4-2014

Bio-Butadiene from Waste Carbon Monoxide

Courtney Bender
University of Pennsylvania

Steven Hellstern
University of Pennsylvania

Gus Roman
University of Pennsylvania

Bio-Butadiene from Waste Carbon Monoxide

Abstract

This report describes a two-step process that creates 1,550 lb/hr 1,3-butadiene from a feed of effluent steel mill gas. The goal for this plant was 100,000 gallons of 1,3- butadiene per year, but preliminary economic analysis suggested a 20x scale up was necessary for economic viability. The first step of this process uses fermenters inoculated with cl. autoethanogenum to convert carbon monoxide-rich effluent gas to 2,3-butanediol. This intermediate is fed to a thermo-catalytic converter to produce 1,3- butanediene. Ethanol and MEK are both byproducts of this process that were initially isolated and sold for greater profit.

In the pages to follow, a detailed design and economic analysis for this process is presented for a plant in China. Process flow sheets, energy and utility requirements, and equipment summaries are provided and analyzed. Process profitability is highly sensitive to the pricing of butadiene and ethanol. It is shown that the plant is likely will be unprofitable at prevailing commodities prices. The investment has an internal rate of return of 0.7%, and net present value of $-74.4MM using a discount rate of 15%. This project has a capital investment of $126.2MM. The return on investment (ROI) is 2.0%, with a payback period of 10.3 years. Alternatives can be explored for different process configurations and varying product goals. A few possibilities are presented within this paper.

Disciplines

Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering

Department of Chemical & Biomolecular Engineering

Senior Design Reports (CBE)

University of Pennsylvania *Year* 2014

BIO-BUTADIENE FROM WASTE CARBON MONOXIDE

Courtney Bender
University of Pennsylvania

Steven Hellstern
University of Pennsylvania

Gus Roman
University of Pennsylvania

CBE 459 Senior Design Project:

BIO-BUTADIENE FROM WASTE CARBON MONOXIDE

By:

Courtney Bender, Steven Hellstern, Gus Roman

Presented To:

Mr. Leonard Fabiano and Dr. Daeyeon Lee

April 15, 2014

Department of Chemical and Biomolecular Engineering
University of Pennsylvania
School of Engineering & Applied Science

Professor Leonard Fabiano
Dr. Daeyeon Lee
University of Pennsylvania
School of Engineering & Applied Science
220 S 33rd Street
Philadelphia, PA 19104
April 15, 20124

Dear Professor Fabiano and Dr. Lee,

We researched a two-step fermentation and reaction process to convert carbon monoxide to 1,3- butadiene. Our report on the solution to the design problem given by Mr. Steven Tieri is enclosed. Our design of the process includes a series of batch reactors to grow up cells, then transporting these cells to ten CSTRs that operate at steady state. Our process takes the intermediate 2,3-butanediol produced in the reactors through a thermo-catalytic converter to produce 1,3-butadiene.

This project includes detailed equipment designs and a preliminary economic analysis of the plant. The plant must be located at a medium sized steel mill to provide enough carbon monoxide to the bacteria. The overall production rate of 1,3-butanediol is 1,550 lbs/hr. This plant operates 24 hours a day for 330 days of the year.

This process introduces a novel separation scheme that is the most expensive piece of equipment for our plant. The separation unit uses a moving bed chromatography to extract the alcohols 2,3-Butadiene and ethanol from the fermentation broth. Our initial problem asked for a production rate of 100,000 gallons/year, however we increased the production by 20 fold to make the process more economically feasible. We produce 12.3 million pounds 1,3-butadiene per year.

Our economic analysis suggests we need to scale up the plant or modify current operation to become more economically feasible. The internal rate of return (IRR) is 0.7% under current conditions. The net present value (NPV) of the project is $(74.4MM). Additionally, we explore various product price environments, demonstrating circumstances in which this can be a more profitable investment at current scale in this report.

Sincerely,

Courtney Bender Steven Hellstern Gus Roman

1.0 ABSTRACT

This report describes a two-step process that creates 1,550 lb/hr 1,3-butadiene from a feed of effluent steel mill gas. The goal for this plant was 100,000 gallons of 1,3-butadiene per year, but preliminary economic analysis suggested a 20x scale up was necessary for economic viability. The first step of this process uses fermenters inoculated with *cl. autoethanogenum* to convert carbon monoxide-rich effluent gas to 2,3-butanediol. This intermediate is fed to a thermo-catalytic converter to produce 1,3-butanediene. Ethanol and MEK are both byproducts of this process that were initially isolated and sold for greater profit.

In the pages to follow, a detailed design and economic analysis for this process is presented for a plant in China. Process flow sheets, energy and utility requirements, and equipment summaries are provided and analyzed. Process profitability is highly sensitive to the pricing of butadiene and ethanol. It is shown that the plant is likely will be unprofitable at prevailing commodities prices. The investment has an internal rate of return of 0.7%, and net present value of $-74.4MM using a discount rate of 15%. This project has a capital investment of $126.2MM. The return on investment (ROI) is 2.0%, with a payback period of 10.3 years. Alternatives can be explored for different process configurations and varying product goals. A few possibilities are presented within this paper.

2.0 INTRODUCTION

1,3-Butadiene is a chemical compound used a variety of ways in the synthetic materials field, especially in the formation of polymers. It is used as an additive to make adiponitrile, a prominent component of nylon, as well as stiffer plastics such as polybutadiene rubber and styrene-butadiene rubber, most commonly used as automobile tires (Morrow, 1990). This report focuses on the use of 1,3-butadiene as the feedstock for adiponitrile.

The bioplastic market is expected to expand 17-20% in the next two years due to a variety of factors. The important ones for this report are consumer demands of our Company, a desire for feedstock diversification, the increasing cost of 1,3-butadiene from fossil materials, and a desire to produce the chemical in a more environmentally friendly manner.

The most common method for producing 1,3-butadiene is as a byproduct of steam cracking that produces ethylene and other olefins. This process occurs when heavier hydrocarbons are used, however ethane has become cheaper and thus a more common feed in recent years. This has resulted in a gradual reduction in the amount of 1,3-butadiene extracted from steam cracking plants throughout the United States, Europe, and Japan (Morrow, 1990).

During World War II, 1,3-butadiene was in high demand. Competition to supply this chemical to the war efforts sparked the development of new ways of creating 1,3-butadiene. One of these processes involved the catalytic conversion of 1,3-butadiene using 2,3-butanediol. 2,3-Butanediol is a chemical that can be produced by anaerobic fermentation with a *clostridium* bacteria. Not only can this process create a desired compound, but also it creates 1,3-butadiene using an environmentally friendly process. This report takes lab-scale research of the fermentation of 2,3-butanediol and applies it to a large-scale production plant to create 1,3-butadiene.

This process is split into two main sections: CO Fermentation for the Formation of BDO and Formation of 1,3-Butadiene via Thermo-Catalytic Conversion of BDO. The fermentation process uses *cl. autoethanogenum* bacteria grown in a carbon monoxide-rich environment. Carbon monoxide is a primary product of steel mill production. Therefore, this chemical plant will be located next to a steel mill that will provide the gas feed needed for the fermentation process. A typical steel mill composition of 42% CO, 36% N_2, 20 CO_2, and 2% H_2 is assumed for this plant. The basis for the industrial-sized process described in this report is based off of a pilot plant by LanzaTech (LanaTech, 2012).

During the fermentation process, the *cl. autoethanogenum* cells are grown in batches to the desired operating concentration of 2 g/L. Continuous stirred-tank reactors (CSTRs) are operated in parallel at steady state to produce 10 g/L of 2,3-butanediol in solution broth. The broth also contains 20 g/L ethanol and 5 g/L cell mass, of which the former is sold as a fuel-grade product and 40% of the latter is recycled to the CSTR to maintain the desired cell density. 2,3-Butanediol and ethanol are both extracted from the fermentation broth using a separation unit that utilizes Simulated Moving Bed Chromatography (SMB). This is an Orochem product.

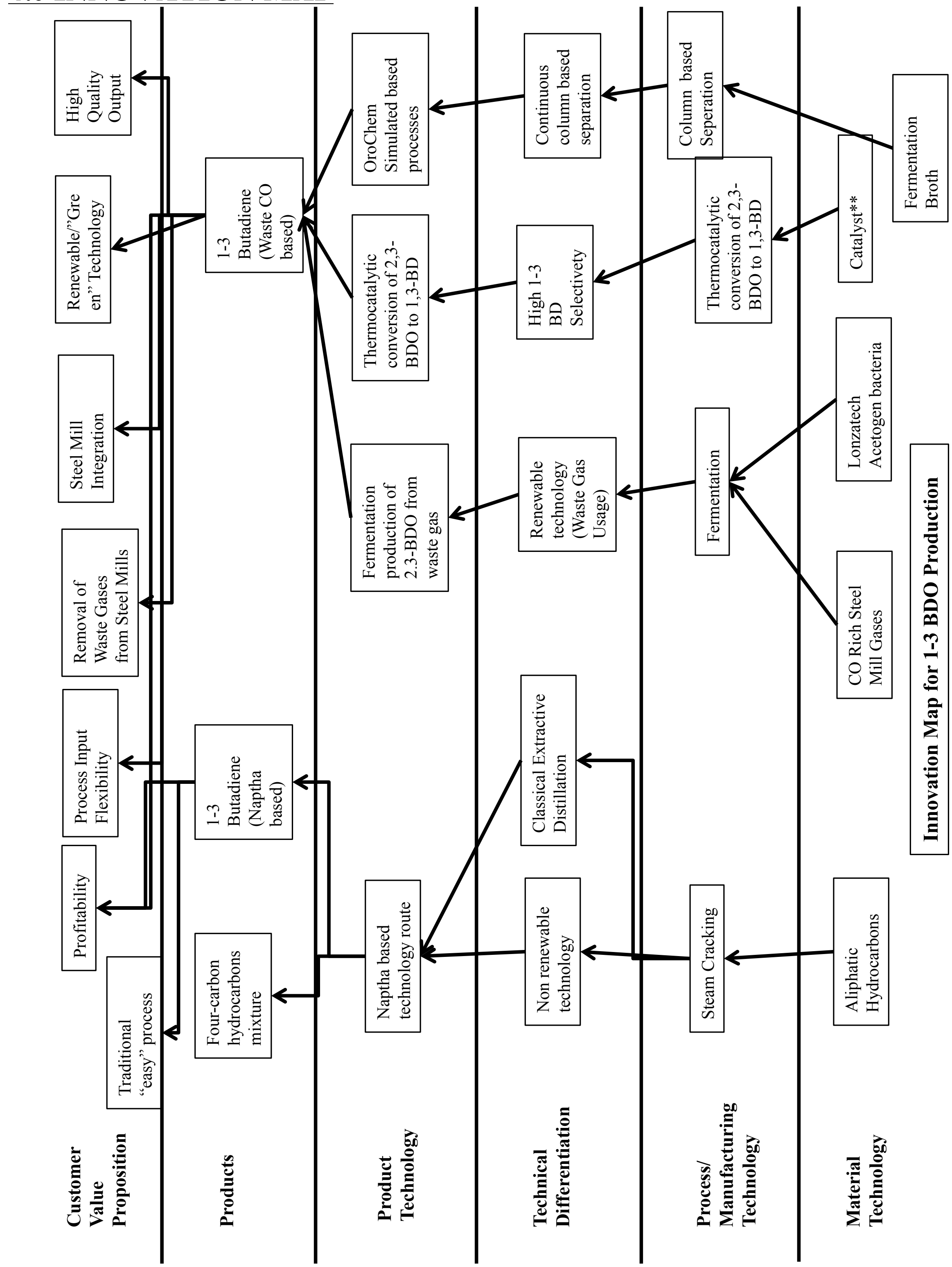
2,3-Butanediol, once recovered from fermentation broth, then enters the reaction process of the plant. We chose to use a thorium oxide catalyst, which has a 62% selectivity for 1,3-butadiene and is most commonly used for this reaction. Byproducts include methyl ethyl ketone (MEK), methyl vinyl carbinol (MVC), and water. A rigorous separation system was developed to perform the separation of these products. We assess the profitability of purifying MEK versus installing the required equipment in this paper.

Our primary objective was to design a plant that produced 1,3-butadiene using fermentation from waste steel mill gas. Our original problem statement proposed a yearly production of 100,000 gallons. However, the final scale is much larger to make the process more economically feasible, meaning we have an excess of 1,3-butadiene that can be put on the market. We chose to build our plant in China, where 1,3-butadiene is more profitable to produce, at $2100/ton USD, and we assume the plant will be operational 330 days out of the year.

3.0 PROJECT CHARTER

Project Name	Bio-Butadiene from Waste CO
Project Champions	Mr. S. Tieri, Dr. D. Lee, Prof. L. Fabiano
Project Members	C. Bender, S. Hellstern, G. Roman
Specific Goals	• Economically synthesize 1,3-butadiene using 2,3-butanediol (BDO) as an intermediary in a 2-step process o Covert waste CO to BDO via fermentation o Thermo-catalytically convert BDO to 1,3-butadiene • Create a minimum-energy plant that exceeds safety and environmental standards
Project Scope	In-scope • Production of polymer-grade 1,3-Butadiene • Concentration and purity of CO feed stream is correct for the fermentation process • Water recycle / storage and integration into the steel mill • Air purification / integration with existing furnace in steel mill • Existing environmental and safety standards Out-of-scope • 1,3-Butadiene for processes other than making adiponitrile • New facilities for water and air treatment
Deliverables	• Detailed process design and accompanying flow sheets o Includes material and energy balances o *How is this process completed?* • Written and oral design reports o Economic viability o Environmental and safety analysis
Time Line	Milestones • *February 4* Preliminary material balance, computer-drawn block flow diagram • *February 25* Complete process synthesis, including material and energy balances for the most promising flow sheet • *March 25* Detailed design of process units • *April 8* Complete rough draft of written report • *April 15* Complete final draft of written report • *April 23* Final report oral presentation

4.0 INNOVATION MAP



5.0 CONCEPT ASSESSMENT

5.1 MARKET AND COMPETATIVE ANALYISIS

Global 1,3-butadiene demand was around 10.5 million tons in 2011, which amounted to over $40 billion in revenues. It is expected that by 2017, these annual revenues will increase to $180 billion. The Asia-Pacific market consumes around 45% of the 1,3-Butadiene produced annually, which is expected to grow as the Chinese and Indian economies continue to develop (Transparency Market Research, n.d.). The North American use accounts for 23% of production (IARC, 1997).

In major markets, such as the United States, Europe, and Japan, butadiene is obtained as a by-product from the steam cracking of a naphtha cut, which produces ethylene and other olefins. An additional mode of production, primarily used in South America and Eastern Europe, is to use ethanol as a feedstock in small-capacity plants. Other production pathways use either n-butenes or n-butane as reactants. Our company will attempt to reap the benefits of a new bio-based LanzaTech technology, which utilizes the carbon monoxide in a steel mill gas to produce 2,3-butanediol, which is then thermo-catalytically converted to 1,3-butadiene. Current forecasts estimate 17-20% average annual growth in demand for bioplastics through 2016.

1,3-Butadiene is used in the production of many polymers. For our company, it is a critical feedstock in the production of adiponitrile, which is used in the production of Nylon 6,6. Other major end uses, by volume of annual consumption, of butadiene are butadiene rubber (27%), styrene butadiene rubber (32%), styrene butadiene latex (10%), acrylonitrile butadiene styrene (9%). Since we will be producing polymer grade butadiene with a purity of >99% by mass, our product can be used as a versatile precursor to all of these end uses.

In addition to our main butadiene project, ethanol and methyl ethyl ketone (MEK) will be produced in significant quantities as valuable side products. In Asia, ethanol is a valuable commodity, with a consumption of 4.6 billion liters while only having a production value of 4.0 billion liters (Ng, 2013). Our process at full capacity produces

36.5 million liters of synthetic grade ethanol per year, lowering this gap in the regional supply by 6.5% and providing valuable revenues to our company.

In addition to the strong revenues produced by ethanol sales, MEK is a valuable chemical in the Asia-Pacific market with over 50% of the global volumes consumed in 2012. This consumption is driven by robust growth in the paints and coatings market from the manufacturing and construction industries (Wood, 2014). MEK is used as a solvent in paints and coatings, printing inks, adhesive for PVC pipes, industrial cements, and resin thinners. In 2010, China's annual MEK production was 670 million pounds. Our process produces which produces 6.4 million tons per year and would be able to capture approximately 1% of the Chinese market.

The proposed bio-butadiene process will be valuable our Company's continued growth. The Company interested in biopolymers for several reasons, including increasing consumer demand, a business desire for feedstock diversification, the increasing price of fossil materials, a hedge for petroleum market volatility, and to positively impact global climate change. Additionally, there is potential to earn waste gas credits since this process repurposes carbon monoxide from steel mill gas exhaust. Our process is very trend-resistant since it utilizes three different chemicals as revenue generators. Especially notable is our ability to produce a significant amount of ethanol, a chemical with a growing market as more countries are beginning to integrate ethanol into their gasoline. In addition, our production of ethanol is outside the food chain using steel mill gas and bacteria as the main inputs instead of the current sugarcane and yeast based production model, allowing for a more sustainable ethanol supply chain

Value Chain Analysis: Our Company is towards the beginning of the value chain. It is a producer and retailer of plastics, which are used in the production of a wide host of consumer products. Consumer products are sold via online and brick and mortar retailers. Negotiating better terms with suppliers of the inputs to our process, the steel mill owners, and negotiating better terms with our customers could increase the strength of our position in the value chain.

Value Proposition: A 1,3-butadiene production process that offers our company the ability to fulfill consumer demand, diversify its feedstock, transition away from fossil materials, which are increasing in price, hedge petroleum market volatility, and positively impact global climate change by using a typical waste product in a new, innovative way.

Market Segmentation: We can look at our own company's needs for 1,3-butadiene production as well as the market, which can offer insight to the best location for the production plant.

5.2 CUSTOMER REQUIREMENTS

Since the first butadiene plants began production in the 1940's (Vernon, 1985), consumers have been demanding butadiene of various purities for their processes. Therefore, butadiene can be classified as a fitness-to-standard (FTS) product rather than a new-unique-difficult (NUD) product. In this process, polymer-grade butadiene is created with a purity of >99% by mass, necessary for its usage as adiponitrile feedstock. In addition, customers will obtain competitively priced 1,3-butadiene created by a green process. We only use waste material, steel mill gas from the steel mill industry, and bacteria, a non-environmentally damaging resource, as the main inputs to the process.

5.3 PRELIMINARY PROCESS SYNTEHSIS

This project is highly based off of LanzaTech's new technology, where bacteria, *cl. autoethanogenum*, is used to produce useful materials from waste steel mill gas. The two main products from this process, ethanol and butadiene, are classically created using valuable hydrocarbons as their feed sources. In this process, steel mill gas, considered a waste product of steel production, is used to feed bacteria that are capable of fixating the carbon monoxide and hydrogen gas from feed gas to produce 2,3-butanediol (BDO) and ethanol. This new technology enables BDO and ethanol to be created through renewable green pathways instead of the classic energy-intensive technologies of the past.

Low levels of BDO and ethanol are present at steady state in the fermentation broth, 10 g/L and 20 g/L respectively. To produce enough BDO to use for the second stage of the process, a series of five batch fermenters grow enough cells to inoculate five continuous stirred tank reactors (CSTRs). This batch fermentation is run twice a year, enough to inoculate a total of ten CSTRs that work in parallel. Under continuous operation at steady state, this process can produce enough quantities of BDO. The output streams from the CSTRs are filtered for solid materials, then combined and fed to a simulated moving bed chromatography unit (SMB). This is an Orochem unit that extracts the process alcohols from the fermentation broth. The alcohols are then separated to near purity using a small distillation tower. The ethanol is stored and the BDO is pumped to the thermo-catalytic conversion portion of the process. An alternative separation scheme using a distillation tower is presented later in this paper.

The second stage of our process will require the conversion of BDO to 1,3-butadiene using a thermo-catalytic conversion reaction. To achieve this we will use a catalyst that has high conversion and selectivity of 1,3-butadiene. Preliminary conversion data are provided in the problem statement, however a better conversion was found using thorium oxide. The three reactions that take place in the reactor are:

(1) $C_4H_{10}O_2 \rightarrow CH_2{=}CHCH{=}CH_2 + H_2O$.
(2) $C_4H_{10}O_2 \rightarrow CH_3C(O)CH_2CH_3 + H_2O$.
(3) $C_4H_{10}O_2 \rightarrow CH_2{=}CHCH(OH)CH_3 + 2{*}H_2O$

5.4 ASSEMBLY OF DATABASE

In order to perform the economic analysis, the following values were found for the chemicals consumed or sold in this process. Using pricing resources, the price of the following chemicals in the Asian market were found in US dollars: $2100/ton for 1,3-butadiene, $1700/ton for MEK, and ethanol is $1400/ton (Research China, 2012). The price of thorium oxide is $5.75/g when bought in quantities of 50 grams or more (Isis.com, 2014).

All systems were drawn using Visio. The process simulation was run in ASPEN PLUS for the reaction section. In order to obtain thermodynamic data and other physical properties data, the ASPEN databanks were used. Additionally, UNIQUAC and NRTL were used to estimate any missing properties data.

Conversion data and reactor operating conditions were obtained from literature. The simple pass conversion of BDO to 1,3-Butadiene over a reactor operating at 70mmHG and 1 bar is 62.1%. Additionally, 26.2% is converted to MEK and 8.3% is converted to methyl vinyl carbinol.

5.5 BENCH-SCALE LABORATORY WORK

There was no experimental component performed for this project. Bench-scale and pilot plant information was obtained from various patents belonging to LanzaTech (LanzaTech, 2012).

6.0 PROCESS FLOW DIAGRAMS & MATERIAL BALANCES

This process is divided into two steps, with eight sections overall:

CO Fermentation for the Formation of BDO

Section 000: Steel Mill Gas Cooling

Section 100: Media Mixing System

Section 200: Batch Fermentation

Section 300: CSTR and Cell Recycle Close-up

Section 400: Moving Bed Chromatography Separation

Formation of 1,3-Butadiene via Thermo-Catalytic Conversion of BDO

Section 500: Thermo Catalytic Conversion

Section 600: Distillation Separation: 1,3-Butadiene Recovery

Section 700: Distillation Separation: Pressure-Swing Distillation

An overall flow diagram is shown below. The individual blocks and accompanying material balances are shown in the following pages. Unit specifications and process descriptions are presented later on in the report. Each group contains separation methods to purify products. All batch processes are denoted with asterisks.

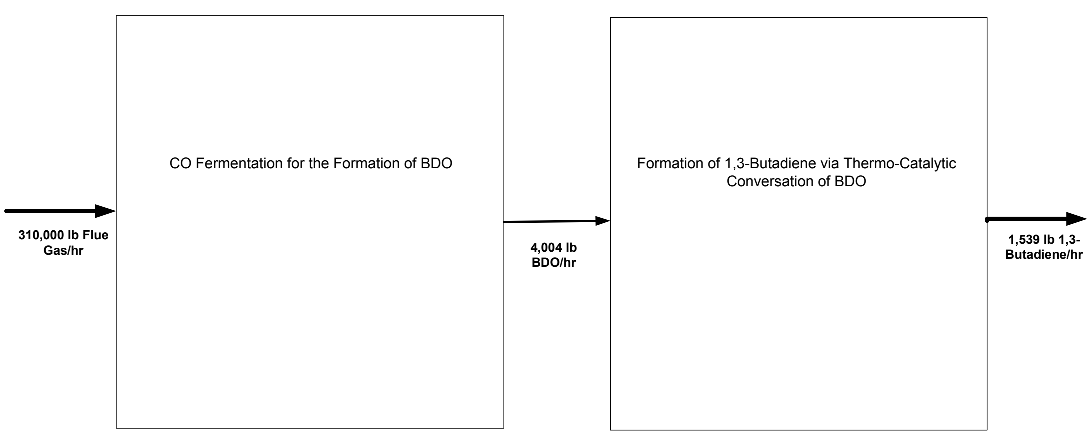


Figure 6-1: Block flow diagram.

Figure 6-2: Overall Detailed Process Flow Diagram

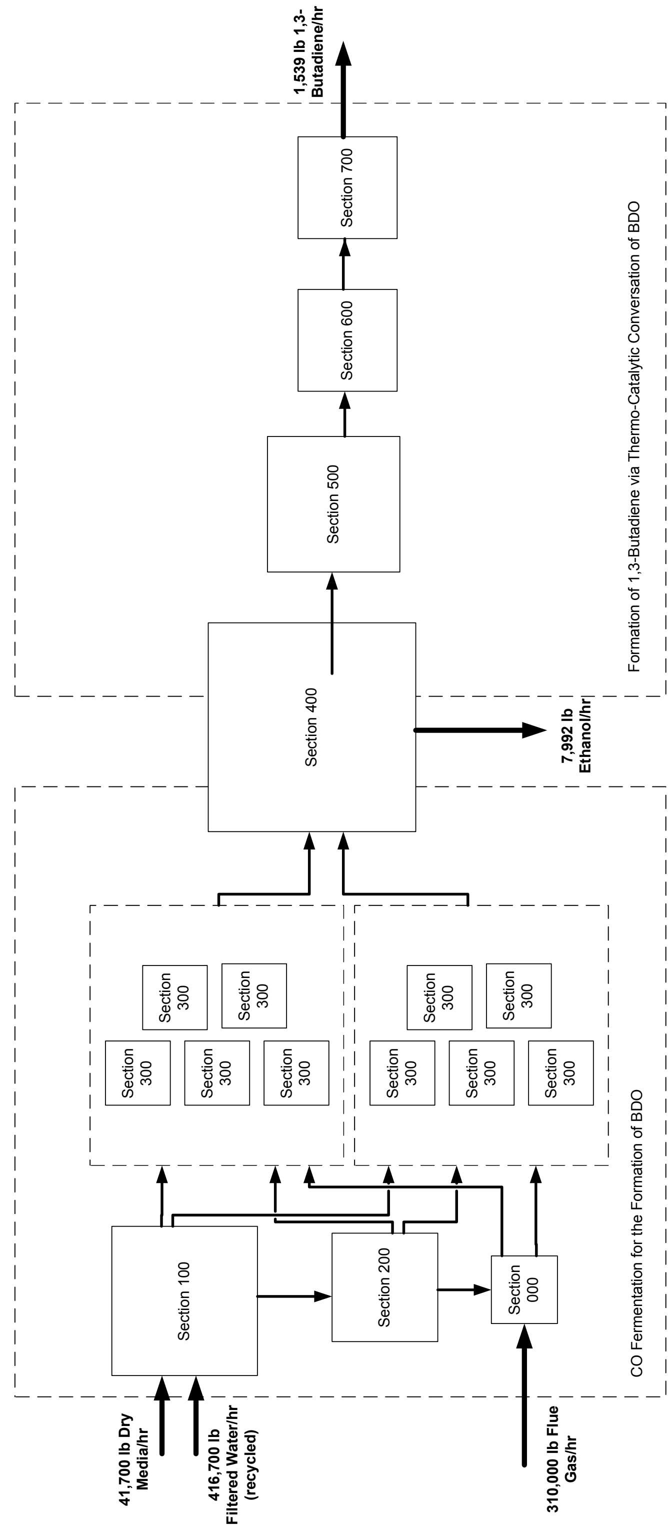
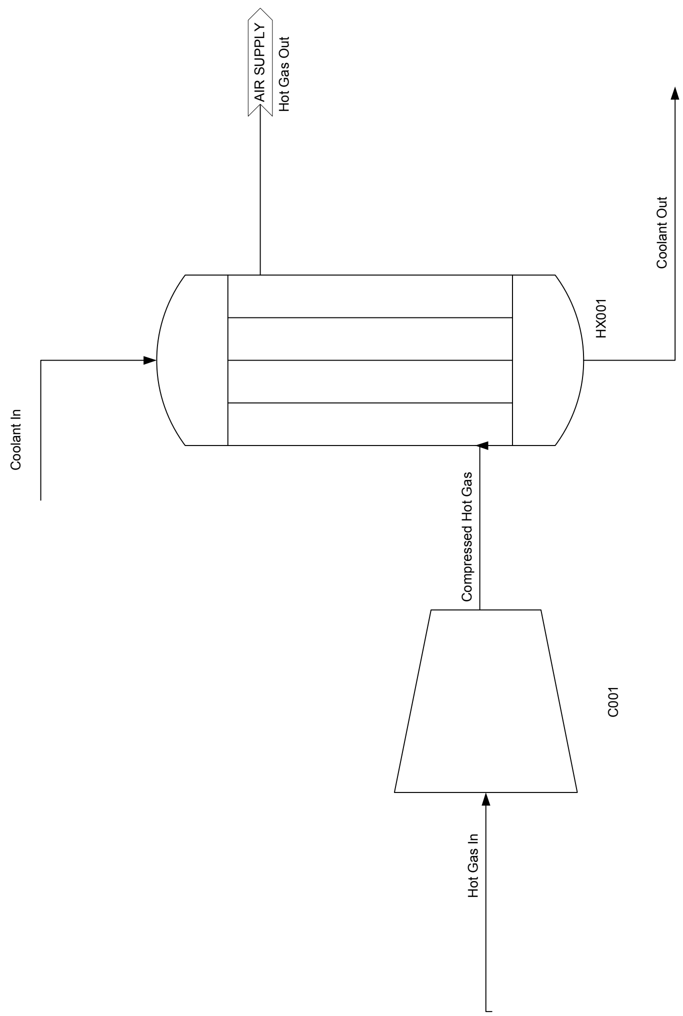
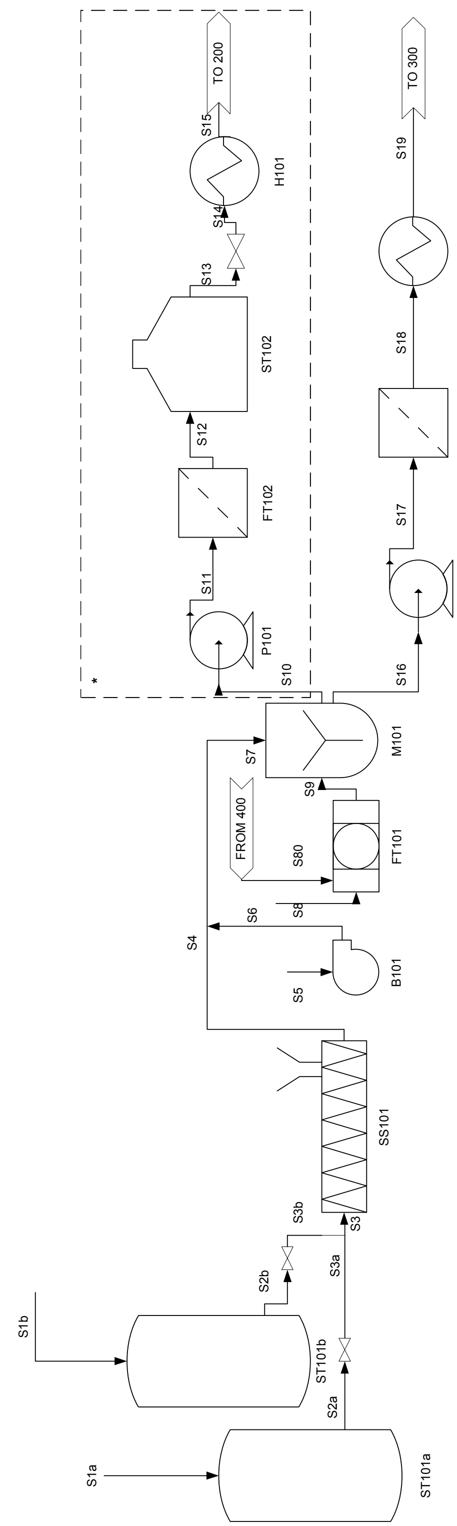


Figure 6-3: Section 000: Steel Mill Gas Cooling



			Streams (lb/hr)				
Name	**Formula**	**MW (g/mol)**	**Hot Gas In**	**C.Hot Gas**	**Hot Gas Out**	**Coolant In**	**Coolant Out**
Water	H_2O	18	0	0	0	849,600	849,600
Media (dry)	-	-	0	0	0	0	0
Media (wet)	-	-	0	0	0	0	0
Carbon Monoxide	CO	28	130,200	13,020	130,200	0	0
Carbon Dioxide	CO_2	44	62,000	3,200	62,000	0	0
Nitrogen	N_2	28	111,600	11,160	111,600	0	0
Hydrogen	H_2	2	6,200	620	6,200	0	0
Cell Mass	-	-	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	0	0	0	0	0
Ethanol	C_2H_6O	46	0	0	0	0	0
1,3-Butadiene	C_4H_6	54	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	0	0	0	0	0
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0
Total			310,000	310,000	310,000	849,600	849,600
Phase			Vapor	Vapor	Vapor	Liquid	Liquid
Temperature (°F)			482	770	98	45	88
Pressure (psi)			14	30	22	14	14

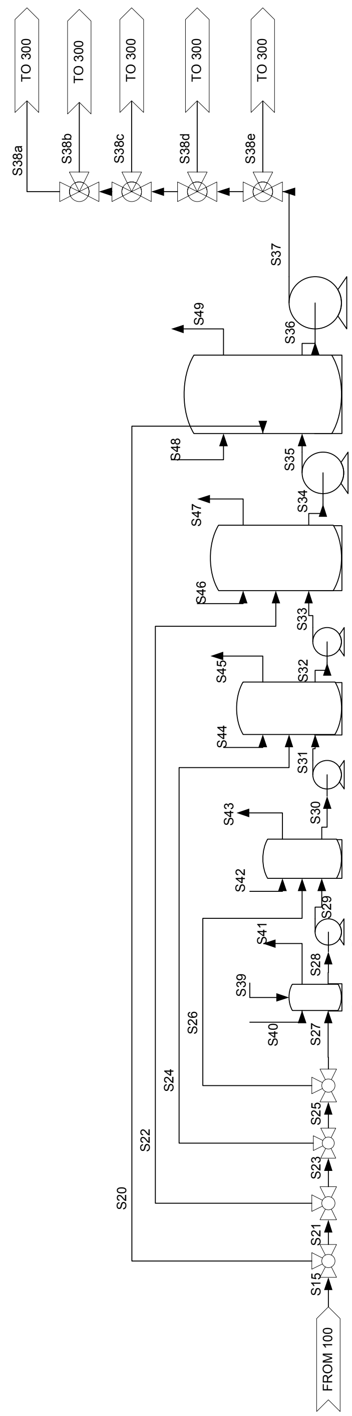
Figure 6-4: Section 100: Media Mixing System



			Streams (lb/hr) *(lb/batch)												
Name	**Formula**	**MW (g/mol)**	**S1***	**S2***	**S3***	**S4***	**S4**	**S5***	**S5**	**S6***	**S6**	**S7***	**S7**	**S8***	**S62**
Water	H_2O	18	0	0	0	0	0	0	0	0	0	0	0	300,240**	0
Media (dry)	-	-	960000**	Max capac	Max capac	33,360	33,360	0	0	0	0	33,360	41,700	0	0
Media (wet)	-	-	0	0	0	0	0	0	0	0	0	0	0	0	416,700
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	5,837	5,837	5,837	5,837	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0	0	0	0
Cell Mass	-	-	0	0	0	0	0	0	0	0	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	0	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	C_2H_6O	46	0	0	0	0	0	0	0	0	0	0	0	0	0
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0	0	0
Total			0	0	0	33,360	33,360	5,837	5,837	5,837	5,837	33,360	41,700	0	416,700
Phase			Solid	Solid	Solid	Solid	Solid	Vapor	Vapor	Vapor	Vapor	Mixed	Mixed	Liquid	Liquid
Temperature (°F)			68	68	68	68	68	68	68	68	68	68	68	68	68
Pressure (psi)			14	14	14	14	14	14	14	14	14	14	14	14	14

			Streams (lb/hr) *(lb/batch)										
Name	**Formula**	**MW (g/mol)**	**S9***	**S9**	**S10***	**S11***	**S12***	**S13***	**S14***	**S15***	**S16**	**S17**	**S18**	**S19**
Water	H_2O	18	330,240	375,000	0	0	0	0	0	0	0	0	0	0
Media (dry)	-	-	0	0	0	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	0	0	333,600	333,600	333,600	Variable	Variable	Variable	416,700	416,700	416,700	416,700
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0	0	0
Cell Mass	-	-	0	0	0	0	0	0	0	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	C_2H_6O	46	0	0	0	0	0	0	0	0	0	0	0	0
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0	0
Total			330,240	375,000	333,600	333,600	333,600	-	-	-	416,700	416,700	416,700	416,700
Phase			Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°F)			68	68	68	68	68	68	68	98	68	68	68	98
Pressure (psi)			14	14	14	14	14	14	14	14	14	50	22	22

Figure 6-5: Section 200: Batch Fermentation

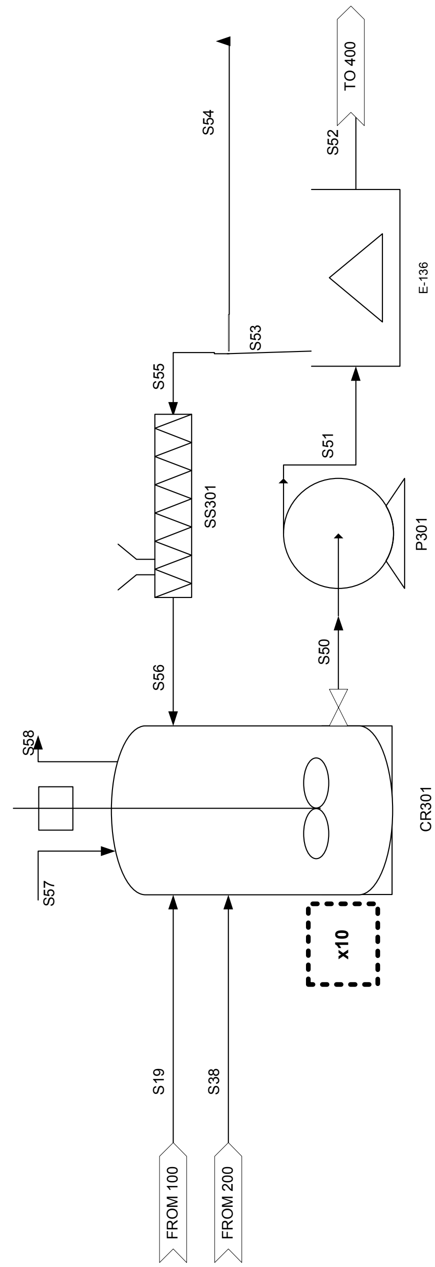


			Streams (lb/batch)										
Name	**Formula**	**MW (g/mol)**	**S15**	**S20**	**S21**	**S22**	**S23**	**S24**	**S25**	**S26**	**S27**	**S28**	**S29**
Water	H_2O	18	0	0	0	0	0	0	0	0	0	0	0
Media (dry)	-	-	0	0	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	Variable	304,166	Variable	16,272	Variable	9,034	Variable	784	92	92	92
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0	0
Cell Mass	-	-	0	0	0	0	0	0	0	0	0	0.018	0.018
2,3-Butanediol	$C_4H_{10}O_2$	90	0	0	0	0	0	0	0	0	0	0	0
Ethanol	C_2H_6O	46	0	0	0	0	0	0	0	0	0	0	0
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0
Total			0	304,166	0	16,272	0	9,034	0	784	92	92	92
Phase			Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Mixed	Mixed
Temperature (°F)			98	98	98	98	98	98	98	98	98	98	98
Pressure (psi)			22	22	22	22	22	22	22	22	22	22	22

			Streams (lb/batch)									
Name	**Formula**	**MW (g/mol)**	**S30**	**S31**	**S32**	**S33**	**S34**	**S35**	**S36**	**S37**	**S38**	**S39**
Water	H_2O	18	0	0	0	0	0	0	0	0	0	0
Media (dry)	-	-	0	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	876	876	9,910	9,910	26,182	26,182	330,348	330,348	66,073	0
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0
Cell Mass	-	-	0.18	0.18	2	2	18	18	67	67	13	$2.2*10^{-7}$
2,3-Butanediol	$C_4H_{10}O_2$	90	0	0	0	0	0	0	0	0	0	0
Ethanol	C_2H_6O	46	0	0	0	0	0	0	0	0	0	0
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0
Total			876	876	9,912	9,912	26,200	26,200	330,415	330,415	66,086	$2.2*10^{-7}$
Phase			Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Solid
Temperature (°F)			98	98	98	98	98	98	98	98	98	98
Pressure (psi)			22	22	22	22	22	22	22	22	22	14

