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Abstract

Tetrahydrofuran (THF) is an extremely valuable solvent that can also be polymerized into polytetramethylene ether glycol (PTMEG), which is the precursor for spandex fibers. Lycra®, a recognized top producer of spandex, has experienced a recent increase in Lycra® demand. Thus, the INVISTA Company has increased the production capabilities of their Gulf Coast Lycra® plant and has commissioned another THF production plant to be built on the same premises. The proposed plant will utilize a maleic acid byproduct from an internal upstream plant and will produce 100 million tons of THF per year. The THF must be at least 99.95% by mass THF, since lower purity THF contains more –OH groups that would terminate the polymerization reaction required to synthesize spandex fibers.

This report provides a thorough design and economic analysis for the manufacture of THF in the Gulf Coast. Process flow sheets and a detailed description of all utility requirements and equipment are provided and analyzed. It is shown that the plant is extremely profitable for its expected 15 year lifespan, with an expected investor's rate of return of 32.7%, return on investment of 45.9%, and net present value of $54.3 million (at a discount rate of 15%). With design commencing in 2009, construction in 2010, and operation beginning 2011, the breakeven year is expected to be 2015.

Disciplines

Chemical Engineering

HYDROGENATION OF MALEIC ACID TO TETRAHYDROFURAN

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April 14, 2009

Table of Contents

1.0 Abstract

Tetrahydrofuran (THF) is an extremely valuable solvent that can also be polymerized into polytetramethylene ether glycol (PTMEG), which is the precursor for spandex fibers. Lycra®, a recognized top producer of spandex, has experienced a recent increase in Lycra® demand. Thus, the INVISTA Company has increased the production capabilities of their Gulf Coast Lycra® plant and has commissioned another THF production plant to be built on the same premises. The proposed plant will utilize a maleic acid byproduct from an internal upstream plant and will produce 100 million tons of THF per year. The THF must be at least 99.95% by mass THF, since lower purity THF contains more –OH groups that would terminate the polymerization reaction required to synthesize spandex fibers.

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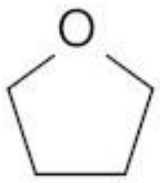
2.0 Introduction

2.1 Project Charter

Project Name	Hydrogenation of Maleic Acid to Tetrahydrofuran (THF)
Project Advisors	Mr. Wayne Robbins and Professor Warren Seider
Specific Goals	To produce 100 million pounds per year of at least 99.95 % pure THF product by mass.
Project Scope	• Develop a process to produce and purify the THF • Evaluate the economic feasibility of the design
Deliverables/Timeline	• Material Balance — Feb 3 • Flow-sheet — Feb 26 • Design of Major Equipment — Mar 24 • Completed Finances — Mar 31 • Written Report — Apr 6 • Revised Report — Apr 14 • Design Presentation — Apr 21

2.2 Product Description

Tetrahydrofuran is a colorless, water-miscible, flammable liquid with an odor resembling that of ether. Its IUPAC name is Oxacyclopentane. It is a volatile general purpose organic solvent and can be used as starting material for various chemical syntheses.



In industry, it is primarily used as a solvent for numerous polymers and resins. It also has extensive uses in the production of rubber, cellophane, adhesives, magnetic tape and printing inks. Under strongly acidic conditions, THF polymerizes to form Polytetramethylene Ether Glycol (PTMEG), which is utilized in the manufacture of various flexible and elastic fibers. THF is also present in the adhesives used to join plastic pipes for well construction and water treatment systems, and since THF is a component of food packaging adhesives, it can be an indirect food additive. It is also frequently used as a solvent in numerous pharmaceutical synthesis procedures.

THF reacts readily with oxygen to form peroxides, which are unstable and decompose in stages to produce organic acids. Therefore, to maintain the purity of THF, it must be stored away from the presence of oxygen. An increase in peroxide concentration can be detected by the appearance of color in the liquid as well as the formation of peroxide residues on the tank walls (Tetrahydrofuran (THF), 2009).

2.3 Methods of Production

The internal research and development division recommended a vapor-only reactor effluent method of producing THF. This chemical reaction process was chosen because it prevents downstream separation equipment from fouling since only volatile compounds are able to leave the reactor. The plant uses maleic acid produced in an internally-owned, upstream facility and hydrogen from pipelines in the Gulf Coast. Maleic acid is hydrogenated in an aqueous environment within a single back-mix tank reactor to form THF. Intermediates include succinic acid, gamma-butyrolactone (GBL), and 1,4-butanediol (BDO). Unfortunately, several side reactions lead to the formation of undesired products including methane, propane, n-butane, propanol, and n-butanol. Thus, an extensive separation train is required to remove the liquid intermediates, alkanes, and alcohols, and to ultimately break a water-THF azeotrope. The final product stream consists of 99.97% pure THF by mass.

2.3.1 Raw Materials

The two raw materials used in this process are hydrogen and maleic acid. Hydrogen is readily available by pipeline at 68°F and 250 psig and costs $0.75/lb. The maleic acid is produced in an internally-owned plant and is transported via pipeline at a transfer price of $0.45/lb maleic acid, on an anhydrous basis. It is available at 94°F and 5 psig and at a maximum 60% by weight maleic acid in water. At purities greater than 60%, the maleic acid begins to separate from the solution.

2.3.2 Reaction Train

Maleic acid is hydrogenated to THF via a series of simultaneous reactions in a back-mix tank reactor. The reactions are a series of hydrogenations in which bonds are broken in the reacting maleic acid and chemical intermediates. Since hydrogen gas does not readily react with the compounds, the reactor contains palladium-rhenium (Pd-Re) catalyst coated on carbon support. The carbon maximizes the available surface area for the reaction to occur and the palladium and rhenium metals provide active sites for the hydrogen to be adsorbed. Thus, hydrogen is more readily available to react when intermediates comes in contact with it.

Operating conditions of 2000 psig and 480°F were provided by the internal R&D department as ideal for the reaction. A tank reactor was selected in order to provide maximum agitation and exposure of the catalyst and hydrogen to the liquid reactants. Agitation is provided by the hydrogen bubbling from the bottom of the reactor. All reaction occurs in the liquid phase, but it was found desirable to only take a vapor product off the top of the reactor to keep downstream separation processes clean. The hydrogenation reactions are highly exothermic, and the heat of reaction is used to vaporize the THF product and other liquid compounds, allowing the reactor to operate adiabatically.

First, maleic acid (MAC) is nearly completely converted to succinic acid (SAC), which is then converted into gamma-butyrolactone (GBL), a heavy liquid intermediate. GBL is then simultaneously hydrogenated to either 1,4-butanediol (BDO), another heavy liquid intermediate, or THF. GBL is also hydrogenated into the byproducts propane, n-butane, propanol, and n-butanol, with a byproduct split of 0.15 butane and 0.85 butanol and 0.10 propane and 0.90 propanol. Byproduct splits were provided by the internal R&D department as reasonable splits given the reactor conditions. BDO is further hydrogenated to THF and forms the same byproducts with the same splits as GBL. THF also undergoes undesirable hydrogenation at the reactor conditions, forming the same alkane and alcohol byproducts. The reactions are summarized below as Reactions 0 through 7b.

Reaction 0	$MAC + H_2 \xrightarrow{k_0} SAC$
Reaction 1	$SAC + 2H_2 \xrightarrow{k_1} GBL$
Reaction 2	$GBL + 2H_2 \xrightarrow{k_2} BDO$
Reaction 3	$GBL + 2H_2 \xrightarrow{k_3} THF + H_2O$
Reaction 4a	$GBL + 3.15H_2 \xrightarrow{k_{4a}} 0.15C_4H_{10} + 0.85C_4H_9OH + 1.15H_2O$
Reaction 4b	$GBL + 4.1H_2 \xrightarrow{k_{4b}} 0.1C_3H_8 + 0.9C_3H_7OH + CH_4 + 1.1H_2O$
Reaction 5	$BDO + 2H_2 \xrightarrow{k_5} THF + H_2O$
Reaction 6a	$BDO + 1.15H_2 \xrightarrow{k_{6a}} 0.15C_4H_{10} + 0.85C_4H_9OH + 1.15H_2O$
Reaction 6b	$BDO + 2.1H_2 \xrightarrow{k_{6b}} 0.1C_3H_8 + 0.9C_3H_7OH + CH_4 + 1.1H_2O$
Reaction 7a	$THF + 1.15H_2 \xrightarrow{k_{7a}} 0.15C_4H_{10} + 0.85C_4H_9OH + 0.15H_2O$
Reaction 7b	$THF + 2.1H_2 \xrightarrow{k_{7b}} 0.1C_3H_8 + 0.9C_3H_7OH + CH_4 + 0.1H_2O$

2.3.3 Plant Location

The plant will be constructed in the Gulf Coast area in order to be in close proximity to the maleic acid and Lycra® production facilities. In addition, the Gulf Coast is home to numerous other chemical plants, which results in the widespread availability of most utilities. As a result, it is the cheapest location to construct a plant and its site factor is 1.0 (Seider, Seader, Lewin, & Widagdo, 2009, p. 552).

2.3.4 Plant Capacity

The project objective is to develop a plant to produce 100 million lbs of THF per year at least 99.95% mass purity. We assume that the plant will run approximately 8000 hours per year, or 333 days per year. This is to allow the plant to shut down for one month for maintenance purposes. As a result, the plant must have a minimum capacity of 12,500 lbs of THF product per hour.

