alcohol 200 Proof TSCA 8(b) inventory: Ethyl alcohol 200 Proof

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

Other Classifications:

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

DSCL (EEC):
R11- Highly flammable. S7- Keep container tightly closed. S16- Keep away from sources of ignition - No smoking.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: E

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:
-SAX, N.I. Dangerous Properties of Industrial Materials. Toronto, Van Nostrand Reinold, 6e ed. 1984. -Material safety data sheet emitted by: la Commission de la Santé et de la Sécurité du Travail du Québec. -Hawley, G.G.. The Condensed Chemical Dictionary, 11e ed., New York N.Y., Van Nostrand Reinold, 1987. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II. HSDB, RTECS, and LOLI databases.

Other Special Considerations: Not available.

Created: 10/09/2005 05:28 PM

Last Updated: 05/21/2013 12:00 PM

Ethylene Glycol

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Chemicals & Laboratory Equipment

Health	1
Fire	1
Reactivity	0
Personal Protection	C

Material Safety Data Sheet
Ethylene glycol MSDS

Section 1: Chemical Product and Company Identification

Product Name: Ethylene glycol

Catalog Codes: SLE1072

CAS#: 107-21-1

RTECS: KW2975000

TSCA: TSCA 8(b) inventory: Ethylene glycol

CI#: Not available.

Synonym: 1,2-Dihydroxyethane; 1,2-Ethanediol; 1,2-Ethandiol; Ethylene dihydrate; Glycol alcohol; Monoethylene glycol; Tescol

Chemical Name: Ethylene Glycol

Chemical Formula: HOCH2CH2OH

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Ethylene glycol	107-21-1	100

Toxicological Data on Ingredients: Ethylene glycol: ORAL (LD50): Acute: 4700 mg/kg [Rat]. 5500 mg/kg [Mouse]. 6610 mg/kg [Guinea pig]. VAPOR (LC50): Acute: >200 mg/m 4 hours [Rat].

Section 3: Hazards Identification

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

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Non-mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to kidneys, liver, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure to a highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

Section 4: First Aid Measures

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

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 immediately.

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. 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:
Medical Conditions Aggravated by Exposure: Persons with pre-existiing kidney, respiratory, eye, or neurological problems might be more sensitive to Ethylene Glycol. Notes to Physician: 1. Support vital functions, correct for dehydration and shock, and manage fluid balance. 2. The currently recommended medical management of Ethylene Glycol poisoning includes elimination of Ethylene Glycol and metabolites. Elimination of Ethylene Glycol may be achieved by the following methods: a. Emptying the stomach by gastric lavage. It is useful if initiated within < 1 of ingestion. b. Correct metabolic acidosis with intravenous administration of sodium bicarbonate, adjusting the administration rate accoridng to repeated and frequent measurement of acid/base status. c. Administer ethanol (orally or by IV (intravenously)) or fomepizole (4-methylpyrazole or Antizol)) therapy by IV as an antidote to inhibit the ormation of toxic metabolites. d. If patients are diagnosed and treated early in the course with the above methods, hemodialysis may be avoided if fomepizole or ethanol therapy is effective and has corrected the metabolic acidosis, and no renal failure is present. However, once severe acidosis and renal failure occured, however, hemodialysis is necessary. It is effective in removing Ethylene Glycol and toxic metabolites, and correcting metabolic acidosis.

Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.

Auto-Ignition Temperature: 398°C (748.4°F)

Flash Points: CLOSED CUP: 111°C (231.8°F). (Tagliabue.)

Flammable Limits: LOWER: 3.2%

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

Fire Hazards in Presence of Various Substances:
Slightly flammable to flammable in presence of open flames and sparks, 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:
Explosive decomposition may occur if combined with strong acids or strong bases and subjected to elevated temperatures.

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. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

Large Spill:
Stop leak if without risk. Do not get water inside container. Do not touch spilled material. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system. 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. 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. Keep away from incompatibles such as oxidizing agents, acids, alkalis.

Storage: Keep container tightly closed. Keep container in a cool, well-ventilated area. Hygroscopic

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:
Safety glasses. Synthetic apron. Gloves (impervious). For most conditions, no respiratory protection should be needed. However, if material is heated or sprayed and if atmospheric levels exceed exposure guidelines, use an approved vapor (air purifying) respirator.