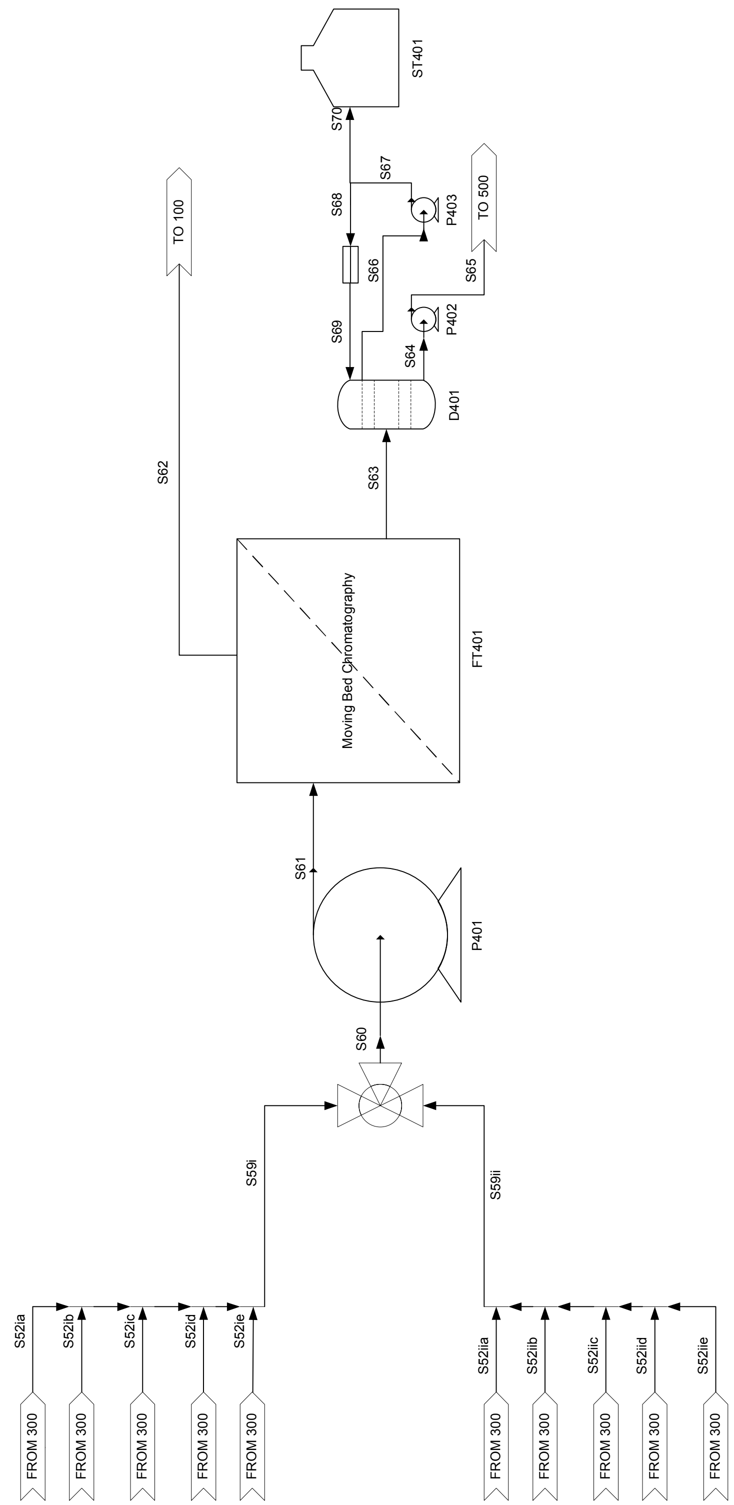
			Streams (lb/hr)									
Name	**Formula**	**MW (g/mol)**	**S40**	**S41**	**S42**	**S43**	**S44**	**S45**	**S46**	**S47**	**S48**	**S49**
Water	H_2O	18	0	0	0	0	0	0	0	0	0	0
Media (dry)	-	-	0	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	CO	28	4	4	33	33	339	339	3,385	3,385	11,541	11,541
Carbon Dioxide	CO_2	44	2	2	16	16	161	161	1,612	1,612	5,496	5,496
Nitrogen	N_2	28	3	3	28	28	290	290	2,902	2,902	9,892	9,892
Hydrogen	H_2	2	0	0	2	2	16	16	161	161	550	550
Cell Mass	-	-	0	0	0	0	0	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	0	0	0	0	0	0	0	0	0	0
Ethanol	C_2H_6O	46	0	0	0	0	0	0	0	0	0	0
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0
Total			9	9	79	79	806	806	8,060	8,060	27,479	27,479
Phase			Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature (°F)			98	98	98	98	98	98	98	98	98	98
Pressure (psi)			22	22	22	22	22	22	22	22	22	22

Figure 6-6: Section 300: CSTR Close-up



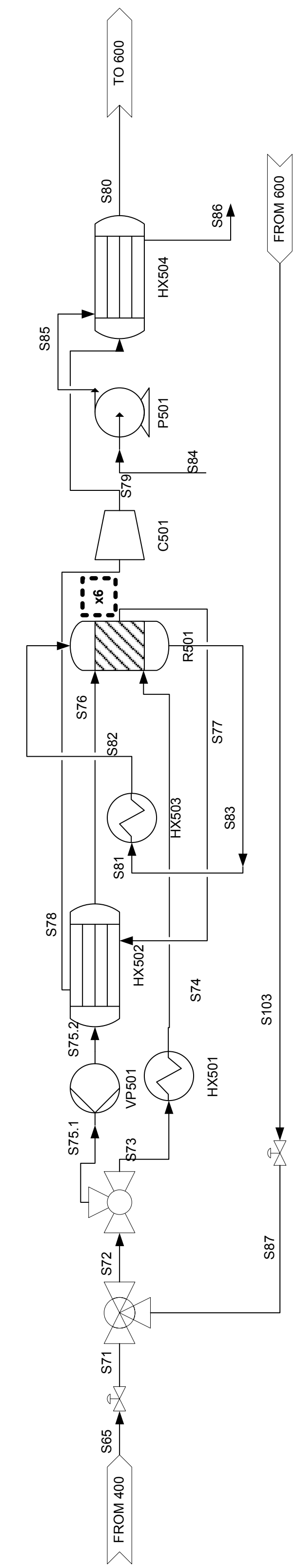
			Streams (lb/hr) *(lb/batch)											
Name	**Formula**	**MW (g/mol)**	**S19***	**S19**	**S38***	**S50**	**S51**	**S52**	**S53**	**S54**	**S55**	**S56**	**S57**	**S58**
Water	H_2O	18	0	0	0	0	0	0	0	0	0	0	0	0
Media (dry)	-	-	0	0	0	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	264,240	41,670	66,060	41,670	41,671	41,671	0	0	0	0	0	0
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0	0	12,823	12,403
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0	0	6,106	5,906
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0	10,992	10,632
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0	611	591
Cell Mass	-	-	0	0	13	200	200	0	200	120	80	80	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	0	0	0	400	400	400	0	0	0	0	0	0
Ethanol	C_2H_6O	46	0	0	0	800	800	800	0	0	0	0	0	0
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0	0
Total			264,240	41,670	66,073	43,070	43,071	42,871	200	120	80	80	30,532	29,532
Phase			Liquid	Liquid	Mixed	Mixed	Mixed	Liquid	Solid	Solid	Solid	Solid	Vapor	Vapor
Temperature (°F)			98	98	98	98	98	98	98	98	98	98	98	98
Pressure (psi)			22	22	22	22	50	22	22	22	22	22	22	22

Figure 6-7: Section 400: Moving Bed Chromatography Separation



			Streams (lb/hr)												
Name	**Formula**	**MW (g/mol)**	**S52**	**S59**	**S60**	**S61**	**S62**	**S63**	**S64**	**S65**	**S66**	**S67**	**S68**	**S69**	**S70**
Water	H_2O	18	0	0	0	0	0	0	0	0	0	0	0	0	0
Media (dry)	-	-	0	0	0	0	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	41,671	208,355	416,710	416,710	416,710	0	0	0	0	0	0	0	0
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0	0	0	0
Cell Mass	-	-	0	0	0	0	0	0	0	0	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	400	2,000	4,000	4,000	0	4,000	3,996	3,996	8	8	8	8	4
Ethanol	C_2H_6O	46	800	4,000	8,000	8,000	0	8,000	8	8	15,984	15,984	15,984	15,984	7,992
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0	0	0
Total			42,871	214,355	428,710	428,710	416,710	12,000	4,004	4,004	15,992	15,992	15,992	15,992	7,996
Phase			Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°F)			98	98	98	98	98	98	389	389	206	206	206	206	206
Pressure (psi)			22	22	22	80	22	22	29	29	29	29	29	29	29

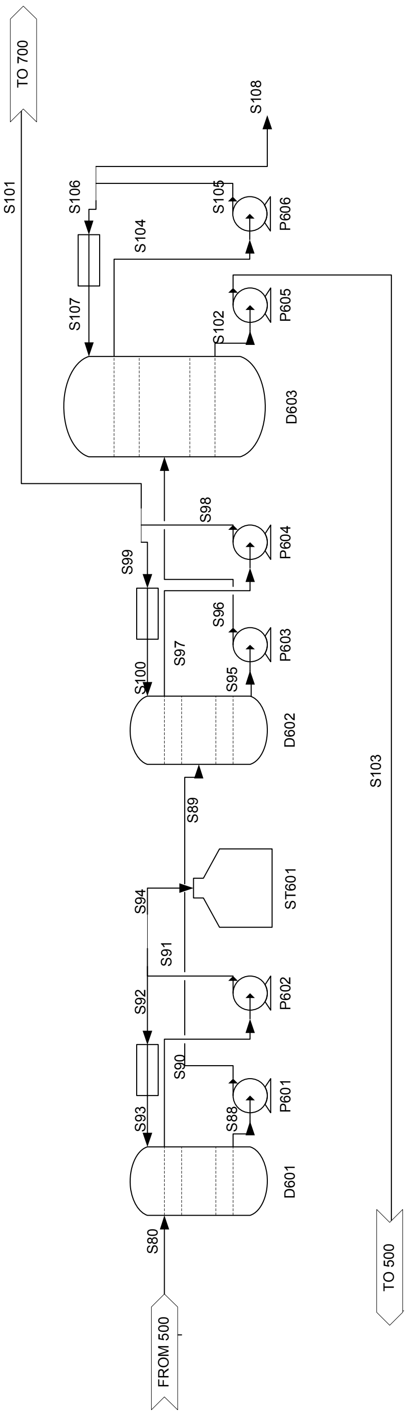
Figure 6-8: Section 500: Thermo Catalytic Conversion



			Streams (lb/hr) *(lb/batch)										
Name	**Formula**	**MW (g/mol)**	**S65**	**S71**	**S87**	**S103**	**S72**	**S73***	**S74***	**S75**	**S72.2**	**S76**	**S77**
Water	H_2O	18	0	0	4	4	4	4	4	4	4	4	4
Media (dry)	-	-	0	0	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0	0
Cell Mass	-	-	0	0	0	0	0	0	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	3,996	3,996	128	128	4,124	4,124	4,124	4,124	4,124	4,127	4,124
Ethanol	C_2H_6O	46	8	8	0	0	8	8	8	8	8	8	8
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	0	0	0	0	0
Total			4,004	4,004	7,996	132	4,136	4,136	4,136	4,136	4,136	4,136	4,136
Phase			Liquid	Mixed	Mixed	Liquid	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed
Temperature (°F)			98	98	290	61	89	245	245	245	245	572	247
Pressure (psi)			22	1	1	1	1	1	1	1	1	1	1

			Streams (lb/hr)											
Name	**Formula**	**MW (g/mol)**	**S78**	**S79**	**S80**	**S78**	**S79**	**S80**	**S81**	**S82**	**S83**	**S84**	**S85**	**S86**
Water	H_2O	18	4	1,316	1,316	1,316	1,316	1,316	20,000	20,000	20,000	3,000	3,000	3000
Media (dry)	-	-	0	0	0	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	0	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0	0	0
Cell Mass	-	-	0	0	0	0	0	0	0	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	4,124	128	128	128	128	128	0	0	0	0	0	0
Ethanol	C_2H_6O	46	8	8	8	8	8	8	0	0	0	0	0	0
1,3-Butadiene	C_4H_6	54	0	1,539	1,539	1,539	1,539	1,539	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	0	865	865	865	865	865	0	0	0	0	0	0
Methyl Vinyl Carbinol	C_4H_8O	72	0	284	284	284	284	284	0	0	0	0	0	0
Total			4,136	4,140	4,140	4,140	4,140	4,140	20,000	20,000	20,000	3,000	3,000	3,000
Phase			Vapor	Vapor	Vapor	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed
Temperature (°F)			572	932	651	1,340	1341	194	992	1,200	992	90	90	760
Pressure (psi)			1	1	1	73	73	73	15	15	15	15	23	23

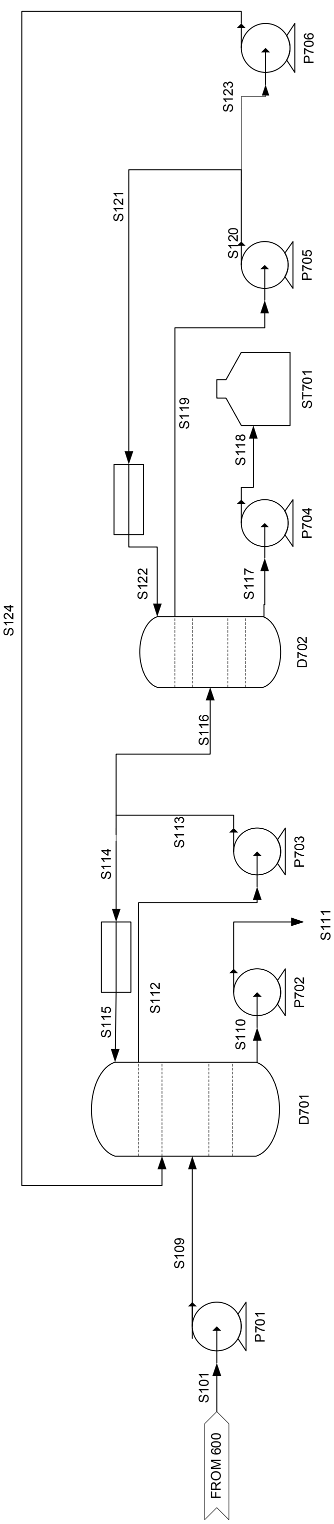
Figure 6-9: Section 600: Distillation Separation: 1,3-Butadiene Recovery



			Streams (lb/hr)										
Name	**Formula**	**MW (g/mol)**	**S80**	**S88**	**S89**	**S90**	**S91**	**S92**	**S93**	**S94**	**S95**	**S96**	**S97**
Water	H_2O	18	1,316	1,311	1,311	20	20	15	3,612	5	1,204	1,204	428
Media (dry)	-	-	0	0	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0	0
Cell Mass	-	-	0	0	0	0	0	0	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	128	128	128	0	0	0	0	0	128	128	0
Ethanol	C_2H_6O	46	8	8	8	0	0	0	0	0	8	8	0
1,3-Butadiene	C_4H_6	54	1,539	0	0	6,156	6,156	4,617	0	1,539	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	865	859	859	0	0	0	0	6	37	37	3,292
Methyl Vinyl Carbinol	C_4H_8O	72	284	284	284	0	0	0	0	0	284	284	0
Total			4,140	2,590	2,590	6,176	6,176	4,632	3,612	1,550	1,661	1,661	3,720
Phase			Mixed	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°F)			162	254	254	109	109	109	109	109	203	203	169
Pressure (psi)			73	66	66	65	65	65	65	65	19	19	17

			Streams (lb/hr)										
Name	**Formula**	**MW (g/mol)**	**S98**	**S99**	**S100**	**S101**	**S102**	**S103**	**S104**	**S105**	**S106**	**S107**	**S108**
Water	H_2O	18	428	321	963	107	4	4	3,600	3,600	2,400	2,400	1,200
Media (dry)	-	-	0	0	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0	0
Cell Mass	-	-	0	0	0	0	0	0	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	0	0	0	0	128	128	0	0	0	0	0
Ethanol	C_2H_6O	46	0	0	0	0	0	0	24	24	16	16	8
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	3,292	2,469	2,469	823	0	0	111	111	74	74	37
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	852	852	568	568	284
Total			3,720	2,790	3,432	930	132	132	4,587	4,587	3,058	3,058	1,529
Phase			Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°F)			169	169	169	169	293	293	192	192	192	192	192
Pressure (psi)			17	17	17	17	17	17	16	16	16	16	16

Figure 6-10: Section 700: Distillation Separation: Pressure-Swing Distillation



			Streams (lb/hr)								
Name	**Formula**	**MW (g/mol)**	**S101**	**S109**	**S110**	**S111**	**S112**	**S113**	**S114**	**S115**	**S116**
Water	H_2O	18	121	121	95	95	104	140	78	78	26
Media (dry)	-	-	0	0	0	0	0	0	0	0	0
Media (wet)	-	-	0	0	0	0	0	0	0	0	0
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0
Cell Mass	-	-	0	0	0	0	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	0	0	0	0	0	0	0	0	0
Ethanol	C_2H_6O	46	0	0	0	0	0	0	0	0	0
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	809	809	714	714	408	408	306	306	102
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	0	0	0
Total			930	930	809	809	512	548	384	384	128
Phase			Liquid	Mixed	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°F)			170	170	309	309	279	279	279	279	279
Pressure (psi)			17	109	106	106	102	102	102	102	102

			Streams (lb/hr)							
Name	**Formula**	**MW (g/mol)**	**S117**	**S118**	**S119**	**S120**	**S121**	**S122**	**S123**	**S124**
Water	H_2O	18	26	26	0	0	0	0	0	0
Media (dry)	-	-	0	0	0	0	0	0	0	0
Media (wet)	-	-	0	0	0	0	0	0	0	0
Carbon Monoxide	CO	28	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0
Cell Mass	-	-	0	0	0	0	0	0	0	0
2,3-Butanediol	$C_4H_{10}O_2$	90	0	0	0	0	0	0	0	0
Ethanol	C_2H_6O	46	0	0	0	0	0	0	0	0
1,3-Butadiene	C_4H_6	54	0	0	0	0	0	0	0	0
Methyl Ethyl Keytone	C_4H_8O	72	95	95	32	32	24	24	8	8
Methyl Vinyl Carbinol	C_4H_8O	72	0	0	0	0	0	0	0	0
Total			121	121	32	32	24	24	8	8
Phase			Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°F)			188	188	178	178	178	178	178	102
Pressure (psi)			24	24	18	18	18	18	18	109

7.0 PROCESS DESCRIPTION

Overview

Our process is divided into two steps with eight overall sections, as described in Section 6. The first step is the fermentation section of the plant, where carbon monoxide-rich gas is fed into continuous stirred tank reactors (CSTRs) to produce 2,3-butanediol during steady state operation. The gaseous feed is cooled in section 000 using a shell and tube heat exchanger with water as coolant. Section 100 is a mixing process for media, which supplies fresh media to sections 200 and 300. The cells are grown in sequential fermentation tanks in section 200, then provided to ten CSTRs (section 300) working in tandem, organized in two blocks of five, as shown in the Figure 6-2. The overall fermentation process concludes at the separation processes in section 400, where simulation moving bed chromatography is used to extract the alcohols 2,3-butanediol and ethanol from the fermentation broth. A small distillation tower is used to create a stream of nearly pure 2,3-butanediol. The ethanol effluent from the distillation tower is sold as a secondary product.

The second step of our process coverts 2,3-butanediol to 1,3-butadiene using a thermo catalytic converter. The reaction products are then separated in a series of distillation towers. Section 500 describes the reactor, producing 1,3-butadiene and byproducts. In sections 600 and 700, the reaction products are separated. First, 1,3-butadiene is isolated in section 600. Then, the byproduct methyl ethyl ketone is isolated in section 700 to sell as a secondary product

CO Fermentation for the Formation of BDO

Section 000: Steel Mill Gas Cooling

A shell and tube heat exchanger is used to cool excess steel mill gas from 500°F to 98°F using water as a coolant. The steel mill gas temperature can be variable depending on whether or not the steel mill recovers energy from the waste gas. We initially assume a temperature of 500°F, though a situation with a hotter feed is considered. This steel mill gas will be fed to the cells in the batch fermenters in section

200 as needed. In addition, once our overall process is running at steady state, gas will be added continuously to each CSTR at 31,000 lb/hr. There are ten of these compressor/heat exchanger units.

Section 100: Media Mixing System

The media mixing section creates wet media liquid and pumps the media to either section 100 or 200, depending on demand. The dry media powder is held in two vertical silos, with a minimum holding volume of 950,000 lbs dry media per day. The duplicity allows the plant to store enough media between refilling. For the batch fermentation process, 333,600 lbs of wet media is created in the ratio of one part dry media in nine parts pure water, which is first purchased from a water supplier for the fermentation media in the batch fermenters. Media is distributed to the batch fermenters at varying volumes and is held at 40°F in a 50,000 gallon storage vessel with a cooling jacket in the intermediary time.

333,600 lbs of media are also made to preliminary fill each CSTR in section 300. The media is fed to section 300 at 98°F, with water again purchased from a supplier. When the CSTRs are operating continuously, wet media is made and then distributed continuously at a total rate of 416,700 lbs/hr at 98°F. Under continuous operation, water is recycled after undergoing microfiltration and simulated moving bed chromatography in section 400 back into section 100 to recover and reuse media water.

Section 200: Batch Fermentation

This section utilizes five sequential fermenters to grow bacteria. The incoming media is provided from the batch system of section 100 at 98°F. The 15-gallon seed fermenter holds 312 lbs of media, growing *cl. autoethanogenum* cells from a concentration of 0.01 mg/L to 0.2 g/L. This takes 4 days including loading and transferring to the next vessel. All 92 lbs of the seed fermenter F201 are moved to the next batch vessel F202, with a capacity of 130 gallons. In addition, 784 lbs of wet media is supplied to the reactor from section 100. The cells grow from a concentration of 0.02 g/L to 0.2 g/L in the fermenter over the course of 3 days including loading and transfer.

The third vessel F203 operates at a capacity of 1,320 gallons. The fermenter contains 876 lbs of media and cells from the previous vessel in addition 9,034 lbs of fresh media. Again, it grows cells from 0.02 g/L to 0.2 g/L over the course of 3 days including loading and transfer. The fourth fermenter F204 has a volume of 13,200 gallons. From the previous fermenter, 9,910 lbs of wet media and cells are added in addition to 16,272 lbs of fresh wet media from section 100. This fermenter takes 3 days to operate including loading and transfer. The fermenter grows the cells from 0.02 g/L to 0.2 g/L and all 26,182 pounds of wet media and cells is used to fill up the last fermenter. The fifth fermenter F505 is the largest, with a volume of 45,000 gallons. The entirety of the previous fermenter, 26,182 pounds, is mixed with 304,166 lbs of fresh media from section 100. This fermenter grows the cells from a concentration of 0.06 g/L to 0.2 g/L over the course of 5 days including loading and transfer. This produces a batch with a total mass of 330,367 pounds including 67 pounds of cell mass. This is enough to inoculate five CSTRs like block 300 with 66,073 pounds of broth each. The fermenters are kept at 98°F using a dimple jacket. The batch length of section 200 is 18 days from inoculation of the seed fermenter to transferring the contents of the final vessel into section 300. Two batches are needed to inoculate all ten CSTRs.

The batch fermentation process provides enough cells to run five CSTRs at once. Since the CSTRs in section 300 grow cells themselves, they can operate with a cell recycle in steady state. Therefore, each block in section 300 needs to be seeded with cells once a year leading to section 200 only being in operation twice a year. Each seed reactor is inoculated with 0.01 mg/L of *cl. autoethanogenum* per batch, purchased fresh each year.

Section 300: CSTR and Cell Recycle Close-up

There are ten CSTRs in total in the plant. Each CSTR will have the same set up: a fermenter, filter, and cell recycle. The volume of each CSTR is 50,000 gallons. When first filled, the CSTR is operated as a batch fermenter, seeded with 66,060 lbs of media and 13 g of cells from section 200, in addition to 336,000 lbs of wet media from section 100. It takes 13 days for the cell culture to reach 2 g/L once seeded.

Once the cell concentration reaches 2 g/L in the tank, the continuous reaction begins. Fermentation broth is cycled through the CSTR at 41,670 lbs/hr. The fermentation broth contains 200 lbs/hr of cell mass, 400 lbs/hr of BDO, and 800 lbs/hr ethanol. The cell mass is collected using a disk-stack centrifuge. 120 lbs/hr of the cell mass is deposited in a settling pond, and 80 lbs/hr of the cell mass is returned to the reactor to ensure a constant concentration of 2 g/L in the vessel. The effluent from the centrifuge, which has no cell mass, is combined with the effluent from the other CSTRs to form a stream of 4000 lbs/hr of 2,3-butanediol and 8,000 lbs/hr of ethanol, which is sent to section 400.

Section 400: Simulated Moving Bed Chromatography Separation

Orochem has developed a separation technique using simulated moving bed chromatography. The feed to the separation unit is 428,355 lbs/hr, the total flow rate from all ten CSTRs. The composition of the feed is 416,710 lbs/hr used media, 4,000 lbs/hr of BDO and 8,000 lbs/hr ethane. The separation unit works by extracting alcohols and hydrocarbons from water for high purity and high recovery rates of greater than 99% (Orochem, 2012). The exit stream of used media is 416,710 lbs/hr, and the exit stream of the alcohol/hydrocarbon stream is 12,000 lbs/hr, in a ratio of 2:1 ethanol to BDO

A simple 5-tray distillation tower is used to separate ethanol from 2,3-butanediol into two pure streams due to significant differences in boiling temperatures. The separation produces 4,000 lb/hr of BDO and 8,000 lb/hr of ethanol that can be sold as a byproduct. The alternative to the simulated moving bed chromatography is to use a distillation tower to separate the output to section 300, discussed later in the report.

Formation of 1,3-Butadiene via Thermo-Catalytic Conversion of BDO

Section 500: Thermo Catalytic Conversion

The feed to this section is pure BDO at a flow rate of 4000 lb/hr, pressure of 70mmHg obtained by passing the feed through a valve, and temperature of 248°F. This stream is combined with a recycle from Section 600, which contains unreacted BDO. The reactor preheater operates at 572°F, and the reactor operates at 932°F and 70 mmHg in order to ensure high conversions of BDO to 1,3-Butadiene. Additionally, a fired heater, which uses No 4. Fuel Oil, is used to heat steam used to maintain the reactor at 932°F.

Once the effluent leaves the reactor, it passes through a heat exchanger to preheat the reactant gas to 572°F. This heat exchanger operates at steady state. However, on start-up an electric heater is used to preheat the feed to the reactor. The reactor effluent leaves the heat exchanger at a pressure of 70mmHg and 651°F Celsius. The effluent then enters section 600. The last unit in this section is a multi-stage compressor, which raises the pressure of the inlet stream to 73 psi.

The catalyst is regenerated every two months by passing high-pressure steam through the reactor for two hours. The exit steam is then treated at a waste treatment facility to remove contaminants.

Section 600: Distillation Separation: 1,3-Butadiene Recovery

Pressurized vapor from section 500 enters a heat exchanger HX601, which creates low-pressure steam to drive the reboiler of D602 in this section. The first distillation column D601 operates at 70 psi and separates out the 1,3-Butadiene from the inlet stream at a polymer grade purity of 99.3%. The distillate is then stored in a storage vessel. The bottoms product is feed to the second column D602 operating at 19 psi. The distillate from this column is a mixture of MEK and water at its azeotropic composition and is sent to section 700 to recover the MEK for sale. The bottoms product from the second column is fed to the third distillation column D603, which operates as a slightly lower pressure than the previous column. The distillate from this column contains approximately 78% by mass water, 19% methyl vinyl carbinol, and 5% MEK, and is sent off site to a wastewater treatment center. The bottoms product contains pure unreacted BDO, which is recycled to section 500.

Section 700: Distillation Separation: Pressure-Swing Distillation

The feed at the azeotropic composition of MEK/water from section 600 is sent to the first of two columns D701 for pressure-swing distillation. The first column operates at 106 psi and removes the MEK as a 99.99% pure product. The distillate is sent to the second column, which removes water as the bottoms product. The second column D602 operates at a pressure of 23 psi. Two pumps are needed in order to ensure that the feeds to the first column are at high enough pressure.

8.0 ENERGY BALANCE AND UTILITY REQUIREMENTS

Six different utilities are used in the process: electricity, cooling water, process water, steam, wastewater treatment, and fuel oil. Costs in the year 2006 were obtained from Seider et. Al. and adjusted based on an assumed CE Index of 570.

Electricity costs were assumed to be $0.06/kWh. The overall electricity requirement of the system was calculated to be 16.7 MW.

The main cooling water requirement was to drive the condensers. Cooling water costs were assumed to $0.075/1,000 gal. The overall cooling water requirements of the system were calculated to be 3921.4 gpm.

The process water costs were assumed to be $0.75/1,000 gal. The overall process water requirements of the system were quite high because the fermentation broth was a large feedstock to the batch system. 748.9 gpm of process water was required.

The main steam costs were to drive the distillation column reboilers. The cost of low-pressure steam (50 psi) was assumed to be $3.00/1000 lb. The cost of the medium-pressure steam (150 psi) was assumed to be $4.50 / 1000 lb. The cost of the medium-pressure steam (450 psi) was assumed to be $6.00 / 1000 lb. The overall steam requirement of the system were 28 lb/hr.

The wastewater treatment was required to treat the methyl vinyl carbinol stream leaving section 600 of the process. A rate of 336.3 lb/hr of organic waste needed to be treated at an assumed cost of $0.15/lb organic waste removed.

Finally, No. 4 Fuel Oil was used to drive the fired heater, which provided the heat duty to the steam used to heat the reactor. The fuel oil was assumed to cost $0.22/lb. The duty required by the fired heater was 2181.1 MBtu/hr. The HHV of the oil was 18701 Btu/lb, and the density of the oil was assumed to be 59 lb/ft^3.

Below are the detailed energy balance and utility requirements of each unit by section of the process. Please see Appendix A for example calculations.

CO Fermentation for the Formation of BDO

Section 000: Steel Mill Gas Cooling

Unit	**Type**	**Utility type**	**Utilities cost ($/yr)**	**Requirement**	**Units**
HX001	Cool Gas Feed to Fermenters	Cooling Water	$69,065	1700	gpm
C001	Compresses Air	Electricity	$4,740,662	8751	kW
Total			*$4,809,727*		

Section 100: Media Mixing System

Unit	**Type**	**Utility type**	**Utilities cost ($/yr)**	**Requirement**	**Units**
ST101a	Storage Tank	NA	NA	NA	NA
ST101b	Storage Tank	NA	NA	NA	NA
SS101	pneumatic conveying system	Electricity	$128,637	237.5	kW
B101	Blower	Electricity	$27,086	50.0	kW
FT101	Water Filter	NA	NA	NA	NA
M101	Mixing Tank	Electricity	$202,400	373.6	kW
M101'	Mixing Tank agitator	Electricity	$1,614	3.0	kW
P101	Pump	Electricity	$5,989	11.1	kW
P102	Pump	Electricity	$7,302	13.5	kW
FT102	Ultra filtration	Electricity	$24,000	44.3	kW
FT103	Ultra filtration	Electricity	$240,000	443.0	kW
H101	HTX	Electricity	$6,575	12.1	kW
H102	HTX	Electricity	$1,985,975	3666.0	kW
ST102	Storage Tank	NA	NA	NA	NA
Total			*$2,629,578*		

Section 200: Batch Fermentation

Unit	Type	Utility type	Utilities cost ($/yr)	Requirement	Units
P201*	Pump	Electricity	$0	0.0	kW
P202*	Pump	Electricity	$0	0.0	kW
P203*	Pump	Electricity	$1	0.0	kW
P204*	Pump	Electricity	$4	0.0	kW
P205*	Pump	Electricity	$19	0.0	kW
F201*	Horizontal Column	Cooling Water	$0	0.0	gpm
F202*	Horizontal Column	Cooling Water	$0	0.0	gpm
F203*	Horizontal Column	Cooling Water	$5	0.1	gpm
F204*	Horizontal Column	Cooling Water	$44	1.1	gpm
F205*	Horizontal Column	Cooling Water	$90	2.2	gpm
Total			*$163*		

Section 300: CSTR and Cell Recycle Close-up

Unit	**Type**	**Utility type**	**Utilities cost ($/yr)**	**Requirement**	**Units**
CR301	CSTR	Cooling Water	$110	2.7	gpm
CR302	CSTR	Cooling Water	$110	2.7	gpm
CR303	CSTR	Cooling Water	$110	2.7	gpm
CR304	CSTR	Cooling Water	$110	2.7	gpm
CR305	CSTR	Cooling Water	$110	2.7	gpm
CR306	CSTR	Cooling Water	$110	2.7	gpm
CR307	CSTR	Cooling Water	$110	2.7	gpm
CR308	CSTR	Cooling Water	$110	2.7	gpm
CR309	CSTR	Cooling Water	$110	2.7	gpm
CR310	CSTR	Cooling Water	$110	2.7	gpm
P301	Pump	Electricity	$1,079	2.0	kW
P302	Pump	Electricity	$1,079	2.0	kW
P303	Pump	Electricity	$1,079	2.0	kW
P304	Pump	Electricity	$1,079	2.0	kW
P305	Pump	Electricity	$1,079	2.0	kW
P306	Pump	Electricity	$1,079	2.0	kW
P307	Pump	Electricity	$1,079	2.0	kW
P308	Pump	Electricity	$1,079	2.0	kW
P309	Pump	Electricity	$1,079	2.0	kW
P310	Pump	Electricity	$1,079	2.0	kW
TF301	Disk Stack Centrifuge	NA	NA	NA	NA
TF302	Disk Stack Centrifuge	NA	NA	NA	NA
TF303	Disk Stack Centrifuge	NA	NA	NA	NA
TF304	Disk Stack Centrifuge	NA	NA	NA	NA
TF305	Disk Stack Centrifuge	NA	NA	NA	NA
TF306	Disk Stack Centrifuge	NA	NA	NA	NA
TF307	Disk Stack Centrifuge	NA	NA	NA	NA
TF308	Disk Stack Centrifuge	NA	NA	NA	NA
TF309	Disk Stack Centrifuge	NA	NA	NA	NA
TF310	Disk Stack Centrifuge	NA	NA	NA	NA
SS301	pneumatic c.s.	Electricity	$47,892	88.4	kW

Cont.					
Unit	**Type**	**Utility type**	**Utilities cost ($/yr)**	**Requirement**	**Units**
SS302	pneumatic c.s.	Electricity	$47,892	88.4	kW
SS303	pneumatic c.s.	Electricity	$47,892	88.4	kW
SS304	pneumatic c.s.	Electricity	$47,892	88.4	kW
SS305	pneumatic c.s.	Electricity	$47,892	88.4	kW
SS306	pneumatic c.s.	Electricity	$47,892	88.4	kW
SS307	pneumatic c.s.	Electricity	$47,892	88.4	kW
SS308	pneumatic c.s.	Electricity	$47,892	88.4	kW
SS309	pneumatic c.s.	Electricity	$47,892	88.4	kW
SS310	pneumatic c.s.	Electricity	$47,892	88.4	kW
SS311	pneumatic c.s.	Electricity	$47,892	88.4	kW
SS312	pneumatic c.s.	Electricity	$47,892	88.4	kW
Total			*$586,592*		

Section 400: Moving Bed Chromatography Separation

Unit	**Type**	**Utility type**	**Utilities cost ($/yr)**	**Requirement**	**Units**
P401	Pump	Electricity	$5,657	10.4	kW
FT401	Membrane Separation Unit	Electricity	$499,450	922.0	kW
ST401	Storage tank	NA	NA	NA	NA
D401	Separation of Ethanol from 2,3-BDO	NA	NA	NA	NA
D401 C.A	Condenser Accumulator	NA	NA	NA	NA
D401 CHX	Condenser HX	Cooling Water	$1,430	35.2	gpm
D401 RB	Reboiler	Low Pressure Steam	$236,041	8.7	lb/hr
D401 RP	Reflux Pump	Electricity	$764	1.4	kW
Total			*$743,342*		

Formation of 1,3-Butadiene via Thermo-Catalytic Conversion of BDO

Section 500: Thermo-Catalytic Conversion

Unit	**Type**	**Utility type**	**Utilities cost ($/yr)**	**Requirement**	**Units**
VS501	Two-stage Steam-jet ejector	86% HP Steam, 14% Cooling Water	$600,000.00	HPS: 9.52, CW: 2067.5	lb/hr, gpm
HX502 (1)	Reactor Vessel	NA - See Fired Heater	NA	NA	NA
HX502 (2)	Reactor Vessel	NA - See Fired Heater	NA	NA	NA
HX502 (3)	Reactor Vessel	NA - See Fired Heater	NA	NA	NA
HX502 (4)	Reactor Vessel	NA - See Fired Heater	NA	NA	NA
HX502 (5)	Reactor Vessel	NA - See Fired Heater	NA	NA	NA
HX502 (6)	Reactor Vessel	NA - See Fired Heater	NA	NA	NA
HX504	Heat Source for Reactors	Fuel Oil	$203,715.63	923686.2	lb/hr
Recycled Water	Reactor HX/Fired Heater System	NA	NA	NA	NA
Catalyst	Catalyst	NA	NA	NA	NA
C501	Compressor to D601	Electricity	$281,236.21	519.1	kW
HX502	Reactor Effluent Heat Recovery	NA	NA	NA	NA
HX503	Compressor Effluent Heat Recovery	Cooling Water	$243.88	6.0	gpm
HX501	Startup Heater	Electricity	$307,352.18	567.4	kW
P501	Pressure increase of Cooling Water to HX	Electricity	$41.49	0.1	kW
Total			*$1,392,589*		

Section 600: Distillation Separation: 1,3-Butadiene Recovery

Unit	Type	Utility type	Utilities cost ($/yr)	Requirement	Units
ST501	Storage Tank	NA	NA	NA	NA
D601	Tray tower for Separation of 1,3-Butadiene	NA	NA	NA	NA
D601 C.A	Condenser Accumulator	NA	NA	NA	NA
D601 CHX	Condenser HX	Cooling Water	$202.11	5.0	gpm
D601 RB	Reboiler	Medium Pressure Steam	$33,148.53	0.8	lb/hr
D601 RP	Reflux Pump	Electricity	$343.96	0.6	kW
D602	Tray tower for Separation of MEK/water	NA	NA	NA	NA
D602 C.A	Condenser Accumulator	NA	NA	NA	NA
D602 CHX	Condenser HX	Cooling Water	$212.74	5.2	gpm
D602 RB	Reboiler	Low Pressure Steam	$25,041.68	0.9	lb/hr
D602 RP	Reflux Pump	Electricity	$365.89	0.7	kW
D603	Tray Tower for Recycle of 2,3-BDO	NA	NA	NA	NA
D603 C.A	Condenser Accumulator	NA	NA	NA	NA
D603 CHX	Condenser HX	Cooling Water	$721.38	17.8	gpm
D603 RB	Reboiler	Low Pressure Steam	$97,563.24	3.6	lb/hr
D603 RP	Reflux Pump	Electricity	$262.21	0.5	kW
Total			*$157,861.74*		

Section 700: Distillation Separation: Pressure-Swing Distillation

Unit	**Type**	**Utility type**	**Utilities cost ($/yr)**	**Requirement**	**Units**
ST701	MEK Storage Tank	NA	NA	NA	NA
P701	Feed Pressure increase	Electricity	$177.05	0.3	kW
P706	Recycle Pressure increase	Electricity	$242.09	0.4	kW
D701	Tray Tower for Separation of MEK	NA	NA	NA	NA
D701 C.A	Condenser Accumulator	NA	NA	NA	NA
D701 CHX	Condenser HX	Cooling Water	$615.86	15.2	gpm
D701 RB	Reboiler	Medium Pressure Steam	$82,077.22	2.0	lb/hr
D701 RP	Reflux Pump	Electricity	$764.16	1.4	kW
D702	Tray Tower for Separation of Water	NA	NA	NA	NA
D702 C.A	Condenser Accumulator	NA	NA	NA	NA
D702 CHX	Condenser HX	Cooling Water	$588.91	14.5	gpm
D702 RB	Reboiler	Low Pressure Steam	$35,217.58	1.3	lb/hr
D702 RP	Reflux Pump	Electricity	$326.49	0.6	kW
Total			*$120,009.36*		

Unaccounted For Energy Balance and Utility Requirements

	Utility Type	**Relevant Quantity (lb/hr)**	**Cost ($/yr)**
Section 500			
Cooling Water Used to Drive P501	Cooling Water	3000	$213.93
High Pressure Steam Used In Generation of Catalyst	High Pressure Steam	1000*	$75,240.00
Treatment of High Pressure Steam	Wastewater treatment	20*	$1,504.80
Section 600			
Treatment of S108	Wastewater treatment	336.3	$399,474.76

Overall Utilities by Section

Amount of Utilities Used

Utilities	**Quantity per Section**			
	000	**100**	**200**	**300**
Steam, 450 psig (lb/hr)	0	0	0	0
Steam, 150 psig (lb/hr)	0.00	0	0	0
Steam, 50 psig (lb/hr)	0.0	0	0	0
Cooling Water (gpm)	1700	0	3.4	27.0
Electricity (kW)	8751.0	4854.1	0.0	1080.8
Wastewater Treatment (lb organic/hr)	0	0	0	0
Fuel Oil (lb/hr)	0.0	0	0	0

Utilities	**Quantity per Section**				
	400	**500**	**600**	**700**	**Total**
Steam, 450 psig (lb/hr)	0	10.9	0	0	10.9
Steam, 150 psig (lb/hr)	0	0	0.8	2.0	2.8
Steam, 50 psig (lb/hr)	8.7	0	4.5	1.3	14.5
Cooling Water (gpm)	35.2	2073.5	33.97	48.5	3921.4
Electricity (kW)	933.8	1086.6	1.8	1.4	16709.4
Wastewater Treatment (lb organic/hr)	0	0.028	336.3	0.0	336.3
Fuel Oil (lb/hr)	0	923686.2	0		923686.2

Price of Utilities Used

Utilities	**Cost per Section**			
	000	**100**	**200**	**300**
Steam, 450 psig (lb/hr)	$-	$-	$-	$-
Steam, 150 psig (lb/hr)	$-	$-	$-	$-
Steam, 50 psig (lb/hr)	$-	$-	$-	$-
Cooling Water (gpm)	$69,065	$-	$139	$1,098
Electricity (kW)	$4,740,662	$2,629,578	$24	$585,494
Wastewater Treatment (lb organic/hr)	$-	$-	$-	$-
Fuel Oil (lb/hr)	$-	$-	$-	$-

Utilities	**Cost per Section**				
	400	**500**	**600**	**700**	**Total**
Steam, 450 psig (lb/hr)	$-	$591,240	$-	$-	$591,240
Steam, 150 psig (lb/hr)	$-	$-	$33,149	$82,077	$115,226
Steam, 50 psig (lb/hr)	$236,041	$-	$122,605	$35,218	$393,863
Cooling Water (gpm)	$1,430	$84,458	$1,136	$1,969	$159,296
Electricity (kW)	$505,871	$588,630	$972	$746	$9,051,976
Wastewater Treatment (lb organic/hr)	$-	$1,505	$399,475	$-	$400,980
Fuel Oil (lb/hr)	$-	$203,716	$-	$-	$203,716

9.0 UNIT DESCRIPTIONS

9.1 Fermentation Vessels

The front end of our process contains five fermentation vessels made to grow the cells to their required mass for continuous operation in the CSTRs. Each fermenter operates for long enough time for the cells to grow during their logarithmic phase to a concentration of 200 mg/L. The batch fermentation vessels only need to perform two runs a year, each time with fresh *cl. autoethanogenum* from the supplier. One batch vessel run takes eighteen days.