3.0 Process Flow Diagram and Material Balances

The process is divided into 6 sections as follows:

Section 100: Preparation of Reactants and Reactor

Section 200: Hydrogen Recycle Loop

Section 300: Liquid Intermediate Recycle Loop

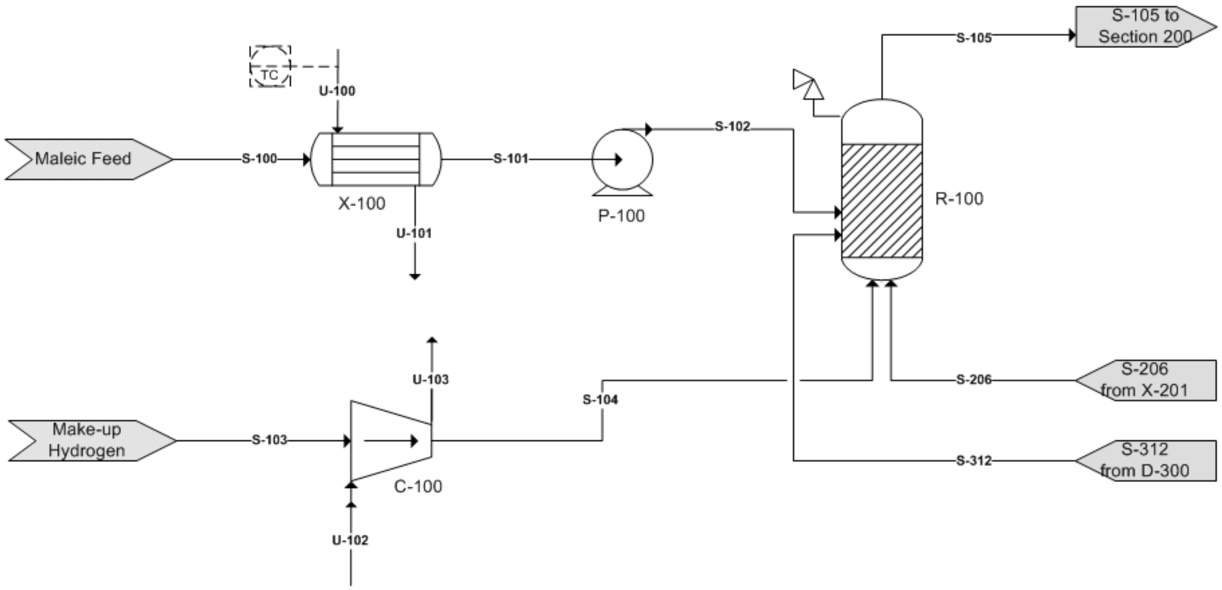
Section 400: THF Recovery from Incineration Streams

Section 500: Pressure-Swing Distillation

Section 600: Product Production and Storage

To explain the function of the various sections, each will be presented with a process flow diagram, and a material balance. The description will summarize key elements and equipment choices. For a full description of the process flow diagram and equipment, refer to Sections 4 and 6, respectively.

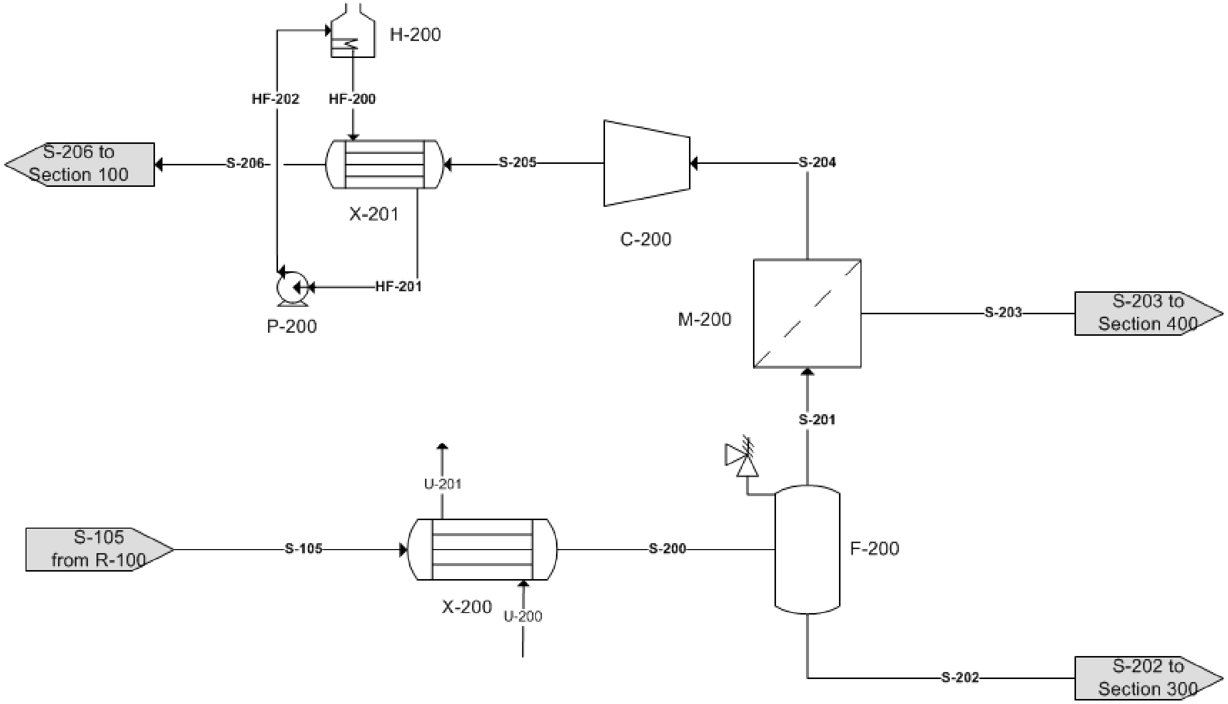
3.1 Section 100: Preparation of Reactants and Reactor



Section 100 Material Balance

	S-100	S-101	S-102	S-103	S-104	S-105	S-206	S-312	U-100	U-101	U-102	U-103
Component Flow (lb/hr)												
MALEIC ACID	22,209.45	22,209.45	22,209.45	-	-	5.09	-	5.09	-	-	-	-
HYDROGEN	-	-	-	2,142.88	2,142.88	11,622.88	11,454.41	-	-	-	-	-
SUCCINIC ACID	-	-	-	-	-	39.23	-	39.23	-	-	-	-
GBL	-	-	-	-	-	3,846.23	-	3,753.50	-	-	-	-
BDO	-	-	-	-	-	232.99	-	232.97	-	-	-	-
THF	-	-	-	-	-	12,702.00	181.90	-	-	-	-	-
METHANE	-	-	-	-	-	86.42	17.19	-	-	-	-	-
NBUTANE	-	-	-	-	-	116.61	13.44	-	-	-	-	-
WATER	14,806.30	14,806.30	14,806.30	-	-	25,716.31	103.05	447.86	2,901.00	2,901.00	57,348.28	57,348.28
PROPANE	-	-	-	-	-	14.89	1.77	-	-	-	-	-
NBUTANOL	-	-	-	-	-	781.23	-	-	-	-	-	-
PROPANOL	-	-	-	-	-	241.48	-	-	-	-	-	-
Total Flow (lb/hr)	37,015.76	37,015.76	37,015.76	2,142.88	2,142.88	55,405.37	11,771.76	4,478.65	2,901.00	2,901.00	57,348.28	57,348.28
Vapor Fraction	0.00	0.00	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00
Temperature (°F)	104.00	201.20	218.84	68.00	389.67	480.40	572.00	286.77	300.15	300.15	90.00	120.00
Pressure (psig)	5.00	0.00	2,040.00	250.00	2,040.00	2,000.00	2,040.00	2,040.00	50.00	50.00	65.00	60.00