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:
STEL: 120 (mg/m3) [Australia] TWA: 100 (mg/m3) from ACGIH (TLV) [United States] CEIL: 125 (mg/m3) from OSHA (PEL) [United States] CEIL: 50 (ppm) from OSHA (PEL) [United States] TWA: 52 STEL: 104 (mg/m3) [United Kingdom (UK)] Inhalation TWA: 10 (mg/m3) [United Kingdom (UK)] SKIN3 Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (syrupy)

Odor: Odorless.

Taste: Mild sweet

Molecular Weight: 62.07 g/mole

Color: Clear Colorless.

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

Boiling Point: 197.6°C (387.7°F)

Melting Point: -13°C (8.6°F)

Critical Temperature: Not available.

Specific Gravity: 1.1088 (Water = 1)

Vapor Pressure: .06 mmHg @ 20 C; .092 mmHg at 25 C

Vapor Density: 2.14 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: The product is more soluble in water; log(oil/water) = -1.4

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, acetone.

Solubility:
Soluble in cold water, hot water, acetone. Slightly soluble in diethyl ether. Miscible with lower aliphatic alcohols, glycerol, acetic acid, acetone and similar ketones, aldehydes, pyridine, similar coal tar bases. Practically insoluble in benzene and its homologs, chlorinated hydrocarbons, petroleum ether.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Excess heat, incompatible materials.

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

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Hygroscopic. Absorbs moisture from the air. Avoid contamination with materials with hydroxyl compounds. Also incompatible with aliphatic amines, isocyanates, chlorosulfonic acid, and oleum

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Ingestion.

Toxicity to Animals:
Acute oral toxicity (LD50): 4700 mg/kg [Rat]. Acute toxicity of the vapor (LC50): >200 mg/m3 4 hours [Rat].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Non-mutagenic for bacteria and/or yeast. May cause damage to the following organs: kidneys, liver, central nervous system (CNS).

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

Special Remarks on Toxicity to Animals:
Lowest Published Toxic Dose/Conc: TDL [Man] - Route: oral; Dose: 15gm/kg Lethal Dose/Conc 50% Kill LD50 [Rabbit] - Route: dermal; Dose: 9530 ul/kg

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects and birth defects (teratogenic) based on animal test data. No human data has been reported at this time. May affect genetic material (mutagenic)

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: May cause skin irritation. May cause more severe response if skin is abraded. A single prolonged exposure is not likely to result in material being absorbed through skin in harmful amounts. Massive contact with damaged skin may result in absorption of potentially harmful amounts Eyes: Vapors or mist may cause temporary eye irritation (mild temporary conjunctival inflammation) and lacrimation. Corneal injury is unlikely or insignificant.. Ingestion: It is rapidly absorbed from the gastrointestinal tract. Oral toxicity is expected to be moderate in humans due to Ethylene Glycol even though tests with animals show a lower degree of toxicity. Excessive exposure (swallowing large amounts) may cause gastrointestinal tract irritation with nausea, vomiting, abdominal discomfort, diarrhea. It can affect behavior/central nervous system within 0.5 to 12 hours after ingestion. A transient inebriation with excitement, stupor, headache, slurred speech, ataxia, somnolence, and euphoria, similar to ethanol intoxication, can occur within the first several hours. As sthe Ethylene Glycol is metabolized, metabolic acidosis and further central nervous system depression (convulsions, muscle weakness) develop. Serious intoxication may develop to coma associated with hypotonia, hyporeflexia, and less commonly seizures, and meningismus. 12 to 24 hours

Section 12: Ecological Information

Ecotoxicity:
Ecotoxicity in water (LC50): 41000 mg/l 96 hours [Fish (Trout)]. 46300 mg/l 48 hours [water flea]. 34250 mg/l 96 hours [Fish (bluegill fish)]. 34250 mg/l 72 hours [Fish (Goldfish)].