F201 is the seed fermenter in this process. It is a carbon steel, vertical vessel with a total volume of 15 gallons. It is inoculated with 0.1 mg of *cl. Autoethanogenum* and charged with 83.4 pounds of water, 8.3 pounds of media, and 9.2 lbs/hr of steel mill gas. The gas is fed through a fermenter bubbler to enable cell growth. A dimple jacket is used to maintain the vessel at the optimum temperature of 98.6 °F. The batch schedule of this vessel is as follows:

0.5 Days to fill and inoculate
3 Days of Cell Growth
0.5 Days to Harvest
1 Day to Clean and Sterilize

The total f.o.b. cost of this vessel was calculated to be $5,897 with a total bare module cost of $24,532. The contents of F201 are used to inoculate F202.

F202 is the second fermentation vessel in this process. It is a carbon steel, vertical vessel with a total volume of 130 gallons. It is inoculated with 0.018 pounds of *cl. autoethanogenum* and charged with 796 pounds of water, 80 pounds of media, and 79 lbs/hr of steel mill gas. The gas is fed to the broth through a fermenter bubbler to enable cell growth to its desired mass of 0.18 lbs. A dimple jacket is used to maintain the vessel at the optimum temperature of 98.6 °F. The batch schedule of this vessel is as follows:

0.5 Days to fill and inoculate
2 Days of Cell Growth
0.5 Days to Harvest
1 Day to Clean and Sterilize

The total f.o.b. cost of this vessel was calculated to be $11,837 with a total bare module cost of $49,240. The contents of F202 are used to inoculate F203.

F203 is the third fermentation vessel in this process. It is a carbon steel, vertical vessel with a total volume of 1,320 gallons. It is inoculated with 0.18 pounds of *cl. autoethanogenum*. It is charged with 9009 pounds of water, 9009 pounds of media, and 806 lbs/hr of steel mill gas that is fed to the broth through a fermenter bubbler to enable cell growth to its desired mass of 2 lbs. A dimple jacket is used to maintain the vessel at the optimum temperature of 98.6 °F. The batch schedule of this vessel is as follows:

0.5 Days to fill and inoculate
2 Days of Cell Growth
0.5 Days to Harvest
1 Day to Clean and Sterilize

The total f.o.b. cost of this vessel was calculated to be $29,677 with a total bare module cost of $123,592. The contents of F203 are used to inoculate F204.

F205 is the fourth fermentation vessel this our process. It is a carbon steel, vertical vessel with a total volume of 13,200 gallons. It is inoculated with 2 pounds of *cl. autoethanogenum*. It is charged with 23,800 pounds of water, 2,380 pounds of media, and 8060 lbs/hr of steel mill gas fed through a fermenter bubbler to enable cell growth to its desired mass of 2 pounds. A dimple jacket is used to maintain the vessel at the optimum temperature of 98.6 °F. The batch schedule of this vessel is as follows:

0.5 Days to fill and inoculate
2 Days of Cell Growth
0.5 Days to Harvest
1 Day to Clean and Sterilize

The total f.o.b. cost of this vessel was calculated to be $86,528 with a total bare module cost of $360,322. The contents of F204 are used to inoculate F205.

F204 is the fifth and final fermentation vessel in this process. It is a carbon steel, vertical vessel with a total volume of 45,000 gallons. It is inoculated with 18 pounds of *cl. autoethanogenum* and is charged with 300,300 pounds of water, 30,030 pounds of media, and 27,479 lbs/hr of steel mill gas. The gas is fed through a fermenter bubbler to enable cell growth to 67 pounds. A dimple jacket is used to maintain the vessel at the optimum temperature of 98.6 °F. The batch schedule of this vessel is as follows:

1 Day to fill and inoculate
3 Days of Cell Growth
1 Day to Harvest
2 Days to Clean and Sterilize

The total f.o.b. cost of this vessel was calculated to be $157,852 with a total bare module cost of $656,555. The contents of F205 are used to inoculate five CSTRs. A batch takes 18 days to produce one batch of cells including the loading of the seed fermenter. Two batches of cells are grown per year.

9.2 Continuous Stirred Tank Reactors

2,3-Butanediol production occurs in the continuous stirred tank reactors. The CSTRs are organized in two blocks of five, for a total of ten CSTRs operating in parallel. Each CSTR is a carbon steel horizontal vessel with a total volume of 50,000 gallons and an aspect ratio of five. CSTRs are first operated as batch processes and initially filled with 40,000 gallons of fresh wet media. Each CSTR takes 1 day to fill to capacity.

Each CSTR is also charged with 66,066 lbs of broth and cells at a concentration of 2 mg/L. This gives a starting concentration of 33 mg/L of cells for each CSTR. Steel mill gas flows at 31,000 lb/hr through a CSTR bubbler. This batch operation continues until the cells reach 2 g/L, the desired concentration for maximum BDO production. This batch production takes 13 days.

Continuous operation is started once the desired steady state concentration is achieved. Fresh media is fed at 5,000 gallons/hr, and fermentation broth is remove from the reactor at the same rate. The gas flow rate constant at 30,532 pounds per hour. The CSTR effluent contains 200 lb/hr of biomass, which is separated used a disk-stacked centrifuge. Of the biomass collected, 120 lbs/hr is sent to a settling pond and 80 lbs/hr is recycled back to the CSTR to maintain steady-state concentration. The cells are hearty and can withstand the force of the centrifuge before being sterilized and disposed of at the end of each year. The cell-free fermentation broth contains 400 lbs/hr of BDO and 800 lbs/hr of ethanol per CSTR.

Besides the difference in loading times, all of the ten CSTRs are identical and operated continuously once the cells reach the desired cell concentration. The f.o.b. cost of each vessel was calculated to be $177,920 with a bare module cost of $737,790. This leads to a total f.o.b. cost of $1,779,200 and total bare module cost of $7,377,900.

9.3 Simulated Moving Bed Chromatography

A simulated moving bed chromatography unit (SMB) is used to separate the cell products from the fermentation broth leaving the CSTRs. The broth is free of cells and contains mostly water with 4,000 lbs/hr of BDO and 8,000 lbs/hr ethanol. The SMB works by separating alcohols and hydrocarbons from water. Please see Appendix C for information on the corporate contact. The output to the SMB unit is be two streams- an extract phase consisting of the alcohols butanediol and ethanol at a rate of 12,000 lbs/hr and a raffinate phase consisting of water and any leftover salts at a rate of 37,500 lbs/hr. The extract, stream S81, is sent to a small distillation column for further separation and the raffinate S80 is reused in the process. A typical unit is shown below.

Figure 9-1: (Orochem, 2012)

9.4 Storage Tanks

S101a is a storage tank designed to hold and transport dry media. It cylindrical, carbon steel, vessel with a volume of 50,000 gallons, a height of 41.3 ft, and a diameter of 13.8 ft. This vessel is designed to provide enough media for block 300 to operate continuously for 1 day or to provide sufficient media for a fermentation batch. Dry powder media leaves the storage tank at 4,170 lbs/hr and is sent to the mixer through the use of blower SS101. It has a total f.o.b purchase cost of $165,626 and total bare module cost of $689,003. A duplicate vessel exists to ensure adequate media storage.

ST102 is a storage tank designed to store the water media mixture until it is supplied to a batch fermentation vessel in block 200. It is a cylindrical, carbon steel, pressurized vessel with a volume of 50,000 gallons, a height of 41.3 feet and a diameter of 13.8 feet. It is maintained at 40 °F through the use of a dimple jacket. ST102 keeps water/media mixture stored at cool temperature until it is needed by components of block 200. Since one batch through block 200 takes approximately 18 days, media is kept at ST102 for a maximum of approximately 19 days to include for loading time. It has a total f.o.b purchase cost of $182,189 and total bare module cost of $757,903.

ST601 is a storage tank is designed to store 1,3-butadiene before it can be shipped and sold. It is cylindrical, carbon steel, pressurized vessel with a volume of 50,000 gallons, a diameter of 23.4 feet. The hold-up time for this vessel is 7 days, accounting for a shipping rate of once a week. It is highly pressurized at 65 psi to ensure the 1,3-butadiene remains a liquid product. It is stored at room temperature. This vessel has a total f.o.b. cost of $226,185 and total bare module cost of $940,923.

ST701 is a storage tank is designed to store methyl ethyl ketone before it can be shipped and sold. It is a carbon steel, cylindrical, pressurized storage tank with a volume of 21,000 gallons, a height of 31.8 feet and a diameter of 10.6 feet. The hold-up time for this vessel is 7 days, accounting for a shipping rate of once a week. In order to keep this product liquid, the tank is pressurized at 58 psi and kept at room temperature. This vessel has a total f.o.b. cost of $115,638 and total bare module cost of $481,052.

ST401 is a storage tank is designed to store ethanol before it can be shipped and sold. It is a carbon steel, cylindrical, pressurized storage tank with a volume of 116,717 gallons, a height of 56.3 feet and a diameter of 18.8 feet. The hold-up time for this vessel is 4 days. In order to keep this product liquid, the tank is pressurized at 40 psi and kept at room temperature. This vessel has a total f.o.b. cost of $267,531 and a total bare module cost of $1,112,928.

9.5 Pumps

P101 is a carbon steel, centrifugal pump used to pressurize stream S10 at 921.5 gpm. The pressure of S10 is increased from 22 psi to 50 psi to allow the stream to pass through the microfiltration unit, FT102, and then to the ST102 where it is kept for storage until needed by the batch fermenters. Therefore, this pump is only needed twice a year during batch operation. The pump is 74% efficient and uses 11.05 kW of electricity. The estimated purchase cost of P101 is $4797 and the total purchase and installation cost is $18,406.

P102 is a carbon steel, centrifugal pump used to pressurize stream S16 at 738 gpm. The pressure of S16 is increased from 22 psi to 50 psi to allow the stream to pass through FT103, a microfiltration unit, to block 300. At full capacity, this pump operates continuously to allow for the CSTRs to operate at steady state. The pump is 75% efficient and uses 13.5 kW of electricity. The estimated purchase cost of P102 is $4475 and the total purchase and installation cost is $16,836.

Pumps P201 to P205 are used to move the media and cell product between batch fermenters. These pumps are in operation twice a year and only change the pressure of the streams enough to pass the material to the next fermenter. Since the streams are mostly water, the solid cell mass can be moved by a centrifugal pump.

P201 is a carbon steel, centrifugal pump, which is used to pressurize stream S28 at 0.02 gpm. The pressure of stream S28 is increased from 22 psi to 23 psi to ensure enough pressure to traverse the pipeline from F201 to F202. This pump is also needed once each batch fermentation cycle. The pump is 30% efficient and uses $2.3 * 10^{-5}$ kW of electricity. The estimated purchase cost is $3000 and the total purchase and installation cost is $11,285.

P202 is a carbon steel, centrifugal pump, which is used to pressurize stream S30, which is at .16 gpm. The pressure of stream S28 is increased from 22 psi to 23 psi, so it has enough pressure to traverse the pipeline from F202 to F203. This pump is also needed twice as year or once for each batch fermentation cycle. The pump is 30% efficient and uses $2.9*10^{-4}$ kW of electricity. The estimated purchase cost of P202 is $4390 and the total purchase and installation cost is $16,517.

P203 is a carbon steel, centrifugal pump which is used to pressurize stream S32, The pressure of stream S32 is increased from 22 psi to 23 psi, so it has enough pressure to traverse the pipeline from F203 to F204. This pump is also needed twice as year or once for each batch fermentation cycle. The pump is 30% efficient and uses $2.4*10^{-3}$ kW of electricity. The estimated purchase cost of P203 is $9478 and the total purchase and installation cost is $35,658.

P204 is a carbon steel, centrifugal pump, which is used to pressurize stream S34, which is at 4.8 gpm. The pressure of stream S32 is increased from 22 psi to 23 psi, so it has enough pressure to traverse the pipeline from F204 to F205. This pump is also needed twice as year or once for each batch fermentation cycle. The pump is 30% efficient and uses electricity at $6.5 * 10^{-3}$ kW. The estimated purchase cost of P203 is $6152 and the total purchase and installation cost is $23,146.

P205 is a carbon steel, centrifugal pump used to pressurize stream S32. The pressure of stream S32 is increased from 22 psi to 23 psi, so it has enough pressure to traverse the pipeline from F204 to F205. This pump is needed twice as year or once for each batch fermentation cycle. The pump is 35% efficient and uses 0.3 kW of electricity. The estimated purchase cost of P203 is $3540 and the total purchase and installation cost is $13,317.

P301 is a carbon steel, centrifugal pump that is used to pressurize stream S50. The pressure of stream S50 is increased from 22 psi to 50 psi so as to pass through the stacked-disk centrifuge and continue to block 400. This pump operates continuously. The pump is 50% efficient and uses 2 kW of electricity. The estimated purchase cost of P301 is $3000 and the total purchase and installation cost is $11,283. Each CSTR has a this pump.

P401 is a carbon steel, centrifugal pump that is used to pressurize stream S60. The pressure of stream S50 is increased from 22 psi to 50 psi so it has enough pressure to travel through FT401, the simulated moving bed chromatography unit and onwards. This pump operates continuously. The pump is 73% efficient and uses 10 kW of electricity. The estimated purchase cost of P301 is $4391 and the total purchase and installation cost is $16,520.

9.6 Heaters

H101 is a carbon steel, electricity-power heater with horizontal carbon steel tubes. It is used to heat wet media in stream S14 from 68 °F to the optimal temperature of 98 °F before being used in the batch fermenters in section 200. The flowrate through H101 can vary depending on the fermentation batch vessel, but the maximum flow rate is 304,166 lbs/hr. It uses electricity to heat the wet media with a power usage of 111 kW and a thermal efficiency of 80% only during the batch fermentation period. H101 costs $3,308 and has a total purchase and installation cost of $3,561.

H102 is a carbon steel, electricity-power heater with horizontal carbon steel tubes. It is used to heat cold wet media in stream S17 from 68 °F to its optimal temperature of 98 °F before being used in the continuous CSTR reactions in section 300. The flowrate through H102 is 417,600 lbs/hr. It uses electricity to continuously heat the wet media with a power usage of 3666 kW and a thermal efficiency of 80%. H102 costs $25,232 and has a total purchase and installation cost of $90,981.

H505 is designed to heat a mixed water and steam stream flowing at 20,000lb/hr to steam at 14 psi and 1200°F. During plant startup, the water is heated from cooling water to steam. This cooling water, at 14 psi and 86°F is then passed through the heater several times to bring the temperature to 1202°F. This heating technique f.o.b. cost is $27,889, with a bare module cost of $69,629. Once the desired temperature of steam is achieved, the heater is then to heat the reactors in this section, modeled as catalyst-packed heat exchangers. The heater is designed to deliver a duty of 2181.08 MBTU/hr, which will heat the reactor exit stream from 911°F to1202°F. The steam is then recycled back to the heater to bring the temperature back to 648.89 Celsius. It assumed that 2,000,000 lbs of water will be sufficient to fill the piping of the system and achieve the desired flow rate of 20,000 lbs/hr. The initial cost of this water at $0.075/1000 gallons will be negligible at $1,424.43. We will use No 4. Fuel Oil, which has a higher heating value of 18,701 BTU/lb and costs $0.22/lb. Therefore, using the required duty, the annual cost will be $203,715.63.

9.7 Reactors

The six reactors operate at 932°F and 70mmHg. Due to the low operating pressure of the reactor, a large volume is needed, too large for one reactor alone. The total calculated reactor volume was 509.5 ft^3, which was obtained using the reactor residence time of 1.4s, the density of the effluent gas, 0.00315 lb/ft^3, and the flow rate of the effluent, 4127.9 lbs/hr (Winfield, 1945). Each individual reactor has a volume of 170 ft^3. The multiple reactors ensure that 1,3-butadiene will continuously be produced. At any one time, three reactors are in operation while the catalyst in the other three is being regenerated. Regeneration is performed by passing steam at 932°F over the catalyst for two hours.

In a single reactor, there are 1557 tubes of 1-inch diameter that are 20 ft long, for a surface area of 8152 ft^2. The shell side pressure is 0.304 psi. Using these specifications, the f.o.b. cost of a single reactor vessel is calculated to be $58,694 and the total bare module cost was calculated to be $212,110. Three reactions occur in the reactor, two of which are endothermic and one of which is exothermic. There is 62.1% conversion of BDO to 1,3-Butadiene and water, 26.2% conversion to MEK and water, and 8.4% conversion to methyl vinyl carbinol and water. The heats of reaction for these reactions respectively are 107904 kJ/kmol, 1482 kJ/kmol, and -21,6755 kJ/kmol.

The amount of thorium oxide catalyst used in each reactor was calculated using the reactor volume, surface area of catalyst, 55 m^2/gram, and density of the catalyst, 8.6 g/cm^3. The amount of catalyst used per reactor is 336 kg, which at a price of $5.745/g results in a catalyst price of $1.93MM.

9.8 Distillation Columns

The purpose of D401 is to remove 1,3-butadiene as the distillate product at a purity of 99.3%, flow rate 1550 lb/hr, temperature of 107°F, and pressure of 65 psi. The condenser duty is -1065.6 MBtu/hr and the reboiler duty is 794.2 MBtu/hr. The bottoms product leaves at a temperature of 282°F and pressure of 70 psi. There are 21 stages and 19 sieve trays. The height of the column is 56 ft and it has a diameter is 1.5 ft. The column is made of carbon steel, has a tray efficiency of 0.7, tray spacing of 2 ft, and theoretical stage pressure drop of 0.1 psi. The feed to the column is on stage 9. There is a total condenser and a kettle reboiler. Additionally, the pressure drop in the condenser is 3 psi.

The purpose of C603 is to remove the MEK as distillate product at its azeotropic composition of approximately 13% water and 87% MEK at 17 psi. The flow rate of this stream is 929.8 lb/hr. The condenser duty is -1121.6 MBtu/hr and the reboiler duty is 961.4 MBtu/hr. The bottoms product leaves at a temperature of 232°F and a pressure of 23 psi. There are 39 stages and 37 sieve trays. The height of the column is 114 ft and diameter is 2 ft. It is made of carbon steel, has a tray efficiency of 0.7, tray spacing of 2 ft, and theoretical stage pressure drop of 0.1 psi. The feed to the column is on stage 32. There is a total condenser and a kettle reboiler. Additionally, the pressure drop in the condenser is 3 psi.

Columns C701 and C702 separate the MEK from water at the azeotropic concentration. The first column C701 removes the MEK as a 99.99% pure product in the bottoms. The flow rate of the MEK product is 809lb/hr at 106 psi. The column has 23 stages and 21 sieve trays. The feed stage is stage 6 for both the recycle from the lower pressure column C702 as well as the feed from the previous tower C603. The height and diameter of the column are 68 ft and 2 ft, respectively. The column is made of carbon steel, with a tray efficiency of 0.7 and tray spacing of 2 ft, and a theoretical stage pressure drop of 0.1 psi. The reflux ratio is 3. There is a total condenser and a kettle reboiler. Additionally, the pressure drop in the condenser is designed to be 3 psi.

The distillate is sent to the second column, which removes the water as the bottoms product at a flow rate of 120 lb/hr. The second column operates at a pressure of 1.6 bar. The column has 33 stages and 31 trays. The feed stage is stage 15. The height and diameter of the column are 96ft and 2.5ft respectively. The column is made of carbon steel, with a tray efficiency of .7 and tray spacing of 2ft, and theoretical stage pressure drop of .1 psi. The reflux ratio is 3. There is a total condenser and a kettle reboiler. Additionally, the pressure drop in the condenser is 3 psi. The pressure-swing distillation towers are only useful to recover MEK as a product for sale. We consider not separating MEK for profit in the next sections.

9.9 Mixing Tanks

M101 is a mixing tank designed to agitate the dry media and water to a wet media mixture. It is a cylindrical, carbon steel, pressurized vessel with a volume of 15,000 gallons, a height of 27.8 ft and a diameter of 9.3 ft. During continuous operation, 416,700 pounds/hr goes through the mixer with a residence time of 18 minutes before exiting as wet media in stream S16. During batch operation, 333,600 pounds/hr goes through the mixer with a residence time of 22 minutes before exiting as wet media in stream S10. There is also an agitator that runs at 3 kW in order to mix the solids and liquids efficiently. The agitator costs $4,170 and is included in the purchase cost of the tank. M101 has a total purchase cost of $95,706 and a total purchase and installation cost of $384,960.

9.10 Compressors

C001 is a cast iron, centrifugal compressor that is used to compress hot flue gas from steel mill to 30 psi. The flowrate into the compressor is 310,000 lb/hr and it has an efficiency of 72%. The compressor has an electricity usage of 8751 kW. C001 has an estimated purchase cost of $3,528,002 and a total purchase and instillation cost of $7,585,376.

C501 is carbon steel, centrifugal, compressor, which is used to compress cooled reactor effluent from the distillation columns. The flowrate into the compressor is 4321 lbs/hr and an efficiency of 72%. The compressor has an electricity usage of 519 kW. C501 has an estimated purchase cost of $368,126 and a total purchase and installation cost of $902,278.

9.11 Heat Exchangers

HX001 is a shell-and-tube heat exchanger fabricated from cast iron. It is used to cool the steel mill gas to 98 °F at 22 psi. The flue gas enters at 770 °F and exits at 98 °F. The cold stream enters at 45 °F and exits at 88 °F. This process transfers 6,710,000 BTU/hr of heat. HX001 has an estimated purchase cost of $21,211 and a total purchase and installation cost of $68,301.

HX502 is a shell and tube heat exchanger fabricated from carbon steel. It is used to recover heat from compression to use for a reboiler. The hot stream enters at 1341 °F and exits at 194 °F. The cold stream enters at 90 °F and exits at 760 °F. This process transfers 4,061,080 BTU/hr of heat. HX502 has an estimated purchase cost of $58,694 and a total purchase and installation of $212,109.

D603 is a total condenser for the distillation tower D603 fabricated from carbon steel. It uses water, at a flowrate of 3,000 lb/hr to condense the distillate of the THIRD DISTILLATION tower. The distillation tower's distillate exits at 240 °F with a flowrate of 71 lbs/hr. The cooling water enters at 90 °F and exits at 120 °F. This process transfers 226,218 BTU/hr of heat. The estimated purchase cost is $550,689 and the total purchase and estimation cost of $627,786.

D601 is a total condenser for distillation tower D601 fabricated from carbon steel. It uses water at a flowrate of 8,880 lbs/hr as the cold stream. The distillate is at a flowrate of 137 and enters the condenser at 137 °F and exits at 107 °F. This process transfers 74,586 BTU/hr of heat. The estimated purchase cost of D601 is $25,190 and it has a total purchase and installation cost of $57,214.

D602 is a total condenser to for the distillation tower D602 tower fabricated from carbon steel. It uses water at a flowrate of 2,487 lbs/hr that enters the condenser at 90 °F and exits at 120 °F. The distillate is cooled from 198 °F to 170 °F and it is a flowrate of 930 lbs/hr. This process transfers 78,150 BTU/hr. The estimated purchase cost of D602 is $4,469 and it has a total purchase and installation cost of $5,340.

D401 is a total condenser for the distillation tower D401. It uses water at a flowrate of 17,902 lbs/hr that enters the condenser at 90 °F and exits the condenser at 120 °F. The distillate enters the condenser at a flowrate of 7,996 lbs/hr at 198 °F and exits at 170 °F. This process transfers 78,510 BTU/hr of heat. The estimated purchase cost of D401 is $502,838 and the total purchase and installation cost is $593,755.

HX501 is carbon steel, electric heat exchanger used to heat feed to the reactor, R501, during start-up conditions. This feed is 4,132 lbs/hr of 1,3- butanediol that is heated from 257 °F to 572 °F. It uses electricity at a rate of 47,334 BTU/hr to provide the heat. This unit is a conditional, continuous unit that is only in operation during project start up. The estimated purchase cost of HX501 is $4724 and the total purchase and installation cost is $5,669.

D701 is a carbon steel total condenser used to condense the distillate from distillation tower, D701. Water is used on the cold side at a flowrate of 7,579 lbs/hr and enters at 90 °F and exits at 120 °F. The distillate has a flowrate of 1,475 lbs/hr and enters at 310 °F and exits at 278 °F. D701 has a heat duty of 227,278 BTU/hr. The estimated purchase cost of D701 is $4,724 and the total purchase and installation cost is $5,669.

D702 is a carbon steel total condenser used to condense the distillate from the distillation tower, D702. Water is used on the cold side at a flowrate of 7,250 lbs/hr and enters at 90 °F and exits at 120 °F. The distillate has a flowrate of 1,255 lbs/hr and enters at 205 °F and exits at 173 °F. D701 has a heat duty of 210,330 BTU/hr. The estimated purchase cost of D701 is $4,348 and the total purchase and installation cost is $5,089.

HX502 is carbon steel, shell and tube heat exchanger used to preheat the feed to the reactor, R501 with effluent heat from the reactor. This feed is 4,132 lbs/hr of that is heated from that is heated from 245 °F to 572 °F. The hot stream is at 4,132 lbs/hr and is cooled from 932 °F to 652 °F. This unit is has a heat duty of 47,334 BTU/hr. The estimated purchase cost of HX501 is $3,854 and the total purchase and installation cost is $7,584.

10.0 COSTING SUMMARIES

10.1 EQUIPMENT COST SUMMARY

The total bare module costs were calculated for each process unit using the Guthrie method. This estimation involves finding the f.o.b. equipment cost and modifying the price by a bare module factor, which adjusts for indirect costs associated with the setup of equipment on site. The correlation equation used to calculate bare module cost was obtained in Seider et al. and based on 2006 costing data. Correspondingly, the bare module costs were adjusted using the CE index of today, which is taken to be 570. The total bare module cost for the process was calculated to be $58,175,107.

Section	Total Bare Module Investment
000	$7,653,677
100	$3,599,764
200	$1,314,344
300	$12,178,958
400	$14,016,860
500	$13,938,042
600	$3,363,827.86
700	$2,109,634.63
Total	**$58,175,107**

Table 10-1: Total bare module investment.

Additionally, the itemized bare module costs are shown for the each of the seven plant sections in the following tables.

CO Fermentation for the Formation of BDO

Section 000: Steel Mill Gas Cooling

Unit	**Type**	**F.o.b Purchase Cost**	**Bare Module Cost ($)**
HX001	Cool Gas Feed to Fermenters	$21,211	$68,301
C001	Compresses Air	$3,528,082	$7,585,376
Total		*$3,549,293*	*$7,653,677*

Section 100: Media Mixing System

Unit	**Type**	**F.o.b Purchase Cost**	**Bare Module Cost ($)**
ST101a	Storage Tank	$165,626	$689,003
ST101b	Storage Tank	$165,626	$689,003
SS101	pneumatic conveying system		$827,361
B101	Blower		$9,320
FT101	Water Filter		$50,600
M101	Mixing Tank	$91,536	$380,790
M101'	Mixing Tank agitator	$4,177	(Contained in M101 BM)
P101	Pump	$4,797	$18,406
P102	Pump		$16,836
FT102	Ultra filtration		$6,000
FT103	Ultra filtration		$60,000
H101	HTX		$3,561
H102	HTX		$90,981
ST102	Storage Tank	$182,189	$757,903
Total		*$613,951*	*$3,599,764*

Section 200: Batch Fermentation

Unit	**Type**	**F.o.b Purchase Cost**	**Bare Module Cost ($)**
P201	Pump	$3,000	$11,285
P202	Pump	$4,390	$16,517
P203	Pump	$9,478	$35,658
P204	Pump	$6,152	$23,146
P205	Pump	$3,540	$13,317
F201	Horizontal Column	$5,897	$24,532
F202	Horizontal Column	$11,837	$49,420
F203	Horizontal Column	$29,677	$123,592
F204	Horizontal Column	$86,528	$360,322
F205	Horizontal Column	$157,852	$656,555
Total		*$318,351*	*$1,314,344*

Section 300: CSTR and Cell Recycle Close-up

Unit	**Type**	**F.o.b Purchase Cost**	**Bare Module Cost ($)**
CR301	CSTR	$177,920	$737,790
CR302	CSTR	$177,920	$737,790
CR303	CSTR	$177,920	$737,790
CR304	CSTR	$177,920	$737,790
CR305	CSTR	$177,920	$737,790
CR306	CSTR	$177,920	$737,790
CR307	CSTR	$177,920	$737,790
CR308	CSTR	$177,920	$737,790
CR309	CSTR	$177,920	$737,790
CR310	CSTR	$177,920	$737,790
P301	Pump	$3,000	$11,283
P302	Pump	$3,000	$11,283
P303	Pump	$3,000	$11,283
P304	Pump	$3,000	$11,283
P305	Pump	$3,000	$11,283
P306	Pump	$3,000	$11,283
P307	Pump	$3,000	$11,283
P308	Pump	$3,000	$11,283
P309	Pump	$3,000	$11,283
P310	Pump	$3,000	$11,283
TF301	Disk Stack Centrifuge	$125,000	$170,672
TF302	Disk Stack Centrifuge	$125,000	$170,672
TF303	Disk Stack Centrifuge	$125,000	$170,672
TF304	Disk Stack Centrifuge	$125,000	$170,672
TF305	Disk Stack Centrifuge	$125,000	$170,672
TF306	Disk Stack Centrifuge	$125,000	$170,672
TF307	Disk Stack Centrifuge	$125,000	$170,672
TF308	Disk Stack Centrifuge	$125,000	$170,672
TF309	Disk Stack Centrifuge	$125,000	$170,672
TF310	Disk Stack Centrifuge	$125,000	$170,672
SS301	pneumatic c.s.	$200,567	$248,459
SS302	pneumatic c.s.	$200,567	$248,459
SS303	pneumatic c.s.	$200,567	$248,459
SS304	pneumatic c.s.	$200,567	$248,459
SS305	pneumatic c.s.	$200,567	$248,459
SS306	pneumatic c.s.	$200,567	$248,459
SS307	pneumatic c.s.	$200,567	$248,459
SS308	pneumatic c.s.	$200,567	$248,459
SS309	pneumatic c.s.	$200,567	$248,459
SS310	pneumatic c.s.	$200,567	$248,459

Cont.			
Unit	**Type**	**F.o.b Purchase Cost**	**Bare Module Cost ($)**
SS311	pneumatic c.s.	$200,567	$248,459
SS312	pneumatic c.s.	$200,567	$248,459
Total		*$5,466,004*	*$12,178,958*

Section 400: Moving Bed Chromatography Separation

Unit	**Type**	**F.o.b Purchase Cost**	**Bare Module Cost ($)**
P401	Pump	$4,391	$16,520
FT401	Membrane Separation Unit	$6,000,000	$12,000,000
ST401	Storage Tank	$267,531	$1,112,928
D401	Separation of Ethanol from 2,3-BDO	$520,838	$593,755
D401 C.A	Condenser Accumulator	$20,020	$52,347
D401 CHX	Condenser HX	$27,098	$99,231
D401 RB	Reboiler	$37,922	$131,080
D401 RP	Reflux Pump	$2,924	$10,999
Total		*$6,880,724*	*$14,016,860*

Formation of 1,3-Butadiene via Thermo-Catalytic Conversion of BDO

Section 500: Thermo Catalytic Conversion

Unit	**Type**	**F.o.b Purchase Cost**	**Bare Module Cost ($)**
VS501	Two-stage Steam-jet ejector	$17,991.28	$17,991.28
HX502 (1)	Reactor Vessel	$58,694.42	$212,109.91
HX502 (2)	Reactor Vessel	$58,694.42	$212,109.91
HX502 (3)	Reactor Vessel	$58,694.42	$212,109.91
HX502 (4)	Reactor Vessel	$58,694.42	$212,109.91
HX502 (5)	Reactor Vessel	$58,694.42	$212,109.91
HX502 (6)	Reactor Vessel	$58,694.42	$212,109.91
HX504	Heat Source for Reactors	$27,889.63	$69,629.25
Recycled Water	Used in Reactor HX/Fired Heater System		$1,424.43
Catalyst	Catalyst		$11,566,212.70
C501	Compressor to First Distillation Column	$368,126.54	$902,278.15
HX502	Reactor Effluent Heat Recovery	$3,196.78	$3,853.87
HX503	Compressor Effluent Heat Recovery	$28,003.36	$101,566.86
HX501	Startup Heater	$4,724.71	$5,669.44
P501	Pressure increase of Cooling Water to HX	$3,920.12	$14,747.49
Total		*$788,028*	*$13,938,042*

Section 600: Distillation Separation: 1,3-Butadiene Recover

Unit	Type	F.o.b Purchase Cost	Bare Module Cost ($)
ST601	storage tank	$226,185.00	$940,923.00
D601	Tray tower for Separation of 1,3-Butadiene	$531,370.98	$605,762.92
D601 C.A	Condenser Accumulator	$21,615.52	$57,214.79
D601 CHX	Condenser HX	$25,190.45	$91,445.51
D601 RB	Reboiler	$4,516.94	$5,335.77
D601 RP	Reflux Pump	$2,941.41	$11,065.59
D602	Tray tower for Separation of MEK/water	$624,635.34	$712,084.29
D602 C.A	Condenser Accumulator	$21,615.52	$57,214.79
D602 CHX	Condenser HX	$4,468.90	$5,339.75
D602 Reboiler	Reboiler	$4,110.86	$4,870.15
D602 RP	Reflux Pump	$2,983.78	$11,224.98
D603	Tray Tower for Recycle of 2,3-BDO	$550,689.18	$627,785.67
D603 C.A	Condenser Accumulator	$21,615.52	$57,214.79
D603 CHX	Condenser HX	$4,769.38	$5,698.80
D603 RB	Reboiler	$43,800.50	$159,328.95
D603 RP	Reflux Pump	$3,008.54	$11,318.14
Total		*$2,093,517.84*	*$3,363,827.86*

Section 700: Distillation Separation: Pressure-Swing Distillation

Unit	Type	F.o.b Purchase Cost	Bare Module Cost ($)
ST701	MEK Storage Tank	$115,638.00	$481,052.00
P701	Feed Pressure increase	$3,574.87	$13,448.66
P706	Recycle Pressure increase	$3,360.55	$12,642.39
D701	Separation of MEK	$552,961.59	$630,376.21
D701 C.A	Condenser Accumulator	$21,615.52	$57,214.79
D701 CHX	Condenser HX	$4,724.71	$5,669.44
D701 Reboiler	Reboiler	$35,081.02	$126,323.16
D701 RP	Reflux Pump	$2,923.80	$10,999.32
D702	Separation of Water	$608,087.12	$693,219.32
D702 C.A	Condenser Accumulator	$21,615.52	$57,214.79
D702 CHX	Condenser HX	$4,347.56	$5,089.38
D702 RB	Reboiler	$4,408.86	$5,223.19
D702 RP	Reflux Pump	$2,967.03	$11,161.98
Total		*$1,381,306.16*	*$2,109,634.63*

10.2 FIXED CAPITAL SUMMARY

The total capital investment was calculated to be $126.2MM. To calculate the total of direct permanent investment (DPI), three additional costs, the Cost of site preparation, cost of service facilities, and allocated costs for utility plants and related facilities, were calculated. The cost of site preparation was assumed to be 7% of the total bare-module cost since the plant is being integrated with an existing steel mill plant facility. The cost of service facilities was assumed to be 6% of TBM since these costs are considered to be some of the largest in the construction of the plant. The allocated costs for utility plants and related facilities was calculated using the total steam requirement of 28 lb/hr, electricity requirement of 16.7 MW, cooling water of 3921.4 gpm, and total process water of 748.9 gpm. These values were used in the correlations presented in Seider et. Al. From DPI, the total depreciable capital (TDC) is calculated by adding the cost of contingencies and contractor's feed, which is assumed to be 18% of DPI. The next important number calculated is the total permanent investment, TPI. This is calculated by adding the cost of land, cost of initial royalties, and cost of plant startup, each assumed to be 2% of TDC. Since the site is in China, there is no adjustment made to the TPI number. Finally, working capital is added to the TPI to get the total capital investment

Working capital is calculated as the sum of cash reserves inventory and accounts receivable minus accounts payable, as presented in Seider, et. Al.

Total Bare-Module Investment, TBM	$58,175,107.50
Cost Of Site Preparation ("substantial": 0.07*TBM)	$4,072,257.52
Cost of Service Facilities ("substantial": 0.06*TBM)	$3,490,506.45
Allocated Costs for Steam	$12,292.73
Allocated Costs for Electricity	$26,917,326.23
Allocated Costs for Cooling Water	$277,677.63
Allocated Costs for Process Water	$862,083.38
Total of Direct Permanent Investment, DPI	$93,807,251.44
Cost of Contingencies and Contractor's fees (0.18*DPI)	$16,885,305.26
Total Depreciable Capital, TDC	$110,692,556.70
Cost of land (0.02*TDC)	$2,213,851.13
Cost of royalties (0.02*TDC)	$2,213,851.13
Cost of plant startup (0.02*TDC)	2,213,851.13
Total Permanent Investment, TPI	$117,334,110.10
Working Capital (See Working Capital Table)	$8,874,233.54
Total Capital Investment, TCI	$126,208,343.65

Working Capital Calculation	**Cost**
Cash Reserves	$3,828,365.78
Inventories	$1,091,860.08
Accounts Receivable	$4,737,080.43
Accounts Payable	$783,072.7475
Working Capital	$8,874,233.54

10.3 COMPUTATION OF ANNUAL GROSS PROFIT

Annual gross profit was calculated by taking the difference between annual sales and annual production costs. Sales and costs were estimated using prices for the Asian Market in accordance with the theoretical location of our plant. The process produces 1550 lb/hr of 1,3-butadiene at $2100/metric ton, 810 lb/hr of MEK at $1700/metric ton, and 8000 lb/hr of ethanol at $1400/metric ton, to produce annual revenues of $11.7 MM/yr, $4.9 MM/yr, and $40.2 MM/yr respectively. Therefore total annual sales are $56.9 MM/yr.

Sales(China)	
1,3-Butadiene ($2100/metric ton)	$11,690,456.72
MEK ($1700/metric ton)	$4,941,385.10
Ethanol - Commodity ($1400/metric ton)	$40,235,870.45
Total	*$56,867,712.28*

Total production costs were calculated using the method outlined in Seider et. Al to be $52.7MM/yr. Total production costs were calculated by summing feedstock, utilities, operations, maintenance, property taxes and insurance, depreciation, and general expense costs.

Cost Factor	**Annual Cost**	
Feedstock (Raw Materials)		$9,400,633.22
Dry Media	$9,260,633.22	
Steel Mill Gas	$-	
Cells	$140,000.00	
Water	$267406.96	
Utilities		$10,916,296.11
Steam, 450 psig	$591,240.00	
Steam, 150 psig	$115,225.76	
Steam, 50 psig	$393,863.14	
Cooling Water	$159,295.56	
Electricity	$9,051,976.46	
Wastewater Treatment	$400,979.56	
Fuel Oil	$203,715.63	
Operations (O)		$2,642,640.00
Direct wages and benefits (DW&B)	$2,184,000.00	
Direct salaries and benefits (0.15*DW&B)	$327,600.00	
Operating supplies and services (0.06*DW&B)	$131,040.00	
Technical Assistance to Manufacturing	$-	
Control Laboratory	$-	
Maintenance (M)		$11,456,679.62
Wages and benefits (MW&B), Solids-fluids handling process	$4,981,165.05	
Salaries and benefits	$1,245,291.26	
Materials and Services	$4,981,165.05	
Maintenance Overhead	$249,058.25	
Operating Overhead		$1,135,705.63
General plant overhead	$353,662.72	
Mechanical department services	$119,547.96	
Employee Relations Department	$293,888.74	
Business Services	$368,606.21	
Property taxes and insurance		$2,213,851.13

Contd.		
Depreciation		$8,192,967.17
Direct Plant	$6,205,655.07	
Allocated Plant	$1,987,312.10	
COM		$45,958,772.88
General Expenses		$6,710,390.05
Selling (or transfer) expense	$1,706,031.37	
Direct research	$2,729,650.19	
Allocated research	$284,338.56	
Administrative expense	$1,137,354.25	
Management incentive compensation	$853,015.68	
Total Production Cost		$52,669,162.93

Feedstock costs was comprised of dry media, steel mill gas, process water, and cells, presented in the tables below.

Total Feedstock Cost	**Quantity**	**Cost ($/yr)**
Dry Media	333600 lb/hr	$9,260,633.22
Process Water	375,000 lb/hr	$267,406.96
Cells	0.1mg/twice a year	$140,000.00
Flue Gas	305,320 lb/hr	$-

Media Calculations	
Media (L)	10
	2.64
Density (lbs/gallon)	18
lbs	47.55
total lbs needed	333600
total loads	7015.63
cost per unit	$4.00
cost per day	$28,062.52
cost (yr)	$9,260,633.22

Utilities used were steam at 450 psi, 150 psi and 50 psi, cooling water, electricity, wastewater treatment, and No. 4. fuel oil. Per unit costs are available from Seider, et. Al.