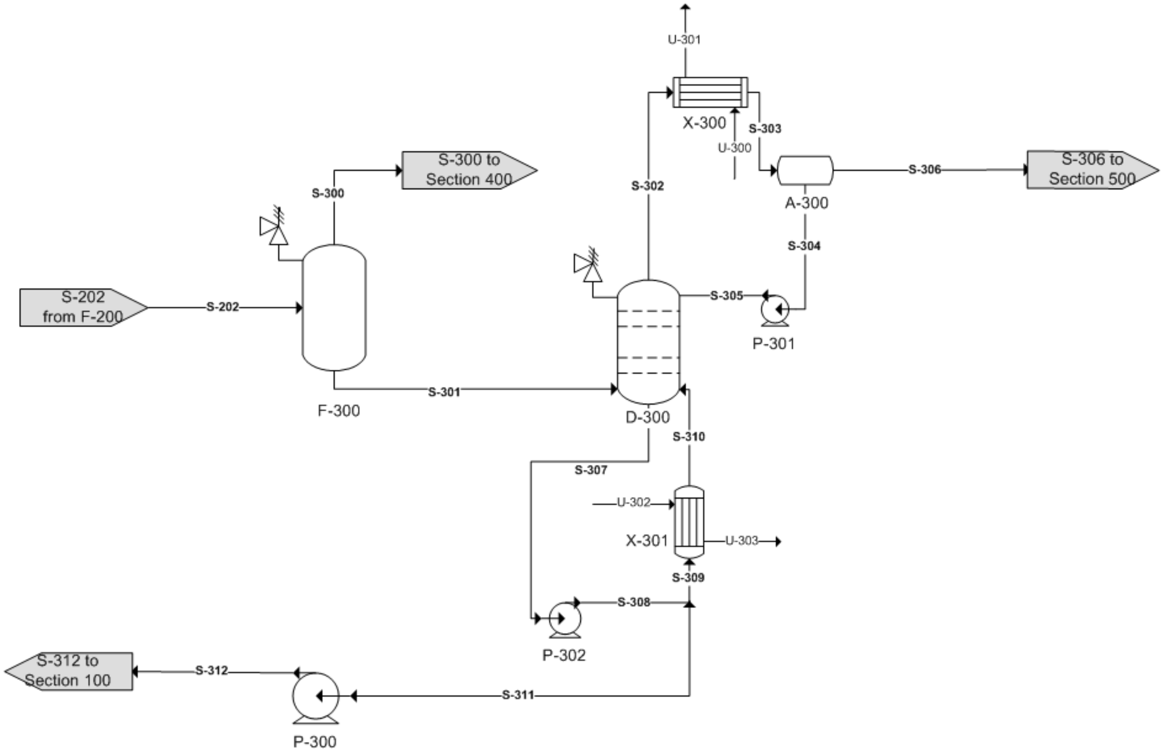
3.2 Section 200: Hydrogen Recycle Loop



Section 200 Material Balance

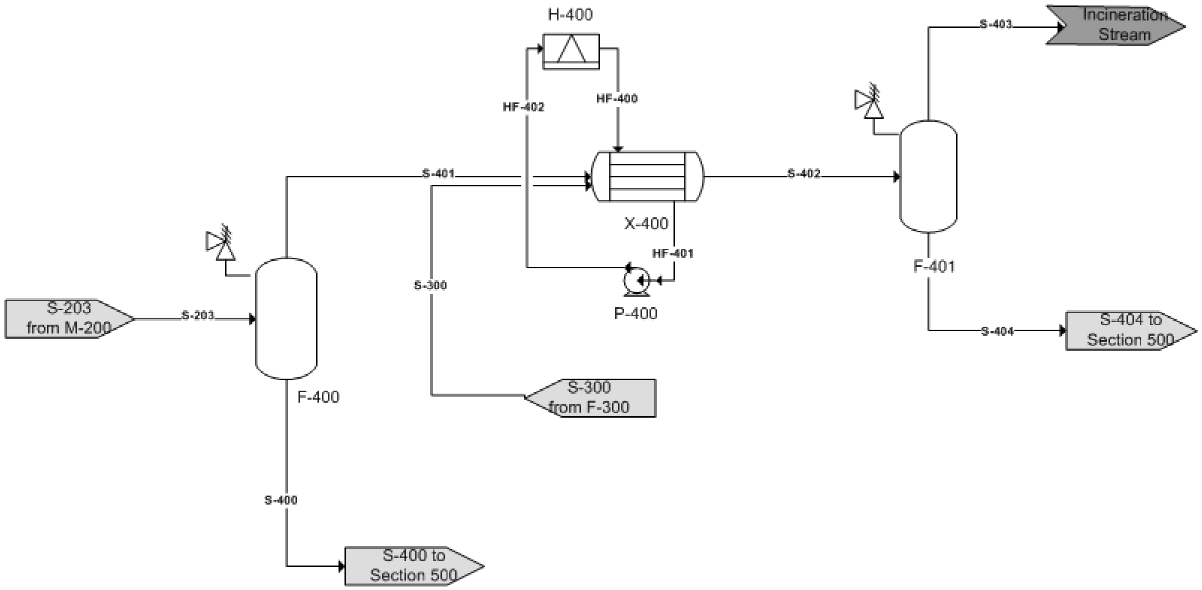
	S-105	S-200	S-201	S-202	S-203	S-204	S-205	S-206	U-200	U-201	HF-200	HF-201	HF-202
Component Flow (lb/hr)													
MALEIC ACID	5.09	5.09	-	5.09	-	-	-	-	-	-	-	-	-
HYDROGEN	11,622.88	11,622.88	11,570.12	52.76	115.70	11,454.41	11,454.41	11,454.41	-	-	-	-	-
SUCCINIC ACID	39.23	39.23	-	39.23	-	-	-	-	-	-	-	-	-
GBL	3,846.23	3,846.23	8.03	3,838.20	8.03	-	-	-	-	-	-	-	-
BDO	232.99	232.99	-	232.99	-	-	-	-	-	-	-	-	-
THF	12,702.00	12,702.00	1,455.18	11,246.82	1,273.29	181.90	181.90	181.90	-	-	-	-	-
METHANE	86.42	86.42	85.94	0.48	68.75	17.19	17.19	17.19	-	-	-	-	-
NBUTANE	116.61	116.61	107.54	9.08	94.09	13.44	13.44	13.44	-	-	-	-	-
WATER	25,716.31	25,716.31	104.09	25,612.22	1.04	103.05	103.05	103.05	43,274.39	43,274.39	-	-	-
PROPANE	14.89	14.89	14.15	0.73	12.39	1.77	1.77	1.77	-	-	-	-	-
NBUTANOL	781.23	781.23	5.20	776.03	5.20	-	-	-	-	-	-	-	-
PROPANOL	241.48	241.48	2.42	239.06	2.42	-	-	-	-	-	-	-	-
DOWTHERM-A	-	-	-	-	-	-	-	-	-	-	68,093.37	68,093.37	68,093.37
Total Flow (lb/hr)	55,405.37	55,405.37	13,352.67	42,052.70	1,580.91	11,771.76	11,771.76	11,771.76	43,274.39	43,274.39	68,093.37	68,093.37	68,093.37
Vapor Fraction	1.00	0.78	1.00	0.00	0.74	1.00	1.00	1.00	0.00	1.00	0.00	0.00	0.00
Temperature (°F)	480.40	104.00	104.01	104.01	105.25	105.25	148.79	572.00	90.00	297.72	660.00	163.79	163.79
Pressure (psig)	2,000.00	1,998.00	1,995.00	1,995.00	1,985.00	1,695.00	2,040.00	2,040.00	50.00	47.00	45.00	42.00	45.00

3.3 Section 300: Liquid Intermediate Recycle Loop



Section 300 Material Balance	S-202	S-300	S-301	S-302	S-303	S-304	S-305	S-306	S-307	S-308	S-309	S-310	S-311	S-312	U-300	U-301	U-302	U-303
Component Flow (lb/hr)																		
MALEIC ACID	5.09	-	5.09	-	-	-	-	-	68.81	68.81	63.72	63.72	5.09	5.09	-	-	-	-
HYDROGEN	52.76	52.50	0.27	-	-	-	-	-	-	-	-	-	-	-	-	-		
SUCCINIC ACID	39.23	-	39.23	-	-	-	-	-	530.67	530.67	491.44	491.44	39.23	39.23	-	-		
GBL	3,838.20	0.01	3,838.19	135.51	135.51	50.82	50.82	84.69	50,769.16	50,769.16	47,015.66	47,015.66	3,753.50	3,753.50	-	-		
BDO	232.99	-	232.99	0.04	0.04	0.02	0.02	0.03	3,151.05	3,151.05	2,918.08	2,918.08	232.97	232.97	-	-		
THF	11,246.82	208.88	11,037.94	17,660.70	17,660.70	6,622.76	6,622.76	11,037.94	0.00	0.00	0.00	0.00	-	-	-	-		
METHANE	0.48	0.45	0.03	-	-	-	-	-	-	-	-	-	-	-	-	-		
NBUTANE	9.08	8.15	0.93	-	-	-	-	-	-	-	-	-	-	-	-	-		
WATER	25,612.22	0.49	25,611.73	40,262.19	40,262.19	15,098.32	15,098.32	25,163.87	6,057.74	6,057.74	5,609.87	5,609.87	447.86	447.86	1,517,566.04	1,517,566.04	51,829.34	51,829.34
PROPANE	0.73	0.63	0.11	-	-	-	-	-	-	-	-	-	-	-	-	-		
NBUTANOL	776.03	1.19	774.83	1,239.73	1,239.73	464.90	464.90	774.83	0.00	0.00	0.00	0.00	-	-	-	-		
PROPANOL	239.06	0.16	238.90	382.23	382.23	143.34	143.34	238.90	0.00	0.00	0.00	0.00	-	-	-	-		
Total Flow (lb/hr)	42,052.70	272.46	41,780.24	59,680.41	59,680.41	22,380.15	22,380.15	37,300.26	60,577.42	60,577.42	56,098.77	56,098.77	4,478.65	4,478.65	1,517,566.04	1,517,566.04	51,829.34	51,829.34
Vapor Fraction	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	1.00	0.00
Temperature (°F)	104.01	78.16	78.16	222.18	168.53	168.53	168.53	168.53	234.49	234.49	234.49	255.19	255.19	286.77	90.00	120.00	297.70	297.70
Pressure (psig)	1,995.00	585.30	585.30	20.00	20.00	20.00	20.00	20.00	22.00	25.00	25.00	20.00	22.00	2,040.00	65.00	55.00	50.00	50.00

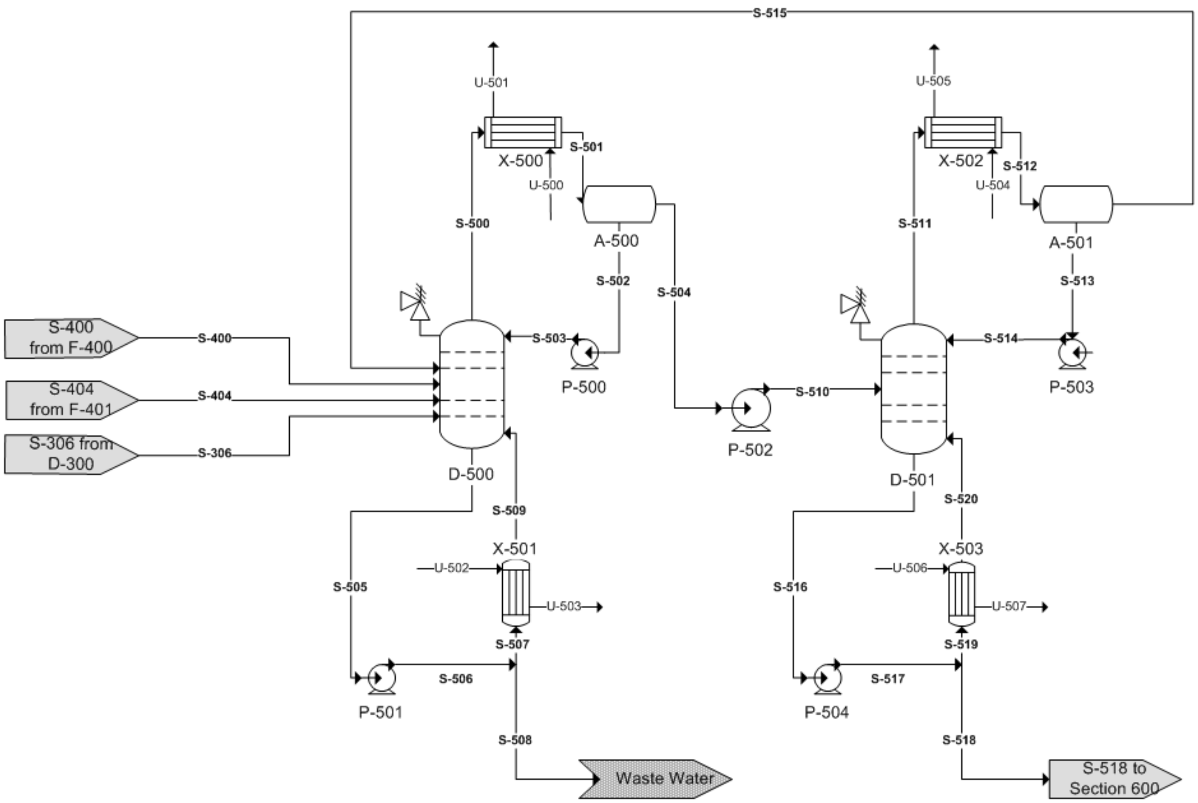
3.4 Section 400: THF Recovery from Incineration Streams