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: 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:
Illinois toxic substances disclosure to employee act: Ethylene glycol Illinois chemical safety act: Ethylene glycol New York release reporting list: Ethylene glycol Rhode Island RTK hazardous substances: Ethylene glycol Pennsylvania RTK: Ethylene glycol Minnesota: Ethylene glycol Massachusetts RTK: Ethylene glycol Massachusetts spill list: Ethylene glycol New Jersey: Ethylene glycol Louisiana spill reporting: Ethylene glycol TSCA 8(b) inventory: Ethylene glycol TSCA 4(a) proposed test rules: Ethylene glycol SARA 313 toxic chemical notification and release reporting: Ethylene glycol CERCLA: Hazardous substances.: Ethylene glycol: 5000 lbs. (2268 kg)

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

Other Classifications:

WHMIS (Canada): CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

DSCL (EEC):
R22- Harmful if swallowed. S46- If swallowed, seek medical advice immediately and show this container or label.

HMIS (U.S.A.):

Health Hazard: 1

Fire Hazard: 1

Reactivity: 0

Personal Protection: C

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

Health: 1

Flammability: 1

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Not applicable. Safety glasses.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 08:18 PM

Last Updated: 05/21/2013 12:00 PM

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Hydrogen

Material Safety Data Sheet

Hydrogen

Section 1. Chemical product and company identification

Product name : Hydrogen

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : Dihydrogen; o-Hydrogen; p-Hydrogen; Molecular hydrogen; H2; UN 1049; UN 1966; Liquid hydrogen (LH2 or LH2)

MSDS # : 001026

Date of Preparation/Revision : **3/7/2013.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas or Liquid.

Emergency overview : WARNING!

GAS:
CONTENTS UNDER PRESURE.
Extremely flammable
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely flammable
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Do not puncture or incinerate container. May cause target organ damage, based on animal data.

Contact with rapidly expanding gases or liquids can cause frostbite.

Target organs : May cause damage to the following organs: lungs.

Routes of entry : Inhalation

Potential acute health effects

Eyes : Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Skin : Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Inhalation : Acts as a simple asphyxiant.

Ingestion : Ingestion is not a normal route of exposure for gases Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Potential chronic health effects

Chronic effects : May cause target organ damage, based on animal data.

Target organs : May cause damage to the following organs: lungs.

Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (Section 11)

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Hydrogen	1333-74-0	100	Oxygen Depletion [Asphyxiant]

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 500 to 571°C (932 to 1059.8°F)

Flammable limits : Lower: 4% Upper: 76%

Products of combustion : No specific data.

Fire hazards in the presence of various substances : Extremely flammable in the presence of the following materials or conditions: oxidizing materials.

Fire-fighting media and instructions : Use an extinguishing agent suitable for the surrounding fire.

Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.
Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.

Hydrogen

Storage : Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).
For additional information concerning storage and handling refer to Compressed Gas Association pamphlets P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

When working with cryogenic liquids, wear a full face shield.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Insulated gloves suitable for low temperatures

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name

hydrogen Oxygen Depletion [Asphyxiant]

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight : 2.02 g/mole
Molecular formula : H2
Boiling/condensation point : -253°C (-423.4°F)
Melting/freezing point : -259.15°C (-434.5°F)
Critical temperature : -240.15°C (-400.3°F)
Vapor density : 0.07 (Air = 1) Liquid Density@BP: 4.43 lb/ft3 (70.96 kg/m3)
Specific Volume (ft ^{3}/lb) : 191.9386
Gas Density (lb/ft ^{3}) : 0.00521

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.
Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Hydrogen

Section 11. Toxicological information

Toxicity data

Chronic effects on humans : May cause damage to the following organs: lungs.
Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.
Mutagenic effects : No known significant effects or critical hazards.
Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Environmental fate : Not available.
Environmental hazards : No known significant effects or critical hazards.
Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1049 UN1966	HYDROGEN, COMPRESSED Hydrogen, refrigerated liquid	2.1	Not applicable (gas).		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: Forbidden. **Cargo aircraft** Quantity limitation: 150 kg
TDG Classification	UN1049 UN1966	HYDROGEN, COMPRESSED Hydrogen, refrigerated liquid	2.1	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **ERAP Index** 3000 **Passenger Carrying Ship Index** Forbidden

						Passenger Carrying Road or Rail Index Forbidden
Mexico Classification	UN1049 UN1966	HYDROGEN, COMPRESSED Hydrogen, refrigerated liquid	2.1	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations : **TSCA 8(a) IUR**: This material is listed or exempted.
United States inventory (TSCA 8b): This material is listed or exempted.
SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: hydrogen
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: hydrogen: Fire hazard, Sudden release of pressure
Clean Air Act (CAA) 112 accidental release prevention - Flammable Substances: Hydrogen
Clean Air Act (CAA) 112 regulated flammable substances: hydrogen

State regulations : **Connecticut Carcinogen Reporting**: This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.
CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is not listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

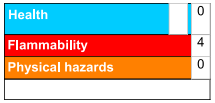
United States

Label requirements : GAS:
CONTENTS UNDER PRESURE.
Extremely flammable
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely flammable
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

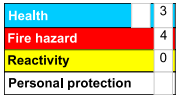
Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.