The largest operations cost was direct wages and benefits (DW&B), which was calculated assuming two operators/per plant section, three plant sections, and an hourly wage of 35$/hr. Please refer to the following table. for more details about assumptions. In addition to DW&B, direct salaries and benefits (15% of DW&B) and operating supplies and services (6% of DW&B) were calculated.

Operations	**Value**
Process Type	Continuous, Solids-fluids Processing
Number of Operators Per Process Section	2
Number of Sections	3
Number of Operators/shift	6
Shifts	5
Hours Worked/(Operator*Year)	2080
Hourly Wage	35
DW&B ($/year)	$2,184,000.00

There were four contributions to maintenance costs. Wages and benefits (MW&B) was assumed to be 4.5% of TCI because our process requires handling of both solids and fluids. Salaries and benefits were assumed to be 25% of MW&B. Materials and services cost was assumed to be equal to MW&B. Maintenance overhead was assumed to be 5% of MW&B.

There were four contributions to operating overhead as well. The four contributors are general plant overhead, mechanical department services, employee relation's department costs, and business services costs. The cost associated with these factors was assumed to be 7.1%, 2.4%, 5.9%, and 7.4% of MW&B, respectively.

Property taxes were assumed to be 2% of TCI.

Depreciation was assumed to be comprised only of direct and allocated plant costs. Direct plant costs were assumed to be 8% of the difference between allocated costs for utility plants and related faculties subtracted from TCI.

Finally, there were five contributors to general expenses, all of which were assumed to cost a certain percentage of sales. Selling expense, direct research, allocated research, administrative expense, and management incentive compensation were assumed to be 3%, 4.8%, 0.5%, 2%, and 1.5% of sales, respectively.

Therefore, gross profit is the difference in sales and total production costs, estimated to be $4.2MM/yr in China.

11.0 ECONOMIC ANALYSIS

11.1 Economic Overview

The centerpiece of the economic analysis of the plant is the cash flow analysis. Additionally, two profitability ratios, ROI and payback period, were calculated to determine the profitability of our system. Additionally, the sensitivity of the profitability to product pricing was examined.

Using the costs and sales numbers previously calculated in section 10, as well as assuming a required rate of return of 15% and a tax rate of 40%, ROI was calculated to be 2%. ROI is defined as after-tax profit/TCI. The payback period was calculated to be 10.3 years.

Ratio	**Value**
Return on Investment (ROI)	2.00%
Payback Period	10.33
Assumptions	**Value**
Tax rate	40%
Required Return on Investment	15%

Finally, a cash flow analysis was performed, from which and IRR and NPV were calculated. We assume a plant life of 30 years and that plant construction is evenly spread out over three years. In addition, the initial working capital is assumed to be bought at the end of year three. The cost of land is incurred at the end of year one. Startup costs are incurred at the end of year three. Additionally, since we are using a proprietary LanzaTech technology, we assume that 3% of sales will be required to pay royalties for the first ten years of operation. We also assume that the first year's sales and production costs are 50% of the maximum sales and the second year's sales and production costs are 75% of the maximum sales.

For the NPV calculation, the required rate of return was assumed to be 15%. Given the above assumption, a negative NPV of 74.4 MM was obtained. The IRR was calculated by setting the NPV of the project to $0, and the IRR obtained was 0.7%.

Total Depreciable Capital (over 3 years)	$	110,692,556.70
Working Capital (at end of 3rd year)	$	8,874,233.54
Sales / 1st year	$	28,433,856.14
Sales / 2nd year	$	42,650,784.21
Sales / 3rd year +	$	56,867,712.28

Tax Rate		0.40
Required Rate of Return		0.15
C(Excl Dep) / 1st Year	$	25,227,655.90
C(Excl Dep) / 2nd Year	$	37,841,483.85
C(Excl Dep) / 3rd Year +	$	50,455,311.80

#	Year	fC_{TDC}	C_{WC}	C_{land}	$C_{startup}$	$C_{royalties}$	D	$C_{Excl\ Dep}$	S	Net Earnings	Discounted Cash Flow	Cash Flow (PV)	Cummulative PV
1	2014	$ (36,897,518.90)		$ (2,213,851.13)							$ (39,111,370.03)	$ (39,111,370.03)	$ (39,111,370.03)
2	2015	$ (36,897,518.90)									$ (36,897,518.90)	$ (32,084,799.04)	$ (71,196,169.08)
3	2016	$ (36,897,518.90)	$ (8,874,233.54)		$ (2,213,851.13)	$ (2,213,851.13)					$ (50,199,454.71)	$ (37,957,999.78)	$ (109,154,168.86)
4	2017					$ (853,015.68)	$ 22,138,511.34	$ 25,227,655.90	$ 28,433,856.14	$ (11,359,386.66)	$ 9,926,109.00	$ 6,526,577.79	$ (102,627,591.07)
5	2018					$ (1,279,523.53)	$ 35,421,618.14	$ 37,841,483.85	$ 42,650,784.21	$ (18,367,390.67)	$ 15,774,703.95	$ 9,019,238.18	$ (93,608,352.89)
6	2019					$ (1,706,031.37)	$ 21,252,970.89	$ 50,455,311.80	$ 56,867,712.28	$ (8,904,342.25)	$ 10,642,597.27	$ 5,291,251.77	$ (88,317,101.13)
7	2020					$ (1,706,031.37)	$ 12,751,782.53	$ 50,455,311.80	$ 56,867,712.28	$ (3,803,629.23)	$ 7,242,121.93	$ 3,130,969.16	$ (85,186,131.96)
8	2021					$ (1,706,031.37)	$ 12,751,782.53	$ 50,455,311.80	$ 56,867,712.28	$ (3,803,629.23)	$ 7,242,121.93	$ 2,722,581.88	$ (82,463,550.08)
9	2022					$ (1,706,031.37)	$ 6,375,891.27	$ 50,455,311.80	$ 56,867,712.28	$ 21,905.53	$ 4,691,765.42	$ 1,533,746.44	$ (80,929,803.64)
10	2023					$ (1,706,031.37)		$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 2,141,408.92	$ 608,722.06	$ (80,321,081.58)
11.00	2024					$ (1,706,031.37)		$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 2,141,408.92	$ 529,323.53	$ (79,791,758.04)
12	2025					$ (1,706,031.37)		$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 2,141,408.92	$ 460,281.33	$ (79,331,476.71)
13	2026					$ (1,706,031.37)		$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 2,141,408.92	$ 400,244.64	$ (78,931,232.07)
14	2027							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 625,316.61	$ (78,305,915.46)
15	2028							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 543,753.57	$ (77,762,161.89)
16	2029							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 472,829.19	$ (77,289,332.70)
17	2030							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 411,155.82	$ (76,878,176.88)
18	2031							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 357,526.80	$ (76,520,650.08)
19	2032							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 310,892.87	$ (76,209,757.21)
20	2033							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 270,341.63	$ (75,939,415.58)
21	2034							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 235,079.67	$ (75,704,335.91)
22	2035							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 204,417.11	$ (75,499,918.80)
23	2036							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 177,754.01	$ (75,322,164.79)
24	2037							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 154,568.70	$ (75,167,596.09)
25	2038							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 134,407.57	$ (75,033,188.52)
26	2039							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 116,876.15	$ (74,916,312.38)
27	2040							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 101,631.43	$ (74,814,680.95)
28	2041							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 88,375.16	$ (74,726,305.79)
29	2042							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 76,847.96	$ (74,649,457.83)
30	2043		$ 8,874,233.54					$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 12,721,673.83	$ 220,956.55	$ (74,428,501.27)

Total Depreciable Capital (over 3 years)	$	110,692,556.70
Working Capital (at end of 3rd year)	$	8,874,233.54
Sales / 1st year	$	28,433,856.14
Sales / 2nd year	$	42,650,784.21
Sales / 3rd year +	$	56,867,712.28

Tax Rate	0.40
Required Rate of Return	0.007062113
C(Excl Dep) / 1st Year	$ 25,227,655.90
C(Excl Dep) / 2nd Year	$ 37,841,483.85
C(Excl Dep) / 3rd Year +	$ 50,455,311.80

#	Year	fC_{TDC}	C_{WC}	C_{land}	$C_{startup}$	$C_{royalties}$	D	$C_{Excl\ Dep}$	S	Net Earnings	Discounted Cash Flow	Cash Flow (PV)	Cummulative PV
1	2014	$ (36,897,518.90)		$ (2,213,851.13)							$ (39,111,370.03)	$ (39,111,370.03)	$ (39,111,370.03)
2	2015	$ (36,897,518.90)									$ (36,897,518.90)	$ (36,638,771.77)	$ (75,750,141.80)
3	2016	$ (36,897,518.90)	$ (8,874,233.54)		$ (2,213,851.13)	$ (2,213,851.13)					$ (50,199,454.71)	$ (49,497,867.06)	$ (125,248,008.86)
4	2017					$ (853,015.68)	$ 22,138,511.34	$ 25,227,655.90	$ 28,433,856.14	$ (11,359,386.66)	$ 9,926,109.00	$ 9,718,746.80	$ (115,529,262.06)
5	2018					$ (1,279,523.53)	$ 35,421,618.14	$ 37,841,483.85	$ 42,650,784.21	$ (18,367,390.67)	$ 15,774,703.95	$ 15,336,850.63	$ (100,192,411.44)
6	2019					$ (1,706,031.37)	$ 21,252,970.89	$ 50,455,311.80	$ 56,867,712.28	$ (8,904,342.25)	$ 10,642,597.27	$ 10,274,633.55	$ (89,917,777.89)
7	2020					$ (1,706,031.37)	$ 12,751,782.53	$ 50,455,311.80	$ 56,867,712.28	$ (3,803,629.23)	$ 7,242,121.93	$ 6,942,698.22	$ (82,975,079.67)
8	2021					$ (1,706,031.37)	$ 12,751,782.53	$ 50,455,311.80	$ 56,867,712.28	$ (3,803,629.23)	$ 7,242,121.93	$ 6,894,011.93	$ (76,081,067.74)
9	2022					$ (1,706,031.37)	$ 6,375,891.27	$ 50,455,311.80	$ 56,867,712.28	$ 21,905.53	$ 4,691,765.42	$ 4,434,924.51	$ (71,646,143.23)
10	2023					$ (1,706,031.37)		$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 2,141,408.92	$ 2,009,987.19	$ (69,636,156.04)
11.00	2024					$ (1,706,031.37)		$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 2,141,408.92	$ 1,995,891.98	$ (67,640,264.06)
12	2025					$ (1,706,031.37)		$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 2,141,408.92	$ 1,981,895.61	$ (65,658,368.45)
13	2026					$ (1,706,031.37)		$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 2,141,408.92	$ 1,967,997.39	$ (63,690,371.06)
14	2027							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,511,078.52	$ (60,179,292.54)
15	2028							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,486,456.77	$ (56,692,835.77)
16	2029							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,462,007.68	$ (53,230,828.08)
17	2030							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,437,730.05	$ (49,793,098.04)
18	2031							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,413,622.66	$ (46,379,475.38)
19	2032							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,389,684.33	$ (42,989,791.05)
20	2033							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,365,913.86	$ (39,623,877.19)
21	2034							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,342,310.09	$ (36,281,567.10)
22	2035							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,318,871.85	$ (32,962,695.25)
23	2036							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,295,597.96	$ (29,667,097.29)
24	2037							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,272,487.29	$ (26,394,610.00)
25	2038							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,249,538.68	$ (23,145,071.32)
26	2039							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,226,751.00	$ (19,918,320.32)
27	2040							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,204,123.12	$ (16,714,197.20)
28	2041							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,181,653.92	$ (13,532,543.27)
29	2042							$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 3,847,440.29	$ 3,159,342.29	$ (10,373,200.98)
30	2043		$ 8,874,233.54					$ 50,455,311.80	$ 56,867,712.28	$ 3,847,440.29	$ 12,721,673.83	$ 10,373,200.98	$ 0.00

11.2 Alternative Process Considerations

Moving Bed Chromatography Separation

The fermentation product contains 1% BDO at the exit of the CSTR. Since the reaction is held in nearly vacuum conditions, the BDO must be concentrated to keep the reactor as small as possible. Two primary methods were examined- classic separation using a large distillation tower and the simulated moving bed chromatography unit presented earlier in this report. Since the primary objective in this process was to increase profitability, capital costs and operating costs were compared. For the classic distillation method, there is total purchase and installation cost of $4,127,090 but a staggering yearly operating cost of $3,114,380. This was a result of the energy intensive process of boiling out the water in the CSTR output stream. The SMB system had a high initial capital investment of $12,539,600, but had a much lower yearly operating cost of $737,685. The large disparity in the yearly operating costs were compared against the lifetime of our plant. By year six, the SMB process is cheaper than the distillation process with a total capital and operating cost of $15,490,340 compared to $16,584,610 respectively. After twenty years, the SMB process is cheaper than the classic distillation process by $36 million. With these results in mind, the SMB process with the small distillation tower was chosen to be the process of choice for creating a nearly pure BDO stream from the CSTR outputs.

Variable Product Pricing

A sensitivity analysis was run to determine the profitability of the process under variable ethanol and 1,3-butadiene prices. If there is a 50% increase in both the price of ethanol and 1,3-Butadiene, the IRR of the process rises to 14.3%, which is very close to the required rate of return of 15%. Another point of note is that the process actually becomes more profitable if the price of ethanol decreases by 10% and the price of 1,3-Butadiene increases by 40%, with the IRR going from 0.7% to 1.3%, which shows that profitability of the process mainly depends on the price of ethanol, which is to be expected because ethanol comprises over 70% of annual revenues. The main take away from this analysis is that under certain circumstances, it is not unreasonable to believe that this process may be profitable enough to be a viable investment.

IRR

Ethanol Price Change		**1,3-Butadiene Price Increase**										
		-50.00%	-40.00%	-30.00%	-20.00%	-10.00%	***.00%***	10.00%	20.00%	30.00%	40.00%	50.00%
		0.5	0.6	0.7	0.8	0.9	1	1.1	1.2	1.3	1.4	1.5
-50.00%	1	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
-40.00%	1	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
-30.00%	1	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
-20.00%	1	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
-10.00%	1	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	0.2%	1.3%	2.2%
.00%	1	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	0.7%	1.7%	2.6%	3.4%	4.2%	5.0%
10.00%	1	[redacted]	0.1%	1.2%	2.1%	3.0%	3.8%	4.6%	5.3%	6.0%	6.6%	7.3%
20.00%	1	2.5%	3.3%	4.1%	4.9%	5.6%	6.3%	6.9%	7.5%	8.1%	8.7%	9.3%
30.00%	1	5.2%	5.9%	6.6%	7.2%	7.8%	8.4%	9.0%	9.5%	10.1%	10.6%	11.1%
40.00%	1	7.5%	8.1%	8.6%	9.2%	9.8%	10.3%	10.8%	11.3%	11.8%	12.3%	12.8%
50.00%	2	9.5%	10.0%	10.5%	11.0%	11.5%	12.0%	12.5%	13.0%	13.4%	13.9%	14.3%

12.0 OTHER IMPORTANT CONSIDERATIONS

12.1 PLANT STARTUP

This plant begins with a batch process, then transitions to a steady-state continuous operation. Each complete fermentation takes 18 days to complete, and it can inoculate five CSTRs at once. It is reasonable to conclude startup time until continuous operation will be less than two months. The reactor must be preheated using a heating recycle system while the CSTRs are growing cells to the correct concentration. Since equipment is being used for two purposes, it is also important to maintain constant and clear communication so that the valves direct the material flow in the right direction.

12.2 PROCESS SAFETY

During batch preparation, it is important that all the valves are switched for the appropriate directions so that the equipment can be used correctly. In addition, the media must be made without oxygen entering the system, since the cells grow in anaerobic conditions. To do this, the blower must use nitrogen gas and be monitored to ensure no oxygen can enter the system. Since hydrogen is present in the steel mill gas, we must be mindful to stay well below flammability limits.

Parts of our process operate at very high temperatures and relatively high pressures. This means potentials for burns or material leaks are possible and preventative measures should be taken to ensure they do not happen during operation. Additionally, the chemicals present throughout this process may be harmful to humans. Full details can be found in the MSDS sheets for each compound located in the appendix.

12.3 ENVIRONMENTAL CONCERNS

During continuous operation, wastewater and excess cell mass must be properly disposed of as to not contaminate the surrounding area. It is our understanding that we can place some of our biologic waste in settling ponds while it is being sanitized. We must also take precautions to see that our water with hydrocarbons is properly treated at water treatment facilities.

Also, excess flue gas must get returned to the furnace that the steel mill uses to traditionally clean the gas. We cannot be responsible for releasing excess carbon monoxide into the atmosphere, especially since we feed our gas in excess to all batch fermenters and CSTRs.

12.4 PROCESS CONTROLLABILITY

As shown in Figures 1-2 to 1-8, control valves are very common in our process. Other instrumentation must also be utilized to ensure temperatures and pressures are correct throughout the plant. This project does not take into account process control, however if this project were to come into fruition, it would be paramount to install control systems into the plant.

13.0 CONCLUSIONS

This process is not profitable enough in a reasonable amount of operation time at current capacity to justify its installation. Bioprocesses generally need additional government funding in order to come into fruition. According to our sensitivity analysis, 1,3-butadiene and ethanol must be worth 50% more, either by market demand or tax incentives, for an ideal IRR of 14.3%. The current design produces 9500 tons of polymer grade 1,3-butadiene yearly along with 30,000 tons of industrial grade ethanol per year, 3,250 tons of MEK. At current market prices, we calculated an ROI of 0.7%, an IRR of 2.0%, and a NPV of -$74 million. Though the project requires a significant initial total capital investment of $124.2MM and has high production expenses of $52.7 MM yearly, the potential for large profit exists depending on the future prices of the products.

With butadiene's importance in the global rubber industry, in our case for the production of adiponitrile, demand and prices will only confidently increase in the future. This growth can be expected in the growing economy of China, and in combination with their extensive steel production, allows for multiple potential locations in the future (Researching China, 2012).

The overall economics show that this process will still be only slightly profitable at current prices after 30 years, with a gross profit of $4.1 MM/yr. This is assuming that the prices of BDO and ethanol will remain constant, two sensitive values for our calculations. Steel mill gas and *cl. autoethanogenum* cultures are likely a stable costs from now into the future and do not play into the sensitivity of our profits.

We recommend two areas of further research. It is possible that one if not all of these areas can make this a profitable process at current market values. The assumed concentrations of BDO and ethanol in broth from CSTRs were obtained from patent literature. Experimental work should be done in order to see if it is possible to create more productive bacteria that could create higher levels of BDO in solution. It is possible other bacteria can be made to be more successful converters of CO to BDO.

Also, the reaction data on the thermo-catalytic reaction section information was gathered from an outdated process. Though thorium oxide was regularly used to perform this conversion, not much research has been performed on this catalyst since the steam cracking became a better way to create 1,3-butadiene. It is possible a more selective catalyst could be found.

14.0 ACKNOWLEDGEMENTS

We appreciate the extensive amount of advice given to us in order for this report to be a success. In particular, we would like to thank Mr. Leonard Fabiano, Dr. Daeyeon Lee, and Mr. Steven Tieri for their ever-available guidance. Mr. Fabiano was a tremendous help in the process design of our report, and we would not have had any ASPEN convergence without his input. Dr. Lee and Mr. Tieri were great assets in keeping us on track and enhancing our deeper understanding of the process. We would also like to thank all of the consultants that devoted their Tuesday afternoons to help us with our task.

15.0 WORKS CITED

Abrini et al., "Clostridium autoethanogenum, sp. Nov., an Anerobic Bacterium that Produces Ethanol from Carbon Monoxide", *Archives of Microbiology*, Vol. 161, No. 4, pp. 345-351.

Choo, Clement. "Asian Butadiene: Price Analysis." *Platts: McGraw Hill Financial*. Published March 1, 2013. Retrieved April 2, 2014.

"Ethanol." *Trading Economics*. Published 2012. Retrieved April 2, 2014.

"Global and China Methyl Ethyl Ketone Industry Report, 2010-2012." *Researching China*. Published 2012. Retrieved April 1, 2014.

Herbert, Vernon, "Synthetic Rubber: A Project That Had to Succeed", Greenwood Press, 1985, ISBN 0-313-24634-3.

Junyang, Jiang and Ryan R. Scott. "China- Peoples Republic of Biofuels 2011 Annual Report." *USDA Foreign Agricultural Service*. Published 07/21/2011. Retrieved April 2, 2014.

Lanzatech New Zealand Limited. *US20120045807 A1*. Washington, DC: U.S. Patent and Trademark Office, 2012.

Morrow NL. "The industrial production and use of 1,3-butadiene." *Environ. Health Prospect*. 1990; 86:7–8

Ng, Esther. "Asian Ethanol Mandates Shifting Goalposts." *Asia Ethanol,* October 2013, pp. 34-39.

Orochem. "SMB (Simulated Moving Bed) Chromatography Overview." Orochem Technologies, 2012.

Soh, Angeline. "Tight Supply Supports Uptrend in Asia MEK prices." *ICIS*. Published December 12, 2013. Retrieved March 28, 2014.

Source Research and Markets. "Methyl Ethyl Ketone Market - Global Industry Analysis, Size, Share, Growth, Trends and Forecast to 2019." January 2014.

Transparency Market Research. "Synthetic and Bio-Based Butadiene Market: Industry Overview, Applications and Downstream Potential Opportunities, 2010 – 2018," 2013. Retrieved April 1, 2014 from *Transparency Market Research*: http://www.transparencymarketresearch.com/synthetic-and-bio-based-butadiene-market.html

International Agency for Research On Cancer (IARC). “1,3-Butadiene”. *Review of Human Carcinogens*. 1992. Vol. 54, No. 11, pp 237-285.

“Vacuum Systems.” *IPIECA, the global oil and gas industry association for environmental and social issues,* 2013.

Winfield, M. E. "The Catalytic Dehydration of 1,3-Butanediol to 1,3-Butadiene." *Journal of the Council for Scientific and Industrial Research* 18.4 (1945): 412-23. Print.

APPENDICES

Appendix A: Sample Calculations

Please note an example of heat exchanger sizing is given in Appendix E

Equations can be found in Chapter 22 of Seider et. Al.

Carbon Monoxide Feed Capacity

Typical steel mill product from scrubber: $1.7x10^6$ lb CO_2/hr
Carbon mass balance across the scrubber
$100\%\ CO_2 = 42\%\ (CO_2\ inlet) + 20\%\ (CO\ inlet)$
From the carbon exiting, 68% was converted from CO (assuming 1:1 conversion)

$$1.7x10^7 lb\ CO_2/hr * 0.68\left(\frac{28}{44}\right) = 7.36x10^7 lb\ CO/hr$$

We have $7.36x10^7$ lb CO/hr available as gaseous feed from a medium steel mill

Density of CO air: 0.0727 lbm/ft^3

From LanzaTech: $\frac{10^7 ft^3/\min CO}{250\ ft^3 reactor} = 2.4\ ft^3\ CO/hr/ft^3 reactor$

Maximum volume of reactors based on feed availability

$$\frac{10^7 ft^3\ CO/hr\ total}{2.4\ ft^3 CO/hr/ft^3 reactor} = 4x10^6\ ft^3 reactor$$

$$= 3x10^7\ gallons\ max$$

The problem statement calls for 100,000 gallons of BDO. We have the capacity to scale up 3000 times.

Batch Schedule Calculation

Seed Fermenter:

$$\frac{200\ \frac{mg\ cells}{L} - .007\frac{mg\ cells}{L}}{3.7\ \frac{mg\ dry\ cells}{L * hr}} = 3\ days$$

Fermenter #2:

$$\frac{200\ \frac{mg\ cells}{L} - 20\frac{mg\ cells}{L}}{3.7\ \frac{mg\ dry\ cells}{L * hr}} = 2\ days$$

Fermenter #3:

$$\frac{200\ \frac{mg\ cells}{L} - 20\frac{mg\ cells}{L}}{3.7\ \frac{mg\ dry\ cells}{L * hr}} = 2\ days$$

Fermenter #4:

$$\frac{200\ \frac{mg\ cells}{L} - 20\frac{mg\ cells}{L}}{3.7\ \frac{mg\ dry\ cells}{L * hr}} = 2\ days$$

Fermenter #5:

$$\frac{200\ \frac{mg\ cells}{L} - 40\frac{mg\ cells}{L}}{3\ .1\frac{mg\ dry\ cells}{L * hr}} = 3\ days$$

Number of CSTRs for target production

$$200\ \frac{lbs}{hr}(original\ target) * 20(scale\ up\ factor) = 4{,}000\ \frac{lbs\ BDO}{hr} = 1814368\ \frac{grams}{hr}$$

$$Flow\ needed = 1814368\frac{grams\ BDO}{hr} * 10\ \frac{grams}{Liter} = 181{,}436.8\ \frac{L}{hr}$$

$$Total\ CSTR\ Volume = \frac{181{,}436.8\ \frac{L}{hr}}{0.1dilution\ factor\ hr\hat{}-1} = 1814368\ L = 479{,}035\ gallons$$

$$\#\ of\ CSTRS = \frac{479{,}035\ gallons}{50{,}000\ gallon\ (assumed\ \max CSTR\ volume)} = \ 10\ CSTRs$$

Example Costing: Bare Module cost from f.o.b. cost
The bare module cost used in the Guthrie Method is calculated using:

$$C_{BM} = C_{P_b} * \left(\frac{I}{I_b}\right) * (F_{BM} + (F_d * F_p * F_m - 1))$$

Where:

C_{P_b} is the f.o.b cost.
$\frac{I}{I_b}$ is the ratio of the current cost index to the base year cost index. I is taken to be 570
and I_b is taken to be 500.
F_{BM} is the bare-module factor
F_d is equipment design factor
F_p is the pressure factor
F_m is the material factor

Example Costing: Centrifugal Compressor

In a few places our process requires the pressure of a vapor stream to change pressure. The bare module cost for C501 is shown below.

F_D=1
F_M=1
From ASPEN, driver horsepower = 969 HP

$$C_B = \exp(7.5800 + 0.80 \ln(driver\ horsepower))$$
= \$368,127

$$C_P = C_B F_D F_M = \$368{,}127$$

Assuming a CE of 570, F_{bm} of 2.15, and F_P of 1

$$C_{bm} = \$902{,}278$$

Utilities Cost

From ASPEN, utilities requirement is 519 kW

Operation of 24 hours per day for 330 days at \$0.06/kWh

$Cost = kWh * price * \frac{570}{500}$ (to adjust for money value today)
= \$281,236/year

Example Costing: Vacuum System

The air leakage in the system is found using the following equation:

$W = 5 + (0.0298 + 0.03088 * \ln(P) - 0.00057333 * \ln(P)^2) * V^{.66}$

Where: W is the air leakage rate in lb/hr, P is the absolute pressure in torr (70 torr), V is the vessel volume in ft^3 (509.5).

Therefore W = 14.2lb/hr.
$C_p = 2 * 1690 * S^{.41}$
Where:
S is the size factor in units of (lb/hr*torr). S is calculated by giving the Flow at suction (4132.23 lb/hr) by the vacuum pressure (70 torr) to get 59.03 lb/hr*torr. Note: This cost equation is a modification of the single-stage steam-jet cost equation. We assume that the two-stage Steam-jet ejector is twice the cost.

Therefore $C_p = \$17{,}991.28$. F_{BM}, F_d, F_p, F_m all taken to be 1 so $C_{bm} = \$17{,}991.28$

Example Costing: Reactor Vessel

We model the Reactor Vessel as a shell and tube heat exchanger with H = 20ft long, R = .5 inch radius tubes. Therefore the single tube volume and surface area are:

$V_{one\ tube} = \pi * H * R^2 = 0.109 ft^3$
$SA_{one\ tube} = 2 * \pi * R * H = 5.24 ft^2$

The total flow through the reactor is:

$$q = \frac{q'}{\rho * 3600}$$

Where : q is flow rate in ft^3/s, q' is flow rate in lb/hr (4127.9), ρ is density in lb/ft^3 (.0031505).
Therefore q = 364 ft^3/s.
$V = \tau * q$

Where: τ is the residence time in seconds (1.4s). V is volume in ft^3.

Therefore V = 509.5 ft^3/s. Therefore the number of tubes required was:

$$N_{tubes,total} = \frac{509.5}{0.109} = 4671$$

In order to purchase a commercially available heat exchanger, the total volume was divided by 3. Therefore the number of tubes/reactor:

$$N_{tubes,1\ Reactor} = \frac{4671}{3} = 1557$$

Therefore the surface area per reactor was:

$$SA_{\ 1\ Reactor} = 1557 * 5.24 = 8152.55\ ft^2$$

Using the fixed head shell and tube HX equation:

$$C_b = \exp(11.2927 - 0.9228 * ln(SA_{\ 1\ Reactor}) + 0.09861 * ln(SA_{\ 1\ Reactor})^2) = \$59{,}694.42$$

$$C_p = F_p * F_m * F_L * C_b$$

Since we are using carbon steel/carbon steel, $F_p, F_m, F_L, F_d = 1$, and $F_{bm} = 3.17$
$C_b = \$212109.90$

Example Costing: Catalyst

For literature the values for the following properties of thorium oxide were obtained:

$SA_{\ catalyst} = 55\ m^2/gram$
$\rho_{catalyst} = 8.6\ g/cm^3$

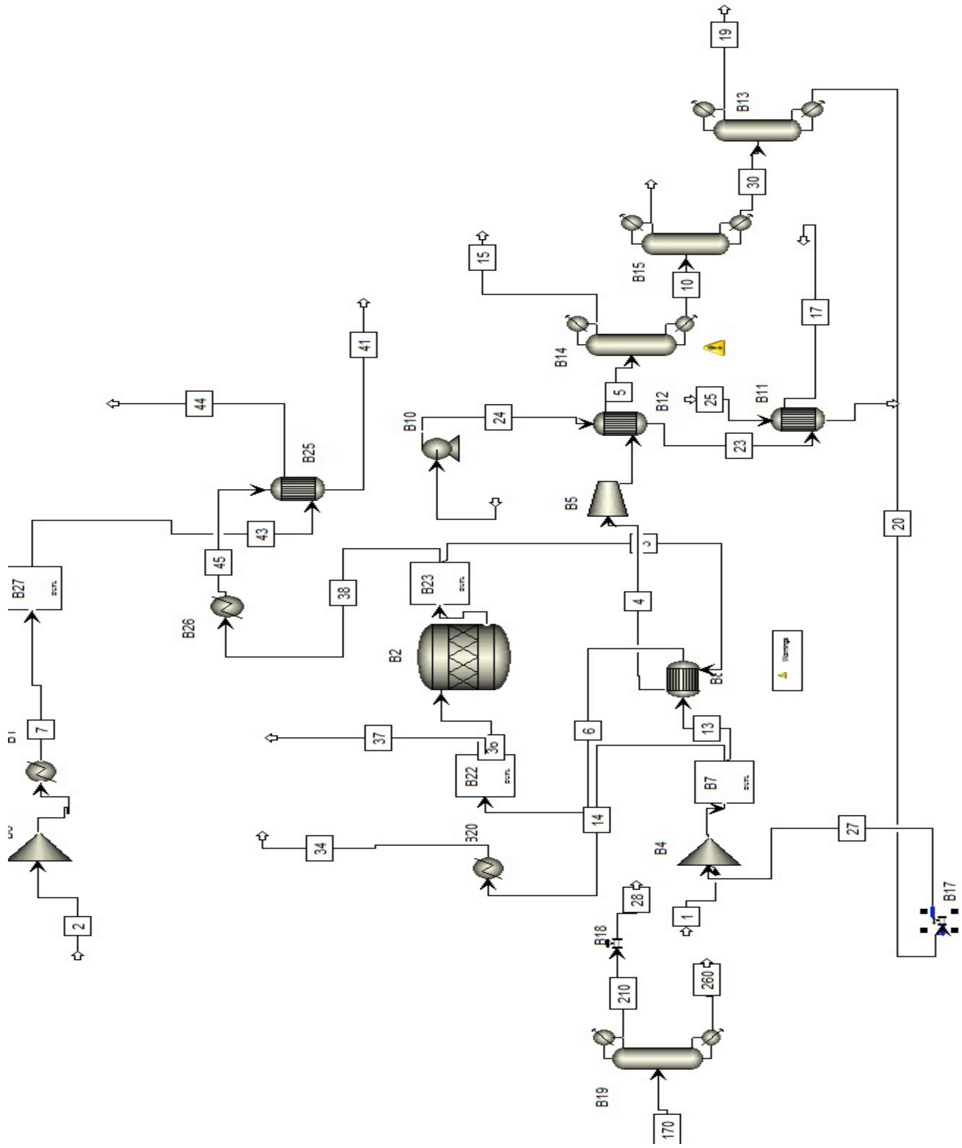
Assuming a void fraction of .4, the amount of catalyst in grams was calculated as follows:

$$Amount = V * \frac{28316.85\ cm^3}{ft^3} * \frac{(1 - .4)}{\rho_{catalyst}} = 509.5 * 28316.85 * \frac{0.6}{8.6} = 1{,}006{,}632.96\ grams$$

Finally, the cost is taken to be $287.25/50 grams, so the overall cost is $5,783,106.35. Since the reactors were bought in duplicate, the total cost was doubled to be $11,566,212.70.

Appendix B: Relevant ASPEN Reports

Block Flow Diagram



Streams

210

STREAM ID 210
FROM : B19
TO : B18

SUBSTREAM: MIXED
PHASE: LIQUID

COMPONENTS: LBMOL/HR	
H2O	0.0
MEK	0.0
2:3-B-01	4.4384-02
1:3-B-01	0.0
3-BUT-01	0.0
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	173.4791
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: MOLE FRAC	
H2O	0.0
MEK	0.0
2:3-B-01	2.5578-04
1:3-B-01	0.0
3-BUT-01	0.0
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.9997
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: LB/HR	
H2O	0.0
MEK	0.0
2:3-B-01	4.0000
1:3-B-01	0.0
3-BUT-01	0.0
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	7992.0160
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: MASS FRAC	
H2O	0.0
MEK	0.0
2:3-B-01	5.0025-04
1:3-B-01	0.0
3-BUT-01	0.0
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.9995
2-BUT-01	0.0
BENZENE	0.0

TOTAL FLOW:
LBMOL/HR 173.5235
LB/HR 7996.0159
L/MIN 85.2454
STATE VARIABLES:
TEMP C 96.6605
PRES BAR 2.0000
VFRAC 0.0
LFRAC 1.0000
SFRAC 0.0
ENTHALPY:
CAL/MOL -6.3932+04
CAL/GM -1387.4112
CAL/SEC -1.3978+06
ENTROPY:
CAL/MOL-K -75.8501
CAL/GM-K -1.6460
DENSITY:
MOL/CC 1.5389-02
GM/CC 0.7091
AVG MW 46.0803

260

STREAM ID 260
FROM : B19
TO : ----

SUBSTREAM: MIXED
PHASE: LIQUID
COMPONENTS: LBMOL/HR
H2O 0.0
MEK 0.0
2:3-B-01 44.3396
1:3-B-01 0.0
3-BUT-01 0.0
2-MET-01 0.0
ACETO-01 0.0
ETHAN-01 0.1737
2-BUT-01 0.0
BENZENE 0.0
COMPONENTS: MOLE FRAC
H2O 0.0
MEK 0.0
2:3-B-01 0.9961

```
  1:3-B-01        0.0
  3-BUT-01        0.0
  2-MET-01        0.0
  ACETO-01        0.0
  ETHAN-01        3.9012-03
  2-BUT-01        0.0
  BENZENE         0.0
COMPONENTS: LB/HR
  H2O             0.0
  MEK             0.0
  2:3-B-01        3995.9840
  1:3-B-01        0.0
  3-BUT-01        0.0
  2-MET-01        0.0
  ACETO-01        0.0
  ETHAN-01        8.0000
  2-BUT-01        0.0
  BENZENE         0.0
COMPONENTS: MASS FRAC
  H2O             0.0
  MEK             0.0
  2:3-B-01        0.9980
  1:3-B-01        0.0
  3-BUT-01        0.0
  2-MET-01        0.0
  ACETO-01        0.0
  ETHAN-01        1.9980-03
  2-BUT-01        0.0
  BENZENE         0.0
TOTAL FLOW:
  LBMOL/HR        44.5133
  LB/HR           4003.9841
  L/MIN           38.0459
STATE VARIABLES:
  TEMP   C        198.1946
  PRES   BAR      2.0276
  VFRAC           0.0
  LFRAC           1.0000
  SFRAC           0.0
ENTHALPY:
  CAL/MOL         -1.2160+05
  CAL/GM          -1351.8934
  CAL/SEC         -6.8202+05
ENTROPY:
  CAL/MOL-K       -126.6372
  CAL/GM-K        -1.4079
```

DENSITY:
MOL/CC 8.8450-03
GM/CC 0.7956
AVG MW 89.9503

39
--

STREAM ID 39
FROM : B2
TO : B23

SUBSTREAM: MIXED
PHASE: VAPOR

COMPONENTS: LBMOL/HR	
H2O	73.0743
MEK	12.0000
2:3-B-01	1.4198
1:3-B-01	28.4427
3-BUT-01	3.9389
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0

COMPONENTS: MOLE FRAC	
H2O	0.6147
MEK	0.1009
2:3-B-01	1.1944-02
1:3-B-01	0.2393
3-BUT-01	3.3135-02
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0

COMPONENTS: LB/HR	
H2O	1316.4533
MEK	865.2824
2:3-B-01	127.9597
1:3-B-01	1538.5138
3-BUT-01	284.0240
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0

```
  BENZENE            0.0
COMPONENTS: MASS FRAC
  H2O               0.3186
  MEK               0.2094
  2:3-B-01          3.0966-02
  1:3-B-01          0.3723
  3-BUT-01          6.8734-02
  2-MET-01          0.0
  ACETO-01          0.0
  ETHAN-01          0.0
  2-BUT-01          0.0
  BENZENE           0.0
TOTAL FLOW:
  LBMOL/HR          118.8758
  LB/HR             4132.2332
  L/MIN             6.1901+05
STATE VARIABLES:
  TEMP   C          500.0000
  PRES   BAR        9.3326-02
  VFRAC             1.0000
  LFRAC             0.0
  SFRAC             0.0
ENTHALPY:
  CAL/MOL           -3.0065+04
  CAL/GM            -864.9111
  CAL/SEC           -4.5032+05
ENTROPY:
  CAL/MOL-K         -5.1801
  CAL/GM-K          -0.1490
DENSITY:
  MOL/CC            1.4518-06
  GM/CC             5.0466-05
AVG MW              34.7609

15
--

STREAM ID           15
FROM :              B14
TO   :              ----

SUBSTREAM: MIXED
PHASE:              LIQUID
COMPONENTS: LBMOL/HR
  H2O               0.3839
  MEK               5.7559-02
```

2:3-B-01	8.6441-14
1:3-B-01	28.4427
3-BUT-01	9.8657-05
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: MOLE FRAC	
H2O	1.3291-02
MEK	1.9927-03
2:3-B-01	2.9927-15
1:3-B-01	0.9847
3-BUT-01	3.4156-06
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: LB/HR	
H2O	6.9163
MEK	4.1504
2:3-B-01	7.7903-12
1:3-B-01	1538.5136
3-BUT-01	7.1139-03
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: MASS FRAC	
H2O	4.4633-03
MEK	2.6784-03
2:3-B-01	5.0273-15
1:3-B-01	0.9929
3-BUT-01	4.5908-06
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
TOTAL FLOW:	
LBMOL/HR	28.8843
LB/HR	1549.5875
L/MIN	19.6485
STATE VARIABLES:	

```
  TEMP   C            41.6329
  PRES   BAR           4.5000
  VFRAC               0.0
  LFRAC               1.0000
  SFRAC               0.0
ENTHALPY:
  CAL/MOL             2.0348+04
  CAL/GM              379.2932
  CAL/SEC             7.4055+04
ENTROPY:
  CAL/MOL-K             -49.1404
  CAL/GM-K              -0.9160
DENSITY:
  MOL/CC              1.1113-02
  GM/CC               0.5962
AVG MW                 53.6481

19
--

STREAM ID              19
FROM :                B13
TO   :               ----

SUBSTREAM: MIXED
PHASE:                LIQUID
COMPONENTS: LBMOL/HR
  H2O                65.7449
  MEK                 0.7212
  2:3-B-01           2.5357-03
  1:3-B-01            0.0
  3-BUT-01              3.9389
  2-MET-01              0.0
  ACETO-01              0.0
  ETHAN-01              0.0
  2-BUT-01              0.0
  BENZENE               0.0
COMPONENTS: MOLE FRAC
  H2O                 0.9338
  MEK                1.0243-02
  2:3-B-01           3.6014-05
  1:3-B-01            0.0
  3-BUT-01           5.5944-02
  2-MET-01              0.0
  ACETO-01              0.0
  ETHAN-01              0.0
```

2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: LB/HR	
H2O	1184.4131
MEK	52.0009
2:3-B-01	0.2285
1:3-B-01	0.0
3-BUT-01	284.0184
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: MASS FRAC	
H2O	0.7789
MEK	3.4196-02
2:3-B-01	1.5028-04
1:3-B-01	0.0
3-BUT-01	0.1868
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
TOTAL FLOW:	
LBMOL/HR	70.4075
LB/HR	1520.6608
L/MIN	12.8438
STATE VARIABLES:	
TEMP C	88.3460
PRES BAR	1.1000
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
CAL/MOL	-6.7179+04
CAL/GM	-3110.4475
CAL/SEC	-5.9596+05
ENTROPY:	
CAL/MOL-K	-43.4903
CAL/GM-K	-2.0136
DENSITY:	
MOL/CC	4.1442-02
GM/CC	0.8951
AVG MW	21.5980