Section 400 Material Balance

	S-203	S-300	S-400	S-401	S-402	S-403	S-404	HF-400	HF-401	HF-402
Component Flow (lb/hr)										
MALEIC ACID	-	-	-	-	-	-	-	-	-	-
HYDROGEN	115.70	52.50	0.30	115.40	167.90	167.82	0.08	-	-	-
SUCCINIC ACID	-	-	-	-	-	-	-	-	-	-
GBL	8.03	0.01	8.02	-	0.02	-	0.02	-	-	-
BDO	-	-	0.00	-	-	-	-	-	-	-
THF	1,273.29	208.88	1,143.24	130.04	338.92	13.54	325.39	-	-	-
METHANE	68.75	0.45	0.62	68.13	68.58	68.38	0.21	-	-	-
NBUTANE	94.09	8.15	34.33	59.76	67.90	40.08	27.82	-	-	-
WATER	1.04	0.49	0.99	0.05	0.54	-	0.54	-	-	-
PROPANE	12.39	0.63	1.80	10.59	11.21	9.82	1.39	-	-	-
NBUTANOL	5.20	1.19	5.13	0.06	1.26	-	1.26	-	-	-
PROPANOL	2.42	0.16	2.33	0.09	0.25	-	0.25	-	-	-
50% ETHYLENE GLYCOL	-	-	-	-	-	-	-	2,047.05	2,047.05	2,047.05
Total Flow (lb/hr)	1,580.91	272.46	1,196.78	384.13	656.59	299.64	356.94	2,047.05	2,047.05	2,047.05
	-									
Vapor Fraction	0.74	1.00	0.00	1.00	0.95	1.00	0.00	0.00	0.00	0.00
Temperature (°F)	105.25	78.16	89.99	89.99	0.00	0.00	0.00	-22.00	63.16	63.16
Pressure (psig)	1,985.00	600.00	150.00	150.00	150.00	150.00	150.00	3.00	0.00	3.00

3.5 Section 500: Pressure-Swing Distillation



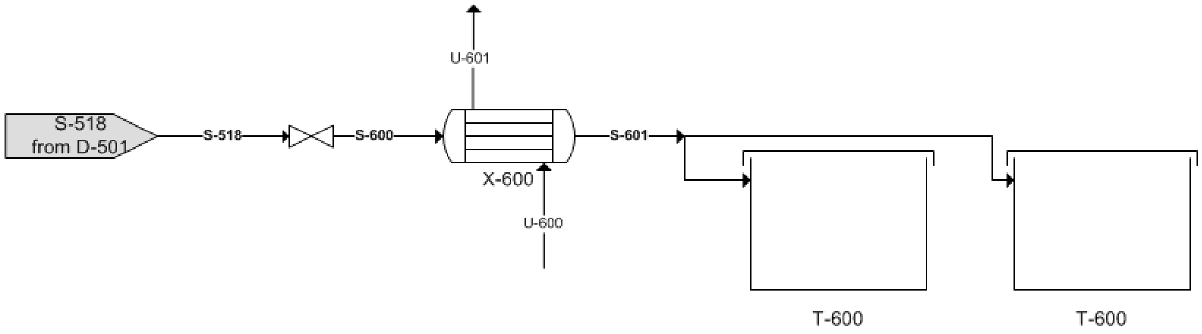
Section 500 Material Balance

	S-306	S-400	S-404	S-500	S-501	S-502	S-503	S-504	S-505	S-506	S-507	S-508	S-509	S-510	S-511	S-512
Component Flow (lb/hr)																
MALEIC ACID	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
HYDROGEN	-	0.30	0.08	-	-	-	-	-	-	-	-	-	-	-	-	-
SUCCINIC ACID	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GBL	84.69	8.02	0.02	0.09	0.09	0.04	0.04	0.05	148.90	148.90	56.16	92.73	56.16	0.05	0.08	0.08
BDO	0.03	0.00	-	-	-	-	-	-	0.05	0.05	0.02	0.03	0.02	-	-	-
THF	11,037.94	1,143.24	325.39	48,042.56	48,042.56	22,815.73	22,815.73	25,226.83	0.62	0.62	0.24	0.39	0.24	25,226.83	23,614.72	23,614.72
METHANE	-	0.62	0.21	-	-	-	-	-	-	-	-	-	-	-	-	-
NBUTANE	-	34.33	27.82	-	-	-	-	-	-	-	-	-	-	-	-	-
WATER	25,163.87	0.99	0.54	2,485.15	2,485.15	1,180.21	1,180.21	1,304.94	40,406.27	40,406.27	15,241.19	25,165.09	15,241.19	1,304.94	2,419.85	2,419.85
PROPANE	-	1.80	1.39	-	-	-	-	-	-	-	-	-	-	-	-	-
NBUTANOL	774.83	5.13	1.26	1.56	1.56	0.74	0.74	0.82	1,253.09	1,253.09	472.66	780.43	472.66	0.82	0.04	0.04
PROPANOL	238.90	2.33	0.25	6.89	6.89	3.27	3.27	3.62	383.46	383.46	144.64	238.82	144.64	3.62	1.54	1.54
Total Flow (lb/hr)	37,300.26	1,196.78	356.94	50,536.24	50,536.24	24,000.00	24,000.00	26,536.24	42,192.39	42,192.39	15,914.91	26,277.48	15,914.91	26,536.24	26,036.24	26,036.24
	-	-	-													
Vapor Fraction	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00	0.00
Temperature (°F)	168.53	89.99	-	147.29	147.26	147.26	147.26	147.26	200.78	200.78	200.78	210.82	210.82	148.43	275.53	274.48
Pressure (psig)	20.00	150.00	150.00	0.30	0.30	0.30	0.30	0.30	2.30	5.30	5.30	2.30	0.30	100.30	100.30	100.30

Section 500 Material Balance

	S-513	S-514	S-515	S-516	S-517	S-518	S-519	S-520	U-500	U-501	U-502	U-503	U-504	U-505	U-506	U-507
Component Flow (lb/hr)																
MALEIC ACID	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
HYDROGEN	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
SUCCINIC ACID	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GBL	0.04	0.04	0.04	0.00	0.00	-	-	-	-	-	-	-	-	-	-	-
BDO	-	-	-	0.00	0.00	-	-	-	-	-	-	-	-	-	-	-
THF	10,883.93	10,883.93	12,730.79	64,468.15	64,468.15	12,496.03	51,972.12	51,972.12	-	-	-	-	-	-	-	-
METHANE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NBUTANE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
WATER	1,115.30	1,115.30	1,304.55	1.97	1.97	0.38	1.59	1.59	367,268.51	367,268.51	12,281.01	12,281.01	191,683.89	191,683.89	8,916.64	8,916.64
PROPANE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NBUTANOL	0.02	0.02	0.02	4.11	4.11	0.80	3.31	3.31	-	-	-	-	-	-	-	-
PROPANOL	0.71	0.71	0.83	14.38	14.38	2.79	11.59	11.59	-	-	-	-	-	-	-	-
Total Flow (lb/hr)	12,000.00	12,000.00	14,036.24	64,488.61	64,488.61	12,500.00	51,988.61	51,988.61	367,268.51	367,268.51	12,281.01	12,281.01	191,683.89	191,683.89	8,916.64	8,916.64
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00	0.00
Temperature (°F)	274.48	274.48	274.48	298.13	298.13	298.48	298.13	298.48	90.00	120.00	297.70	297.70	90.00	120.00	365.90	365.90
Pressure (psig)	100.30	100.30	100.30	102.30	105.30	102.30	105.30	100.30	65.00	55.00	50.00	50.00	65.00	65.00	150.00	150.00

3.6 Section 600: Product Production and Storage



Section 600 Material Balance					
	S-518	**S-600**	**S-601**	**U-600**	**U-601**
Component Flow (lb/hr)					
MALEIC ACID	-	-	-	-	-
HYDROGEN	-	-	-	-	-
SUCCINIC ACID	-	-	-	-	-
GBL	-	-	-	-	-
BDO	-	-	-	-	-
THF	12,496.03	12,496.03	12,496.03	-	-
METHANE	-	-	-	-	-
NBUTANE	-	-	-	-	-
WATER	0.38	0.38	0.38	34,705.03	34,705.03
PROPANE	-	-	-	-	-
NBUTANOL	0.80	0.80	0.80	-	-
PROPANOL	2.79	2.79	2.79	-	-
Total Flow (lb/hr)	12,500.00	12,500.00	12,500.00	34,705.03	34,705.03
	-				
Vapor Fraction	0.00	0.38	0.00	0.00	0.00
Temperature (°F)	298.48	171.33	104.00	90.00	120.00
Pressure (psig)	102.30	6.70	5.30	65.00	55.00

3.7 Brief Process Descriptions

Section 100

In this section, the maleic acid feed and make-up hydrogen streams are preheated and pressurized to the specified conditions that enable the back-mix tank reactor to operate adiabatically. The maleic acid stream is heated using low pressure steam in a shell-and-tube heat exchanger, and pumped up to the reactor pressure via a reciprocating pump. The hydrogen stream is compressed in a two-stage compressor with an intercooler. The reactor catalytically hydrogenates the maleic acid to produce THF and a number of intermediates and byproducts, which are carried out with the hydrogen in the vapor phase out the top of the reactor. In addition to the feed streams, a hydrogen recycle stream from Section 200 and a liquid intermediate recycle stream from Section 300 are fed into the bottom of the reactor.

Section 200

In this section, the vapor effluent from the reactor passes through a shell-and-tube heat exchanger and is cooled the maximum extent with boiler feed water. The partially condensed stream then moves into a flash vessel, where the liquid is drawn off the bottom and sent to the liquid intermediate recycle loop (Section 300), and the hydrogen-rich vapor is sent into a hydrogen separation membrane. The membrane separates hydrogen into the permeate and leaves the alkanes, alcohols, and other low-boilers in the retentate. The retentate contains a significant amount of THF and is sent to the THF recovery train (Section 400). The hydrogen-rich permeate then is compressed to reactor pressures and heated to an elevated temperature by a Dowtherm A fired heater and heat exchanger. The heated and compressed hydrogen recycle stream is sent back to the reactor.

Section 300

In this section, the heavy liquid intermediates are removed from the liquid product from the first flash separation. First, the pressure of the liquid stream is dropped significantly and flashed to remove more of the dissolved hydrogen to stabilize the downstream distillation columns. The vapor product from the second flash separation contains a significant amount of THF and is sent to the THF recovery train (Section 400). The liquid product is then sent into the middle tray of a standard distillation column, which easily separates the GBL and BDO components into the bottoms and sends the water, THF, and most of the alcohols into the distillate. The liquid intermediates are recycled back into the reactor. The THF and water form an azeotrope at the conditions of the first tower, and must be sent to a pressure-swing distillation train to be separated.