Hazardous Material Information System (U.S.A.) :

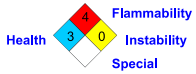


liquid:



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

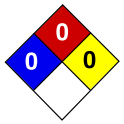
liquid:



Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

Water



Material Safety Data Sheet
Water MSDS

Section 1: Chemical Product and Company Identification

Product Name: Water

Catalog Codes: SLW1063

CAS#: 7732-18-5

RTECS: ZC0110000

TSCA: TSCA 8(b) inventory: Water

CI#: Not available.

Synonym: Dihydrogen oxide

Chemical Name: Water

Chemical Formula: H2O

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Water	7732-18-5	100

Toxicological Data on Ingredients: Not applicable.

Section 3: Hazards Identification

Potential Acute Health Effects:
Non-corrosive for skin. Non-irritant for skin. Non-sensitizer for skin. Non-permeator by skin. Non-irritating to the eyes. Non-hazardous in case of ingestion. Non-hazardous in case of inhalation. Non-irritant for lungs. Non-sensitizer for lungs. Non-corrosive to the eyes. Non-corrosive for lungs.

Potential Chronic Health Effects:
Non-corrosive for skin. Non-irritant for skin. Non-sensitizer for skin. Non-permeator by skin. Non-irritating to the eyes. Non-hazardous in case of ingestion. Non-hazardous in case of inhalation. Non-irritant for lungs. Non-sensitizer for lungs. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available.

Section 4: First Aid Measures

Eye Contact: Not applicable.

Skin Contact: Not applicable.

Serious Skin Contact: Not available.

Inhalation: Not applicable.

Serious Inhalation: Not available.

Ingestion: Not Applicable

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: Not applicable.

Explosion Hazards in Presence of Various Substances: Not Applicable

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

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

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

Section 7: Handling and Storage

Precautions: No specific safety phrase has been found applicable for this product.

Storage: Not applicable.

Section 8: Exposure Controls/Personal Protection

Engineering Controls: Not Applicable

Personal Protection: Safety glasses. Lab coat.

Personal Protection in Case of a Large Spill: Not Applicable

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Odorless.

Taste: Not available.

Molecular Weight: 18.02 g/mole

Color: Colorless.

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

Boiling Point: 100°C (212°F)

Melting Point: Not available.

Critical Temperature: Not available.

Specific Gravity: 1 (Water = 1)

Vapor Pressure: 2.3 kPa (@ 20°C)

Vapor Density: 0.62 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: Not applicable

Solubility: Not Applicable

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Not available.

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.

Toxicity to Animals:
LD50: [Rat] - Route: oral; Dose: > 90 ml/kg LC50: Not available.

Chronic Effects on Humans: Not available.

Other Toxic Effects on Humans:
Non-corrosive for skin. Non-irritant for skin. Non-sensitizer for skin. Non-permeator by skin. Non-hazardous in case of ingestion. Non-hazardous in case of inhalation. Non-irritant for lungs. Non-sensitizer for lungs. Non-corrosive to the eyes. Non-corrosive for lungs.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

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: TSCA 8(b) inventory: Water

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):
This product is not classified according to the EU regulations. Not applicable.

HMIS (U.S.A.):

Health Hazard: 0

Fire Hazard: 0

Reactivity: 0

Personal Protection: a

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

Health: 0

Flammability: 0

Reactivity: 0

Specific hazard:

Protective Equipment:
Not applicable. Lab coat. Not applicable. Safety glasses.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 08:33 PM

Last Updated: 05/21/2013 12:00 PM

Hexanol

ScienceLab.com
Chemicals & Laboratory Equipment

Health	2
Fire	2
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
Hexanol MSDS

Section 1: Chemical Product and Company Identification

Product Name: Hexanol

Catalog Codes: SLH2575

CAS#: 111-27-3

RTECS: MQ4025000

TSCA: TSCA 8(b) inventory: Hexanol

CI#: Not available.