20
--

STREAM ID 20
FROM : B13
TO : B17

SUBSTREAM: MIXED
PHASE: LIQUID
COMPONENTS: LBMOL/HR

H2O	0.2499
MEK	7.8607-10
2:3-B-01	1.4173
1:3-B-01	0.0
3-BUT-01	2.1317-07
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0

COMPONENTS: MOLE FRAC

H2O	0.1499
MEK	4.7149-10
2:3-B-01	0.8501
1:3-B-01	0.0
3-BUT-01	1.2786-07
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0

COMPONENTS: LB/HR

H2O	4.5018
MEK	5.6681-08
2:3-B-01	127.7315
1:3-B-01	0.0
3-BUT-01	1.5371-05
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0

COMPONENTS: MASS FRAC

H2O	3.4044-02
MEK	4.2865-10
2:3-B-01	0.9660

1:3-B-01	0.0
3-BUT-01	1.1624-07
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
TOTAL FLOW:	
LBMOL/HR	1.6672
LB/HR	132.2333
L/MIN	1.1676
STATE VARIABLES:	
TEMP C	162.0657
PRES BAR	1.3827
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
CAL/MOL	-1.1511+05
CAL/GM	-1451.3368
CAL/SEC	-2.4181+04
ENTROPY:	
CAL/MOL-K	-115.6397
CAL/GM-K	-1.4580
DENSITY:	
MOL/CC	1.0795-02
GM/CC	0.8562
AVG MW	79.3145

8
-

STREAM ID 8
FROM : B3
TO : ----

SUBSTREAM: MIXED
PHASE: LIQUID
COMPONENTS: LBMOL/HR

H2O	5.2631
MEK	9.9060
2:3-B-01	0.0
1:3-B-01	1.1282-18
3-BUT-01	2.1036-07
2-MET-01	0.0
ACETO-01	0.0

ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: MOLE FRAC	
H2O	0.3470
MEK	0.6530
2:3-B-01	0.0
1:3-B-01	7.4375-20
3-BUT-01	1.3868-08
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: LB/HR	
H2O	94.8164
MEK	714.2877
2:3-B-01	0.0
1:3-B-01	6.1026-17
3-BUT-01	1.5168-05
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: MASS FRAC	
H2O	0.1172
MEK	0.8828
2:3-B-01	0.0
1:3-B-01	7.5424-20
3-BUT-01	1.8747-08
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
TOTAL FLOW:	
LBMOL/HR	15.1691
LB/HR	809.1041
L/MIN	9.2425
STATE VARIABLES:	
TEMP C	154.0302
PRES BAR	7.3309
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0

ENTHALPY:
CAL/MOL -6.1688+04
CAL/GM -1156.5241
CAL/SEC -1.1790+05
ENTROPY:
CAL/MOL-K -64.1523
CAL/GM-K -1.2027
DENSITY:
MOL/CC 1.2407-02
GM/CC 0.6618
AVG MW 53.3391

9
-

STREAM ID 9
FROM : B6
TO : ----

SUBSTREAM: MIXED
PHASE: LIQUID
COMPONENTS: LBMOL/HR
H2O 1.4424
MEK 1.3123
2:3-B-01 0.0
1:3-B-01 6.8097-09
3-BUT-01 1.8137-09
2-MET-01 0.0
ACETO-01 0.0
ETHAN-01 0.0
2-BUT-01 0.0
BENZENE 0.0
COMPONENTS: MOLE FRAC
H2O 0.5236
MEK 0.4764
2:3-B-01 0.0
1:3-B-01 2.4720-09
3-BUT-01 6.5842-10
2-MET-01 0.0
ACETO-01 0.0
ETHAN-01 0.0
2-BUT-01 0.0
BENZENE 0.0
COMPONENTS: LB/HR
H2O 25.9850
MEK 94.6263

```
  2:3-B-01          0.0
  1:3-B-01        3.6835-07
  3-BUT-01         1.3078-07
  2-MET-01           0.0
  ACETO-01           0.0
  ETHAN-01           0.0
  2-BUT-01          0.0
  BENZENE            0.0
COMPONENTS: MASS FRAC
  H2O             0.2154
  MEK              0.7846
  2:3-B-01          0.0
  1:3-B-01        3.0540-09
  3-BUT-01         1.0843-09
  2-MET-01           0.0
  ACETO-01           0.0
  ETHAN-01           0.0
  2-BUT-01          0.0
  BENZENE            0.0
TOTAL FLOW:
  LBMOL/HR            2.7547
  LB/HR            120.6113
  L/MIN             1.1842
STATE VARIABLES:
  TEMP   C          86.8378
  PRES   BAR           1.6410
  VFRAC              0.0
  LFRAC              1.0000
  SFRAC             0.0
ENTHALPY:
  CAL/MOL          -6.4973+04
  CAL/GM          -1483.9529
  CAL/SEC         -2.2551+04
ENTROPY:
  CAL/MOL-K          -60.8474
  CAL/GM-K           -1.3897
DENSITY:
  MOL/CC          1.7586-02
  GM/CC            0.7700
AVG MW              43.7840

21
--

STREAM ID           21
FROM :             B9
```

TO : B3

SUBSTREAM: MIXED
PHASE: LIQUID

COMPONENTS: LBMOL/HR	
H2O	6.6955
MEK	11.2213
2:3-B-01	1.6928-27
1:3-B-01	6.7326-09
3-BUT-01	2.1217-07
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: MOLE FRAC	
H2O	0.3737
MEK	0.6263
2:3-B-01	9.4482-29
1:3-B-01	3.7577-10
3-BUT-01	1.1842-08
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: LB/HR	
H2O	120.6219
MEK	809.1306
2:3-B-01	1.5256-25
1:3-B-01	3.6417-07
3-BUT-01	1.5299-05
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0
2-BUT-01	0.0
BENZENE	0.0
COMPONENTS: MASS FRAC	
H2O	0.1297
MEK	0.8703
2:3-B-01	1.6409-28
1:3-B-01	3.9169-10
3-BUT-01	1.6455-08
2-MET-01	0.0
ACETO-01	0.0
ETHAN-01	0.0

```
  2-BUT-01           0.0
  BENZENE            0.0
 TOTAL FLOW:
  LBMOL/HR           17.9168
  LB/HR              929.7524
  L/MIN              9.1457
 STATE VARIABLES:
  TEMP   C           76.5195
  PRES   BAR         7.5000
  VFRAC              0.0
  LFRAC              1.0000
  SFRAC              0.0
 ENTHALPY:
  CAL/MOL            -6.4685+04
  CAL/GM             -1246.5085
  CAL/SEC            -1.4602+05
 ENTROPY:
  CAL/MOL-K          -69.8677
  CAL/GM-K           -1.3464
 DENSITY:
  MOL/CC             1.4810-02
  GM/CC              0.7685
 AVG MW              51.8928
```

Blocks

```
 BLOCK:  B2      MODEL: RSTOIC
 ------------------------------
  INLET STREAM:         36
  OUTLET STREAM:        39
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

              ***  MASS AND ENERGY BALANCE  ***
                   IN         OUT       GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)        46.0514      118.876       72.8244     -0.119544E-15
  MASS(LB/HR   )        4132.23      4132.23                   0.220098E-15
  ENTHALPY(CAL/SEC )    -603003.     -450318.                  -0.253207

              ***  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  ***
```

```
STOICHIOMETRY MATRIX:

 REACTION #   1:
  SUBSTREAM MIXED   :
  H2O        1.00    MEK        1.00    2:3-B-01  -1.00

 REACTION #   2:
  SUBSTREAM MIXED   :
  H2O        2.00    2:3-B-01  -1.00    1:3-B-01   1.00

 REACTION #   3:
  SUBSTREAM MIXED   :
  H2O        1.00    2:3-B-01  -1.00    3-BUT-01   1.00


REACTION CONVERSION SPECS: NUMBER=    3
  REACTION #   1:
  SUBSTREAM:MIXED    KEY COMP:2:3-B-01 CONV FRAC: 0.2620
  REACTION #   2:
  SUBSTREAM:MIXED    KEY COMP:2:3-B-01 CONV FRAC: 0.6210
  REACTION #   3:
  SUBSTREAM:MIXED    KEY COMP:2:3-B-01 CONV FRAC: 0.8600E-01



TWO    PHASE  TP  FLASH
SPECIFIED TEMPERATURE C                          500.000
SPECIFIED PRESSURE    BAR                        0.093326
MAXIMUM NO. ITERATIONS                            50
CONVERGENCE TOLERANCE                              0.000100000
SIMULTANEOUS REACTIONS
GENERATE COMBUSTION REACTIONS FOR FEED SPECIES           NO

                  ***  RESULTS  ***
OUTLET TEMPERATURE    C                           500.00
OUTLET PRESSURE       BAR                        0.93326E-01
HEAT DUTY             CAL/SEC                    0.15268E+06
VAPOR FRACTION                                   1.0000



HEAT OF REACTIONS:

  REACTION        REFERENCE        HEAT OF
  NUMBER          COMPONENT         REACTION
```

		CAL/MOL
1	2:3-B-01	353.97
2	2:3-B-01	25772.
3	2:3-B-01	-5177.0

REACTION EXTENTS:

REACTION NUMBER	REACTION EXTENT LBMOL/HR
1	12.000
2	28.443
3	3.9389

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
H2O	0.61471	0.73991	0.61471	10383.
MEK	0.10095	0.13416	0.10095	9403.5
2:3-B-01	0.11944E-01	0.15122E-01	0.11944E-01	9870.9
1:3-B-01	0.23926	0.94461E-01	0.23926	31655.
3-BUT-01	0.33135E-01	0.16347E-01	0.33135E-01	25331.

BLOCK: B19 MODEL: RADFRAC

INLETS - 170 STAGE 3
OUTLETS - 210 STAGE 1
260 STAGE 5
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	218.037	218.037	0.00000
MASS(LB/HR)	12000.0	12000.0	0.235393E-09
ENTHALPY(CAL/SEC)	-0.218629E+07	-0.207981E+07	-0.487024E-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                              5
  ALGORITHM OPTION                            STANDARD
  ABSORBER OPTION                             NO
  INITIALIZATION OPTION                       STANDARD
  HYDRAULIC PARAMETER CALCULATIONS            NO
  INSIDE LOOP CONVERGENCE METHOD              BROYDEN
  DESIGN SPECIFICATION METHOD                 NESTED
  MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS      25
  MAXIMUM NO. OF INSIDE LOOP ITERATIONS       10
  MAXIMUM NUMBER OF FLASH ITERATIONS          30
  FLASH TOLERANCE                             0.000100000
  OUTSIDE LOOP CONVERGENCE TOLERANCE          0.000100000

 ****   COL-SPECS   ****

  MOLAR VAPOR DIST / TOTAL DIST               0.0
  MASS REFLUX RATIO                           1.00000
  MASS DISTILLATE TO FEED RATIO               0.66000

 ****   PROFILES   ****

  P-SPEC         STAGE   1  PRES, BAR         2.00000

 **** TRAY VAPORIZATION EFFICIENCY ****

         SEGMENT   2  4  EFFICIENCY           0.70000

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


 ***   COMPONENT SPLIT FRACTIONS   ***

              OUTLET STREAMS
              --------------
          210        260
  COMPONENT:
  2:3-B-01    .10000E-02   .99900
  ETHAN-01    .99900       .10000E-02
```

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	C	96.6605
BOTTOM STAGE TEMPERATURE	C	198.195
TOP STAGE LIQUID FLOW	LBMOL/HR	280.855
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	44.5133
TOP STAGE VAPOR FLOW	LBMOL/HR	0.0
BOILUP VAPOR FLOW	LBMOL/HR	345.821
MOLAR REFLUX RATIO		1.61854
MOLAR BOILUP RATIO		7.76895
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-527,905.
REBOILER DUTY	CAL/SEC	634,382.

**** MANIPULATED VARIABLES ****

	BOUNDS LOWER	BOUNDS UPPER	CALCULATED VALUE
MASS DISTIL TO FEED RATIO	0.10000	1.0000	0.66633
MASS REFLUX RATIO	0.10000	3.0000	1.6185

**** DESIGN SPECIFICATIONS ****

NO	SPEC-TYPE	QUALIFIERS	UNIT	SPECIFIED VALUE	CALCULATED VALUE
1	MASS-RECOV	STREAMS: 210 COMPS: ETHAN-01		0.99900	0.99900
2	MASS-RECOV	STREAMS: 260 COMPS: 2:3-B-01		0.99900	0.99900

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

DEW POINT 0.14501E-04 STAGE= 4
BUBBLE POINT 0.60032E-05 STAGE= 4
COMPONENT MASS BALANCE 0.16035E-05 STAGE= 2 COMP=2:3-B-01
ENERGY BALANCE 0.28329E-03 STAGE= 4

**** PROFILES ****

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

```
                              ENTHALPY
STAGE TEMPERATURE   PRESSURE          CAL/MOL          HEAT DUTY
   C           BAR         LIQUID      VAPOR       CAL/SEC

 1   96.660       2.0000     -63932.     -54902.     -.52790+06
 2   107.71       2.0069     -64307.     -54711.
 3   116.27       2.0138     -79905.     -54990.
 4   164.69       2.0207    -0.11712E+06  -63882.
 5   198.19       2.0276    -0.12160E+06 -0.10198E+06    .63438+06

STAGE     FLOW RATE              FEED RATE             PRODUCT RATE
        LBMOL/HR              LBMOL/HR              LBMOL/HR
   LIQUID    VAPOR      LIQUID    VAPOR    MIXED      LIQUID    VAPOR
 1  454.4      0.000                        173.5234
 2  283.2      454.4
 3  474.5      456.7       218.0367
 4  390.3      430.0
 5  44.51      345.8                         44.5132

 ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE              FEED RATE             PRODUCT RATE
        LB/HR                LB/HR                LB/HR
   LIQUID    VAPOR      LIQUID    VAPOR    MIXED      LIQUID    VAPOR
 1 0.2094E+05  0.000                           7996.0159
 2 0.1320E+05 0.2094E+05
 3 0.2726E+05 0.2120E+05   .12000+05
 4 0.3331E+05 0.2326E+05
 5  4004.     0.2930E+05                       4003.9840

                ****   MOLE-X-PROFILE     ****
 STAGE     2:3-B-01     ETHAN-01
   1    0.25578E-03   0.99974
   2    0.12616E-01   0.98738
   3    0.25843       0.74157
   4    0.89111       0.10889
   5    0.99610       0.39012E-02

                ****   MOLE-Y-PROFILE     ****
 STAGE     2:3-B-01     ETHAN-01
   1    0.38116E-05    1.0000
   2    0.25578E-03   0.99974
   3    0.79197E-02   0.99208
   4    0.18206       0.81794
   5    0.87760       0.12240
```

```
                **** K-VALUES          ****
 STAGE    2:3-B-01     ETHAN-01
   1   0.14902E-01   1.0003
   2   0.28963E-01   1.4465
   3   0.43779E-01   1.9112
   4   0.29187       10.731
   5   0.88103       31.377

                **** MASS-X-PROFILE    ****
 STAGE    2:3-B-01     ETHAN-01
   1   0.50025E-03  0.99950
   2   0.24386E-01  0.97561
   3   0.40538      0.59462
   4   0.94121      0.58793E-01
   5   0.99800      0.19980E-02

                **** MASS-Y-PROFILE    ****
 STAGE    2:3-B-01     ETHAN-01
   1   0.74564E-05  0.99999
   2   0.50025E-03  0.99950
   3   0.15376E-01  0.98462
   4   0.30335      0.69665
   5   0.93345      0.66554E-01

                **** VAPORIZATION EFF  ****
 STAGE    2:3-B-01     ETHAN-01
   1    1.0000       1.0000
   2   0.70000      0.70000
   3   0.70000      0.70000
   4   0.70000      0.70000
   5    1.0000       1.0000

BLOCK:  B14     MODEL: RADFRAC
-------------------------------
  INLETS   - 5       STAGE   9
  OUTLETS  - 15      STAGE   1
           10     STAGE  16
 PROPERTY OPTION SET:   NRTL     RENON (NRTL) / IDEAL GAS



**********************************************************************
   *                                              *
   *   INCOMPLETE OR INCONSISTENT KEY SPECS. APPROXIMATIONS ARE
USED.  *
   *                                              *
```

```
**********************************************************************

*** MASS AND ENERGY BALANCE ***
                         IN          OUT       RELATIVE DIFF.
TOTAL BALANCE
  MOLE(LBMOL/HR)        118.876      118.876     0.119544E-15
  MASS(LB/HR   )        4132.23      4132.23     0.174735E-07
  ENTHALPY(CAL/SEC )   -657939.     -676934.     0.280596E-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                                  16
ALGORITHM OPTION                                  STANDARD
ABSORBER OPTION                                   NO
INITIALIZATION OPTION                             STANDARD
HYDRAULIC PARAMETER CALCULATIONS                  NO
INSIDE LOOP CONVERGENCE METHOD                    BROYDEN
DESIGN SPECIFICATION METHOD                       NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS            200
MAXIMUM NO. OF INSIDE LOOP ITERATIONS             10
MAXIMUM NUMBER OF FLASH ITERATIONS                30
FLASH TOLERANCE                                   0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE                0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST                     0.0
MASS REFLUX RATIO                                 3.00000
MASS DISTILLATE TO FEED RATIO                     0.37500

**** PROFILES ****
```

```
P-SPEC        STAGE   1  PRES, BAR                4.50000

**** TRAY VAPORIZATION EFFICIENCY ****

          SEGMENT   2 16  EFFICIENCY              0.70000

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


*** COMPONENT SPLIT FRACTIONS  ***

                  OUTLET STREAMS
                  --------------
          15          10
COMPONENT:
H2O        .52538E-02   .99475
MEK        .47966E-02   .99520
2:3-B-01   .60881E-13   1.0000
1:3-B-01   1.0000       .23671E-09
3-BUT-01   .25047E-04   .99997


***  SUMMARY OF KEY RESULTS  ***

TOP STAGE TEMPERATURE           C                    41.6329
BOTTOM STAGE TEMPERATURE        C                    138.928
TOP STAGE LIQUID FLOW           LBMOL/HR             86.6529
BOTTOM STAGE LIQUID FLOW        LBMOL/HR             89.9915
TOP STAGE VAPOR FLOW            LBMOL/HR             0.0
BOILUP VAPOR FLOW               LBMOL/HR             56.1427
MOLAR REFLUX RATIO                                   3.00000
MOLAR BOILUP RATIO                                   0.62387
CONDENSER DUTY (W/O SUBCOOL)    CAL/SEC              -74,588.5
REBOILER DUTY                   CAL/SEC              55,593.9

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

DEW POINT                   0.88909E-05  STAGE=  4
BUBBLE POINT                0.25420E-03  STAGE=  5
COMPONENT MASS BALANCE      0.39691E-05  STAGE=  4 COMP=3-BUT-01
ENERGY BALANCE              0.17236E-04  STAGE=  5
```

**** PROFILES ****

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

STAGE	TEMPERATURE	PRESSURE	ENTHALPY CAL/MOL		HEAT DUTY
	C	BAR	LIQUID	VAPOR	CAL/SEC
1	41.633	4.5000	20348.	26102.	-.74588+05
2	58.340	4.7068	17045.	25472.	
3	64.304	4.7137	15.161	22770.	
4	86.273	4.7206	-41700.	11618.	
7	119.50	4.7413	-59731.	-23518.	
8	120.09	4.7482	-59832.	-23724.	
9	134.37	4.7551	-64973.	-49358.	
10	136.95	4.7620	-65113.	-54922.	
11	137.26	4.7689	-65126.	-55486.	
12	137.35	4.7758	-65128.	-55541.	
13	137.45	4.7827	-65135.	-55550.	
15	138.03	4.7965	-65226.	-55612.	
16	138.93	4.8034	-66232.	-55755.	.55594+05

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	115.5	0.000		28.8843			
2	91.18	115.5					
3	72.76	120.1					
4	53.17	101.6					
7	51.79	80.76					
8	53.97	80.68	40.1575				
9	145.2	42.69	78.7181				
10	146.3	55.18					
11	146.4	56.30					
12	146.4	56.42					
13	146.4	56.44					
15	146.1	56.28					
16	89.99	56.14		89.9914			

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR

1	6198.	0.000			1549.5874
2	4827.	6198.			
3	3744.	6376.			
4	2566.	5294.			
7	2416.	3971.			
8	2556.	3965.		2101.4060	
9	5142.	2004.	2030.8271		
10	5190.	2559.			
11	5195.	2608.			
12	5194.	2612.			
13	5189.	2612.			
15	5160.	2585.			
16	2583.	2578.			2582.6456

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

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.13291E-01	0.19927E-02	0.29927E-14	0.98471	0.34156E-05
2	0.41256E-01	0.18405E-01	0.17249E-12	0.94031	0.31530E-04
3	0.13395	0.12224	0.12125E-10	0.74353	0.27824E-03
4	0.35404	0.38324	0.10104E-08	0.26096	0.17648E-02
7	0.45541	0.47845	0.20674E-04	0.46099E-01	0.20023E-01
8	0.44220	0.46995	0.51248E-03	0.45999E-01	0.41340E-01
9	0.68059	0.26807	0.99702E-02	0.28429E-02	0.38534E-01
10	0.68033	0.27092	0.98996E-02	0.27538E-03	0.38576E-01
11	0.68037	0.27103	0.98917E-02	0.26248E-04	0.38676E-01
12	0.68057	0.27056	0.98909E-02	0.24954E-05	0.38981E-01
13	0.68114	0.26905	0.98929E-02	0.23632E-06	0.39911E-01
15	0.68359	0.25473	0.10126E-01	0.20309E-08	0.51553E-01
16	0.80775	0.13271	0.15778E-01	0.74813E-10	0.43769E-01

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

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.35549E-02	0.17905E-03	0.35549E-16	0.99627	0.30941E-06
2	0.13291E-01	0.19927E-02	0.29927E-14	0.98471	0.34156E-05
3	0.34529E-01	0.14457E-01	0.13171E-12	0.95099	0.24767E-04
4	0.99663E-01	0.88069E-01	0.86802E-11	0.81207	0.20014E-03
7	0.29601	0.31345	0.53743E-06	0.38429	0.62560E-02
8	0.29713	0.30787	0.13272E-04	0.38214	0.12856E-01
9	0.44050	0.45679	0.45438E-03	0.74204E-01	0.28047E-01
10	0.47319	0.48884	0.49847E-03	0.74795E-02	0.29995E-01
11	0.47665	0.49185	0.50336E-03	0.71559E-03	0.30275E-01
12	0.47722	0.49166	0.50428E-03	0.68111E-04	0.30554E-01
13	0.47780	0.49034	0.50505E-03	0.64739E-05	0.31348E-01
15	0.48424	0.47437	0.51747E-03	0.57220E-07	0.40879E-01
16	0.48459	0.45031	0.10662E-02	0.51662E-08	0.64030E-01

**** K-VALUES ****

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.26747	0.89849E-01	0.11879E-01	1.0117	0.90591E-01
2	0.46029	0.15467	0.24785E-01	1.4960	0.15476
3	0.36835	0.16892	0.15513E-01	1.8271	0.12715
4	0.40242	0.32816	0.12271E-01	4.4442	0.16198
7	0.92876	0.93572	0.37138E-01	11.906	0.44629
8	0.96006	0.93574	0.36998E-01	11.866	0.44423
9	0.92471	2.4338	0.65100E-01	37.277	1.0396
10	0.99370	2.5772	0.71926E-01	38.791	1.1106
11	1.0009	2.5921	0.72691E-01	38.938	1.1181
12	1.0018	2.5957	0.72831E-01	38.986	1.1196
13	1.0021	2.6033	0.72928E-01	39.130	1.1220
15	1.0120	2.6603	0.73007E-01	40.250	1.1328
16	0.85704	4.8476	0.96537E-01	98.651	2.0899

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

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.44633E-02	0.26784E-02	0.50273E-14	0.99285	0.45908E-05
2	0.14040E-01	0.25071E-01	0.29366E-12	0.96085	0.42949E-04
3	0.46889E-01	0.17127	0.21232E-10	0.78145	0.38983E-03
4	0.13217	0.57267	0.18871E-08	0.29252	0.26372E-02
7	0.17590	0.73965	0.39945E-04	0.53461E-01	0.30955E-01
8	0.16818	0.71539	0.97504E-03	0.52528E-01	0.62930E-01
9	0.34615	0.54570	0.25367E-01	0.43413E-02	0.78443E-01
10	0.34544	0.55059	0.25146E-01	0.41983E-03	0.78399E-01
11	0.34544	0.55079	0.25124E-01	0.40014E-04	0.78598E-01
12	0.34564	0.54998	0.25129E-01	0.38052E-05	0.79241E-01
13	0.34624	0.54741	0.25156E-01	0.36069E-06	0.81202E-01
15	0.34875	0.52014	0.25842E-01	0.31108E-08	0.10527
16	0.50705	0.33343	0.49546E-01	0.14101E-09	0.10997

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

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.11867E-02	0.23923E-03	0.59366E-16	0.99857	0.41342E-06
2	0.44633E-02	0.26784E-02	0.50273E-14	0.99285	0.45908E-05
3	0.11713E-01	0.19629E-01	0.22351E-12	0.96862	0.33627E-04
4	0.34471E-01	0.12192	0.15019E-10	0.84333	0.27707E-03
7	0.10845	0.45964	0.98499E-06	0.42273	0.91739E-02
8	0.10891	0.45166	0.24336E-04	0.42055	0.18860E-01
9	0.16902	0.70154	0.87219E-03	0.85490E-01	0.43075E-01
10	0.18378	0.75990	0.96848E-03	0.87221E-02	0.46628E-01
11	0.18538	0.76567	0.97936E-03	0.83564E-03	0.47129E-01
12	0.18568	0.76568	0.98155E-03	0.79570E-04	0.47583E-01
13	0.18603	0.76413	0.98368E-03	0.75681E-05	0.48851E-01
15	0.18996	0.74483	0.10155E-02	0.67398E-07	0.64187E-01

16	0.19014	0.70721	0.20927E-02	0.60863E-08	0.10056

**** VAPORIZATION EFF ****

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	1.0000	1.0000	1.0000	1.0000	1.0000
2	0.70000	0.70000	0.70000	0.70000	0.70000
3	0.70000	0.70000	0.70000	0.70000	0.70000
4	0.70000	0.70000	0.70000	0.70000	0.70000
7	0.70000	0.70000	0.70000	0.70000	0.70000
8	0.70000	0.70000	0.70000	0.70000	0.70000
9	0.70000	0.70000	0.70000	0.70000	0.70000
10	0.70000	0.70000	0.70000	0.70000	0.70000
11	0.70000	0.70000	0.70000	0.70000	0.70000
12	0.70000	0.70000	0.70000	0.70000	0.70000
13	0.70000	0.70000	0.70000	0.70000	0.70000
15	0.70000	0.70000	0.70000	0.70000	0.70000
16	0.70000	0.70000	0.70000	0.70000	0.70000

****

***** COLUMN TARGETING RESULTS *****

****

*** THERMAL ANALYSIS ***

STAGE	TEMPERATURE	PRESSURE	ENTHALPY DEFICIT	EXERGY LOSS	CARNOT FACTOR
	C	BAR	CAL/SEC	CAL/SEC	
1	41.633	4.5000	74588.	601.79	0.52839E-01
2	58.340	4.7068	55941.	76.598	0.10058
3	64.304	4.7137	52314.	2272.3	0.11647
4	86.273	4.7206	45573.	3516.5	0.17048
7	119.50	4.7413	251.90	31.887	0.24067
8	120.09	4.7482	-589.52	1558.6	0.24181
9	134.37	4.7551	-24445.	417.77	0.26838
10	136.95	4.7620	-2844.0	1.8285	0.27298
11	137.26	4.7689	-383.13	3.9164	0.27353
12	137.35	4.7758	-60.607	4.7584	0.27369
13	137.45	4.7827	-90.772	5.7336	0.27386
15	138.03	4.7965	2866.6	40.068	0.27490
16	138.93	4.8034	55594.	-.25880E+28	0.27647

```
BLOCK:  B15      MODEL: RADFRAC
-------------------------------
   INLETS   - 10       STAGE  32
   OUTLETS  - 29       STAGE   1
             30        STAGE  36
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                 ***  MASS AND ENERGY BALANCE  ***
                              IN            OUT       RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(LBMOL/HR)           89.9915        89.9915        0.00000
     MASS(LB/HR   )          2582.65        2582.64       0.387507E-06
     ENTHALPY(CAL/SEC )      -750989.       -762205.       0.147155E-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                              36
   ALGORITHM OPTION                             3P-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
   MASS REFLUX RATIO                             3.00000
   MASS DISTILLATE TO FEED RATIO                    0.36000

  **** L2-STAGES SPECIFICATIONS ****
```

TWO LIQUID PHASE CALCULATIONS ARE PERFORMED FOR STAGE TO STAGE
1 9

**** L2-COMPS SPECIFICATIONS ****

KEY COMPONENTS IN THE SECOND LIQUID PHASE COMPONENT
H2O

**** PROFILES ****

P-SPEC STAGE 1 PRES, BAR 1.15000

**** TRAY VAPORIZATION EFFICIENCY ****

SEGMENT 2 36 EFFICIENCY 0.70000

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

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	29	30
COMPONENT:		
H2O	.92110E-01	.90789
MEK	.93961	.60387E-01
2:3-B-01	0.0000	1.0000
1:3-B-01	1.0000	.12147E-09
3-BUT-01	.53867E-07	1.0000

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	C	76.3741
BOTTOM STAGE TEMPERATURE	C	110.980
TOP STAGE LIQUID FLOW	LBMOL/HR	71.6672
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	72.0747
TOP STAGE VAPOR FLOW	LBMOL/HR	0.0
BOILUP VAPOR FLOW	LBMOL/HR	58.3740
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		0.80991

CONDENSER DUTY (W/O SUBCOOL) CAL/SEC -78,511.7
REBOILER DUTY CAL/SEC 67,295.8

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

DEW POINT 0.39984E-03 STAGE= 1 PHASE=L1
BUBBLE POINT 0.39968E-03 STAGE= 1 PHASE=L1
COMPONENT MASS BALANCE 0.24404E-09 STAGE= 8 COMP=3-BUT-01
ENERGY BALANCE 0.21316E-11 STAGE= 9

**** PROFILES ****

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

STAGE	TEMPERATURE	PRESSURE	ENTHALPY CAL/MOL		HEAT DUTY
	C	BAR	LIQUID	VAPOR	CAL/SEC
1	76.374	1.1500	-64719.	-56292.	-.78512+05
2	91.958	1.3568	-64194.	-56025.	
8	92.899	1.3982	-64173.	-56009.	
9	93.054	1.4051	-64313.	-56006.	
10	93.043	1.4120	-64282.	-56054.	
30	96.871	1.5499	-64574.	-56116.	
31	97.634	1.5568	-64860.	-56191.	
32	98.684	1.5637	-66580.	-56297.	
33	100.19	1.5706	-66817.	-56456.	
35	106.90	1.5844	-67415.	-57250.	
36	110.98	1.5913	-67843.	-57737.	.67296+05

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	71.67	0.000			17.9167		
2	57.18	71.67					
8	57.19	75.10					
9	56.65	75.10					
10	56.84	74.56					
30	56.11	74.35					
31	55.78	74.03		13.3582			
32	133.8	60.33	76.6332				
33	132.6	61.75					
35	130.4	59.21					

36	72.07	58.37		72.0746

STAGE	FLOW RATE LBMOL/HR		ENTHALPY CAL/MOL	
	LIQUID1	LIQUID2	LIQUID1	LIQUID2
1	61.01	10.66	-64308.	-67073.
2	49.72	7.465	-63811.	-66743.
8	49.57	7.618	-63781.	-66723.
9	46.31	10.34	-63776.	-66719.
10	56.84	0.000	-64282.	-64282.
30	56.11	0.000	-64574.	-64574.
31	55.78	0.000	-64860.	-64860.
32	0.000	133.8	-66580.	-66580.
33	0.000	132.6	-66817.	-66817.
35	0.000	130.4	-67415.	-67415.
36	0.000	72.07	-67843.	-67843.

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	3719.	0.000		929.7524			
2	2966.	3719.					
8	2959.	3890.					
9	2832.	3888.					
10	2840.	3762.					
30	2748.	3712.					
31	2689.	3678.	647.6005				
32	4625.	2971.	1935.0440				
33	4422.	2972.					
35	3886.	2485.					
36	1653.	2233.		1652.8922			

STAGE	FLOW RATE LB/HR	
	LIQUID1	LIQUID2
1	3494.	224.6
2	2808.	158.3
8	2797.	161.6
9	2613.	219.3
10	2840.	0.000
30	2748.	0.000
31	2689.	0.000
32	0.000	4625.
33	0.000	4422.

35	0.000	3886.
36	0.000	1653.

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

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.37370	0.62630	0.94482E-28	0.37577E-09	0.11842E-07
2	0.37412	0.62588	0.26713E-26	0.23971E-10	0.23826E-07
8	0.37660	0.62340	0.21202E-23	0.60626E-11	0.42848E-06
9	0.40877	0.59123	0.20695E-22	0.57372E-11	0.62471E-06
10	0.40917	0.59083	0.59313E-21	0.57278E-11	0.10804E-05
30	0.42755	0.52466	0.16512E-04	0.54342E-11	0.47774E-01
31	0.44197	0.47951	0.50474E-03	0.50879E-11	0.78017E-01
32	0.69772	0.22555	0.10749E-01	0.14863E-12	0.65976E-01
33	0.72042	0.18001	0.10862E-01	0.52501E-14	0.88713E-01
35	0.78622	0.56790E-01	0.11650E-01	0.27045E-17	0.14534
36	0.91565	0.10006E-01	0.19700E-01	0.11346E-19	0.54649E-01

**** MOLE-X1-PROFILE ****

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.27420	0.72580	0.10000E-32	0.44005E-09	0.13735E-07
2	0.28900	0.71100	0.47713E-28	0.27486E-10	0.27081E-07
8	0.28988	0.71012	0.22990E-23	0.69723E-11	0.48835E-06
9	0.29002	0.70998	0.23108E-22	0.69855E-11	0.75077E-06
10	0.40917	0.59083	0.59313E-21	0.57278E-11	0.10804E-05
30	0.42755	0.52466	0.16512E-04	0.54342E-11	0.47774E-01
31	0.44197	0.47951	0.50474E-03	0.50879E-11	0.78017E-01
32	0.69772	0.22555	0.10749E-01	0.14863E-12	0.65976E-01
33	0.72042	0.18001	0.10862E-01	0.52501E-14	0.88713E-01
35	0.78622	0.56790E-01	0.11650E-01	0.27045E-17	0.14534
36	0.91565	0.10006E-01	0.19700E-01	0.11346E-19	0.54649E-01

**** MOLE-X2-PROFILE ****

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.94343	0.56571E-01	0.63547E-27	0.77004E-11	0.10024E-08
2	0.94098	0.59021E-01	0.20144E-25	0.56202E-12	0.21494E-08
8	0.94083	0.59169E-01	0.95684E-24	0.14387E-12	0.38951E-07
9	0.94081	0.59193E-01	0.98827E-23	0.14436E-12	0.59930E-07
10	0.40917	0.59083	0.59313E-21	0.57278E-11	0.10804E-05
30	0.42755	0.52466	0.16512E-04	0.54342E-11	0.47774E-01
31	0.44197	0.47951	0.50474E-03	0.50879E-11	0.78017E-01
32	0.69772	0.22555	0.10749E-01	0.14863E-12	0.65976E-01
33	0.72042	0.18001	0.10862E-01	0.52501E-14	0.88713E-01
35	0.78622	0.56790E-01	0.11650E-01	0.27045E-17	0.14534
36	0.91565	0.10006E-01	0.19700E-01	0.11346E-19	0.54649E-01

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

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.34136	0.65864	0.46239E-29	0.73298E-08	0.57714E-08
2	0.37370	0.62630	0.17684E-27	0.37577E-09	0.11842E-07
8	0.37559	0.62440	0.65058E-25	0.94254E-10	0.21399E-06
9	0.37591	0.62409	0.65904E-24	0.94260E-10	0.32909E-06
10	0.40035	0.59965	0.14790E-22	0.94653E-10	0.47744E-06
30	0.40993	0.56835	0.41763E-06	0.94813E-10	0.21724E-01
31	0.41451	0.54926	0.12515E-04	0.95069E-10	0.36211E-01
32	0.42278	0.52391	0.28498E-03	0.76367E-11	0.53028E-01
33	0.44336	0.47714	0.30277E-03	0.32211E-12	0.79197E-01
35	0.55732	0.24347	0.43928E-03	0.30936E-15	0.19877
36	0.62642	0.11456	0.17101E-02	0.60296E-17	0.25731

**** K-VALUES: V-L1 ****

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	1.2444	0.9071	2.0732-02	16.6502	0.4200
2	1.8472	1.2584	3.9757-02	19.5300	0.6247
8	1.8510	1.2561	4.0427-02	19.3120	0.6260
9	1.8516	1.2558	4.0537-02	19.2766	0.6262
10	1.3978	1.4499	3.5621-02	23.6075	0.6313
30	1.3697	1.5475	3.6133-02	24.9249	0.6496
31	1.3398	1.6364	3.5422-02	26.6934	0.6631
32	MISSING	MISSING	MISSING	MISSING	MISSING
33	MISSING	MISSING	MISSING	MISSING	MISSING
35	MISSING	MISSING	MISSING	MISSING	MISSING
36	MISSING	MISSING	MISSING	MISSING	MISSING

**** K-VALUES: V-L2 ****

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.3617	11.6381	4.8920-02	951.4966	5.7555
2	0.5673	15.1591	9.5436-02	955.1500	7.8707
8	0.5703	15.0756	9.7133-02	935.9155	7.8483
9	0.5708	15.0620	9.7414-02	932.8020	7.8446
10	MISSING	MISSING	MISSING	MISSING	MISSING
30	MISSING	MISSING	MISSING	MISSING	MISSING
31	MISSING	MISSING	MISSING	MISSING	MISSING
32	0.8656	3.3182	3.7874-02	73.4022	1.1482
33	0.8792	3.7867	3.9819-02	87.6467	1.2753
35	1.0127	6.1246	5.3869-02	163.4065	1.9537
36	0.9773	16.3557	0.1240	759.1551	6.7263

**** K-VALUES: L2-L1 ****

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.2906	12.8299	2.3596	57.1464	13.7029
2	0.3071	12.0464	2.4005	48.9068	12.5994
8	0.3081	12.0016	2.4027	48.4628	12.5376

9	0.3083	11.9943	2.4031	48.3904	12.5274
10	MISSING	MISSING	MISSING	MISSING	MISSING
30	MISSING	MISSING	MISSING	MISSING	MISSING
31	MISSING	MISSING	MISSING	MISSING	MISSING
32	MISSING	MISSING	MISSING	MISSING	MISSING
33	MISSING	MISSING	MISSING	MISSING	MISSING
35	MISSING	MISSING	MISSING	MISSING	MISSING
36	MISSING	MISSING	MISSING	MISSING	MISSING

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

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.12974	0.87026	0.16409E-27	0.39169E-09	0.16455E-07
2	0.12994	0.87006	0.46413E-26	0.24998E-10	0.33122E-07
8	0.13114	0.86886	0.36933E-23	0.63387E-11	0.59719E-06
9	0.14730	0.85270	0.37305E-22	0.62072E-11	0.90099E-06
10	0.14750	0.85250	0.10696E-20	0.61997E-11	0.15588E-05
30	0.15725	0.77238	0.30381E-04	0.60013E-11	0.70331E-01
31	0.16516	0.71721	0.94356E-03	0.57087E-11	0.11669
32	0.36371	0.47061	0.28031E-01	0.23263E-12	0.13766
33	0.38935	0.38938	0.29367E-01	0.85194E-14	0.19190
35	0.47548	0.13747	0.35244E-01	0.49110E-17	0.35181
36	0.71929	0.31460E-01	0.77416E-01	0.26762E-19	0.17183

**** MASS-X1-PROFILE ****

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.86248E-01	0.91375	0.15735E-32	0.41559E-09	0.17292E-07
2	0.92193E-01	0.90781	0.76141E-28	0.26327E-10	0.34578E-07
8	0.92549E-01	0.90745	0.36718E-23	0.66837E-11	0.62405E-06
9	0.92608E-01	0.90739	0.36913E-22	0.66974E-11	0.95953E-06
10	0.14750	0.85250	0.10696E-20	0.61997E-11	0.15588E-05
30	0.15725	0.77238	0.30381E-04	0.60013E-11	0.70331E-01
31	0.16516	0.71721	0.94356E-03	0.57087E-11	0.11669
32	0.36371	0.47061	0.28031E-01	0.23263E-12	0.13766
33	0.38935	0.38938	0.29367E-01	0.85194E-14	0.19190
35	0.47548	0.13747	0.35244E-01	0.49110E-17	0.35181
36	0.71929	0.31460E-01	0.77416E-01	0.26762E-19	0.17183

**** MASS-X2-PROFILE ****

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.80645	0.19355	0.27174E-26	0.19764E-10	0.34295E-08
2	0.79933	0.20067	0.85602E-25	0.14335E-11	0.73080E-08
8	0.79890	0.20110	0.40645E-23	0.36681E-12	0.13238E-06
9	0.79883	0.20117	0.41978E-22	0.36803E-12	0.20367E-06
10	0.14750	0.85250	0.10696E-20	0.61997E-11	0.15588E-05
30	0.15725	0.77238	0.30381E-04	0.60013E-11	0.70331E-01
31	0.16516	0.71721	0.94356E-03	0.57087E-11	0.11669

32	0.36371	0.47061	0.28031E-01	0.23263E-12	0.13766
33	0.38935	0.38938	0.29367E-01	0.85194E-14	0.19190
35	0.47548	0.13747	0.35244E-01	0.49110E-17	0.35181
36	0.71929	0.31460E-01	0.77416E-01	0.26762E-19	0.17183

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

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	0.11464	0.88536	0.77684E-29	0.73912E-08	0.77581E-08
2	0.12974	0.87026	0.30712E-27	0.39169E-09	0.16455E-07
8	0.13065	0.86935	0.11321E-24	0.98442E-10	0.29793E-06
9	0.13080	0.86920	0.11472E-23	0.98480E-10	0.45833E-06
10	0.14296	0.85704	0.26419E-22	0.10148E-09	0.68238E-06
30	0.14790	0.82073	0.75377E-06	0.10271E-09	0.31371E-01
31	0.15030	0.79713	0.22701E-04	0.10350E-09	0.52552E-01
32	0.15467	0.76716	0.52156E-03	0.83886E-11	0.77648E-01
33	0.16595	0.71483	0.56692E-03	0.36200E-12	0.11865
35	0.23923	0.41832	0.94330E-03	0.39872E-15	0.34151
36	0.29501	0.21593	0.40288E-02	0.85260E-17	0.48503

**** VAPORIZATION EFF ****

STAGE	H2O	MEK	2:3-B-01	1:3-B-01	3-BUT-01
1	1.0000	1.0000	1.0000	1.0000	1.0000
2	0.70000	0.70000	0.70000	0.70000	0.70000
8	0.70000	0.70000	0.70000	0.70000	0.70000
9	0.70000	0.70000	0.70000	0.70000	0.70000
10	0.70000	0.70000	0.70000	0.70000	0.70000
30	0.70000	0.70000	0.70000	0.70000	0.70000
31	0.70000	0.70000	0.70000	0.70000	0.70000
32	0.70000	0.70000	0.70000	0.70000	0.70000
33	0.70000	0.70000	0.70000	0.70000	0.70000
35	0.70000	0.70000	0.70000	0.70000	0.70000
36	0.70000	0.70000	0.70000	0.70000	0.70000

BLOCK: B16 MODEL: PUMP

INLET STREAM: 31
OUTLET STREAM: 18
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	0.118709	0.118709	0.00000
MASS(LB/HR)	8.02844	8.02844	0.00000
ENTHALPY(CAL/SEC)	-949.780	-949.093	-0.722847E-03