Section 400

In this section, THF in two separate incineration streams is condensed out of the vapor phase and recovered via refrigeration. First, the retentate from the membrane in Section 200 is flashed to a much lower pressure in order to condense a significant amount of THF from the vapor, and the liquid product is sent to the pressure-swing distillation train (Section 500). The vapor product is sent along with the vapor product from the Section 300 flash vessel into a refrigeration unit, where the temperature is dropped to condense most of the remaining THF in a fourth flash vessel. The condensed THF and other impurities are sent to Section 500 for further purification. The vapor product contains significant heating value and is incinerated in the fired heater in Section 200.

Section 500

In this section, two pressure-swing distillation columns are used to break the water-THF azeotrope in order to produce the final THF product with 99.97% mass purity. The first column operates at atmospheric conditions and receives feeds from Section 300 and 400. The bottoms stream contains mostly water, which is sent to a waste water treatment plant. The distillate contains the azeotrope at atmospheric conditions and is sent to the second column, which operates at a much higher pressure. The second column operates at an elevated pressure in order to alter the azeotropic composition so that the distillate may be recycled back to the first column to break the azeotrope. The bottoms stream from the second column contains the THF product at the desired purity.

Section 600

In this section, the product stream is dropped to atmospheric pressure and temperature using a valve and cooling water through a shell-and-tube heat exchanger. The final product is sent to one of two floating-roof storage tanks, each with a holdup of 48 hours.

Section 4.0 Detailed Process Description

This section will describe the process in detail by walking through the process flow diagram and rationalizing the selection of each major equipment item. As a rule of thumb for selecting the materials of construction for each piece of equipment, the cheapest option, carbon steel, is used for all equipment involving cooling water or pressurized steam. Maleic acid and succinic acid are weak organic acids, GBL is a lactone, BDO is an alcohol, and THF is an ether, all of which are damaging to carbon steel. Hydrogen is also known to corrode carbon steel. Thus, stainless steel is selected for equipment with these compounds as major components in the feed streams.

This section then continues with a detailed discussion of the reactor and membrane model, which were not modeled in ASPEN Plus 2006. The section concludes with a summary of the key process decisions that were made throughout the design stage of the facility.

4.1 Section 100: Reactor Train

The process begins with the maleic acid feed (S-100), which is 60% maleic acid by weight and is drawn from the bottom of an atmospheric storage tank at 5 psig and 104°F. The feed passes through X-100, a fixed-head shell-and-tube heat exchanger, which heats S-100 to 201.2°F using 50 psig steam (at 297.7°F). The temperature is selected to ensure that the reactor remains adiabatic. A small pressure drop of 5 psi is observed on the cold side and no pressure drop is observed on hot side. (Refer to Page 71 for a full description of **X-100**.)

The maleic acid stream exiting the heat exchanger (S-101) is now pumped through a stainless steel, reciprocating plunger pump (P-100) up to 2040 psig. This pressure is 40 psi greater than the 2000 psig pressure required in the reactor in order to overcome the liquid head present at the bottom of the reactor. A reciprocating pump is selected because the large pressure increase of 2040 psig implies a developed head of 5,755 ft, which is out of the range of a centrifugal pump. Stainless steel is selected to prevent corrosion from the maleic acid. The exiting stream (S-102) is fed into the bottom of the reactor. (Refer to Page 63 for a full description of **P-100**.)

The hydrogen fed to the reactor is a combination of recycled hydrogen from the process and make-up hydrogen, which is available by pipeline. The make-up hydrogen (S-103) required for this continuous process enters the facility at 250 psig and 68°F from the pipeline, and is compressed using a stainless steel, two-stage compressor to 2040 psig. Like the maleic acid feed, the hydrogen is compressed to 40 psi higher than the reaction pressure in order to overcome the liquid head at the bottom of the reactor. The maximum single-stage compression ratio is 3.75 for a diatomic gas (Seider, Seader, Lewin,

& Widagdo, 2009), and accordingly, bringing the pressure from 250 psig to 2040 psig requires two stages. The first compression raises the pressure to 723 psig and the temperature of the hydrogen stream to 334°F, requiring a carbon steel/stainless steel intercooler after the first stage to bring the temperature down to 104°F with cooling water. The second compressor raises the pressure to 2040 psig and the temperature to 390°F, but no intercooler is required after the second stage because the elevated temperature of the hydrogen is desired to maintain the adiabatic aspect of the reactor. The exiting stream (S-104) is fed into the bottom of the reactor. (Refer to Page 55 for a full description of **C-100**.)

The maleic acid feed (S-102) and the liquid intermediate recycle stream (S-312, see below) are fed into the bottom of a back-mix tank reactor. The reactor is adiabatic at 480°F, and the heat contained in the preheated hydrogen and maleic acid streams combined with the enthalpy of reaction vaporize the THF and its byproducts. Temperature control within the reactor is managed by adjusting the maleic acid feed temperature. The elevated temperature and pressure were suggested by the R&D team as ideal conditions for maximum THF production. Agitation is provided by the large excess of hydrogen from the makeup stream (S-104) and the recycle stream (S-206) (see below), which bubble up through the reactor. The vapor product is carried with the hydrogen out of the top of the reactor. To achieve a target space-time yield (STY) of 600 lbs THF/hr-1000 lb catalyst, the reactor must contain 20833 lbs of palladium-rhenium catalyst on carbon support to aid hydrogenation. The vapor product stream (S-105) is 55,405 lb/hr and leaves the reactor at 2000 psig and 480°F. (Refer to Page 68 for a full description of **R-100**.)

4.2 Section 200: Hydrogen Recycle Loop

The vapor product (S-105) that leaves the reactor is cooled from 480°F to 104°F by passing through X-200, a fixed-head shell-and-tube heat exchanger. The exchanger uses boiler feed water (BFW) and produces 50 psig steam, which reduces the amount of pipeline 50 psig steam required in other parts of the process. The vapor stream is cooled to the maximum extent possible without using refrigeration in order to maximize the liquid fraction at 2000 psig, so that the following flash vessel can effectively separate the low-boilers (hydrogen, methane, propane) from the condensables. A small pressure drop of 2 psi is observed on the hot side and 3 psi on the cold side. (Refer to Page 71 for a full description of **X-200**.)

The cooled reactor effluent leaving X-200 (S-200) contains a vapor fraction of 0.78 and enters a stainless steel, vertical flash vessel (F-200) at a pressure of 1995 psig. This first flash separation utilizes the large temperature drop from 480°F to 104°F with minimal pressure drop in order to minimize the compression work required to bring the recycled hydrogen stream back up to 2040 psig. The vapor effluent (S-201) is 13,353 lb/hr and contains most of the non-condensable compounds, hydrogen and alkanes, and a moderate amount of vaporized and entrained THF, water, and alcohols. Approximately 99.5% of the hydrogen in stream S-200 is removed into this vapor effluent. This stream is fed into a hydrogen membrane to recover the hydrogen and allow it to be recycled back into the reactor. The liquid effluent (S-202) is 42,053 lb/hr and contains the condensable compounds with a small amount of dissolved hydrogen, methane, propane, and butane. This stream passes through another flash separation at a lower pressure in order to remove most of the hydrogen from the stream before it is fed into the downstream distillation columns. The vessel is constructed using stainless steel to prevent corrosion. (Refer to Page 60 for a full description of **F-200**.)

The non-condensables leaving F-200 in S-201 are passed through a shell-and-tube, size-exclusion membrane, which separates the hydrogen and water vapor into the permeate (S-204) and leaves most of the remaining compounds in the retentate (S-203). The membrane removes 99% of the hydrogen into the permeate and is constructed from polysulfonate polymer, due to its stability at high pressures. A pressure drop of 300 psi is observed on the permeate side, while the retentate side has a much less significant drop in pressure of 10 psi. (Refer to Page 62 for a full description of **M-200**.)

The hydrogen-rich permeate (S-204) leaves the membrane at 1695 psig and passes through a stainless steel, reciprocating compressor (C-200) to bring the pressure back up to the required reactor pressure of 2040 psig. The pressure increase requires only a single stage compression. Stainless steel is used as the material of construction to prevent hydrogen-related corrosion. (Refer to Page 56 for a full description of **C-200**.)

The stream leaving C-200 (S-205) enters a fixed-head shell and tube heat exchanger to heat the recycled hydrogen from 104°F to 572°F; the outlet temperature is set to ensure that the reactor operates adiabatically at 480°F. Dowtherm A is selected as the heating fluid in order to prevent ignition of the hydrogen stream and because the desired stream temperature is above temperatures achievable by 700 psig steam. The Dowtherm A is heated by a gas-fired furnace (H-200) that uses the waste incineration stream (S-403) produced in Section 400 and pipeline natural gas. The heating fluid loop is driven by a small, carbon steel centrifugal pump (P-200). The exchanger effluent (S-206) is fed into the bottom of the reactor with the make-up hydrogen. (Refer to Pages 72, 59, and 63 for a full description of **X-201**, **H-200**, and **P-200**, respectively.)

4.3 Section 300: Liquid Intermediate Recycle Loop

The high-pressure liquid effluent leaving F-200 at 104°F (S-202) is flashed across a valve and fed into a stainless steel, vertical flash vessel (F-300) at a pressure of 585.3 psig. This second flash separation utilizes the large pressure drop from 1995 psig to 585.3 psig to further remove the dissolved hydrogen and other non-condensables from the liquid stream, so that it will not disrupt the downstream distillation columns. Approximately 99.5% of the hydrogen is removed into the 272 lb/hr vapor effluent (S-300), which contains mostly non-condensable compounds. This stream has significant heating value and would reduce the amount of natural gas utility that the furnace H-200 requires; however, S-300 contains a significant amount, 209 lb/hr, of THF, and thus, it is proven economically beneficial to install a small refrigerator (Section 400) to recover the precious product in this first incineration stream. The liquid effluent (S-301) is 41,780 lb/hr and is fed to a distillation tower to separate the useful liquid intermediates from the product and water. The intermediates are then recycled back into the reactor to maximize the production of THF. The vessel is constructed using stainless steel to prevent corrosion. (Refer to Page 60 for a full description of **F-300**.)