Synonym: Hexyl Alcohol

Chemical Formula: C6H14O

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Hexanol	111-27-3	100

Toxicological Data on Ingredients: Hexanol: ORAL (LD50): Acute: 720 mg/kg [Rat]. 1950 mg/kg [Mouse]. DERMAL (LD50): Acute: 3100 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion. Hazardous in case of skin contact (permeator), of inhalation. Slightly hazardous in case of skin contact (corrosive). Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to the nervous system, mucous membranes. 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. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.

Skin Contact:
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

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

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate 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. Seek medical attention.

Ingestion:
Do not induce vomiting. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Combustible.

Auto-Ignition Temperature: 293°C (559.4°F)

Flash Points: CLOSED CUP: 63°C (145.4°F). OPEN CUP: 73.9°C (165°F).

Flammable Limits: LOWER: 2.1% UPPER: 7.7%

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

Fire Hazards in Presence of Various Substances: Not available.

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:
Combustible material. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk.

Section 7: Handling and Storage

Precautions:

Keep container dry. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapour/spray. Never add water to this product 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

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. Keep container dry. Keep in a cool place.

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: Sweetish. Characteristic.

Taste: Not available.

Molecular Weight: 102.17 g/mole

Color: Clear Colorless.

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

Boiling Point: 158°C (316.4°F)

Melting Point: -51.6°C (-60.9°F)

Critical Temperature: Not available.

Specific Gravity: 0.8136 (Water = 1)

Vapor Pressure: 1 mm of Hg (@ 20°C)

Vapor Density: 3.52 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: Not available.

Solubility: Very slightly soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Dermal contact. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
Acute oral toxicity (LD50): 720 mg/kg [Rat]. Acute dermal toxicity (LD50): 3100 mg/kg [Rabbit].

Chronic Effects on Humans: The substance is toxic to the nervous system, mucous membranes.

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

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

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 more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Class 3: Flammable liquid.

Identification: : Flammable liquids n.o.s. : UN2282 PG: III

Special Provisions for Transport: No DOT, ref 49CFR, 173.150

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: Hexanol TSCA 8(b) inventory: Hexanol

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada):
CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F). CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R22- Harmful if swallowed. R38- Irritating to skin. R41- Risk of serious damage to eyes.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 2

Reactivity: 0

Personal Protection: h

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

Health: 1

Flammability: 2

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 05:43 PM

Last Updated: 05/21/2013 12:00 PM

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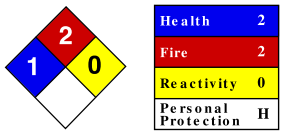
Octanol



Material Safety Data Sheet
1-Octanol MSDS

Section 1: Chemical Product and Company Identification

Product Name: 1-Octanol

Catalog Codes: SLO1090

CAS#: 111-87-5

RTECS: RH6550000

TSCA: TSCA 8(b) inventory: 1-Octanol

CI#: Not available.

Synonym:

Chemical Formula: C8H17OH

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{1-}Octanol	111-87-5	100

Toxicological Data on Ingredients: 1-Octanol: ORAL (LD50): Acute: 1790 mg/kg [Mouse].

Section 3: Hazards Identification

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

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. Do not use an eye ointment. Seek medical attention.

Skin Contact:
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

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

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation: Not available.

Ingestion:
Do not induce vomiting. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Combustible.

Auto-Ignition Temperature: 270°C (518°F)

Flash Points: CLOSED CUP: 81.1°C (178°F). (TAG)

Flammable Limits: LOWER: 1.1% UPPER: 7.4%

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

Fire Hazards in Presence of Various Substances: Not available.

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:
Combustible material. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. 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. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapour/spray. In case of insufficient ventilation, wear suitable respiratory equipment If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. Keep container dry. Keep in a cool place.

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: 130.23 g/mole

Color: Not available.

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

Boiling Point: 194.5°C (382.1°F)

Melting Point: -16.5°C (2.3°F)

Critical Temperature: Not available.

Specific Gravity: 0.827 (Water = 1)

Vapor Pressure: Not available.

Vapor Density: 4.5 (Air = 1)

Volatility: Not available.

Odor Threshold: 0.1 ppm

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: Not available.