```
              ***  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  BAR                          7.50000
  DRIVER EFFICIENCY                           1.00000

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

                  ***  RESULTS  ***
  VOLUMETRIC FLOW RATE  L/MIN                      0.081469
  PRESSURE CHANGE  BAR                          6.25894
  NPSH AVAILABLE   M-KGF/KG                        2.80319
  FLUID POWER  KW                            0.00084985
  BRAKE POWER  KW                            0.0028744
  ELECTRICITY  KW                           0.0028744
  PUMP EFFICIENCY USED                          0.29566
  NET WORK REQUIRED  KW                          0.0028744
  HEAD DEVELOPED M-KGF/KG                          85.6693

BLOCK:  B6      MODEL: RADFRAC
-------------------------------
  INLETS   - 32       STAGE  15
  OUTLETS  - 31       STAGE   1
           9       STAGE  30
 PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS


*********************************************************************
   *                                          *
   *    ERRORS IN BLOCK CALCULATIONS                        *
   *                                          *
   *    COLUMN DRIES UP OR COLUMN FLOWS VIOLATE BUILT-IN LIMITS
*
   *                                          *

*********************************************************************
```

```
*** MASS AND ENERGY BALANCE ***
                        IN          OUT       RELATIVE DIFF.
TOTAL BALANCE
  MOLE(LBMOL/HR)        2.86644     2.87340   -0.242229E-02
  MASS(LB/HR   )        128.677     128.640    0.287973E-03
  ENTHALPY(CAL/SEC )   -22838.6    -23501.1    0.281878E-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                              30
ALGORITHM OPTION                              STANDARD
ABSORBER OPTION                               NO
INITIALIZATION OPTION                         STANDARD
HYDRAULIC PARAMETER CALCULATIONS              NO
INSIDE LOOP CONVERGENCE METHOD                BROYDEN
DESIGN SPECIFICATION METHOD                   NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS        200
MAXIMUM NO. OF INSIDE LOOP ITERATIONS         10
MAXIMUM NUMBER OF FLASH ITERATIONS            30
FLASH TOLERANCE                               0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE            0.000100000

****  COL-SPECS  ****

MOLAR VAPOR DIST / TOTAL DIST                 0.0
MASS REFLUX RATIO                             3.00000
MASS BOTTOMS RATE          LB/HR              120.618

****  PROFILES  ****

P-SPEC      STAGE  1  PRES, BAR               1.24106
```

**** TRAY VAPORIZATION EFFICIENCY ****

SEGMENT 2 10 EFFICIENCY 0.70000

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

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	31	9
COMPONENT:		
H2O	.30104E-07	1.0000
MEK	.78472E-01	.92153
1:3-B-01	.81969	.18031
3-BUT-01	.22978E-03	.99977

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	C	75.8660
BOTTOM STAGE TEMPERATURE	C	86.8378
TOP STAGE LIQUID FLOW	LBMOL/HR	0.33525
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	2.75469
TOP STAGE VAPOR FLOW	LBMOL/HR	0.0
BOILUP VAPOR FLOW	LBMOL/HR	0.286644-04
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		0.104057-04
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-443.307
REBOILER DUTY	CAL/SEC	-160.618

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

DEW POINT	6.0857	STAGE= 10	
BUBBLE POINT	0.84851	STAGE= 10	
COMPONENT MASS BALANCE	0.15332E-01	STAGE= 1	COMP=MEK
ENERGY BALANCE	0.21222	STAGE= 14	

**** PROFILES ****

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

STAGE	TEMPERATURE C	PRESSURE BAR	ENTHALPY CAL/MOL LIQUID	ENTHALPY CAL/MOL VAPOR	HEAT DUTY CAL/SEC
1	75.866	1.2411	-63362.	-55760.	-443.3071
2	60.631	1.4479	-63976.	-56172.	
3	55.619	1.4548	-64174.	-56304.	
12	75.540	1.5168	-65536.	-56137.	
13	84.378	1.5237	-65347.	-56250.	
14	84.700	1.5306	-64816.	-56273.	
15	84.943	1.5375	-65029.	-56217.	
16	85.075	1.5444	-65025.	-56214.	
27	86.505	1.6203	-64979.	-56190.	
28	86.643	1.6272	-64974.	-56190.	
29	86.818	1.6341	-64974.	-56195.	
30	86.838	1.6410	-64973.	-56177.	-160.6184

STAGE	FLOW RATE LBMOL/HR LIQUID	FLOW RATE LBMOL/HR VAPOR	FEED RATE LBMOL/HR LIQUID	FEED RATE LBMOL/HR VAPOR	FEED RATE LBMOL/HR MIXED	PRODUCT RATE LBMOL/HR LIQUID	PRODUCT RATE LBMOL/HR VAPOR
1	0.4470	0.000		0.1187			
2	0.3033	0.4470					
3	0.2977	0.4153					
12	0.2792	0.3747					
13	0.2953	0.3912					
14	0.4841	0.4073	0.5961				
15	2.764	0.2866E-04	2.2703				
16	2.766	0.1002E-01					
27	2.780	0.2402E-01					
28	2.782	0.2540E-01					
29	2.754	0.2751E-01					
30	2.755	0.2866E-04			2.7546		

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR LIQUID	FLOW RATE LB/HR VAPOR	FEED RATE LB/HR LIQUID	FEED RATE LB/HR VAPOR	FEED RATE MIXED	PRODUCT RATE LB/HR LIQUID	PRODUCT RATE LB/HR VAPOR
1	32.23	0.000		8.5597			
2	21.87	32.23					
3	21.46	29.95					
12	11.40	22.31					

13	11.81	19.47		
14	22.57	19.90	30.6468	
15	121.1	0.1446E-02	98.0299	
16	121.2	0.5052		
27	121.9	1.208		
28	122.0	1.276		
29	120.6	1.374		
30	120.6	0.1447E-02		120.6112

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

STAGE	H2O	MEK	1:3-B-01	3-BUT-01
1	0.38856E-06	1.0000	0.27702E-06	0.37304E-11
2	0.13259E-05	1.0000	0.61428E-08	0.67140E-11
3	0.44930E-05	1.0000	0.14514E-08	0.10309E-10
12	0.57851	0.42149	0.17839E-08	0.20026E-09
13	0.59344	0.40656	0.27412E-08	0.26259E-09
14	0.47118	0.52882	0.40133E-08	0.43312E-09
15	0.52316	0.47684	0.26987E-08	0.65718E-09
16	0.52311	0.47689	0.27301E-08	0.65702E-09
27	0.52252	0.47748	0.30889E-08	0.65528E-09
28	0.52248	0.47752	0.30104E-08	0.65503E-09
29	0.52361	0.47639	0.24726E-08	0.65842E-09
30	0.52361	0.47639	0.24720E-08	0.65842E-09

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

STAGE	H2O	MEK	1:3-B-01	3-BUT-01
1	0.47132E-06	0.99999	0.56803E-05	0.18433E-11
2	0.38856E-06	1.0000	0.27702E-06	0.37304E-11
3	0.10721E-05	1.0000	0.79477E-07	0.59063E-11
12	0.23236	0.76764	0.84028E-07	0.13872E-09
13	0.41294	0.58706	0.80556E-07	0.14401E-09
14	0.42993	0.57007	0.78310E-07	0.19127E-09
15	0.40059	0.59941	0.64218E-07	0.31675E-09
16	0.40079	0.59921	0.64842E-07	0.31678E-09
27	0.40330	0.59670	0.71829E-07	0.31696E-09
28	0.40452	0.59548	0.69706E-07	0.31663E-09
29	0.40954	0.59046	0.56685E-07	0.31747E-09
30	0.39975	0.60025	0.57985E-07	0.32057E-09

**** K-VALUES ****

STAGE	H2O	MEK	1:3-B-01	3-BUT-01
1	2.4518	0.72974	12.056	0.54383
2	1.1323	0.37039	7.4308	0.25508
3	0.90611	0.30646	6.5903	0.20501
12	0.45978	1.1332	25.510	0.39362
13	0.63372	1.5462	31.976	0.56509

14	0.82222	1.1639	21.533	0.45700
15	0.74016	1.3015	24.980	0.49340
16	0.74073	1.3007	24.927	0.49351
27	0.74700	1.2922	24.368	0.49471
28	0.74784	1.2919	24.325	0.49502
29	0.74795	1.2965	24.389	0.49695
30	0.74537	1.2919	24.295	0.49522

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

STAGE	H2O	MEK	1:3-B-01	3-BUT-01
1	0.97078E-07	1.0000	0.20781E-06	0.37304E-11
2	0.33126E-06	1.0000	0.46080E-08	0.67140E-11
3	0.11226E-05	1.0000	0.10888E-08	0.10309E-10
12	0.25535	0.74465	0.23642E-08	0.35379E-09
13	0.26723	0.73277	0.37062E-08	0.47328E-09
14	0.18208	0.81792	0.46565E-08	0.66990E-09
15	0.21514	0.78486	0.33322E-08	0.10817E-08
16	0.21510	0.78490	0.33707E-08	0.10814E-08
27	0.21470	0.78530	0.38110E-08	0.10777E-08
28	0.21468	0.78532	0.37139E-08	0.10773E-08
29	0.21544	0.78456	0.30547E-08	0.10843E-08
30	0.21544	0.78456	0.30540E-08	0.10843E-08

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

STAGE	H2O	MEK	1:3-B-01	3-BUT-01
1	0.11776E-06	1.0000	0.42611E-05	0.18433E-11
2	0.97078E-07	1.0000	0.20781E-06	0.37304E-11
3	0.26786E-06	1.0000	0.59620E-07	0.59063E-11
12	0.70310E-01	0.92969	0.76341E-07	0.16800E-09
13	0.14947	0.85053	0.87550E-07	0.20864E-09
14	0.15855	0.84145	0.86711E-07	0.28232E-09
15	0.14308	0.85692	0.68869E-07	0.45283E-09
16	0.14318	0.85682	0.69553E-07	0.45297E-09
27	0.14447	0.85553	0.77256E-07	0.45444E-09
28	0.14510	0.85490	0.75072E-07	0.45457E-09
29	0.14769	0.85231	0.61379E-07	0.45825E-09
30	0.14265	0.85735	0.62129E-07	0.45787E-09

**** VAPORIZATION EFF ****

STAGE	H2O	MEK	1:3-B-01	3-BUT-01
1	1.0000	1.0000	1.0000	1.0000
2	0.70000	0.70000	0.70000	0.70000
3	0.70000	0.70000	0.70000	0.70000
12	1.0000	1.0000	1.0000	1.0000
13	1.0000	1.0000	1.0000	1.0000
14	1.0000	1.0000	1.0000	1.0000

```
   15    1.0000      1.0000      1.0000      1.0000
   16    1.0000      1.0000      1.0000      1.0000
   27    1.0000      1.0000      1.0000      1.0000
   28    1.0000      1.0000      1.0000      1.0000
   29    1.0000      1.0000      1.0000      1.0000
   30    1.0000      1.0000      1.0000      1.0000

BLOCK:  B8      MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:            3
  OUTLET STREAM:           4
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  COLD SIDE:
  ----------
  INLET STREAM:            13
  OUTLET STREAM:           6
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                ***  MASS AND ENERGY BALANCE  ***
                             IN            OUT       RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(LBMOL/HR)           164.927        164.927        0.00000
     MASS(LB/HR   )        8264.47        8264.47        0.00000
     ENTHALPY(CAL/SEC )      -0.110065E+07   -0.110065E+07     0.00000

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

                  ***  INPUT DATA  ***

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

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

```
FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED COLD OUTLET TEMP
  SPECIFIED VALUE          C              300.0000
  LMTD CORRECTION FACTOR                  1.00000

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

HEAT TRANSFER COEFFICIENT SPECIFICATION:
  HOT LIQUID    COLD LIQUID      CAL/SEC-SQCM-K      0.0203
  HOT 2-PHASE   COLD LIQUID      CAL/SEC-SQCM-K      0.0203
  HOT VAPOR     COLD LIQUID      CAL/SEC-SQCM-K      0.0203
  HOT LIQUID    COLD 2-PHASE     CAL/SEC-SQCM-K      0.0203
  HOT 2-PHASE   COLD 2-PHASE     CAL/SEC-SQCM-K      0.0203
  HOT VAPOR     COLD 2-PHASE     CAL/SEC-SQCM-K      0.0203
  HOT LIQUID    COLD VAPOR       CAL/SEC-SQCM-K      0.0203
  HOT 2-PHASE   COLD VAPOR       CAL/SEC-SQCM-K      0.0203
  HOT VAPOR     COLD VAPOR       CAL/SEC-SQCM-K      0.0203

            ***  OVERALL RESULTS  ***

STREAMS:
            --------------------------------------
            |                          |
3     ----->|          HOT             |-----> 4
T=  5.0000D+02  |                      |     T=  3.4433D+02
P=  9.3326D-02  |                      |     P=  9.3326D-02
V=  1.0000D+00  |                      |     V=  1.0000D+00
            |                          |
6     <-----|          COLD            |<----- 13
T=  3.0000D+02  |                      |     T=  1.1938D+02
P=  9.3326D-02  |                      |     P=  9.3326D-02
V=  1.0000D+00  |                      |     V=  9.7220D-01
            --------------------------------------

DUTY AND AREA:
  CALCULATED HEAT DUTY          CAL/SEC         47333.7292
  CALCULATED (REQUIRED) AREA    SQM                1.0767
  ACTUAL EXCHANGER AREA         SQM                1.0767
  PER CENT OVER-DESIGN                          0.0000

HEAT TRANSFER COEFFICIENT:
  AVERAGE COEFFICIENT (DIRTY)   CAL/SEC-SQCM-K       0.0203
  UA (DIRTY)                CAL/SEC-K         218.5849
```

```
 LOG-MEAN TEMPERATURE DIFFERENCE:
  LMTD CORRECTION FACTOR                    1.0000
  LMTD (CORRECTED)         C              216.5462
  NUMBER OF SHELLS IN SERIES                  1

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

                 ***  ZONE RESULTS  ***

 TEMPERATURE LEAVING EACH ZONE:

                         HOT
      -------------------------------------------------------------
      |                    |                    |
HOT IN |       VAP         |        VAP         | HOT OUT
------>|                   |                    |------>
 500.0 |              352.1|                    | 344.3
      |                    |                    |
COLDOUT|       VAP         |        BOIL        | COLDIN
<------|                   |                    |<------
 300.0 |              119.4|                    | 119.4
      |                    |                    |
      -------------------------------------------------------------
                         COLD

 ZONE HEAT TRANSFER AND AREA:

 ZONE    HEAT DUTY     AREA     LMTD     AVERAGE U      UA
          CAL/SEC      SQM       C    CAL/SEC-SQCM-K  CAL/SEC-K
   1    45075.860     1.0281  215.9654   0.0203      208.7179
   2     2257.869     0.0486  228.8315   0.0203        9.8670

BLOCK:  B5      MODEL: COMPR
-----------------------------
 INLET STREAM:         4
 OUTLET STREAM:        12
 PROPERTY OPTION SET:   NRTL     RENON (NRTL) / IDEAL GAS

               ***  MASS AND ENERGY BALANCE  ***
                        IN          OUT       RELATIVE DIFF.
  TOTAL BALANCE
    MOLE(LBMOL/HR)          118.876       118.876       0.00000
    MASS(LB/HR   )       4132.23       4132.23       0.00000
```

```
    ENTHALPY(CAL/SEC )      -497652.       -373656.      -0.249162

              ***  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  ***

  ISENTROPIC CENTRIFUGAL COMPRESSOR
   OUTLET PRESSURE  BAR                            5.00000
   ISENTROPIC EFFICIENCY                           0.72000
   MECHANICAL EFFICIENCY                             1.00000

                   ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  KW                519.146
   BRAKE      HORSEPOWER REQUIREMENT  KW              519.146
   NET WORK REQUIRED                KW              519.146
   POWER LOSSES                  KW                0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  KW                373.785
   CALCULATED OUTLET TEMP  C                        727.249
   ISENTROPIC TEMPERATURE  C                       627.231
   EFFICIENCY (POLYTR/ISENTR) USED                     0.72000
   OUTLET VAPOR FRACTION                           1.00000
   HEAD DEVELOPED,       M-KGF/KG                 73,207.2
   MECHANICAL EFFICIENCY USED                         1.00000
   INLET HEAT CAPACITY RATIO                        1.11524
   INLET VOLUMETRIC FLOW RATE , L/MIN               494,372.
   OUTLET VOLUMETRIC FLOW RATE, L/MIN                 14,949.9
   INLET  COMPRESSIBILITY FACTOR                      1.00000
   OUTLET COMPRESSIBILITY FACTOR                        1.00000
   AV. ISENT. VOL. EXPONENT                        1.10466
   AV. ISENT. TEMP EXPONENT                         1.10466
   AV. ACTUAL VOL. EXPONENT                          1.13792
   AV. ACTUAL TEMP EXPONENT                           1.13792

 BLOCK:  B25      MODEL: HEATX
 -----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:            43
  OUTLET STREAM:           44
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
```

```
COLD SIDE:
----------
INLET STREAM:            45
OUTLET STREAM:           41
PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

              ***  MASS AND ENERGY BALANCE  ***
                        IN             OUT       RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(LBMOL/HR)           1354.39        1354.39        0.00000
   MASS(LB/HR   )           26390.4        26390.4        0.00000
   ENTHALPY(CAL/SEC )      -0.879639E+07   -0.879639E+07   -0.211751E-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               C                 500.0000
  LMTD CORRECTION FACTOR                          1.00000

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

HEAT TRANSFER COEFFICIENT SPECIFICATION:
  HOT LIQUID    COLD LIQUID     CAL/SEC-SQCM-K         0.0203
  HOT 2-PHASE   COLD LIQUID     CAL/SEC-SQCM-K         0.0203
  HOT VAPOR     COLD LIQUID     CAL/SEC-SQCM-K         0.0203
```

```
  HOT LIQUID    COLD 2-PHASE    CAL/SEC-SQCM-K         0.0203
  HOT 2-PHASE   COLD 2-PHASE    CAL/SEC-SQCM-K         0.0203
  HOT VAPOR     COLD 2-PHASE    CAL/SEC-SQCM-K         0.0203
  HOT LIQUID    COLD VAPOR      CAL/SEC-SQCM-K         0.0203
  HOT 2-PHASE   COLD VAPOR      CAL/SEC-SQCM-K         0.0203
  HOT VAPOR     COLD VAPOR      CAL/SEC-SQCM-K         0.0203

              ***  OVERALL RESULTS  ***

 STREAMS:
          -------------------------------------
          |                            |
 43   ----->|          HOT            |-----> 44
 T=  5.9333D+02  |                     |    T=  5.1000D+02
 P=  1.0000D+00  |                     |    P=  1.0000D+00
 V=  1.0000D+00  |                     |    V=  1.0000D+00
          |                            |
 41   <-----|          COLD           |<----- 45
 T=  5.0000D+02  |                     |    T=  5.0000D+01
 P=  9.3326D-02  |                     |    P=  9.3326D-02
 V=  1.0000D+00  |                     |    V=  1.0000D+00
          -------------------------------------

 DUTY AND AREA:
  CALCULATED HEAT DUTY          CAL/SEC          120933.1843
  CALCULATED (REQUIRED) AREA    SQM                   2.5913
  ACTUAL EXCHANGER AREA         SQM                   2.5913
  PER CENT OVER-DESIGN                                0.0000

 HEAT TRANSFER COEFFICIENT:
  AVERAGE COEFFICIENT (DIRTY)   CAL/SEC-SQCM-K         0.0203
  UA (DIRTY)                    CAL/SEC-K            526.0756

 LOG-MEAN TEMPERATURE DIFFERENCE:
  LMTD CORRECTION FACTOR                               1.0000
  LMTD (CORRECTED)              C                    229.8780
  NUMBER OF SHELLS IN SERIES                           1

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

              ***  ZONE RESULTS  ***

 TEMPERATURE LEAVING EACH ZONE:
```

```
                    HOT
      ------------------------------------------------------------
      |                                         |
HOT IN  |                 VAP                   | HOT OUT
------> |                                       |------>
 593.3  |                                       | 510.0
      |                                         |
COLDOUT |                 VAP                   | COLDIN
<------ |                                       |<------
 500.0  |                                       |  50.0
      |                                         |
      ------------------------------------------------------------
                    COLD
```

ZONE HEAT TRANSFER AND AREA:

ZONE	HEAT DUTY CAL/SEC	AREA SQM	LMTD C	AVERAGE U CAL/SEC-SQCM-K	UA CAL/SEC-K
1	120933.184	2.5913	229.8780	0.0203	526.0756

Appendix C: Orochem Contact

We were recommended to consider a relatively new technology that the company Orochem has invented to separate alcohols and hydrocarbons from water. Our team talked to an Orochem representative, Dr. Anil Oroskar, and acquired some theoretical details about this new technology. For our process which produces 14,730 metric tons of BDO per year and 29,460 metric tons of ethanol per year, the approximate capitol cost of such a piece of equipment would be 10-14 million, so the value of $12 million was used for a semi-conservative estimate. In addition, there would be yearly operation costs of approximate $25 dollars per metric ton of BDO produced, which would result in operating expenses of $359,450 per year. The adsorbent used in the process, which is a proprietary Orochem technology, has a guaranteed life of 5 years, but then it needs to be recharged by an Orochem employee at an approximate cost of $700,000 per recharge.

Appendix D: Problem Statement

11. Bio-Butadiene from Waste Carbon Monoxide
(recommended by Stephen M. Tieri, DuPont)

1,3-Butadiene is a material with a wide variety of applications in the arena of synthetic materials and polymers; for the production of synthetic rubbers, as a copolymer additive, and as an ingredient in rocket fuel. For your company, it is a critical feedstock to support and maintain the continuity of Nylon 6,6 production, via nickel-catalyzed hydrocyanation to produce adiponitrile (ADN). Previously, 2,3-butanediol (BDO) was a feedstock for butadiene production for synthetic rubber; however, this production technology was abandoned in favor of the more cost-effective naphtha-based technology route.

Current forecasts estimate 17-20% average annual growth for bioplastics through 2016, driven by a mix of internal and external market forces. Your company's interest in biopolymers is motivated by a number of factors; including consumer demand, a business desire for feedstock diversification, the increasing price of fossil materials, as a hedge for petroleum market volatility, and to positively impact global climate change.

Through research efforts and in cooperation with its partners, your company has developed and acquired innovative technology to produce bio-based 1,3-butadiene by a two-step process from carbon monoxide. The first step converts waste carbon monoxide via fermentation to 2,3-butanediol (BDO). Specifically, the research group developed a microorganism which is the catalyst and basis for this bio-based production route. The second step thermo-catalytically converts the 2,3-butanediol to 1,3-butadiene. As the butadiene from this technology has the identical structure and functionality of traditional petrochemical butadiene, it serves as a direct replacement to produce renewably sourced polymers without modifications to existing downstream equipment or processes. Early technology successes resulted in supplemental research funding awarded through government grants, which have provided partial funding for development and pilot production programs.

There are a variety of potential sources to provide the necessary CO feed, including CO- rich gas streams from thermochemical gasification of forestry and agricultural residues and other types of waste. However, also, the source of CO can be an industrial process, such as ferrous metal products manufacturing. Existing steel mills produce CO-rich gas streams, which are well suited to complement your fermentation technology. An important technology and business advantage is the input gas flexibility of your technology to utilize any single or combination of four waste gasses from an integrated steel mill, a basic oxygen furnace (BOF), a blast furnace, and coke-oven manufacturing processes.

Operation of the company's 2,3-BDO pilot plant has been extremely successful, achieving all of its technology targets and goals. More specifically, the pilot plant demonstrated its target production of 100 M gpy (M = 1,000), the capability to use "raw" steel waste gas, and to tolerate the full range of gas contaminants. Additionally, the technology demonstrated both the ability to tolerate variations in gas composition and achieved production rate targets necessary for commercial viability.

Recovery and isolation of the intermediate 2,3-BDO from fermentation broth using convention distillation separation techniques present significant challenges with respect to process energy consumption, and subsequently economic competitiveness.

Current development studies in the area of separations indicate a high potential for chromatographic separation, and/or membrane technologies, to provide the required 2,3-BDO isolation with a significant reduction in energy requirements compared to distillation alternatives.

Many historical catalysts for dehydration of 2,3-BDO to 1,3-butadiene also produce, and potentially favor, methylethylketone (MEK). While both butadiene and MEK produced from your Bio-BDO are valuable monomers, your main interest is in butadiene to support ADN production. Your partner's catalyst technology group has identified and developed new commercially-viable heterogeneous catalysts for the thermo-catalytic conversion of butadiene, and is continuing work to optimize conversion, selectivity, and yield. Demonstrated conversion data for preliminary catalyst formulations production is included in the table below.

Now that the research, development, and pilot-plant teams have succeeded in achieving their milestone targets, corporate leadership is eager to proceed to design the first commercial-scale production facility. Your company and its technology-development partners intend to use this technology to attract additional investors and industrial partners for both feedstock supply and sustainably branded intermediates and polymers. Your company expects to build and operate this commercial facility, in addition to some future sister facilities, and does not currently plan to license this specific technology as an additional revenue source.

Your project team has been assembled to commercialize this new sustainable technology and design the first commercial-scale plant. Its business objective is to design a commercial-scale facility to produce polymer grade 1,3-butadiene from "raw" steel plant waste gas from an integrated steel manufacturing facility. Your Bio-Butadiene production facility will be co-located with an existing steel/ferrous metal production plant. Your team will need to identify the optimal Bio-Butadiene plant capacity/scale for economic viability, for maximum profitability, and for matching the waste gas supply capacity from an integrated steel mill, and to quantify the economic sensitivity of the process design and scale. While the current business intention is to target medium to large-size steel mills for future facilities, the scope of your team's work includes verifying the extent to which this steel mill capacity range is a reasonable target. The 1,3-butadiene product purity and quality will need to meet or exceed current commercial requirements for polymer grade material, to be acceptable for internal use and for additional sales to perspective external customers. As your technology has the potential for global application, the business team is interested in understanding the potential economic differences between locating on existing steel production sites in China, Japan, and the United States; and to identify the optimal location for the first plant.

Product	*BDO Conversion*	*Selectivity*	*Yield*
1,3-Butadiene	94% ϭϯ– 49%	66% ϭϯ– 33%	61% ϭϯ– 21%

The plant design should be as environmentally-friendly as possible, as required by state and federal emissions legislation. Process materials should be recovered and recycled 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. As the process technology integration and design team, you will be there for the start-up and will have to live with whatever design decisions you have made.

Undoubtedly, you will need additional data and information beyond that given here and listed in the references below. Cite any literature data used. If required, make reasonable assumptions, state them, and quantify the extent to which your design or economics are sensitive to the assumptions you have made.

Appendix E: Heat Exchanger Design

This shell-and-tube heat exchanger is for Section 000. The feed is calculated at one tenth of that actually required, so this is used as a basis but does not appear in our final design.

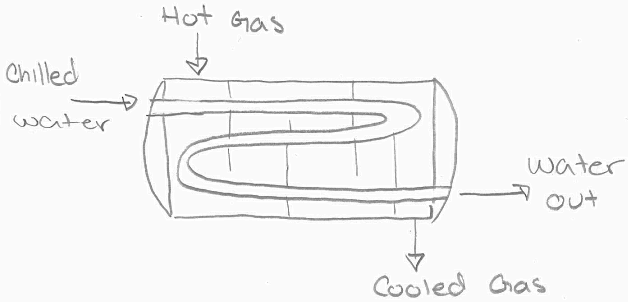
Exhaust gas cooling

Liquid - Gas Heat exchanger

- Shell + tube

tubes : 3/4 inch OD
16 ft long
1-inch triangular spacing
16 BWG ⇒ 0.620 inch ID
} typical assumptions

neglect wall resistance



Assuming the steel mill uses hot exhaust gas to get energy before we use it ⇒ Hot gas @ 482°F

Chilled water is used as a coolant in this exchanger.

Gas comes in @ 482°F, 31,000 lb/hr

Gas leaves @ 98°F, 31,000 lb/hr, 22 psi

⇒ Figure out pressure needed at inlet

	Gas 482°F	Gas 290°F	Gas 98°F	Chilled water 88°F	Chilled water 66.5°F	Chilled water 45°F
C_p (BTU/lb°F)	0.3116	0.3073	0.303	0.998	1.001	1.003
μ (Cp)	0.0260	0.0218	0.0175	0.2381	0.3401	0.4420

Sp. gr. to air = 1.061

density of air = 0.0752 lb/ft³

density of water = 62.4 lb/ft³

Sp. gr. = 1

@ 482, Gas Cp

$(0.42)(0.254371\ \text{BTU/lbR})\,CO + (0.20)(0.246011\ \text{BTU/lbR})\,CO_2$
$+ (0.36)(0.253296\ \text{BTU/lbR})\,N_2 + (0.02)(3.468044\ \text{BTU/lbR})\,H_2$
$= 0.3116$ BTU/lbR

@ 98°F, Gas Cp

$= 0.303$ BTU/lbR

heat duty

$Q = m C_p \Delta T$

$= 31{,}000$ lb gas $\cdot 0.3072 \cdot (482°F - 98°F)$

$= 3.66 \times 10^6$ BTU/hr

$3.66 \times 10^6 \frac{BTU}{hr} = m\,(1.001$ BTU/lb hr$)(88°F - 45°F)$

mass flow of chilled water

= **84,959 lbs/hr** chilled water

ΔT_{Lm}

$= \frac{\Delta T_1 - \Delta T_2}{\ln(\Delta T_1/\Delta T_2)} = \frac{(482-88)-(98-45)}{\ln((482-88)/(98-45))}$

$=$ **170° F**

Note: this side is liquid with a relatively small ΔT, so ΔP is not interesting.

$F_T = \frac{\sqrt{R^2+1}\,\ln[(1-S)/(1-RS)]}{(R-1)\ln\left[\frac{[2-S(R+1-\sqrt{R^2+1})]}{[2-S(R+1+\sqrt{R^2+1})]}\right]}$

$R = \frac{T_{hot,in} - T_{hot,out}}{T_{cold,out} - T_{cold,in}} = \frac{482-98}{88-45} = 8.93$

$S = \frac{T_{cold,out} - T_{cold,in}}{T_{hot,in} - T_{cold,in}} = \frac{88-45}{482-45} = 0.0984$

$F_T = 0.867 > 0.85$

$Q = U A F_T \Delta T_{Lm}$

U for this system ~ 35 BTU/°F-ft²-hr (Table 18.5, Seider et Al)

$A = \frac{Q}{U F_T \Delta T_{Lm}} = \frac{3.66 \times 10^6 \text{ BTU/hr}}{(35 \text{ BTU/°F·ft}^2\text{hr})(0.867)(170)}$

$=$ **709 ft²**

Tube design

$A_t = \pi D_i L$

$= \pi(0.62/12)(16 ft)$

$= 2.60$ ft²/pass

$N_t = \frac{A}{A_t \cdot 4 \text{ passes}} = \frac{709 \text{ ft}^2}{2.60 \text{ ft}^2 \cdot 4} =$ **69 tubes** 4 passes

69 tubes/pass $= \frac{4(A_{c1})}{\pi D_i^2} = \frac{4(A_{c1})}{\pi(0.62/12)^2}$ $A_{c1} = 0.143$ ft²

$A_{c1} = \frac{m_i}{\rho_i v_i} = \frac{84{,}959 \text{ lbs/hr}}{(62.4 \text{ lb/ft}^3)\, v_i \text{ (ft/hr)}}$ **$v_i = 9{,}519$ ft/hr**

Shell design

69 tubes • 4 passes

= 276 tubes

ID = $21\frac{1}{4}$ inch

tubes at centerline = 21

$N_R = 0.5(24\frac{1}{4}) = 10$

baffle spacing

$b_{min} = \frac{1}{5}\ ID = 4\frac{1}{4}$

$b_{max} = ID = 21\frac{1}{4}$

⇒ 18 inch baffle spacing

$\frac{16\ ft}{(18/12)} = 10$ baffles total

Pressure drop

$$-\Delta P = K_S \frac{2N_R f' G_S^2}{g_c \rho \Phi} \qquad \Phi = 1, \quad K_S = 1.10(1 + \#\text{ of baffles}) = 12.1$$

$$b = 0.44 + \frac{0.08\,X_L}{(X_T - 1)^{0.43 + 1.13/X_L}}$$

$$f' = b\left(\frac{D_o G_S}{\mu_b}\right)^{-0.15}$$

$$X_T = X_L = \frac{P_t}{D_o} = \frac{1.00}{0.75} = 1.33$$

$b = 0.4836$

$$G_S = \frac{m_o}{\frac{D_S}{P_t} \cdot c \cdot b_{space}} = \frac{31{,}000\ lb/hr}{(37/1)(0.75/12)(18/12)} = 26{,}811$$

$$f' = 0.4836\left(\frac{0.75/12 \cdot 26{,}811}{0.000672\ ft^s/cp \cdot 0.0218\ cp \cdot 3600\ s}\right)^{-0.15}$$

$= 0.102$

$$-\Delta P_S = \frac{12.1 \cdot 2(10)(0.102)(26{,}811)^2}{32.2 \cdot (3600\ s/hr)^2 (1.061)(0.0752)} \Big/ 144\ inch^2/ft$$

$= 3.70$ psi

Need exit pressure to be at 22 psi, which means the inlet temperature will be greater.

Inlet P = 30 psi, T = 770°F

Assumption: ΔP will not exceed 8 psi

New $T_{hot,in}$

C_p (BTU/lb°F) = 0.322 @ 434 °F
μ (Cp) = 0.0299

c_p = 0.313
μ = 0.0237

$Q = mC_p\Delta T$

= 31,000 lb gas · 0.322 · (770 − 98)

= 6.71×10^6 BTU/hr

$6.71 \times 10^6 \frac{BTU}{hr} = m(1.001\ BTU/hr)(88-45)$

mass flow of chilled water

= **155,842 lbs/hr**

ΔT_{Lm} = 225°F

S = 0.0593
R = 15.6

F_T = 0.877 > 0.85

$Q = UAF_T\,\Delta T_{Lm}$

$$A = \frac{6.71\times10^6\ BTU/hr}{(35\ BTU/F\cdot ft^2\cdot hr)(0.877)(225)}$$

= **972 ft²**

Tube design

$A_t = \pi D_i L$
= 2.60 ft²/pass

$$N_t = \frac{A}{A_t \cdot 4\,passes} = \frac{972\ ft^2}{2.60\ ft^2 \cdot 4} = \boxed{93\ tubes}$$ 4 passes

$$93\ tubes/pass = \frac{4(A_{c1})}{\pi(0.62/12)^2} \qquad A_{c1} = 0.196\ ft^2$$

$$A_{c1} = \frac{m}{\rho U} = \frac{155{,}842\ lbs/hr}{(62.4)(U_i)}$$

U_i = 12,752 ft/hr

Shell design

93 tubes · 4 passes

= 372 tubes

ID = 25 inch

tubes at centerline = 25

$N_R = 0.5(25) = 12$

baffle spacing

$b_{min} = \frac{1}{5} ID = 5$

$b_{max} = ID = 25$

⇒ 20 inch baffle spacing

$\frac{16}{20/12} = 9$ baffles total

Pressure drop

$$-\Delta P = K_s \frac{2 N_R f' G_s^2}{g_c \rho \phi} \quad \phi = 1,\ K_s = 11,\ b = 0.4836$$

$$G_s = \frac{31{,}000 \text{ lb/hr}}{(25/1)(0.25/12)(20/12)} = 35{,}712$$

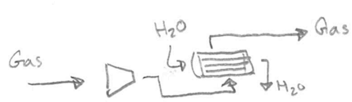
$$f' = 0.4836 \left(\frac{0.75/12 \cdot 35{,}712}{0.000672 \cdot 0.0237 \cdot 3600} \right)^{-0.15}$$

$$= 0.0991$$

$$-\Delta P = 11 \cdot \frac{2(12)(0.0991)(35{,}712)^2}{32.2 \cdot (3600 s/hr)^2 (1.061)(0.0752)} \Big/ 144 \text{ in}^2/\text{ft}$$

$$= 6.96 \text{ psi}$$

Incoming pressure is good!