The liquid effluent leaving F-300 is fed into the middle tray of a stainless steel distillation tower (D-300), which separates the heavy liquid intermediates, GBL and BDO, into the bottoms stream (S-311). The distillate stream (S-306) contains mostly THF and water, which forms an azeotrope at the conditions within the tower. This stream is sent to a pressure-swing distillation process, which utilizes a pressure differential and a distillate recycle to break the azeotrope. The column operates at 5.3 psig and experiences an approximate 2 psi pressure drop across the column. The tower contains 24 Koch Flexitray trays, which are selected due to their widespread use in chemical production processes. The tower operates at a reflux ratio of 0.60 which places 98.0% of the GBL and BDO in the feed into the bottoms stream that is recycled back to the reactor. Also included in the distillation tower are typical centrifugal reflux (P-301) and reboiler (P-302) pumps, a horizontal reflux accumulator (A-300), a shell-and-tube condenser (X-300) and a thermosyphon reboiler (X-301). The pumps are stainless steel, centrifugal pumps that send the stream back into the column. The reflux accumulator is built from stainless steel and designed using a 5 minute desired holdup and an aspect ratio of 2, length to diameter. The condenser uses cooling water to condense the vapor leaving the top tray and cool it from 222°F to a distillate temperature of 169°F, while a small amount of non-condensables are released through a vent at the top of the tower. The thermosyphon reboiler uses 50 psig steam to vaporize and heat the liquid leaving the last stage of the column from 234°F to 255°F, which is within the operational range of 50 psig steam (at 297.7°F). (Refer to Pages 57, 64, 64, 53, 72, and 73 and for **D-300, P-301**, **P-302**, **A-300, X-300**, and **X-301** respectively.)

The bottoms stream leaving D-300 (S-311) is rich in the liquid intermediates GBL and BDO, and is passed through a reciprocating, stainless steel pump (P-300) to bring the stream back up to 2040 psig, the reaction pressure required to overcome the liquid head present at the bottom of the reactor. A reciprocating pump is selected because the large pressure increase of 2,033 psig implies a developed head of 4,619 ft, which is out of the range of a centrifugal pump. The exiting stream (S-312) is fed into the bottom of the reactor in Section 100. Refer to Page 63 for a full description of **P-300**.

4.4 Section 400: THF Recovery from Incineration Streams

The high-pressure vapor retentate (S-203) leaving the membrane at 105°F and 1,985 psig is flashed across a valve and fed into a stainless steel, vertical flash vessel (F-400) at a pressure of 150 psig. This third flash separation utilizes the large pressure drop from 1,985 psig to 150 psig to further remove the dissolved hydrogen and other non-condensables from the liquid stream, to stabilize the downstream pressure-swing distillation columns. Approximately 99.7% of the hydrogen is removed into the vapor effluent (S-401), which is 384 lb/hr, and again, contains mostly hydrogen and other non-condensables. Like the first incineration stream, S-300, this vapor stream has significant heating value and upon incineration, would reduce the amount of natural gas utility that the furnace H-200 requires. However, S-401 also contains a significant amount, 130 lb/hr, of THF, and it was proven economically beneficial to install a small refrigerator to recover the precious product in this second incineration stream and S-300, the vapor effluent produced in F-300. The liquid effluent S-400 is 1,197 lb/hr, contains mostly THF and butane, and is fed into the atmospheric pressure-swing distillation column for further purification. (Refer to Page 61 for a full description of **F-400**.)

The two incineration streams, S-300 and S-401, combined have 339 lb/hr of THF, which is a significant amount and merits another flash separation to further recover the THF from the other components. The pressure and temperature has already been dropped significantly in S-300 to 585.3 psig and 78°F in F-300 and in S-401 to 150 psig and 90°F in F-400. Thus, refrigeration is the only remaining option to further remove the THF out of the vapor phase. Due to the relatively small flow rate of the combined streams, a refrigeration unit is proven economically productive due to the valuable nature of THF. Thus, a stainless steel, air-cooled mechanical refrigeration unit (H-400) and small, centrifugal coolant pump (P-400) is installed to recirculate and cool a 50% ethylene glycol-water coolant to -22°F. The coolant is then fed into the shell side of a fixed head, shell and tube heat exchanger (X-400) to bring the temperatures the incinerations streams down to 0°F. The pressure of S-300 is dropped to 150 psig across a valve before entering the exchanger to match the pressure of S-401. This significant temperature drop causes a large portion of the remaining THF to condense out of the incineration streams, and the outlet stream, S-402, is fed into a flash separation vessel. A small pressure drop of 3 psi is observed on the cold side and no drop is observed on the hot side. Refer to Pages 59, 65, and 73 for a full description of **H-400**, **P-400**, and **X-400** respectively.

As S-402 leaves the refrigeration heat exchanger at 0°F and 150 psig, it is fed into a stainless steel, vertical flash vessel (F-401) at a pressure of 150 psig. This fourth flash separation utilizes the large temperature drop from X-400 to further remove condensed THF from the incineration stream, so that it can be recovered and fed into the first, atmospheric pressure-swing distillation tower. Approximately 96% of the THF is recovered in the liquid effluent (S-404), which is 357 lb/hr, and contains mostly THF and butane. The vapor effluent (S-403) is 300 lb/hr and contains primarily hydrogen and alkanes. It has a heating value of 13,126,528 Btu/hr and is fed into the furnace, H-200. Refer to Page 61 for a full description of **F-401**.

4.5 Section 500: Pressure-Swing Distillation Columns

A pressure-swing distillation train is selected to purify the THF product because of its known effectiveness in breaking aqueous azeotropes, which is present in the distillate leaving the GBL-BDO recycle loop. The first column operates at a near-atmospheric pressure of 0.3 psig while the second column operates at an elevated pressure of 100.3 psig. The pressure differential affects the composition of the THF-water azeotrope by moving it from 83% by mole THF at atmospheric pressure to 71% by mole THF at 100.3 psig. By recycling the distillate from the high pressure column back into the atmospheric column, the bottoms stream from the high pressure column yields very pure THF.

The liquid distillate (S-306) from the GBL-BDO distillation column, D-300, is fed into the middle tray of the first stainless steel, pressure-swing distillation tower (D-500). The liquid streams from F-400 and F-401are fed into stages 2 and 16, respectively, and the distillate recycle stream from the high-pressure column is fed into middle tray. The bottoms stream (S-508) is 26,277 lb/hr and contains 95.8% water, 3% butanol, and 1% propanol by mass, and is sent to a nearby waste water treatment plant. The distillate stream (S-504) is 26,536 lb/hr, contains the THF and water azeotrope at the atmospheric conditions within the tower, and is sent into the high-pressure distillation column. The tower contains 40 Koch Flexitray trays and operates at a reflux ratio of 0.90, which gives the desired purity of the azeotrope through the distillate without losing a significant amount of THF through the bottoms. Also included in the distillation tower are typical centrifugal reflux (P-500) and reboiler (P-501) pumps, a horizontal reflux accumulator (A-500), a shell-and-tube condenser (X-500) and a thermosyphon reboiler (X-501). The pumps are stainless steel, centrifugal pumps that send the stream back into the column. The reflux accumulator is built from stainless steel and designed using a 5 minute desired holdup and an aspect ratio of 2, length to diameter. The condenser uses cooling water to condense the vapor leaving the top tray at 147°F, while a small amount of non-condensables are released through a vent at the top of the tower. The thermosyphon reboiler uses 50 psig steam to vaporize and heat the liquid leaving the last stage of the column from 201 °F to 211°F, which is within the operational range of 50 psig steam (at 297.7°F). (Refer to Pages 57, 65, 65, 73, 74, and 53 for a full description of **D-500**, **P-500**, **P-501**, **X-500**, **X-501**, and **A-500**, respectively.)

The liquid distillate (S-504) from D-500, is fed into the middle tray of the second stainless steel, pressure-swing distillation tower (D-501) after being pumped up to the high pressure of 100.3 psig via pump P-502, a stainless steel, centrifugal pump. The distillate stream (S-515) is 14,036 lb/hr, contains the THF and water azeotrope at the high-pressure conditions within the tower, and is recycled back into the low-pressure distillation column. The bottoms stream (S-518) is 12,500 lb/hr and contains 99.97% pure THF by mass, which is the desired product from the process. It is actually more pure than the required 99.95% purity, but the cost of increasing the purity to 99.97% is negligible. The tower contains 18 Koch Flexitray trays and operates at a reflux ratio of 0.86, which gives the required purity of THF through the bottoms. Also included in the distillation tower are typical centrifugal reflux (P-503) and reboiler (P-504) pumps, a horizontal reflux accumulator (A-501), a shell-and-tube condenser (X-502) and a thermosyphon reboiler (X-503). The pumps are stainless steel, centrifugal pumps that send the stream back into the column. The reflux accumulator is built from stainless steel and designed using a desired 5 minute holdup and an aspect ratio of 2, length to diameter. The condenser uses cooling water to condense the vapor leaving the top tray at 275°F, while a small amount of non-condensables are released through a vent at the top of the tower. The thermosyphon reboiler uses 150 psig steam (at 366°F) to vaporize the liquid leaving the last stage of the column at 298°F, since the temperature is outside of the range of 50 psig steam. (Refer to Pages 58, 66, 66, 74, 75, and 53 for a full description of **D-501**, **P-503**, **P-504**, **X-502**, **X-503**, and **A-501**, respectively.)

4.6 Section 600: Product Production and Storage

The bottoms stream (S-518) from D-501 must be brought to atmospheric conditions before it is sent to the storage tanks. First, the pressure is dropped across a valve down to 6.7 psig, which allows the liquid to have enough head to progress through the pipeline to the storage tanks. Next, the stream (S-600) is fed into the tube side of a fixed head, shell and tube heat exchanger (X-600) to bring the temperatures down to 104°F via cooling water. A small pressure drop of 1.4 psi is observed on the hot side and a pressure drop of 10 psi is observed on the cold side. (Refer to Page 75 for a full description of **X-600**.)

After the product is brought to near-atmospheric conditions, it is sent to one of two storage tanks, each with a 2-day storage capacity of 83,325 gal. Due to the extremely flammable and toxic nature of THF liquid and vapor, the storage tanks are constructed from stainless steel and are floating roof tanks. (Refer to Page 70 for a full description of T-600).