Solubility: Insoluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: No.

Section 11: Toxicological Information

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

Toxicity to Animals: Acute oral toxicity (LD50): 1790 mg/kg [Mouse].

Chronic Effects on Humans: Not available.

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

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

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:

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:
Pennsylvania RTK: 1-Octanol TSCA 8(b) inventory: 1-Octanol

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada):

CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F). CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R38- Irritating to skin. R41- Risk of serious damage to eyes.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 2

Reactivity: 0

Personal Protection: h

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

Health: 1

Flammability: 2

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.

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Last Updated: 05/21/2013 12:00 PM

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Ruthenium(III) acetylacetonate (catalyst)

SIGMA-ALDRICH sigma-aldrich.com

Material Safety Data Sheet

Version 4.1
Revision Date 12/05/2012
Print Date 03/26/2014

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	:	Ruthenium(III) acetylacetonate
Product Number	:	282766
Brand	:	Aldrich
Supplier	:	Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	:	+1 800-325-5832
Fax	:	+1 800-325-5052
Emergency Phone # (For both supplier and manufacturer)	:	(314) 776-6555
Preparation Information	:	Sigma-Aldrich Corporation Product Safety - Americas Region 1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Irritant, Reproductive hazard

GHS Classification
Skin irritation (Category 2)
Eye irritation (Category 2A)
Specific target organ toxicity - single exposure (Category 3)

GHS Label elements, including precautionary statements

Pictogram

Signal word: Warning

Hazard statement(s)

H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

Precautionary statement(s)

P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ eye protection/ face protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P312	Call a POISON CENTER or doctor/ physician if you feel unwell.
P321	Specific treatment (see supplemental first aid instructions on this label).
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

HMIS Classification

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	0
Physical hazards:	0

NFPA Rating

Health hazard:	2
Fire:	0
Reactivity Hazard:	0

Potential Health Effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.
Ingestion	May be harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms	:	2,4-Pentanedioneruthenium(III) derivative Ru(acac)3
Formula	:	$C_{15}H_{21}O_6Ru$
Molecular Weight	:	398.39 g/mol

Component		Concentration
Ruthenium(III) acetylacetonate		
CAS-No.	14284-93-6	-
EC-No.	238-193-0	

4. FIRST AID MEASURES

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, Ruthenium oxide

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

Environmental precautions
Do not let product enter drains.

Methods and materials for containment and cleaning up
Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

Conditions for safe storage
Keep container tightly closed in a dry and well-ventilated place.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection
For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator.For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Hand protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash protection
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an Industrial Hygienist familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Eye protection
Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin and body protection
impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Hygiene measures
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	solid
Colour	dark violet

Safety data

pH	no data available
Melting point/freezing point	Melting point/range: 260 °C (500 °F) - dec.
Boiling point	no data available
Flash point	no data available
Ignition temperature	no data available
Auto-ignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	no data available
Density	no data available
Water solubility	no data available
Partition coefficient: n-octanol/water	no data available
Relative vapor density	no data available
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions
no data available

Conditions to avoid
no data available

Materials to avoid
Strong oxidizing agents

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, Ruthenium oxide
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
no data available

Inhalation LC50
Dermal LD50
no data available

Other information on acute toxicity
no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitization
no data available

Germ cell mutagenicity

no data available

Carcinogenicity

IARC:	No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
ACGIH:	No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
NTP:	No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA:	No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

Overexposure may cause reproductive disorder(s) based on tests with laboratory animals.

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure (Globally Harmonized System)
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion	May be harmful if swallowed.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.

Signs and Symptoms of Exposure
May liberate 2,4-pentanedione upon decomposition. 2,4-Pentanedione has the following toxicological hazards: toxic, irritant, neurological hazard, teratogen, possible mutagen, target organ - thymus. In humans, 2,4-pentanedione is reported to cause contact dermatitis and contact urticaria.