Appendix F: Unit Specification Sheets

SEED FERMENTER		
IDENTIFICATION: F201		
FUNCTION: Start to grow cells		
OPERATION: Batch		
MATERIALS HANDLED:		
(lb)	Feed	Output
Butadiene	0	0
Butanediol	0	0
Cells	2.2*10^-7	0.018
Steel Mill Gas	220	220
Water	83.4	83.4
Media	8.3	8.3
Total	**311.7**	**311.7**
MATERIALS HANDLED:		
(lb/hr)	Feed	Output
Steel Mill Gas	9.2	9.2
Total	9.2	9.2
DESIGN DATA:		
Material:	Carbon Steel	
Pressure:	22 psig	
Temperature:	98.6 F	
Height:	2.8 ft	
Diameter:	0.95 ft	
Volume:	15 gallons	
PURCHASE COST: 5,897		

FERMENTER		
IDENTIFICATION: F202		
FUNCTION: Continue growing cells		
OPERATION: Batch		
MATERIALS HANDLED:		
(lb)	Feed	Output
Butadiene	0	0
Butanediol	0	0
Cells	0.018	0.18
Steel Mill Gas	1896	1896
Water	796	796
Media	80	80
Total	**2772**	**2772**
MATERIALS HANDLED:		
(lb/hr)	Feed	Output
Steel Mill Gas	79	79
Total	**79**	**79**
DESIGN DATA:		
Material:	Carbon Steel	
Pressure:	22 psig	
Temperature:	98.6 F	
Height:	5.8 ft	
Diameter:	1.93 ft	
Volume:	130 gallons	
PURCHASE COST: 11,837		

FERMENTER		
IDENTIFICATION: F203		
FUNCTION: Continue growing cells		
OPERATION: Batch		
MATERIALS HANDLED:		
(lb)	Feed	Output
Butadiene	0	0
Butanediol	0	0
Cells	0.18	2
Steel Mill Gas	19345	19345
Water	9009	9009
Media	901	899
Total	**29255**	**29255**
MATERIALS HANDLED:		
(lb/hr)	Feed	Output
Steel Mill Gas	806	806
Total	**806**	**806**
DESIGN DATA:		
Material:	Carbon Steel	
Pressure:	22 psig	
Temperature:	98.6 F	
Height:	12.5 ft	
Diameter:	4.15 ft	
Volume:	1320 gallons	
PURCHASE COST: 29,677		

FERMENTER		
IDENTIFICATION: F204		
FUNCTION: Continue growing cells		
OPERATION: Batch		
MATERIALS HANDLED:		
(lb)	Feed	Output
Butadiene	0	0
Butanediol	0	0
Cells	2	18
Steel Mill Gas	193440	193440
Water	23800	23800
Media	2380	2364
Total	**45527**	**45527**
MATERIALS HANDLED:		
(lb/hr)	Feed	Output
Steel Mill Gas	8060	8060
Total	**8060**	**8060**
DESIGN DATA:		
Material:	Carbon Steel	
Pressure:	22 psig	
Temperature:	98.6 F	
Height:	26.7 ft	
Diameter:	8.9 ft	
Volume:	13200 gallons	
PURCHASE COST: 86,528		

FERMENTER		
IDENTIFICATION: F205		
FUNCTION: Continue growing cells		
OPERATION: Batch		
MATERIALS HANDLED:		
(lb)	Feed	Output
Butadiene	0	0
Butanediol	0	0
Cells	18	67
Steel Mill Gas	659491	659472
Water	300300	300300
Media	30030	30000
Total	**989839**	**29255**
MATERIALS HANDLED:		
(lb/hr)	Feed	Output
Steel Mill Gas	27479	27478
Total	**27479**	**27478**
DESIGN DATA:		
Material:	Carbon Steel	
Pressure:	22 psig	
Temperature:	98.6 F	
Height:	40 ft	
Diameter:	13.3 ft	
Volume:	45000 gallons	
PURCHASE COST: 157,852		

CONTINUOUS STIRRED TANK REACTOR		
IDENTIFICATION: CR301		
FUNCTION: Enable continuous production of 2,3 Butanediol		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Feed	Output
Cells	80	200
Butanediol	0	400
Steel Mill Gas	30532	29532
Ethanol	0	800
Water	37500	37500
Media	4170	4050
Total	**72282**	**72282**
DESIGN DATA:		
Material:	Carbon Steel	
Pressure:	22 psig	
Temperature:	98.6 F	
Height:	58.2 ft	
Diameter:	11.6 ft	
Volume:	50,000 gallons	
PURCHASE COST: 177,920		

BLOWER	
IDENTIFICATION: B101	
FUNCTION: Provide dry media to the mixer	
OPERATION: Conditional, Continuous	
DESIGN DATA:	
Type:	Centrifugal
Driver Type:	Motor
Material:	Cast Iron
Pressure In:	14 psi
Pressure Out:	16 psi
Temperature:	60 °F
Flow Rate:	5,837 lb/hr
Efficiency:	0.72
Blade Type:	Sheet Metal
UTILITIES: Electricity (50 kW)	
PURCHASE COST: $9,320	

FILTER SCREEN	
IDENTIFICATION: FT103	
FUNCTION: Filter media to ensure it is pure	
OPERATION: Conditional, Continuous	
DESIGN DATA:	
Type:	Ultrafiltration
Flow Rate:	50,000 gallons/hr
Pressure In:	50 psi
Pressure Out:	22 psi
Contact Area:	6000 ft^2
Flux:	200 GFD
PURCHASE COST: $60,000	

FILTER SCREEN	
IDENTIFICATION: FT101	
FUNCTION: Filter media to ensure it is pure	
OPERATION: Conditional, Continuous	
DESIGN DATA:	
Type:	Ultrafiltration
Flow Rate:	50,570 gallons/hr
Pressure In:	50 psi
Pressure Out:	22 psi
Contact Area:	5060 ft^2
Flux:	200 GFD
PURCHASE COST: $50,600	

FILTER SCREEN	
IDENTIFICATION: FT102	
FUNCTION: Filter media to ensure it is pure	
OPERATION: Conditional, Continuous	
DESIGN DATA:	
Type:	Ultrafiltration
Flow Rate:	5,000 gallons/hr
Pressure In:	50 psi
Pressure Out:	22 psi
Contact Area:	600 ft^2
Flux:	200 GFD
PURCHASE COST: $6,000	

Electricity Powered Heater	
IDENTIFICATION: H102	
FUNCTION: To heat wet media before batch usage	
OPERATION: Continuous	
DESIGN DATA:	
(lb/hr)	417,600
DESIGN DATA:	
Material:	Carbon Steel
Power Usage:	3666 kW
Efficiency:	0.8
Pressure:	22
T_{in}:	68 °F
T_{out}:	98 °F
UTILITIES: Electricity (3666 kW)	
PURCHASE COST: $25,232	

Electricity Powered Heater		
IDENTIFICATION: H101		
FUNCTION: To heat wet media before batch usage		
OPERATION: Batch		
DESIGN DATA:		
	(lb/hr)	304,166
DESIGN DATA:		
	Material:	Carbon Steel
	Power Usage:	111 kW
	Efficiency:	0.8
	Pressure:	22
	T_{in}:	68 °F
	T_{out}:	98 °F
UTILITIES: Electricity (111 kW)		
PURCHASE COST: 3,308		

Mixing Tank		
IDENTIFICATION: M101		
FUNCTION: To mix dry media and water to produce wet media		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Feed	Output
Butadiene		
Butanediol		
Media	41700	41700
Methyl Ethyl Ketone		
Water	375000	375000
Total	416700	416700
DESIGN DATA:		
Material:	Carbon Steel	
Pressure:	22 psig	
Temperature:	98 °F	
Height:	27.8 feet	
Diameter:	9.3 feet	
Volume:	15,000 gallons	
PURCHASE COST: $95,706		

STORAGE TANK		
IDENTIFICATION: ST101a & ST101b		
FUNCTION: To store and transport dry media		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Feed	Output
Butadiene		
Butanediol		
Media	41700	41700
Methyl Ethyl Keystone		
Water		
Total	41700	41700
DESIGN DATA:		
Material:	Carbon Steel	
Pressure:	22 psig	
Temperature:	70 °F	
Height:	41.3 ft	
Diameter:	13.8 ft	
Volume:	50,000 gallons	
PURCHASE COST: $165, 626		

PUMP	
IDENTIFICATION: P-101	
FUNCTION: Pump wet media to CSTRs	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	921.5 gpm
Pressure In:	21 psi
Pressure Out:	50 psi
Efficiency:	0.74
UTILITIES: Electricity (11.05 kW)	
PURCHASE COST: $4794	

PUMP	
IDENTIFICATION: P-102	
FUNCTION: Pump wet media to batch fermentation reactors	
OPERATION: Batch	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	737.7 gpm
Pressure In:	21 psi
Pressure Out:	50 psi
Efficiency:	0.75
UTILITIES: Electricity (13.5 kW)	
PURCHASE COST: $4475	

PUMP	
IDENTIFICATION: P-201	
FUNCTION: Pump wet media to batch fermentation reactors	
OPERATION: Batch	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	0.02 gpm
Pressure In:	22 psi
Pressure Out:	23 psi
Efficiency:	0.3
UTILITIES: Electricity (2.3×10^{-5} kW)	
PURCHASE COST: $3000	

PUMP	
IDENTIFICATION: P-202	
FUNCTION: Pump wet media to batch fermentation reactors	
OPERATION: Batch	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	0.02 gpm
Pressure In:	22 psi
Pressure Out:	23 psi
Efficiency:	0.3
UTILITIES: Electricity (2.9×10^{-4} kW)	
PURCHASE COST: $4390	

PUMP	
IDENTIFICATION: P-203	
FUNCTION: Pump wet media to batch fermentation reactors	
OPERATION: Batch	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	1.8 gpm
Pressure In:	22 psi
Pressure Out:	23 psi
Efficiency:	0.3
UTILITIES: Electricity (2.4×10^{-3} kW)	
PURCHASE COST: $9478	

PUMP
IDENTIFICATION: P-204
FUNCTION: Pump wet media to batch fermentation reactors
OPERATION: Batch
DESIGN DATA: Type: Centrifugal Material: Carbon Steel Flow Rate: 4.8 gpm Pressure In: 22 psi Pressure Out: 23 psi Efficiency: 0.3
UTILITIES: Electricity ($6.5x10^{-3}$ kW)
PURCHASE COST: $6152

PUMP
IDENTIFICATION: P205
FUNCTION: Pump wet media to batch fermentation reactors
OPERATION: Batch
DESIGN DATA: Type: Centrifugal Material: Carbon Steel Flow Rate: 30 gpm Pressure In: 22 psi Pressure Out: 23 psi Efficiency: 0.35
UTILITIES: Electricity (0.03 kW)
PURCHASE COST: $3540

\\\

PUMP	
IDENTIFICATION: P-301	
FUNCTION: Pump wet media to batch fermentation reactors	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	92 gpm
Pressure In:	22 psi
Pressure Out:	50 psi
Efficiency:	0.5
UTILITIES: Electricity (2 kW)	
PURCHASE COST: $3000	

PUMP	
IDENTIFICATION: P-401	
FUNCTION: Pump wet media to batch fermentation reactors	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	692 gpm
Pressure In:	22 psi
Pressure Out:	50 psi
Efficiency:	0.73
UTILITIES: Electricity (10 kW)	
PURCHASE COST: $4391	

HEAT EXCHANGER			
IDENTIFICATION: HX001			
FUNCTION: Cool steel mill gas to 98°F at 22 psi			
OPERATION: Continuous			
MATERIALS HANDLED:			
	(lb/hr)	Hot Side	Cold Side
	Steel Mill Gas	0	310,000
	Water	849,600	0
	Total	849,600	310,000
DESIGN DATA:			
	Type:	Shell-and-tube	
	Material:	Carbon Steel	
	Heat Transfer Area:	972	
	Length:	16	
	U:	35 BTU/ft²-hr-°F	
	Heat Duty:	6,710,000 BTU/hr	
	Pressure Drop	7 psi	
		Hot Side	Cold Side
	T_{in}:	770	45
	T_{out}:	98	88
PURCHASE COST: $68,300			

COMPRESSOR		
IDENTIFICATION: C001		
FUNCTION: Compress hot flue gas from steel mill to 30 psi		
OPERATION: Continuous		
DESIGN DATA:		
	Type:	Centrifugal
	Driver Type:	Motor
	Material:	Cast Iron
	Pressure In:	14 psi
	Pressure Out:	30 psi
	Temperature In:	482 °F
	Temperature Out:	770 °F
	Flow Rate:	310,000 lb/hr
	Efficiency:	0.72
	Driver Power:	1301 HP
UTILITIES: Electricity (8751 kW)		
PURCHASE COST: $7,585,000		

REACTOR				
IDENTIFICATION: R501				
FUNCTION: Thermo Catalytic Conversion				
OPERATION: Continuous				
MATERIALS HANDLED:				
	(lb/hr)	Feed	Effluent	
	Butadiene	0	1538	
	Butanediol	4128	129	
	Methyl Vinyl Carbinol	0	284	
	Methyl Ethyl Ketone	0	866	
	Water	5	1316	
	Total	4133	4133	
DESIGN DATA:				
	Type:	Shell-and-packed tube	Tube Diameter:	1 inch
	Material:	Carbon Steel	Tube Length:	20 ft
	Catalyst Type:	Thorium Oxide	Number of Tubes:	1557
	Catalyst Mass:	2219 lb	Shell Diameter:	55 inch
	Temperature:	932 °F	Number of Shells:	1
	Pressure In:	1 psi	Residence Time:	1.4 s
	Pressure Out:	1 psi		
CATALYST COST: $1,927,700				
PURCHASE COST: $212,210				

CENTRIFUGAL PUMP		
IDENTIFICATION: P501		
FUNCTION: Continuous		
OPERATION: Pump higher pressure water to the heat exchanger		
DESIGN DATA:		
	Type:	Centrifugal
	Material:	Carbon Steel
	Flow Rate:	3000 lb/hr
	Pressure In:	15 psi
	Pressure Out:	20 psi
	Efficiency:	0.3
	Head:	19.6 ft
UTILITIES: Electricity (0.055 kW)		
PURCHASE COST: $14,750		

REFLUX PUMP		
IDENTIFICATION: D603		
FUNCTION: Reflux to the third distillation column		
OPERATION: Continuous		
DESIGN DATA:		
	Type:	Centrifugal
	Material:	Carbon Steel
	Flow Rate:	6729 lb/hr
	Efficiency:	0.7
	Head:	100 ft
UTILITIES: Electricity (0.48 kW)		
PURCHASE COST: $11,320		

REFLUX PUMP		
IDENTIFICATION: D601		
FUNCTION: To pump reflux back to the first distillation column		
OPERATION: Continuous		
DESIGN DATA:		
	Type:	Centrifugal
	Material:	Carbon Steel
	Flow Rate:	8202 lb/hr
	Efficiency:	0.7
UTILITIES: Electricity (0.64 kW)		
PURCHASE COST: $11,065		

REFLUX PUMP	
IDENTIFICATION: D602	
FUNCTION: To pump reflux to the second distillation column	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	5440 lb/hr
Efficiency:	0.7
UTILITIES: Electricity (0.68 kW)	
PURCHASE COST: $12,225	

PUMP	
IDENTIFICATION: P706	
FUNCTION: To pump feed at 109 psi to D701	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	1355 lb/hr
Pressure In:	18 psi
Pressure Out:	109 psi
Efficiency:	0.3
UTILITIES: Electricity (0.45 kW)	
PURCHASE COST: $12,640	

REFLUX PUMP	
IDENTIFICATION: D401	
FUNCTION: Pump reflux to the BDO separation distillation column	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	26,612 lb/hr
Efficiency:	0.7
UTILITIES: Electricity (1.41 kW)	
PURCHASE COST: $11,000	

REFLUX PUMP	
IDENTIFICATION: D701	
FUNCTION: Pump reflux to the fourth distillation tower	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	6910 lb/hr
Efficiency:	0.7
UTILITIES: Electricity (0.6 kW)	
PURCHASE COST: $11,160	

REFLUX PUMP	
IDENTIFICATION: D702	
FUNCTION: Pump reflux to the fifth distillation column	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	6041 lb/hr
Efficiency:	0.7
UTILITIES: Electricity (0.66 kW)	
PURCHASE COST: $11,190	

PUMP	
IDENTIFICATION: P701	
FUNCTION: Pump feed to D701 at 109 psi	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Centrifugal
Material:	Carbon Steel
Flow Rate:	930 lb/hr
Pressure In:	17
Pressure Out:	109
Efficiency:	0.3
UTILITIES: Electricity (0.33 kW)	
PURCHASE COST: $13,450	

HEAT EXCHANGER		
IDENTIFICATION: HX504		
FUNCTION: Recover heat from compression to use for a rebuilder		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	1538	0
Butanediol	128	0
Methyl Vinyl Carbinol	284	0
Methyl Ethyl Ketone	865	0
Water	1316	3000
Total	4132	3000
DESIGN DATA:		
Type:	Shell-and-tube	
Material:	Carbon Steel	
Heat Transfer Area:	446 ft^2	
U:	150 (BTU/hr-ft^2-R)	
Length:	20 ft	
Heat Duty:	4,061,080 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	1341	90
T_{out}:	194	760
PURCHASE COST: $101,600		

VACUUM SYSTEM	
IDENTIFICATION: VS501	
FUNCTION: Reduce the pressure of streams leading into the reactor vessel	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Two-stage steam-jet ejector
Material:	Carbon Steel
Flow Rate:	4132 lb/hr
Pressure Out:	70 mmHg
Size Factor:	59.0 lb/hr*torr
Air Leakage:	14.2 lb/hr
UTILITIES: HP Steam ($516,000) CW ($84,000)	
PURCHASE COST: $17,991	

HEAT EXCHANGER		
IDENTIFICATION: D603		
FUNCTION: Condense distillate of third distillation column		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	0	0
Butanediol	4	0
Methyl Vinyl Carbinol	0	0
Methyl Ethyl Ketone	1	0
Water	66	3000
Total	71	3000
DESIGN DATA:		
Type:	Total Condenser	
Material:	Carbon Steel	
Heat Transfer Area:	134 ft^2	
Length:	20 ft	
Heat Duty:	226,218 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	240	90
T_{out}:	191	120
PURCHASE COST: $5700		

HEAT EXCHANGER		
IDENTIFICATION: D601		
FUNCTION: Condense the distillate form the first distillation tower		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	1539	0
Butanediol	0	0
Methyl Vinyl Carbinol	0	0
Methyl Ethyl Ketone	4	0
Water	7	8880
Total	1550	8880
DESIGN DATA:		
Type:	Total Condenser	
Material:	Carbon Steel	
Heat Transfer Area:	244 ft^2	
Length:	20 ft	
Heat Duty:	74586 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	137	90
T_{out}:	107	120
PURCHASE COST: $91,450		

HEAT EXCHANGER		
IDENTIFICATION: D602		
FUNCTION: Totally condense the distillate of the second distillation column		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	0	0
Butanediol	0	0
Methyl Vinyl Carbinol	0	0
Methyl Ethyl Ketone	809	0
Water	121	2487
Total	930	2487
DESIGN DATA:		
Type:	Total Condenser	
Material:	Carbon Steel	
Heat Transfer Area:	89 ft^2	
Length:	20 ft	
Heat Duty:	78,510 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	198	90
T_{out}:	170	120
PURCHASE COST: $5,340		

HEAT EXCHANGER			
IDENTIFICATION: D401			
FUNCTION: Totally condense the distillation column separating ethanol and butanediol			
OPERATION: Continuous			
MATERIALS HANDLED:			
	(lb/hr)	Hot Side	Cold Side
	Butadiene	0	0
	Butanediol	4	0
	Methyl Vinyl Carbinol	0	0
	Methyl Ethyl Ketone	0	0
	Ethanol	7992	0
	Water	0	17,602
	Total	7996	17,902
DESIGN DATA:			
	Type:	Total Condenser	
	Material:	Carbon Steel	
	Heat Transfer Area:	401 ft^2	
	Length:	20 ft	
	Heat Duty:	527,850	
	Pressure Drop	0	
		Hot Side	Cold Side
	T_{in}:	226	90
	T_{out}:	206	120
PURCHASE COST: $99,230			

HEAT EXCHANGER		
IDENTIFICATION: HX501		
FUNCTION: Heat feed to reactor during start-up conditions		
OPERATION: Conditional, Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	0	0
Butanediol	4128	0
Methyl Vinyl Carbinol	0	0
Methyl Ethyl Ketone	0	0
Water	4	0
Total	4132	N/A
DESIGN DATA:		
Type:	Electric	
Material:	Carbon Steel	
Heat Transfer Area:	129	
Length:	20	
Heat Duty:	47,334 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	257	N/A
T_{out}:	572	N/A
PURCHASE COST: $5,70		

HEAT EXCHANGER		
IDENTIFICATION: D701		
FUNCTION: Totally condense the distillate to the fourth distillation tower		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	0	0
Butanediol	0	0
Methyl Vinyl Carbinol	0	0
Methyl Ethyl Ketone	1234	0
Water	241	7579
Total	1475	7579
DESIGN DATA:		
Type:	Total Condenser	
Material:	Carbon Steel	
Heat Transfer Area:	65 ft^2	
Length:	20 ft	
Heat Duty:	227,278 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	310	90
T_{out}:	278	120
PURCHASE COST: $5,090		

HEAT EXCHANGER		
IDENTIFICATION: D702		
FUNCTION: Totally condense the distillate from the fifth distillation tower		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	0	0
Butanediol	0	0
Methyl Vinyl Carbinol	0	0
Methyl Ethyl Ketone	1234	0
Water	121	7250
Total	1255	7250
DESIGN DATA:		
Type:	Total Condenser	
Material:	Carbon Steel	
Heat Transfer Area:	109 ft^2	
Length:	20 ft	
Heat Duty:	210,330 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	205	90
T_{out}:	173	120
PURCHASE COST: $5,560		

HEAT EXCHANGER		
IDENTIFICATION: HX502		
FUNCTION: Preheat the feed to the reactor with the effluent heat from the reactor		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	0	1538
Butanediol	4128	128
Methyl Vinyl Carbinol	0	284
Methyl Ethyl Ketone	0	866
Water	4	1316
Total	4132	4132
DESIGN DATA:		
Type:	Shell-and-tube	
Material:	Carbon Steel	
Heat Transfer Area:	12 ft^2	
Length:	20 ft	
U:	150 BTU/hr-ft^2-R	
Heat Duty:	47,334 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	932	245
T_{out}:	652	572
PURCHASE COST: $3,854		

REFLUX ACCUMULATOR	
IDENTIFICATION: D603	
FUNCTION: Accumulate reflux from the third distillation tower	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Horizontal Drum
Material:	Carbon Steel
Diameter:	3 ft
Length:	9 ft
Capacity:	476 gallons
Temperature:	191 °F
Pressure:	35 psi
PURCHASE COST: $57,215	

REFLUX ACCUMULATOR	
IDENTIFICATION: D601	
FUNCTION: Accumulate reflux from the first distillation tower	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Horizontal Drum
Material:	Carbon Steel
Diameter:	3 ft
Length:	9 ft
Capacity:	476 gallons
Temperature:	107 °F
Pressure:	76 psi
PURCHASE COST: $57,215	

REFLUX ACCUMULATOR	
IDENTIFICATION: D602	
FUNCTION: Accumulate reflux from the second distillation tower	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Horizontal Drum
Material:	Carbon Steel
Diameter:	3 ft
Length:	9 ft
Capacity:	476 gallons
Temperature:	169 °F
Pressure:	35 psi
PURCHASE COST: $57,215	

REFLUX ACCUMULATOR		
IDENTIFICATION: D401		
FUNCTION: Accumulate reflux from the ethanol-butanediol separation tower		
OPERATION: Continuous		
DESIGN DATA:		
	Type:	Horizontal Drum
	Material:	Carbon Steel
	Diameter:	3 ft
	Length:	9 ft
	Capacity:	317 gallons
	Temperature:	206 °F
	Pressure:	35 psi
PURCHASE COST: $52,347		

REFLUX ACCUMULATOR		
IDENTIFICATION: D701		
FUNCTION: Accumulate reflux from the fourth horizontal drum		
OPERATION: Continuous		
DESIGN DATA:		
	Type:	Horizontal Drum
	Material:	Carbon Steel
	Diameter:	3 ft
	Length:	9 ft
	Capacity:	476 gallons
	Temperature:	279 °F
	Pressure:	112 psi
PURCHASE COST: $57,215		

REFLUX ACCUMULATOR		
IDENTIFICATION: D702		
FUNCTION: Accumulate reflux from the fifth distillation tower		
OPERATION: Continuous		
DESIGN DATA:		
	Type:	Horizontal Drum
	Material:	Carbon Steel
	Diameter:	3 ft
	Length:	9 ft
	Capacity:	475 gallons
	Temperature:	173 °F
	Pressure:	35 psi
PURCHASE COST: $57,215		

REBOILER		
IDENTIFICATION: D603		
FUNCTION: Phase change, reboiler for the third column		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	0	4
Butanediol	0	127
Methyl Vinyl Carbinol	0	0
Methyl Ethyl Ketone	0	0
Water	0	1
High Pressure Steam	1863	0
Total	1863	132
DESIGN DATA:		
Type:	U-tube	
Material:	Carbon Steel	
Heat Transfer Area:	1645 ft^2	
Length:	20	
Heat Duty:	3,745,450 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	298	252
T_{out}:	298	324
PURCHASE COST: $159,330		

REBOILER			
IDENTIFICATION: D601			
FUNCTION: Reboiler to the first distillation column			
OPERATION: Continuous			
MATERIALS HANDLED:			
	(lb/hr)	Hot Side	Cold Side
	Butadiene	0	0
	Butanediol	0	128
	Methyl Vinyl Carbinol	0	284
	Methyl Ethyl Ketone	0	861
	Water	0	1309
	Medium Pressure Steam	422	0
	Total	422	2582
DESIGN DATA:			
	Type:	U-tube	
	Material:	Carbon Steel	
	Heat Transfer Area:	88 ft^2	
	Length:	20 ft	
	Heat Duty:	794,185 BTU/hr	
	Pressure Drop	0	
		Hot Side	Cold Side
	T_{in}:	366	280
	T_{out}:	366	282
PURCHASE COST: $5,340			

REBOILER		
IDENTIFICATION: D401		
FUNCTION: Reboiler to the ethanol-butanediol separation tower		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	0	0
Butanediol	0	3996
Methyl Vinyl Carbinol	0	0
Methyl Ethyl Ketone	0	0
Ethanol	0	8
Water	0	0
Low Pressure Steam	4507	0
Total	4507	4004
DESIGN DATA:		
Type:	U-tube	
Material:	Carbon Steel	
Heat Transfer Area:	1034 ft^2	
Length:	20 ft	
Heat Duty:	9,061,920 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	298	328
T_{out}:	298	389
PURCHASE COST: $131,080		

REBOILER		
IDENTIFICATION: D701		
FUNCTION: Reboiler to the fourth distillation tower		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	0	0
Butanediol	0	0
Methyl Vinyl Carbinol	0	0
Methyl Ethyl Ketone	0	809
Water	0	0
Medium Pressure Steam	1045	0
Total	1045	809
DESIGN DATA:		
Type:	U-tube	
Material:	Carbon Steel	
Heat Transfer Area:	933 ft^2	
Length:	20 ft	
Heat Duty:	1,961,140 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	366	346
T_{out}:	366	347
PURCHASE COST: $126,320		

REBOILER		
IDENTIFICATION: D702		
FUNCTION: Reboiler for the fifth distillation column		
OPERATION: Continuous		
MATERIALS HANDLED:		
(lb/hr)	Hot Side	Cold Side
Butadiene	0	0
Butanediol	0	0
Methyl Vinyl Carbinol	0	0
Methyl Ethyl Ketone	0	0
Water	0	121
Low Pressure Steam	673	0
Total	673	121
DESIGN DATA:		
Type:	U-tube	
Material:	Carbon Steel	
Heat Transfer Area:	78 ft^2	
Length:	20 ft	
Heat Duty:	1,352,300 BTU/hr	
Pressure Drop	0	
	Hot Side	Cold Side
T_{in}:	298	236
T_{out}:	298	237
PURCHASE COST: $5,223		

DISTILLTION COLUMN				
IDENTIFICATION: D603				
FUNCTION: Isolate 2,3-butanediol for recycle back to the reactor				
OPERATION: Continuous				
MATERIALS HANDLED:				
	(lb/hr)	Feed	Distillate	Bottoms
	Butadiene	0	0	0
	Butanediol	128	0	128
	Methyl Vinyl Carbinol	284	284	0
	Methyl Ethyl Ketone	52	52	0
	Water	1189	1184	5
	Total	1653	1520	133
DESIGN DATA:				
Number of Stages:	19	Number of Trays:	17	
Overhead Pressure:	16 psi	Feed Stage:	9	
Height:	48 ft	Molar Reflux Ratio:	2	
Diameter:	4 ft	Tray Type:	Sieve	
Material:	Carbon Steel	Op. Temp:	324 °F	
Tray Efficiency:	0.7	Stage Pressure:	13 psi	
Tray Spacing:	2 ft	Pressure Drop:	0.1 psi	
PURCHASE COST: $627,785				

DISTILLTION COLUMN				
IDENTIFICATION: D601				
FUNCTION: Isolate the 1,3-butadiene product at near purity				
OPERATION: Continuous				
MATERIALS HANDLED:				
(lb/hr)	Feed		Distillate	Bottoms
Butadiene	1538		1538	128
Butanediol	127		0	0
Methyl Vinyl Carbinol	284		0	184
Methyl Ethyl Ketone	865		4	861
Water	1316		7	1309
Total	4130		1549	2482
DESIGN DATA:				
Number of Stages:	21	Number of Trays:		19
Overhead Pressure:	65 psi	Feed Stage:		9
Height:	56 ft	Molar Reflux Ratio:		3
Diameter:	1.5 ft	Tray Type:		Sieve
Material:	Carbon Steel	Op. Temp:		282 °F
Tray Efficiency:	0.7	Stage Pressure:		62 psi
Tray Spacing:	2 ft	Pressure Drop:		0.1 psi
PURCHASE COST: $605,760				

DISTILLTION COLUMN			
IDENTIFICATION: D602			
FUNCTION: Isolate the MEK for pressure-swing distillation			
OPERATION: Continuous			
MATERIALS HANDLED:			
(lb/hr)	Feed	Distillate	Bottoms
Butadiene	0	0	0
Butanediol	128	0	128
Methyl Vinyl Carbinol	284	0	284
Methyl Ethyl Ketone	861	809	52
Water	1309	12	1189
Total	2582	821	1653
DESIGN DATA:			
Number of Stages:	38	Number of Trays:	36
Overhead Pressure:	17 psi	Feed Stage:	32
Height:	114 ft	Molar Reflux Ratio:	3
Diameter:	2 ft	Tray Type:	Sieve
Material:	Carbon Steel	Op. Temp:	232 °F
Tray Efficiency:	0.7	Stage Pressure:	14 psi
Tray Spacing:	2 ft	Pressure Drop:	0.1 psi
PURCHASE COST: $712, 080			

DISTILLATION COLUMN				
IDENTIFICATION: D401				
FUNCTION: Separate 2,3-butanediol and ethanol at near purities				
OPERATION: Continuous				
MATERIALS HANDLED:				
(lb/hr)	Feed		Distillate	Bottoms
Butadiene	0		0	0
Butanediol	4000		4	3996
Methyl Vinyl Carbinol	0		0	0
Methyl Ethyl Ketone	0		0	0
Ethanol	8000		7992	8
Water	0		0	0
Total	12000		7996	4004
DESIGN DATA:				
Number of Stages:	7	Number of Trays:		5
Overhead Pressure:	29 psi	Feed Stage:		3
Height:	26 ft	Molar Reflux Ratio:		1
Diameter:	4.5 ft	Tray Type:		Sieve
Material:	Carbon Steel	Op. Temp:		232 °F
Tray Efficiency:	0.7	Stage Pressure:		29 psi
Tray Spacing:	2 ft	Pressure Drop:		0.1 psi
PURCHASE COST: $593,760				

COMPRESSOR	
IDENTIFICATION: C501	
FUNCTION: Compress cooled reactor effluent for distillation columns	
OPERATION: Continuous	
DESIGN DATA:	
Type:	Centrifugal
Driver Type:	Motor
Material:	Carbon Steel
Pressure In:	1.3 psi
Pressure Out:	73 psi
Temperature In:	652 °F
Temperature Out:	1341 °F
Flow Rate:	4321 lb/hr
Efficiency:	0.72
Driver Power:	696 HP
UTILITIES: Electricity (519 kW)	
PURCHASE COST: $902,280	

DISTILLATION COLUMN				
IDENTIFICATION: D701				
FUNCTION: First distillation tower for MEK pressure-swing distillation				
OPERATION: Continuous				
MATERIALS HANDLED:				
(lb/hr)	Feed	Recycle	Distillate	Bottoms
Butadiene	0	0	0	0
Butanediol	0	0	0	0
Methyl Vinyl Carbinol	0	0	0	0
Methyl Ethyl Ketone	809	1234	1234	809
Water	121	121	241	0
Total	930	1355	1475	809
DESIGN DATA:				
Number of Stages:	22		Number of Trays:	20
Overhead Pressure:	102 psi		Feed Stage:	6
Height:	68 ft		Molar Reflux Ratio:	3
Diameter:	2 ft		Tray Type:	Sieve
Material:	Carbon Steel		Op. Temp:	347 °F
Tray Efficiency:	0.7		Stage Pressure:	99 psi
Tray Spacing:	2 ft		Pressure Drop	0.1 psi
PURCHASE COST: $630,380				

DISTILLATION COLUMN			
IDENTIFICATION: D702			
FUNCTION: Second column in MEK pressure-swing distillation			
OPERATION: Continuous			
MATERIALS HANDLED:			
(lb/hr)	Feed	Distillate	Bottoms
Butadiene	0	0	0
Butanediol	0	0	0
Methyl Vinyl Carbinol	0	0	0
Methyl Ethyl Ketone	1234	1234	0
Water	241	121	121
Total	1475	1355	121
DESIGN DATA:			
Number of Stages:	32	Number of Trays:	30
Overhead Pressure:	18 psi	Feed Stage:	15
Height:	96 ft	Molar Reflux Ratio:	3
Diameter:	2.5 ft	Tray Type:	Sieve
Material:	Carbon Steel	Op. Temp:	239 °F
Tray Efficiency:	0.7	Stage Pressure:	15 psi
Tray Spacing:	2 ft	Pressure Drop:	0.1 psi
PURCHASE COST: $693,220			

Appendix F: MSDS Reports

SIGMA-ALDRICH sigma-aldrich.com

Material Safety Data Sheet

Version 5.2
Revision Date 04/19/2013
Print Date 04/08/2014

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	:	2,3-Butanediol
Product Number	:	B84904
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
No known OSHA hazards

Not a dangerous substance or mixture according to the Globally Harmonised System (GHS).

HMIS Classification

Health hazard:	0
Flammability:	0
Physical hazards:	1

NFPA Rating

Health hazard:	0
Fire:	2
Reactivity Hazard:	1

Health hazard:	0
Fire:	2
Reactivity Hazard:	0

Potential Health Effects

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

3. COMPOSITION/INFORMATION ON INGREDIENTS

Formula	:	$C_4H_{10}O_2$
Molecular Weight	:	90.12 g/mol

No ingredients are hazardous according to OSHA criteria.

Aldrich - B84904 Page 1 of 6

4. FIRST AID MEASURES

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

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

In case of eye contact
Flush eyes with water as a precaution.

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

5. FIREFIGHTING MEASURES

Conditions of flammability
Not flammable or combustible.

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

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Avoid dust formation. Avoid breathing vapours, mist or gas.

Environmental precautions
Do not let product enter drains.

Methods and materials for containment and cleaning up
Sweep up and shovel. Keep in suitable, closed containers for disposal.

7. HANDLING AND STORAGE

Precautions for safe handling
Provide appropriate exhaust ventilation at places where dust is formed.

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

Hygroscopic.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection
Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. 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

Aldrich - B84904 Page 2 of 6

Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
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 and safety officer 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
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin and body protection
Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Hygiene measures
General industrial hygiene practice.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	solid
Colour	no data available

Safety data

pH	9.0 - 10.0 at 500 g/l at 20 °C (68 °F)
Melting point/freezing point	Melting point/range: 25 °C (77 °F)
Boiling point	183 - 184 °C (361 - 363 °F)
Flash point	85 °C (185 °F) - closed cup
Ignition temperature	402 °C (756 °F)
Auto-ignition temperature	no data available
Lower explosion limit	3.1 %(V)
Upper explosion limit	11.4 %(V)
Vapour pressure	23 hPa (17 mmHg) at 20 °C (68 °F)
Density	1.002 g/cm3 at 20 °C (68 °F)
Water solubility	soluble
Partition coefficient: n-octanol/water	log Pow: -0.92
Relative vapour density	3.61
Odour	no data available
Odour Threshold	no data available
Evapouration 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
Acid chlorides, Acid anhydrides, Oxidizing agents, Chloroformates, Reducing agents

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

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
LD50 Oral - rat - male and female - > 5,000 mg/kg

Inhalation LC50
no data available

Dermal LD50
no data available

Other information on acute toxicity
LD50 Intraperitoneal - mouse - 6,075 mg/kg

Skin corrosion/irritation
Skin - rabbit - No skin irritation - 24 h

Serious eye damage/eye irritation
Eyes - rabbit - No eye irritation - 72 h

Respiratory or skin sensitisation
Maximisation Test - guinea pig - Does not cause skin sensitisation. - OECD Test Guideline 406

Germ cell mutagenicity

Genotoxicity in vitro - S. typhimurium - with and without metabolic activation - negative

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

no data available

Teratogenicity

no data available

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

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

Signs and Symptoms of Exposure
Gastrointestinal disturbance, Nausea, Headache, Vomiting

Synergistic effects
no data available

Additional Information
RTECS: EK0532000

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Toxicity to daphnia and other aquatic invertebrates	Immobilization EC50 - Daphnia magna (Water flea) - > 100 mg/l - 48 h Method: OECD Test Guideline 202
Toxicity to bacteria	Respiration inhibition EC50 - Sludge Treatment - > 1,000 mg/l - 0.5 h

Persistence and degradability

Biodegradability	aerobic Result: > 90 % - Readily biodegradable. Method: OECD Test Guideline 301A

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.

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
No known OSHA hazards

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
No SARA Hazards

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
Butane-2,3-diol	513-85-9	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Butane-2,3-diol	513-85-9	

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

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Material Safety Data Sheet
The Dow Chemical Company

Product Name: BUTADIENE

Issue Date: 2013.10.29
Print Date: 30 Oct 2013

The Dow Chemical Company encourages and expects you to read and understand the entire (M)SDS, as there is important information throughout the document. We expect you to follow the precautions identified in this document unless your use conditions would necessitate other appropriate methods or actions.

1. Product and Company Identification

Product Name
BUTADIENE

COMPANY IDENTIFICATION
The Dow Chemical Company
2030 Willard H. Dow Center
Midland, MI 48674
United States

For MSDS updates and Product Information: 800-258-2436

Prepared By: Prepared for use in Canada by EH&S, Hazard Communications.
Revision 2013.10.29
Print Date: 10/30/2013

Customer Information Number: 800-258-2436
SDSQuestion@dow.com

EMERGENCY TELEPHONE NUMBER

24-Hour Emergency Contact: 989-636-4400
Local Emergency Contact: 989-636-4400

2. Hazards Identification

Emergency Overview
Color: Colorless
Physical State: Liquefied gas
Odor: Ester

®(TM)*Trademark

Hazards of product:

DANGER! Extremely flammable liquid and vapor - Vapor may cause flash fire. Harmful if inhaled. May cause frostbite. May cause central nervous system effects. May cause anesthetic effects. Do not extinguish. Vapors may travel a long distance; ignition and/or flash back may occur. Evacuate area. Keep upwind of spill. Stay out of low areas. Warn public of downwind explosion hazard. Elevated temperatures can cause hazardous polymerization. Contents under pressure. Cancer hazard. Can cause cancer.

Potential Health Effects
Eye Contact: Vapor may cause eye irritation experienced as mild discomfort and redness. Liquid may cause frostbite.
Skin Contact: No hazard from gas. Liquid may cause frostbite upon skin contact.
Skin Absorption: No adverse effects anticipated by skin absorption.
Inhalation: In confined or poorly ventilated areas, vapor can readily accumulate and can cause unconsciousness and death. Excessive exposure may cause irritation to upper respiratory tract (nose and throat). May cause central nervous system effects. Symptoms of excessive exposure may be anesthetic or narcotic effects; dizziness and drowsiness may be observed.
Ingestion: Swallowing is unlikely because of the physical state. Liquid may cause frostbite of the lips and mouth.
Aspiration hazard: Based on available information, aspiration hazard could not be determined.
Effects of Repeated Exposure: In animals, effects have been reported on the following organs: Blood-forming organs (Bone marrow & Spleen). Kidney. Liver. Ovaries. Respiratory tract. Testes.
Cancer Information: Has caused cancer in laboratory animals. Butadiene epidemiology studies have linked employment in two different chemical operations each with a different type of cancer. The causative factors for these excess cancers have not been determined.
Birth Defects/Developmental Effects: Has caused birth defects in laboratory animals only at doses toxic to the mother. Has been toxic to the fetus in laboratory animals at doses toxic to the mother.

3. Composition/information on ingredients

Component	CAS #	Amount W/W
1,3-Butadiene	106-99-0	> 99.5 %

Amounts are presented as percentages by weight.

4. First-aid measures

Description of first aid measures

General advice: First Aid responders should pay attention to self-protection and use the recommended protective clothing (chemical resistant gloves, splash protection). If potential for exposure exists refer to Section 8 for specific personal protective equipment.
Inhalation: Move person to fresh air. If not breathing, give artificial respiration; if by mouth to mouth use rescuer protection (pocket mask, etc). If breathing is difficult, oxygen should be administered by qualified personnel. Call a physician or transport to a medical facility.
Skin Contact: In case of frostbite, immediately flush skin with plenty of water for 15 minutes. Seek medical attention. Suitable emergency safety shower facility should be immediately available.
Eye Contact: In case of frostbite, immediately flush eyes with water; remove contact lenses, if present, after the first 5 minutes, then continue flushing eyes for at least 15 minutes. Obtain medical attention promptly, preferably from an ophthalmologist. Suitable emergency eye wash facility should be immediately available.

Ingestion: If swallowed, seek medical attention. Do not induce vomiting unless directed to do so by medical personnel. In case of frostbite, immediately rinse lips and mouth with tepid water for at least 15 minutes. Obtain medical attention promptly.

Most important symptoms and effects, both acute and delayed

Aside from the information found under Description of first aid measures (above) and Indication of immediate medical attention and special treatment needed (below), no additional symptoms and effects are anticipated.

Indication of immediate medical attention and special treatment needed

Maintain adequate ventilation and oxygenation of the patient. Treat for frostbite, if present. No specific antidote. Treatment of exposure should be directed at the control of symptoms and the clinical condition of the patient.

5. Fire Fighting Measures

Suitable extinguishing media

Do not extinguish. Stop flow of product and allow fire to burn out. Once product flow has stopped, small fires may be extinguished with: Water fog or fine spray. Dry chemical fire extinguishers. Carbon dioxide fire extinguishers. Foam.

Special hazards arising from the substance or mixture

Hazardous Combustion Products: During a fire, smoke may contain the original material in addition to combustion products of varying composition which may be toxic and/or irritating. Combustion products may include and are not limited to: Carbon monoxide. Carbon dioxide.
Unusual Fire and Explosion Hazards: Container may vent and/or rupture due to fire. Vapors are heavier than air and may travel a long distance and accumulate in low lying areas. Ignition and/or flash back may occur.

Advice for firefighters

Fire Fighting Procedures: Keep people away. Isolate fire and deny unnecessary entry. Stay upwind. Keep out of low areas where gases (fumes) can accumulate. Do not extinguish. If flames are accidentally extinguished, explosive re-ignition may occur. Use water spray to cool fire exposed containers and fire affected zone until fire is out and danger of reignition has passed. Fight fire from protected location or safe distance. Consider the use of unmanned hose holders or monitor nozzles. Immediately withdraw all personnel from the area in case of rising sound from venting safety device or discoloration of the container. Eliminate ignition sources. For spills of liquefied gas, apply appropriate foam or vapor suppressing agent. Warning! Contact of water with liquefied gas can result in boiling, frothing, and rapid generation of vapor. For unignited vapor cloud, use water spray to knock down and control dispersion of vapors.
Special Protective Equipment for Firefighters: Wear positive-pressure self-contained breathing apparatus (SCBA) and protective fire fighting clothing (includes fire fighting helmet, coat, trousers, boots, and gloves). If protective equipment is not available or not used, fight fire from a protected location or safe distance.