4.7 Modeling Considerations

4.7.1 Reactor

The reactor is modeled in ASPEN Plus 2006 as a stoichiometric reactor (RSTOIC) by specifying the reactions described in Section 2.2.2 to occur in series. Fractional conversions of the reactants and intermediates were provided by the R&D department, which used reactor effluent data from a pilot plant constructed in Europe operating at the same conditions as R-100. The original plant was constructed using a kinetic model, which included Langmuir-Hinshelwood adsorption kinetics and a series of empirical rate constants. However, R&D felt that our reactor model effluent would more accurately represent reality if the stoichiometric model was employed. For more information about the reactor kinetic model, refer to Page 184 of A.1 in the Appendix. It is recommended that this model be refined through further experimental and modeling studies prior to setting the operating conditions for this potentially profitable process. A flexible, kinetic model would provide insight into how changes in the catalyst, temperature, and pressure within the reactor can affect the rate of production, reactor effluent composition, and project profitability. This information would be extremely valuable when selecting ideal operating conditions and designing control systems for the process.

The catalyst charge and regeneration cost estimates were provided by correspondence with BASF Catalysts, Inc. The catalyst is a 1% palladium-rhenium catalyst on a carbon support, which must be regenerated annually. To achieve a Space-Time-Yield (STY) of 600 lb lbs THF/hr-lb catalyst, as imposed by the project requirements, the reactor must contain 20833 lb of catalyst. Refer to Page 68 for a full description of the reactor and Page 220 for a description of the catalyst costing.

4.7.2 Hydrogen Separation Membrane

Since the membrane feed almost exclusively involves hydrogen in the noncondensable stream, gas permeation is utilized to achieve the desired separation from alkanes, alcohols, and THF. According to tabulated data, the permeability of hydrogen is 250 barrer at STP (Seader & Henley, Separation Process Principles, 2005, p. 526). According to plasticization pressure graphs, membrane permeability will initially decrease before ultimately increasing as the pressure becomes greater (Katz, et al., 1974, p. 241). Though this value is not indicative of our operating conditions of 1995 psig and 104°F, the plasticization pressure of our membrane can be considered to be negligible because our membrane's fibers are composed of polysulfonate polymer (Histed, 2009).

Furthermore, permeance is defined as the ratio of a substance's permeability to the membrane's thickness (Seader & Henley, Separation Process Principles, 2005, p. 498). In this case, the membrane's suggested thickness is 1000 Å, or 10^{-5} cm, so the permeance is 250 barrer divided by 10^{-5} cm (Histed, 2009). Using ASPEN Plus 2006 data from the simulation flowsheet, hydrogen's molar density was computed by dividing the molar flow rate by the volumetric flow rate. Additionally, the total flow rate of the incoming feed stream (S-201) and each individual component's flow rate were all provided by ASPEN. Each component's permeate split fraction was provided by Mr. Wayne Robbins, the project industrial consultant, and was multiplied by Aspen's flow rate to determine the composition of the retentate stream (S-203) and the permeate recycle stream (S-204) (Robbins, Split Fractions, 2009)

To compute the area, a variety of pressure drops across a certain section of the membrane were considered. The area was essentially computed by dividing the molar flow rate by the molar density, the permeance, and the corresponding pressure drop per section (Seader & Henley, Separation Process Principles, 2005, p. 527). After analyzing the various membrane areas, it was determined that three membranes connected in series, each with an area of approximately 3250 ft^2, would be optimal based on the physical feasibility of maintaining that section of the plant and also from an economic standpoint. According to a Hydrogen Membranes expert at Air Products, each square foot of the membrane costs $10. Thus, the total area amounts to 9745.2 ft^2, resulting in a total cost of $97,452 (Histed, 2009). For more information about the membrane model, refer to Page 202 of A.1 in the Appendix. For email correspondence with Mr. Adam Histed, refer to Pages 339 and 342 in the Appendix.

4.7.3 Distillation Tower Purge Streams

The project team encountered difficulty in converging the distillation tower models in ASPEN Plus 2006 when a partial condenser was employed. However, in reality, it is known that a vapor purge must be allowed out the top in order to prevent the buildup of the low-boilers, hydrogen, methane, propane and n-butane. Thus, a total condenser is employed in each of the distillation towers to ensure convergence, and dummy separators are inserted in the streams entering the first pressure-swing column to remove any residual low-boilers before they enter the total condenser. The vapor streams of these dummy separators are proxies for the vapor purge of the pressure-swing columns.

4.8 Key Process Decisions

In this section, the key process decisions are described in detail and rationalized.

1. **Reactant Preparation**: To ensure that the reactor remains adiabatic at 480°F, the maleic acid feed is heated to 201.2°F and the hydrogen recycle stream is heated to 572°F. These temperatures were selected per guidance from our project advisor, Mr. Wayne Robbins. The hydrogen make-up enters the reactor at the pipeline temperature of 68°F, and thus the recycle stream is heated beyond 480°F to supply the extra heat needed in the reactor. The temperature of the maleic acid stream is carefully controlled to ensure the reactor stays adiabatic and produces the required flow rate of vapor effluent. All feed streams to the reactor enter at 2040 psig to overcome the 40 psi liquid head present at the bottom of the reactor, to ensure that the vapor at the top of the reactor leaves at 2000 psig.
2. **Hydrogen Separation Membrane**: A hydrogen separation membrane is used to purify the hydrogen recycle stream because the non-condensable alkanes (methane, propane) are difficult to separate from hydrogen using flash methods. Dropping the temperature and/or pressure of the recycle stream would not separate hydrogen from the alkanes, and the alkanes would be sent back into the reactor via the recycle loop. This would cause the low-boiling byproducts to build up within the hydrogen recycle loop.
3. **Liquid Intermediate Recovery**: The heavy liquid intermediates are removed very early on in the separation process due to the ease of separation from the THF-water azeotrope at moderate pressure and temperatures. A standard distillation tower is used for this separation.
4. **Preheating Hydrogen**: The hydrogen recycle stream must be heated to the specified 572°F, but it is dangerous to pass a stream of pressurized hydrogen directly through a furnace. With guidance from Professor Fabiano, a Dowtherm A fired heater was selected to heat inert thermal fluid to 660°F so that heat transfer may occur between the thermal fluid and the process stream.
5. **Alcohol Removal**: The alcohol byproducts must be removed to avoid buildup in the final product, and the design team decided to remove them in the first pressure-swing column. The reflux rate and bottoms rate were adjusted until the majority of all alcohols were removed from the system through the waste water stream.
6. **Pressure-Swing Column Pressures**: The two pressure-swing distillation columns operate at 0.3 psig and 100.3 psig, and the pressures were chosen in accordance with *Product and Process Design Principles, 3rd Edition*, where a THF-water azeotrope is used as an example in the section that discusses pressure-swing distillation (Seider, Seader, Lewin, & Widagdo, 2009).

7. **Flash Separation Train Order**: The first flash separation utilizes a large temperature drop to 104°F to separate hydrogen and the other low-boilers from the liquid intermediates, water, and THF. This separation maintains the high pressure at 1995 psig so that the hydrogen recycle stream can pass through the membrane easily and to reduce the compression duty of C-200. The second flash separation, F-300, drops the pressure to 585.3 psig to further remove hydrogen and other low-boilers before the liquid stream enters the liquid intermediate separation column. A pressure of 585.3 psig was selected in order to ensure the column converges with a small amount of non-condensables through the condenser. F-400 utilizes a large pressure drop again to 150 psig, to further remove hydrogen and other low-boilers. At this point, the two incineration streams leaving F-300 and F-400 contain a large amount of THF at relatively low pressures, and only a large temperature drop can condense the THF out of the incineration streams. Thus, the last flash separation, F-401, occurs at 0°F.
8. **THF Recovery Train**: Initially, the THF recovery train did not exist and a large amount of THF was released with the two incineration streams leaving F-300 and F-400. However, upon closer inspection and with guidance from Professor Fabiano, the design group decided that the 325 lb THF/hr was worth recovering by dropping the temperature to 0°F. Since the total flow rate of the incineration streams is only 657 lb/hr, it was found economical to install a small refrigeration unit to cool the stream to recover the valuable product.

5.0 Energy Balance and Utility Requirements

This section outlines the energy balance and overall utility requirements of the production plant. The energy balance includes all energy inputs and outputs that cross the system boundary and excludes heat exchangers that have two internally-contained streams. As revealed in the table below, the overall process requires a net energy removal duty. This is due to the fact that the heat of reaction released by the highly exothermic hydrogenation reactions is used to vaporize the product, and it is not accounted for in the energy balance since it does not cross the system boundary. In the table, note that the duties of X-201 and X-400 are omitted since the exchangers involve two streams contained within the system boundary; its inclusion would result in double counting the heat duties of the fired heater and refrigerator.

Two significant efforts were made to reduce utility requirements by integrating X-200 and X-301 and by incinerating the vapor effluent of F-401 within the fired heater H-200. First, boiler feed water is used in place of cooling water in X-200 so that 50 psig steam may be generated by the exchanger; this steam is applied to the D-300 reboiler, X-301, in order to reduce the utility steam requirement of the reboiler. Second, since the vapor effluent from F-401 contains a significant amount of clean fuel (hydrogen, methane, propane, and n-butane), it is sent to H-200, where it is incinerated and used to heat the Dowtherm A heating fluid. This reduces the natural gas requirement of the fired heater. Other efforts to integrate heat requirements could not be accomplished because the remaining heat removal duties are at temperatures below 300°F, the minimum temperature where steam production is viable. However, significant pressure drops from 2040 psig to 150 psig in both vapor and liquid phases are accomplished by using valves throughout the process. The project team believes that this pressure energy can be harnessed with a turbine (turbines) and should be considered.