Synergistic effects
no data available

Additional Information
RTECS: Not available

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Persistence and degradability
no data available

Bioaccumulative potential
no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

OSHA Hazards
Irritant, Reproductive hazard

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Ruthenium(III) acetylacetonate	14284-93-6	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Ruthenium(III) acetylacetonate	14284-93-6	

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Appendix D. Problem Statement

Ethanol to Butanol (recommended by Bruce M. Vrana, DuPont)

Prior to the advent of the petrochemical industry, which made the process uneconomic, acetone, butanol and ethanol were produced together by fermentation, using one of several Clostridia strains. With the growth in interest of biofuels and the increase in price of petrochemicals, renewable routes to butanol are being revisited by several parties. Butanol is an excellent biofuel, with many advantages over the incumbent biofuel, ethanol. It has higher fuel value, meaning more miles per gallon. It can be blended to higher levels without requiring engine modifications. It has lower vapor pressure than ethanol and comparable octane number. But direct fermentation routes to butanol are challenging, and your company is a newcomer in looking at butanol, so it would be futile to attempt to compete with the companies in various stages of commercializing fermentation routes to butanol.

Your company has instead developed a traditional catalyst to convert ethanol to n-butanol with good selectivity. This so-called Guerbet reaction is enhanced with your catalyst by the addition of hydrogen. Increasing hydrogen pressure improves the selectivity to as high as 95%, but of course increases the capital cost of the plant. You will want to find the optimum pressure, balancing the capital and operating costs of the plant.

The United States and Brazil produce most of the world's ethanol by fermentation of local agricultural feedstocks. The U.S. industry is almost entirely based on corn, while Brazil uses sugar cane. Process efficiencies in both countries have improved significantly in recent years, with increasing ethanol production for use in transportation fuels; thus, do not use process or cost data that are more than 2-3 years old.

Your team has been assembled to develop the most economic process to make n-butanol from ethanol. Management desires to use the entire capacity of the adjoining 100MM gal/yr ethanol plant to make n-butanol. Coincidentally, your company has plants with the same annual capacity in the U.S. and Brazil. Thus, you may locate your plant in either country, using appropriate construction costs for your location, and local ethanol prices and specs.

You will need to focus on the process to make butanol, not the process to make the catalyst, which you can assume will be produced for you by a catalyst vendor.

If you decide to locate in Brazil, one important factor to consider in your economics is that ethanol price increases dramatically during the inter-harvest period, typically 3-4 months of the year when sugar cane cannot be harvested and local ethanol plants shut down. In recent years, Brazil has imported ethanol from the U.S. during this part of the year. Corn ethanol in the U.S. has no such restriction, as corn can be stored year-round.

You may locate your site either in an agricultural region of the U.S. (Iowa) or Brazil (São Paolo state), or in an industrial area, such as the U.S. Gulf Coast or coastal areas of São Paolo. If the plant is built in an agricultural region, hydrogen will be more expensive, and you will need to ship your product to the end use fuel market. Hydrogen would require an onsite production

facility and you would purchase hydrogen for $0.75/lb. Freight for butanol would be $0.05/gal, while the freight for the ethanol would be negligible.

If the plant is built in an industrial area, hydrogen will be less expensive and you will need to ship your feedstock to your site. Hydrogen would be available by pipeline for $0.50/lb in the U.S., $0.60/lb in industrial regions of Brazil. Freight for ethanol to the site would be $0.05/gal, while the freight for the product would be negligible.

Hydrogen pressure from either the pipeline or an onsite plant is 200 psig. If you desire higher pressure, you will need to install a compressor and pay for the energy to compress it.

All prices are forecasts by your marketing organization for long-term average prices, expressed in 2014 dollars for the quantities needed delivered to your site or sold from your site.

Based on your market research, the price per gallon of butanol is 1.3 to 1.5 times the price per gallon of ethanol, both in the U.S. and Brazil. Obviously, you will want to test how sensitive your economics are to this price range.

You will need to make many assumptions to complete your design, since the data you have are far from complete. State them explicitly in your report, so that management may understand the uncertainty in your design and economic projections before approving an expensive pilot plant to provide the scale-up data you need to complete the design. Test your economics to reasonable ranges of your assumptions. If there are any possible "show- stoppers" (i.e., possible fatal flaws, if one assumption is incorrect that would make the design either technically infeasible or uneconomical), these need to be clearly communicated and understood before proceeding.

The plant design should be as environmentally-friendly as possible, at a minimum meeting Federal and state emissions regulations. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate. Remember that, if the plant is approved, you will be there for the plant start-up and will have to live with whatever design decisions you have made.

Reference U.S. Patent 8,318,990, November 27, 2012, assigned to Mitsubishi Chemical Corporation