See Section 9 for related Physical Properties

6. Accidental Release Measures

Personal precautions, protective equipment and emergency procedures: Evacuate area. Refer to Section 7, Handling, for additional precautionary measures. Only trained and properly protected personnel must be involved in clean-up operations. Keep personnel out of low areas. Keep personnel out of confined or poorly ventilated areas. Keep upwind of spill. Ventilate area of leak or spill. No smoking in area. For large spills, warn public of downwind explosion hazard. Check area with

combustible gas detector before reentering area. Ground and bond all containers and handling equipment. Eliminate all sources of ignition in vicinity of spill or released vapor to avoid fire or explosion. Vapor explosion hazard. Keep out of sewers. Spills of this liquefied gas may form ice, which can plug drains and can make valves inoperable. Contact of water with liquefied gas can result in boiling, frothing, and rapid generation of vapor. See Section 10 for more specific information. Use appropriate safety equipment. For additional information, refer to Section 8, Exposure Controls and Personal Protection.

Environmental precautions: Prevent from entering into soil, ditches, sewers, waterways and/or groundwater. See Section 12, Ecological Information.

Methods and materials for containment and cleaning up: Isolate area until gas has dispersed. Stop flow of gas. Ground and bond all containers and handling equipment. Use fine water spray to reduce vapors. If available, use foam to smother or suppress vapors. Apply vapor suppression foams until spill can be cleaned up. Knock down and dilute vapors with water fog or spray. See Section 13, Disposal Considerations, for additional information.

7. Handling and Storage

Handling

General Handling: Keep away from heat, sparks and flame. Avoid contact with eyes, skin, and clothing. Avoid breathing vapor. Never use air pressure for transferring product. No smoking in area. Electrically bond and ground all containers and equipment before transfer or use of material. Contents under pressure. Do not puncture or incinerate container. Containers, even those that have been emptied, can contain vapors. Do not cut, drill, grind, weld, or perform similar operations on or near empty containers. Use of non-sparking or explosion-proof equipment may be necessary, depending upon the type of operation. Wash thoroughly after handling. Keep container closed. Use only with adequate ventilation. See Section 8, EXPOSURE CONTROLS AND PERSONAL PROTECTION. This product is a poor conductor of electricity and can become electrostatically charged, even in bonded or grounded equipment. If sufficient charge is accumulated, ignition of flammable mixtures can occur. Handling operations that can promote accumulation of static charges include but are not limited to mixing, filtering, pumping at high flow rates, splash filling, creating mists or sprays, tank and container filling, tank cleaning, sampling, gauging, switch loading, vacuum truck operations.
Other Precautions: Vapors are heavier than air and may travel a long distance and accumulate in low lying areas. Ignition and/or flash back may occur.

Storage

No smoking, open flames or sources of ignition in handling and storage area. Uninhibited monomer vapors can polymerize and plug relief devices. Maintain inhibitor level. This product is inhibited with: 4-tert-Butylcatechol Purge oxygen from storage vessels before filling. Hold bulk storage under nitrogen blanket. See Section 10 for more specific information.

8. Exposure Controls / Personal Protection

Exposure Limits

Component	List	Type	Value
1,3-Butadiene	CAD AB OEL	TWA	4.4 mg/m3 2 ppm
	CAD BC OEL	TWA	2 ppm
	CAD ON OEL	TWAEV	2 ppm
	ACGIH	TWA	2 ppm
	OEL (QUE)	TWA	4.4 mg/m3 2 ppm Exposure must be minimized.
	OEL (QUE)	TWA	4.4 mg/m3 2 ppm Exposure must be minimized.

Consult local authorities for recommended exposure limits.

Personal Protection

Eye/Face Protection: For handling the gas, wear safety glasses (with side shields). When contact with the liquid (condensed gas) is possible, wear chemical goggles. If exposure causes eye discomfort, use a full-face respirator.
Skin Protection: Wear clean, body-covering clothing.
Hand protection: Use an insulated glove for protection from liquid contact of the skin that may cause frostbite due to rapid cooling.
Respiratory Protection: Respiratory protection should be worn when there is a potential to exceed the exposure limit requirements or guidelines. If there are no applicable exposure limit requirements or guidelines, use an approved respirator. Selection of air-purifying or positive-pressure supplied-air will depend on the specific operation and the potential airborne concentration of the material. For emergency conditions, use an approved positive-pressure self-contained breathing apparatus. In confined or poorly ventilated areas, use an approved self-contained breathing apparatus or positive pressure air line with auxiliary self-contained air supply. The following should be effective types of air-purifying respirators: Organic vapor cartridge.
Ingestion: No precautions necessary due to the physical properties of the material.

Engineering Controls

Ventilation: Use engineering controls to maintain airborne level below exposure limit requirements or guidelines. If there are no applicable exposure limit requirements or guidelines, use only in enclosed systems or with local exhaust ventilation. Exhaust systems should be designed to move the air away from the source of vapor/aerosol generation and people working at this point. Lethal concentrations may exist in areas with poor ventilation.

9. Physical and Chemical Properties

Appearance	
Physical State	Liquefied gas
Color	Colorless
Odor	Ester
Odor Threshold	1.6 ppm *Literature*
pH	Not applicable
Melting Point	-108.9 °C *Literature*
Freezing Point	-108.9 °C *Literature*
Boiling Point (760 mmHg)	-4.41 °C *Literature* .
Flash Point - Closed Cup	-76.2 °C *Literature* Flammable gas., (CRC)
Evaporation Rate (Butyl Acetate = 1)	No test data available
Flammability (solid, gas)	Extremely flammable gas.
Flammable Limits In Air	**Lower**: 2.0 %(V) *Literature* **Upper**: 12.0 %(V) *Literature*
Vapor Pressure	2,170 kPa @ 16.85 °C *Literature*
Vapor Density (air = 1)	1.9 @ 60 °F *Literature*
Specific Gravity (H2O = 1)	0.62 *Literature*
Solubility in water (by weight)	0.735 g/l @ 20 °C *Literature*
Partition coefficient, n-octanol/water (log Pow)	1.99 *Measured*
Autoignition Temperature	1,013 hPa 420 °C *Literature*
Decomposition Temperature	No test data available
Dynamic Viscosity	0.14 mPa.s *Literature*
Explosive properties	no data available
Oxidizing properties	no data available
Liquid Density	5.2 lb/gal @ 15 °C *Literature*
Percent Volatiles	100 %(m) *Literature*

Henry's Law Constant (H)	7.36E-02 atm*m3/mole; 25 °C Measured

10. Stability and Reactivity

Reactivity
No dangerous reaction known under conditions of normal use.

Chemical stability
Stable under recommended storage conditions. See Storage, Section 7. Unstable at elevated temperatures. Dimerizes readily.

Possibility of hazardous reactions
Can occur. Elevated temperatures can cause hazardous polymerization. Maintain inhibitor level. Monomer contaminated with peroxides can form polymer at ambient conditions. Dry polymer containing peroxides at greater than 15% concentration can be detonated by slight mechanical shock or heat. Polymerization can be catalyzed by: Air. Peroxides. Rust. This product is inhibited with: p-Tertiary butylcatechol.

Conditions to Avoid: Avoid contact with air to prevent formation of explosive peroxides. Avoid static discharge.

Incompatible Materials: Avoid contact with: Air. Oxidizers. Rust. Avoid unintended contact with: Peroxides.

Hazardous decomposition products
Decomposition products depend upon temperature, air supply and the presence of other materials. Processing may release fumes and other decomposition products. At temperatures exceeding melt temperatures, polymer fragments can be released. Fumes can be irritating.

11. Toxicological Information

Acute Toxicity
Ingestion
LD50, rat 5,480 mg/kg
Dermal
As product: The dermal LD50 has not been determined.
Inhalation
LC50, 4 h, rat 285 mg/l
Eye damage/eye irritation
Vapor may cause eye irritation experienced as mild discomfort and redness. Liquid may cause frostbite.
Skin corrosion/irritation
No hazard from gas. Liquid may cause frostbite upon skin contact.
Sensitization
Skin
No relevant data found.
Respiratory
No relevant data found.
Repeated Dose Toxicity
In animals, effects have been reported on the following organs: Blood-forming organs (Bone marrow & Spleen). Kidney. Liver. Ovaries. Respiratory tract. Testes.
Chronic Toxicity and Carcinogenicity
Has caused cancer in laboratory animals. Butadiene epidemiology studies have linked employment in two different chemical operations each with a different type of cancer. The causative factors for these excess cancers have not been determined.

Carcinogenicity Classifications:

Component	List	Classification
1,3-Butadiene	ACGIH	Suspected human carcinogen.; Group A2
	IARC	Carcinogenic to humans.; 1

Developmental Toxicity
Has caused birth defects in laboratory animals only at doses toxic to the mother. Has been toxic to the fetus in laboratory animals at doses toxic to the mother.
Reproductive Toxicity
In animal studies, did not interfere with reproduction.
Genetic Toxicology
In vitro genetic toxicity studies were positive. Animal genetic toxicity studies were positive.

12. Ecological Information

Toxicity

Material is slightly toxic to aquatic organisms on an acute basis (LC50/EC50 between 10 and 100 mg/L in the most sensitive species tested).

Fish Acute & Prolonged Toxicity
LC50, Pimephales promelas (fathead minnow), 96 h: 45 mg/l

Persistence and Degradability

Biodegradation may occur under aerobic conditions (in the presence of oxygen).
Indirect Photodegradation with OH Radicals

Rate Constant	Atmospheric Half-life	Method
6.66E-11 cm3/s	1.9 h	Estimated.

Theoretical Oxygen Demand: 3.26 mg/mg

Bioaccumulative potential
Bioaccumulation: Bioconcentration potential is low (BCF < 100 or Log Pow < 3).
Partition coefficient, n-octanol/water (log Pow): 1.99 Measured
Bioconcentration Factor (BCF): 13; Fish; Measured

Mobility in soil
Mobility in soil: Potential for mobility in soil is very high (Koc between 0 and 50).
Partition coefficient, soil organic carbon/water (Koc): 44 - 228 Estimated.
Henry's Law Constant (H): 7.36E-02 atm*m3/mole; 25 °C Measured

13. Disposal Considerations

DO NOT DUMP INTO ANY SEWERS, ON THE GROUND, OR INTO ANY BODY OF WATER. All disposal practices must be in compliance with all Federal, State/Provincial and local laws and regulations. Regulations may vary in different locations. Waste characterizations and compliance with applicable laws are the responsibility solely of the waste generator. AS YOUR SUPPLIER, WE HAVE NO CONTROL OVER THE MANAGEMENT PRACTICES OR MANUFACTURING PROCESSES OF PARTIES HANDLING OR USING THIS MATERIAL. THE INFORMATION PRESENTED HERE PERTAINS ONLY TO THE PRODUCT AS SHIPPED IN ITS INTENDED CONDITION AS DESCRIBED IN MSDS SECTION: Composition Information. FOR UNUSED & UNCONTAMINATED PRODUCT, the preferred options include sending to a licensed, permitted: Incinerator or other thermal destruction device.

14. Transport Information

TDG Small container
Proper Shipping Name: BUTADIENES, STABILIZED
Hazard Class: 2.1 **ID Number:** UN1010

TDG Large container
Proper Shipping Name: BUTADIENES, STABILIZED
Hazard Class: 2.1 **ID Number:** UN1010

IMDG
Proper Shipping Name: BUTADIENES, STABILIZED
Hazard Class: 2.1 **ID Number:** UN1010
EMS Number: F-D,S-U
Marine pollutant: No
Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
Product Name: Butadiene
Ship Type: Not available
Pollution Category: N/A

ICAO/IATA
Proper Shipping Name: BUTADIENES, STABILIZED
Hazard Class: 2.1 **ID Number:** UN1010**Cargo Packing Instruction:** 200

PASSENGER AIRCRAFT SHIPMENTS ARE FORBIDDEN BY ICAO/IATA REGULATIONS.

15. Regulatory Information

US. Toxic Substances Control Act
All components of this product are on the TSCA Inventory or are exempt from TSCA Inventory requirements under 40 CFR 720.30
CEPA - Domestic Substances List (DSL)
All substances contained in this product are listed on the Canadian Domestic Substances List (DSL) or are not required to be listed.
Hazardous Products Act Information: CPR Compliance
This product has been classified in accordance with the hazard criteria of the Canadian Controlled Products Regulations (CPR) and the MSDS contains all the information required by the CPR.

Hazardous Products Act Information: WHMIS Classification

A	Compressed Gas
B1	Flammable Gas
D2A	Material Causes Chronic Toxic Effects at Repeated Low Doses
D2A	Possible, Probable or Known Human Carcinogen According to Classifications By IARC or ACGIH

Hazardous Products Act Information: Hazardous Ingredients
This product contains the following ingredients which are Controlled Products and/or are on the Ingredient Disclosure List (Canadian HPA Section 13 and 14).

Component	CAS #	Amount W/W
1,3-Butadiene	106-99-0	99.5%

16. Other Information

Recommended Uses and Restrictions

Identified uses

A reactive monomer - Raw material for industrial use. We recommend that you use this product in a manner consistent with the listed use. If your intended use is not consistent with the stated use, please contact your sales or technical service representative.

Revision

Identification Number: 79557 / 1001 / Issue Date 2013.10.29 / Version: 4.1
Most recent revision(s) are noted by the bold, double bars in left-hand margin throughout this document.

Legend

N/A	Not available
W/W	Weight/Weight
OEL	Occupational Exposure Limit
STEL	Short Term Exposure Limit
TWA	Time Weighted Average
ACGIH	American Conference of Governmental Industrial Hygienists, Inc.
DOW IHG	Dow Industrial Hygiene Guideline
WEEL	Workplace Environmental Exposure Level
HAZ_DES	Hazard Designation
VOL/VOL	Volume/Volume

The Dow Chemical Company urges each customer or recipient of this (M)SDS to study it carefully and consult appropriate expertise, as necessary or appropriate, to become aware of and understand the data contained in this (M)SDS and any hazards associated with the product. The information herein is provided in good faith and believed to be accurate as of the effective date shown above. However, no warranty, express or implied, is given. Regulatory requirements are subject to change and may differ between various locations. It is the buyer's/user's responsibility to ensure that his activities comply with all federal, state, provincial or local laws. The information presented here pertains only to the product as shipped. Since conditions for use of the product are not under the control of the manufacturer, it is the buyer's/user's duty to determine the conditions necessary for the safe use of this product. Due to the proliferation of sources for information such as manufacturer-specific (M)SDSs, we are not and cannot be responsible for (M)SDSs obtained from any source other than ourselves. If you have obtained an (M)SDS from another source or if you are not sure that the (M)SDS you have is current, please contact us for the most current version.

MATERIAL SAFETY DATA SHEET

1. CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

MATHESON TRI-GAS, INC.
150 Allen Road Suite 302
Basking Ridge, New Jersey 07920
Information: 1-800-416-2505

Emergency Contact:
CHEMTREC 1-800-424-9300
Calls Originating Outside the US:
703-527-3887 (Collect Calls Accepted)

SUBSTANCE: CARBON MONOXIDE

TRADE NAMES/SYNONYMS:
MTG MSDS 18; CARBON OXIDE; CARBONIC OXIDE; CARBON OXIDE (CO); FLUE GAS; UN 1016; CO; MAT04290; RTECS FG3500000

CHEMICAL FAMILY: inorganic, gas

PRODUCT USE: industrial

CREATION DATE: Jan 24 1989
REVISION DATE: Dec 11 2008

2. COMPOSITION, INFORMATION ON INGREDIENTS

COMPONENT: CARBON MONOXIDE
CAS NUMBER: 630-08-0
PERCENTAGE: 100

3. HAZARDS IDENTIFICATION

NFPA RATINGS (SCALE 0-4): HEALTH=3 FIRE=4 REACTIVITY=0

EMERGENCY OVERVIEW:
COLOR: colorless
PHYSICAL FORM: gas
ODOR: odorless
MAJOR HEALTH HAZARDS: harmful if inhaled, blood damage, difficulty breathing
PHYSICAL HAZARDS: Flammable gas. May cause flash fire.

POTENTIAL HEALTH EFFECTS:
INHALATION:

SHORT TERM EXPOSURE: changes in body temperature, changes in blood pressure, nausea, vomiting, chest pain, difficulty breathing, irregular heartbeat, headache, drowsiness, fatigue, dizziness, disorientation, hallucinations, pain in extremities, tremors, loss of coordination, hearing loss, visual disturbances, eye damage, bluish skin color, suffocation, blood disorders, convulsions, coma
LONG TERM EXPOSURE: nausea, vomiting, loss of appetite, headache, dizziness, visual disturbances, blood disorders, heart disorders, heart damage, nerve damage, reproductive effects, birth defects, brain damage
SKIN CONTACT:
SHORT TERM EXPOSURE: blisters, frostbite
LONG TERM EXPOSURE: no information is available
EYE CONTACT:
SHORT TERM EXPOSURE: frostbite, blurred vision
LONG TERM EXPOSURE: no information is available
INGESTION:
SHORT TERM EXPOSURE: ingestion of a gas is unlikely
LONG TERM EXPOSURE: ingestion of a gas is unlikely

4. FIRST AID MEASURES

INHALATION: If adverse effects occur, remove to uncontaminated area. Give artificial respiration if not breathing. If breathing is difficult, oxygen should be administered by qualified personnel. Get immediate medical attention.

SKIN CONTACT: If frostbite or freezing occur, immediately flush with plenty of lukewarm water (105-115 F; 41-46 C). DO NOT USE HOT WATER. If warm water is not available, gently wrap affected parts in blankets. Get immediate medical attention.

EYE CONTACT: Contact with liquid: Immediately flush eyes with plenty of water for at least 15 minutes. Then get immediate medical attention.

INGESTION: If a large amount is swallowed, get medical attention.

NOTE TO PHYSICIAN: For inhalation, consider oxygen.

5. FIRE FIGHTING MEASURES

FIRE AND EXPLOSION HAZARDS: Severe fire hazard. Vapor/air mixtures are explosive. Containers may rupture or explode if exposed to heat.

EXTINGUISHING MEDIA: carbon dioxide, regular dry chemical

Large fires: Use regular foam or flood with fine water spray.

FIRE FIGHTING: Move container from fire area if it can be done without risk. Cool containers with water spray until well after the fire is out. Stay away from the ends of tanks. For fires in cargo or storage area: Cool containers with water from unmanned hose holder or monitor nozzles until well after fire is out. If this is impossible then take the following precautions: Keep unnecessary people away, isolate hazard area and deny entry. Let the fire burn. Withdraw immediately in case of rising sound from venting safety device or any discoloration of tanks due to fire. For tank, rail car or tank truck: Evacuation radius: 800 meters (1/2 mile). Do not attempt to extinguish fire unless flow of material can be stopped first. Flood with fine water spray. Cool containers with water. Apply water from a protected location or from a safe distance. Avoid inhalation of material or combustion by-products. Stay upwind and keep out of low areas.

FIRE FIGHTING PROTECTIVE EQUIPMENT: Wear full protective fire fighting gear including self contained breathing apparatus (SCBA) for protection against possible exposure.

FLASH POINT: Not available
LOWER FLAMMABLE LIMIT: >=12.5 % by volume
UPPER FLAMMABLE LIMIT: 74 % by volume
AUTOIGNITION: 1292 F (700 C)

6. ACCIDENTAL RELEASE MEASURES

WATER RELEASE:
Subject to California Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65). Keep out of water supplies and sewers.

OCCUPATIONAL RELEASE:
Avoid heat, flames, sparks and other sources of ignition. Stop leak if possible without personal risk. Reduce vapors with water spray. Keep unnecessary people away, isolate hazard area and deny entry. Remove sources of ignition.

7. HANDLING AND STORAGE

STORAGE: Store in accordance with all current regulations and standards. Store in a cool, dry place. Store in a well-ventilated area. Avoid direct sunlight. Avoid heat, flames, sparks and other sources of ignition. Subject to storage regulations: U.S. OSHA 29 CFR 1910.101. Keep separated from incompatible substances.

8. EXPOSURE CONTROLS, PERSONAL PROTECTION

EXPOSURE LIMITS:
CARBON MONOXIDE:
50 ppm (55 mg/m3) OSHA TWA
35 ppm (40 mg/m3) OSHA TWA (vacated by 58 FR 35338, June 30, 1993)
200 ppm (229 mg/m3) OSHA ceiling (vacated by 58 FR 35338, June 30, 1993)
25 ppm ACGIH TWA
35 ppm (40 mg/m3) NIOSH recommended TWA 10 hour(s)

200 ppm (229 mg/m3) NIOSH recommended ceiling

VENTILATION: Ventilation equipment should be explosion-resistant if explosive concentrations of material are present. Provide local exhaust or process enclosure ventilation system. Ensure compliance with applicable exposure limits.

EYE PROTECTION: For the gas: Eye protection not required, but recommended. For the liquid: Wear splash resistant safety goggles. Contact lenses should not be worn. Provide an emergency eye wash fountain and quick drench shower in the immediate work area.

CLOTHING: For the gas: Protective clothing is not required. For the liquid: Wear appropriate protective, cold insulating clothing.

GLOVES: Wear insulated gloves.

RESPIRATOR: The following respirators and maximum use concentrations are drawn from NIOSH and/or OSHA.
350 ppm
Any supplied-air respirator.
875 ppm
Any supplied-air respirator operated in a continuous-flow mode.
1200 ppm
Any air-purifying full-facepiece respirator (gas mask) with a chin-style, front-mounted or back-mounted canister providing protection against the compound of concern.
End of service life indicator required (ESLI).
Any self-contained breathing apparatus with a full facepiece.
Any supplied-air respirator with a full facepiece.
Emergency or planned entry into unknown concentrations or IDLH conditions -
Any self-contained breathing apparatus that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode.
Any supplied-air respirator with a full facepiece that is operated in a pressure-demand or other positive-pressure mode in combination with an auxiliary self-contained breathing apparatus operated in pressure-demand or other positive-pressure mode.
Escape -
Any air-purifying full-facepiece respirator (gas mask) with a chin-style, front-mounted or back-mounted canister providing protection against the compound of concern.
End of service life indicator required (ESLI).
Any appropriate escape-type, self-contained breathing apparatus.

9. PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE: gas
COLOR: colorless
ODOR: odorless
TASTE: tasteless
MOLECULAR WEIGHT: 28.01

MATHESON TRI•GAS ask. . .The Gas Professionals™

MOLECULAR FORMULA: C-O
BOILING POINT: -312.7 F (-191.5 C)
FREEZING POINT: -337 F (-205 C)
DECOMPOSITION POINT: Not available
VAPOR PRESSURE: 760 mmHg @ -191 C
VAPOR DENSITY (air=1): 0.968
SPECIFIC GRAVITY: Not applicable
DENSITY: 1.250 g/L @ 0 C
WATER SOLUBILITY: 2.3% @ 20 C
PH: Not applicable
VOLATILITY: Not applicable
ODOR THRESHOLD: Not available
EVAPORATION RATE: Not applicable
VISCOSITY: 0.01657 cP @ 0 C
COEFFICIENT OF WATER/OIL DISTRIBUTION: Not applicable
SOLVENT SOLUBILITY:
Soluble: alcohol, benzene, acetic acid, ethyl acetate, chloroform, cuprous chloride solutions

10. STABILITY AND REACTIVITY

REACTIVITY: Stable at normal temperatures and pressure.

CONDITIONS TO AVOID: Avoid heat, flames, sparks and other sources of ignition. Minimize contact with material. Avoid inhalation of material or combustion by-products. Keep out of water supplies and sewers.

INCOMPATIBILITIES: oxidizing materials, halogens, metal oxides, metals, combustible materials, lithium

HAZARDOUS DECOMPOSITION:
Thermal decomposition products: oxides of carbon

POLYMERIZATION: Will not polymerize.

11. TOXICOLOGICAL INFORMATION

CARBON MONOXIDE:
TOXICITY DATA: 1807 ppm/4 hour(s) inhalation-rat LC50
ACUTE TOXICITY LEVEL:
Toxic: inhalation
TARGET ORGANS: blood, heart, nervous system
MEDICAL CONDITIONS AGGRAVATED BY EXPOSURE: blood system disorders, heart or cardiovascular disorders, hormonal disorders, respiratory disorders
REPRODUCTIVE EFFECTS DATA: Available.

MATHESON TRI•GAS ask. . .The Gas Professionals™

ADDITIONAL DATA: Alcohol may enhance the toxic effects. May cross the placenta. Smoking may enhance the toxic effects.

12. ECOLOGICAL INFORMATION

ECOTOXICITY DATA:
FISH TOXICITY: 75000 ug/L 1 day(s) LC100 (Mortality) Orangespotted sunfish (Lepomis humilis)

INVERTEBRATE TOXICITY: No data available.

ALGAL TOXICITY: No data available.

PHYTOTOXICITY: Absorbed and metabolized by plants in varying rates dependent on ecological conditions.

FATE AND TRANSPORT:
BIODEGRADATION: Oxidation to carbon dioxide in aerobic conditions found to vary between bacteria species.

ATMOSPHERIC PROCESSES: Degraded by photochemical reactions in atmosphere.

13. DISPOSAL CONSIDERATIONS

Dispose in accordance with all applicable regulations. Subject to disposal regulations: U.S. EPA 40 CFR 262. Hazardous Waste Number(s): D001.

14. TRANSPORT INFORMATION

U.S. DOT 49 CFR 172.101:
PROPER SHIPPING NAME: Carbon monoxide, compressed
ID NUMBER: UN1016
HAZARD CLASS OR DIVISION: 2.3
LABELING REQUIREMENTS: 2.3; 2.1
QUANTITY LIMITATIONS:
PASSENGER AIRCRAFT OR RAILCAR: Forbidden
CARGO AIRCRAFT ONLY: 25 kg
ADDITIONAL SHIPPING DESCRIPTION: Toxic-Inhalation Hazard Zone D

CANADIAN TRANSPORTATION OF DANGEROUS GOODS:
SHIPPING NAME: Carbon monoxide, compressed
UN NUMBER: UN1016
CLASS: 2.3; 2.1

15. REGULATORY INFORMATION

U.S. REGULATIONS:
CERCLA SECTIONS 102a/103 HAZARDOUS SUBSTANCES (40 CFR 302.4): Not regulated.

SARA TITLE III SECTION 302 EXTREMELY HAZARDOUS SUBSTANCES (40 CFR 355 Subpart B): Not regulated.

SARA TITLE III SECTION 304 EXTREMELY HAZARDOUS SUBSTANCES (40 CFR 355 Subpart C): Not regulated.

SARA TITLE III SARA SECTIONS 311/312 HAZARDOUS CATEGORIES (40 CFR 370 Subparts B and C):
ACUTE: Yes
CHRONIC: Yes
FIRE: Yes
REACTIVE: No
SUDDEN RELEASE: Yes

SARA TITLE III SECTION 313 (40 CFR 372.65): Not regulated.

OSHA PROCESS SAFETY (29 CFR 1910.119): Not regulated.

STATE REGULATIONS:
California Proposition 65:
Known to the state of California to cause the following:
Carbon monoxide
Developmental toxicity (Jul 01, 1989)

CANADIAN REGULATIONS:
WHMIS CLASSIFICATION: A, B1, D1A, D2A.

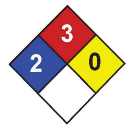
NATIONAL INVENTORY STATUS:
U.S. INVENTORY (TSCA): Listed on inventory.

TSCA 12(b) EXPORT NOTIFICATION: Not listed.

CANADA INVENTORY (DSL/NDSL): Listed on DSL.

16. OTHER INFORMATION

MATHESON TRI-GAS, INC. MAKES NO EXPRESS OR IMPLIED WARRANTIES, GUARANTEES OR REPRESENTATIONS REGARDING THE PRODUCT OR THE INFORMATION HEREIN, INCLUDING BUT NOT LIMITED TO ANY IMPLIED WARRANTY OF MERCHANTABILITY OR FITNESS FOR USE. MATHESON TRI-GAS, INC. SHALL NOT BE LIABLE FOR ANY PERSONAL INJURY, PROPERTY OR OTHER DAMAGES OF ANY NATURE, WHETHER COMPENSATORY, CONSEQUENTIAL, EXEMPLARY, OR OTHERWISE, RESULTING FROM ANY PUBLICATION, USE OR RELIANCE UPON THE INFORMATION HEREIN.



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 similiar 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 Indutrial 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

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.

Build 1.1 **Page: 3/6**

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

Build 1.1 **Page: 4/6**

Hydrogen

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

"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.

Build 1.1 **Page: 5/6**

Hydrogen

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.) :

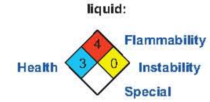
Health	0
Flammability	4
Physical hazards	0

liquid:

Health	3
Fire hazard	4
Reactivity	0
Personal protection	

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.

Build 1.1 **Page: 6/6**

SIGMA-ALDRICH sigma-aldrich.com

Material Safety Data Sheet

Version 4.1
Revision Date 01/19/2012
Print Date 04/08/2014

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	:	3-Buten-2-ol
Product Number	:	B86400
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
Flammable liquid, Irritant

GHS Classification
Flammable liquids (Category 2)
Acute toxicity, Inhalation (Category 4)
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: Danger

Hazard statement(s)

H225	Highly flammable liquid and vapour.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.

Precautionary statement(s)

P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

HMIS Classification
Health hazard: 2
Flammability: 3
Physical hazards: 0

Aldrich - B86400   Page 1 of 7

NFPA Rating
Health hazard: 2
Fire: 3
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 : Methyl vinyl carbinol

Formula : C_4H_8O
Molecular Weight : 72.11 g/mol

Component		Concentration
But-3-en-2-ol		
CAS-No.	598-32-3	-
EC-No.	209-929-8	

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
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Suitable extinguishing media
For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

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

Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

Aldrich - B86400   Page 2 of 7

Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Conditions for safe storage
Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. 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.

Eye protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin and body protection
Complete suit protecting against chemicals, Flame retardant antistatic protective 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	clear, liquid
Colour	light yellow

Safety data

pH	no data available
Melting point/freezing point	no data available
Boiling point	96 - 97 °C (205 - 207 °F) - lit.
Flash point	16 °C (61 °F) - closed cup
Ignition temperature	no data available
Autoignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	no data available
Density	0.832 g/cm3 at 25 °C (77 °F)
Water solubility	no data available
Partition coefficient: n-octanol/water	no data available
Relative vapour 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

Vapours may form explosive mixture with air.

Conditions to avoid
Heat, flames and sparks. Extremes of temperature and direct sunlight.

Materials to avoid
Strong oxidizing agentsStrong oxidizing agents, Strong acids, Acid chlorides, Acid anhydrides

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
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

no data available

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
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Synergistic effects
no data available

Additional Information
RTECS: EM9275050

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
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. 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)
UN number: 1987 Class: 3 Packing group: II
Proper shipping name: Alcohols, n.o.s.
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 1987 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: ALCOHOLS, N.O.S. (But-3-en-2-ol)
Marine pollutant: No

IATA
UN number: 1987 Class: 3 Packing group: II
Proper shipping name: Alcohols, n.o.s. (But-3-en-2-ol)

15. REGULATORY INFORMATION

OSHA Hazards
Flammable liquid, Irritant

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
Fire Hazard, Acute 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
But-3-en-2-ol	598-32-3	

New Jersey Right To Know Components

	CAS-No.	Revision Date
But-3-en-2-ol	598-32-3	

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

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

SIGMA-ALDRICH sigma-aldrich.com

SAFETY DATA SHEET

Version 3.3
Revision Date 02/13/2014
Print Date 03/31/2014

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Thorium oxide

Product Number : 89170
Brand : Aldrich
REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No. : 1314-20-1

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Carcinogenicity (Category 1B), H350
Specific target organ toxicity - repeated exposure (Category 2), H373

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word: Danger

Hazard statement(s)
H301 + H311 + H331 Toxic if swallowed, in contact with skin or if inhaled
H350 May cause cancer.
H373 May cause damage to organs through prolonged or repeated exposure.

Precautionary statement(s)
P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.

P260 Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/ protective clothing.
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.
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.
P308 + P313 IF exposed or concerned: Get medical advice/ attention.
P322 Specific measures (see supplemental first aid instructions on this label).
P330 Rinse mouth.
P361 Remove/Take off immediately all contaminated clothing.
P363 Wash contaminated clothing 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.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS
Radioactive.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances
Formula : O_2Th
Molecular Weight : 264.04 g/mol
CAS-No. : 1314-20-1
EC-No. : 215-225-1

Hazardous components

Component	Classification	Concentration
Thorium dioxide		
	Acute Tox. 3; Carc. 1B; STOT RE 2; H301 + H311 + H331, H350, H373	-

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of 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. Take victim immediately to hospital. Consult a physician.

In case of eye contact
Flush eyes with water as a precaution.

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

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
no data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

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

5.2 Special hazards arising from the substance or mixture
Metal oxides

5.3 Advice for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information
no data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 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.

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 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.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place.

Keep in a dry place.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin 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.

Body Protection
Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: powder Colour: white
b)	Odour	no data available
c)	Odour Threshold	no data available
d)	pH	no data available
e)	Melting point/freezing point	no data available
f)	Initial boiling point and boiling range	no data available
g)	Flash point	no data available
h)	Evapouration rate	no data available
i)	Flammability (solid, gas)	no data available
j)	Upper/lower flammability or explosive limits	no data available
k)	Vapour pressure	no data available
l)	Vapour density	no data available
m)	Relative density	no data available
n)	Water solubility	no data available
o)	Partition coefficient: n-octanol/water	no data available
p)	Auto-ignition temperature	no data available
q)	Decomposition temperature	no data available
r)	Viscosity	no data available
s)	Explosive properties	no data available
t)	Oxidizing properties	no data available

9.2 Other safety information
no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
no data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
no data available

10.4 Conditions to avoid
no data available

10.5 Incompatible materials
no data available

10.6 Hazardous decomposition products
Other decomposition products - no data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
no data available

no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitisation
no data available

Germ cell mutagenicity
Carcinogenicity

Possible human carcinogen

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: Known to be human carcinogen (Thorium dioxide)

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
no data available

no data available

Specific target organ toxicity - single exposure
no data available

Specific target organ toxicity - repeated exposure
May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard
no data available

Additional Information
RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity
no data available

12.2 Persistence and degradability
no data available

12.3 Bioaccumulative potential
no data available

12.4 Mobility in soil
no data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Contact a licensed professional waste disposal service to dispose of this material. After use follow local procedures for radioactive waste. Consult local, state, and federal regulations on the disposal of radioactive waste. Observe all federal, state, and local environmental regulations.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 2910 Class: NONE
Proper shipping name: Radioactive material, excepted package-limited quantity of material
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 2910 Class: 7 EMS-No: F-I, S-S
Proper shipping name: RADIOACTIVE MATERIAL, EXCEPTED PACKAGE - LIMITED QUANTITY OF MATERIAL
Marine pollutant: No

IATA
UN number: 2910 Class: 7.4H
Proper shipping name: Radioactive material, excepted package - limited quantity of material

15. REGULATORY INFORMATION

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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
The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Thorium dioxide	1314-20-1	1993-04-24

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

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Thorium dioxide	1314-20-1	1993-04-24

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Thorium dioxide	1314-20-1	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
Thorium dioxide	1314-20-1	1993-04-24

California Prop. 65 Components

	CAS-No.	Revision Date
WARNING! This product contains a chemical known to the State of California to cause cancer. Thorium dioxide	1314-20-1	2007-09-28

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Carc.	Carcinogenicity
H301	Toxic if swallowed.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled
H311	Toxic in contact with skin.
H331	Toxic if inhaled.
H350	May cause cancer.

HMIS Rating

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

NFPA Rating

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	0

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 3.3 Revision Date: 02/13/2014 Print Date: 03/31/2014

SIGMA-ALDRICH sigma-aldrich.com

SAFETY DATA SHEET

Version 4.9
Revision Date 02/26/2014
Print Date 04/14/2014

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name	:	2-Butanone
Product Number	:	443468
Brand	:	Sigma-Aldrich
Index-No.	:	606-002-00-3
REACH No.	:	A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	:	78-93-3

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company	:	Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	:	+1 800-325-5832
Fax	:	+1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 2), H225
Eye irritation (Category 2A), H319
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)

H225	Highly flammable liquid and vapour.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.

Precautionary statement(s)

P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.

Sigma-Aldrich - 443468 Page 1 of 9

P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
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/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
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.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS
Repeated exposure may cause skin dryness or cracking.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	Methyl ethyl ketone MEK Ethyl methyl ketone
Formula	:	C_4H_8O
Molecular Weight	:	72.11 g/mol
CAS-No.	:	78-93-3
EC-No.	:	201-159-0
Index-No.	:	606-002-00-3

Hazardous components

Component	Classification	Concentration
Ethyl methyl ketone		
	Flam. Liq. 2; Eye Irrit. 2A; STOT SE 3; H225, H319, H336	90 - 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of 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.

Sigma-Aldrich - 443468 Page 2 of 9

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
no data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

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

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Flash back possible over considerable distance., Container explosion may occur under fire conditions.

5.3 Advice for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment.Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Store under inert gas. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Hygroscopic.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Ethyl methyl ketone	78-93-3	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Central Nervous System & Peripheral Nervous System impairment Substances for which there is a Biological Exposure Index or Indices (see BEI® section)		
		STEL	300 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Upper Respiratory Tract irritation Central Nervous System & Peripheral Nervous System impairment Substances for which there is a Biological Exposure Index or Indices (see BEI® section)		
		TWA	200 ppm 590 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	300 ppm 885 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	200 ppm 590 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	200 ppm 590 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	300 ppm 885 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Ethyl methyl ketone	78-93-3	Methyl ethyl ketone (MEK)	2 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

8.2 Exposure controls

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

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin 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.

Splash contact
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 292 min
Material tested:Butoject® (KCL 897 / Aldrich Z677647, 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 and safety officer 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.

Body Protection
impervious clothing, Flame retardant antistatic protective clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid, clear Colour: colourless
b)	Odour	no data available
c)	Odour Threshold	no data available
d)	pH	no data available
e)	Melting point/freezing point	-87 °C (-125 °F)
f)	Initial boiling point and boiling range	80 °C (176 °F) - lit.
g)	Flash point	-3 °C (27 °F) - closed cup
h)	Evapouration rate	no data available
i)	Flammability (solid, gas)	no data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 10.1 %(V) Lower explosion limit: 1.8 %(V)
k)	Vapour pressure	95 hPa (71 mmHg) at 20 °C (68 °F)
l)	Vapour density	2.49 - (Air = 1.0)
m)	Relative density	0.805 g/mL at 25 °C (77 °F)
n)	Water solubility	soluble
o)	Partition coefficient: n-octanol/water	log Pow: 0.29
p)	Auto-ignition temperature	no data available
q)	Decomposition temperature	no data available
r)	Viscosity	no data available
s)	Explosive properties	no data available
t)	Oxidizing properties	no data available

9.2 Other safety information

Surface tension	24.6 mN/m at 20 °C (68 °F)
Relative vapour density	2.49 - (Air = 1.0)

10. STABILITY AND REACTIVITY

10.1 Reactivity
no data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
Vapours may form explosive mixture with air.

10.4 Conditions to avoid
Exposure to moisture.
Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials
Oxidizing agents, Strong reducing agents

10.6 Hazardous decomposition products
Other decomposition products - no data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - rat - 2,737 mg/kg

LC50 Inhalation - mouse - 4 h - 32,000 mg/m3

LC50 Inhalation - Mammal - 38,000 mg/m3

LD50 Dermal - rabbit - 6,480 mg/kg

no data available

Skin corrosion/irritation
Skin - rabbit
Result: No skin irritation
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - rabbit
Result: Irritating to eyes.
(OECD Test Guideline 405)

Respiratory or skin sensitisation
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
no data available

no data available

Specific target organ toxicity - single exposure
May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure
no data available

Aspiration hazard
no data available

Additional Information
RTECS: EL6475000

Central nervous system depression, Gastrointestinal disturbance, narcosis

Liver - Irregularities - Based on Human Evidence
Liver - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	mortality NOEC - Cyprinodon variegatus (sheepshead minnow) - 400 mg/l - 96 h
	LC50 - Pimephales promelas (fathead minnow) - 3,130 - 3,320 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates	LC50 - Daphnia magna (Water flea) - > 520 mg/l - 48 h
	EC50 - Daphnia magna (Water flea) - 7,060 mg/l - 24 h

12.2 Persistence and degradability
no data available

12.3 Bioaccumulative potential
no data available

12.4 Mobility in soil
no data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. 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)
UN number: 1193 Class: 3 Packing group: II
Proper shipping name: Ethyl methyl ketone
Reportable Quantity (RQ): 5000 lbs
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG

UN number: 1193 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: ETHYL METHYL KETONE
Marine pollutant: No

IATA
UN number: 1193 Class: 3 Packing group: II
Proper shipping name: Ethyl methyl ketone

15. REGULATORY INFORMATION

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Ethyl methyl ketone	78-93-3	1993-04-24

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Ethyl methyl ketone	78-93-3	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
Ethyl methyl ketone	78-93-3	1993-04-24

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

Full text of H-Statements referred to under sections 2 and 3.

Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.
STOT SE	Specific target organ toxicity - single exposure

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	3
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	3
Reactivity Hazard:	0

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 4.9 Revision Date: 02/26/2014 Print Date: 04/14/2014