5.1 Energy Balance

ENERGY REQUIREMENTS OF PROCESS

Equipment	Description	Duty (Btu/hr)	Source	Notes
Section 100				
X-100	Heat Exchanger	2,786,743	Steam (50 psig)	S-100 heated 94°F to 201.2°F
P-100	Pump	524,183	Electricity	S-101 pumped 0 psig to 2040 psig
C-100	2-Stage Compressor	4,489,811	Electricity	S-103 compressed 250 psig to 2040 psig
C-100	Compressor Intercooler	(1,713,554)	Cooling Water	S-103 cooled 334°F to 104°F
		6,087,184		**Net Section 100**
Section 200				
X-200	Heat Exchanger	(49,017,997)	Boiler Feed Water	S-105 cooled 480°F to 104°F, 43,274 lb/hr 50 psig steam generated
C-200	Compressor	1,959,896	Electricity	S-204 compressed 1695 psig to 2040 psig
X-201	Heat Exchanger	***	Dowtherm A	S-205 heated 149°F to 572°F
H-200	Fired Heater	17,038,956	Natural gas/ Incin. Streams	HF 202 heated 164°F to 660°F
P-200	Pump	76,452	Electricity	HF-201 pumped 0 psig to 3 psig
F-401	*Incineration Credits*	(13,126,528)	*Incineration Stream*	*Hydrogen and alkanes to be incinerated*
		(43,069,222)		**Net Section 200**
Section 300				
X-300	Condenser	(45,344,534)	Cooling Water	S-302 condensed, cooled 222°F to 169°F
P-301	Pump	547,496	Electricity	S-304 pumped up 62 ft to top of D-300
P-302	Pump	69,561	Electricity	S-307 pumped 22 psig to 25 psig
X-301	Reboiler	47,247,168	Steam (50 psig)	S-309 vaporized, heated 234°F to 255°F
P-300	Pump	89,922	Electricity	S-311 pumped 22 psig to 2040 psig
X-200	*Steam Credits*	(39,436,434)	*Steam (50 psig)*	*From 43,274 lb/hr steam production and* ΔH_v *=911.31 Btu/lb*
		(36,826,820)		**Net Section 300**
Section 400				
X-400	Heat Exchanger	***	Coolant	S-401 cooled 90°F to 0°F, S-300 cooled 78°F to 0°F
P-400	Pump	1,311	Electricity	HF-401 pumped 0°F psig to 3°F psig
H-400	Refrigerator	132,532	Refrige Electricity	HF-402 cooled 63°F to -22°F
		133,842		**Net Section 400**

Section 500				
X-500	Condenser	(10,973,901)	Cooling Water	S-500 condensed
P-500	Pump	714,843	Electricity	S-502 pumped up 94 ft to top of D-500
P-501	Pump	54,768	Electricity	S-505 pumped 2.3 psig to 5.3 psig
X-501	Reboiler	11,195,257	Steam (50 psig)	S-507 vaporized, heated 201°F to211°F
P-502	Pump	20,515	Electricity	S-504 pumped 0.3 psig to 100.3 psig
X-502	Condenser	(5,727,472)	Cooling Water	S-511 condensed
P-503	Pump	230,210	Electricity	S-513 pumped up 50 ft to top of D-501
P-504	Pump	88,118	Electricity	S-516 pumped 102.3 psig to 105.3 psig
X-503	Reboiler	7,640,278	Steam (150 psig)	S-519 vaporized
		3,242,618		**Net Section 500**
Section 600				
X-600	Heat Exchanger	(1,199,440)	Cooling Water	S-600 cooled 171°F to 104°F
		(1,199,440)		**Net Section 600**
Total Net Energy Required		**(71,631,839)**	**Btu/hr**	

5.2 Utility Requirements

All utilities are assumed to be readily available in the Gulf Coast region and are purchased directly from public and private utility companies. The project team deemed in-house utility plants unnecessary, given the relatively small steam and electricity requirements. All utility prices are estimated using Table 23.1 (at CE 2006= 500) of *Product and Process Design Principles, 3rd Edition*, and are adjusted for 2008 prices, where CE 2008 is 548.4 (Seider, Seader, Lewin, & Widagdo, 2009). Brief and full table summaries of all utility requirements follow brief paragraph descriptions of the cost and details associated with each type of utility.

Electricity

The process requires 2,599 kW of electricity to power the various pumps and compressors used throughout the plant. Electricity is available locally at a cost of $0.06582/kW-h, adjusted for 2008 prices.

Cooling Water (CW)

The process requires 2,168,572 lb/hr of cooling water to cool and condense process streams in various heat exchangers. It is available by pipeline at $0.08228/1000 gallons, adjusted for 2008 prices. Cooling water is assumed to enter the plant at a temperature of 90°F and a pressure of 65 psig. It is used to cool streams by absorbing heat until it reaches a temperature of 120°F, at which point it is at the highest allowable temperature for disposal. Since the plant operates in the Gulf Coast, a conservative minimum temperature approach of 14°F is employed whenever cooling water is used in the process.

Steam

The process requires 67,011 lb/hr of 50 psig steam and 8,917 lb/hr of 150 psig steam, which is available by pipeline at $3.291/1000 lb and $5.2656/1000 lb, respectively. However, 43,274 lb/hr of 50 psig steam is produced by the process, and is applied to reduce the amount of pipeline 50 psig steam required to 23,737 lb/hr. The steam is used within various heat exchangers and reboilers to heat the process streams. The higher grade steam is required in the reboiler of the high-pressure distillation column because the reboiler temperature is higher than the temperature of saturated 50 psig steam.

Boiler Feed Water (BFW)

The process requires 43,274 lb/hr of BFW in order to cool and partially condense the vapor effluent from the reactor. Since this stream must be cooled from 480°F to 104°F, the heat can be recovered to produce 50 psig steam, which reduces the amount of utility steam required. BFW is assumed to enter the plant at the same temperature as cooling water, 90°F, and it is highly purified to ensure that upon vaporization, it does not leave residue on the walls of the heat exchanger. It is available at \$1.9746/1000 gallons, adjusted for 2008 prices.

Refrigeration

The process requires 11.04 day-ton/hr of refrigeration at -30°F to power the refrigeration unit in the THF recovery section. It is available at \$2.6328/day-ton, adjusted for 2008 prices.

Natural Gas

The process requires 3,806 SCF/hr of natural gas in the fired Dowtherm A heater in the hydrogen recycle section. This utility supplements the incineration stream from the THF recovery section, which contains hydrogen and small chain alkanes that are incinerated in the heater as well. It is available via pipeline at \$3.5104/1000 SCF, adjusted for 2008 prices.

Waste Water Treatment

The process requires waste water treatment to remove 1,112 lb/hr of organics from 26,277 lb/hr of waste water that leaves through the bottoms of the atmospheric pressure-swing distillation column. Since the plant operates on the Gulf Coast, waste water treatment facilities are close by and readily available to receive the waste water by pipeline from the THF production plant. The treatment facility charges \$0.16455/lb organic removed for its services, adjusted for 2008 prices.

Utility Requirements of Process

Utility	Process Requirement		Cost/hr
Electricity	2,598.7	kW	\$ 202.59
Cooling Water	2,168,571.8	lb/hr	\$ 25.33
Steam (50 psig)	23,737.0	lb/hr	\$ 92.52
Steam (150 psig)	8,916.6	lb/hr	\$ 55.61
Boiler Feed Water	43,274.4	lb/hr	\$ 12.13
Refrigeration (-30°F)	11.0	day-ton/hr	\$ 34.44
Natural Gas	3,805.9	SCF/hr	\$ 15.82
Waste Water Treatment	1,112.4	lb organics/hr	\$ 216.80

Utility Requirements of Process

Electricity

Equipment	*Description*	*Usage (Production)*		*Section Total*	
Section 100				1,469.5	kW
P-100	Reciprocating Pump	153.6	kW		
C-100	2-Stage Compressor + Intercooler	1,315.8	kW		
Section 200				596.8	kW
C-200	Reciprocating Compressor	574.4	kW		
P-200	Centrifugal Pump	22.4	kW		
Section 300				207.2	kW
P-300	Reciprocating Pump	26.4	kW		
P-301	Centrifugal Reflux Pump	160.5	kW		
P-302	Centrifugal Reboiler Pump	20.4	kW		
Section 400				0.4	kW
P-400	Centrifugal Pump	0.4	kW		
Section 500				324.9	kW
P-500	Centrifugal Reflux Pump	209.5	kW		
P-501	Centrifugal Reboiler Pump	16.1	kW		
P-502	Centrifugal Pump	6.0	kW		
P-503	Centrifugal Reflux Pump	67.5	kW		
P-504	Centrifugal Reboiler Pump	25.8	kW		
Total Electricity Requirement				2,598.7	kW

Cooling Water

Equipment	*Description*	*Usage (Production)*		*Section Total*	
Section 100				57,348.3	lb/hr
C-100	2-Stage Compressor + Intercooler	57,348.3	lb/hr		
Section 300				1,517,566.0	lb/hr
X-300	Shell-and-Tube Condenser	1,517,566.0	lb/hr		
Section 500				558,952.4	lb/hr
X-500	Shell-and-Tube Condenser	367,268.5	lb/hr		
X-502	Shell-and-Tube Condenser	191,683.9	lb/hr		
Section 600				34,705.0	lb/hr
X-600	Shell-and-Tube Heat Exchanger	34,705.0	lb/hr		
Total Cooling Water Requirement				2,168,571.8	lb/hr

Steam (50 psig)

Equipment	*Description*	*Usage (Production)*		*Section Total*	
Section 100				2,901.0	lb/hr
X-100	Heat Exchanger	2,901.0	lb/hr		
Section 300				51,829.3	lb/hr
X-301	Thermosyphon Reboiler	51,829.3	lb/hr		
Section 500				12,281.0	lb/hr
X-501	Thermosyphon Reboiler	12,281.0	lb/hr		
Steam Credits (BFW)				(43,274.4)	lb/hr
X-200	Steam Produced by X-200	(43,274.4)	lb/hr		
Total 50 psig Steam Requirement				23,737.0	lb/hr

Steam (150 psig)

Equipment	*Description*	*Usage (Production)*		*Section Total*	
Section 500				8,916.6	lb/hr
X-503	Thermosyphon Reboiler	8,916.6	lb/hr		
Total 150 psig Steam Requirement				8,916.6	lb/hr

Boiler Feed Water

Equipment	*Description*	*Usage (Production)*		*Section Total*	
Section 200				43,274.4	lb/hr
X-200	Heat Exchanger	43,274.4	lb/hr		
Total Boiler Feed Water Requirement				43,274.4	lb/hr

Refrigeration (-30°F)

Equipment	*Description*	*Usage (Production)*		*Section Total*	
Section 400				11.0	ton-day/hr
H-400	Refrigerator	11.0	ton-day/hr		
Total -30°F Refrigeration Requirement				11.0	ton-day/hr

Natural Gas

Equipment	*Description*	*Usage (Production)*		*Section Total*	
Section 200				3,805.9	SCF/hr
H-200	Fired Heater for Dowtherm A	3,805.9	SCF/hr		
Total Natural Gas Requirement				3,805.9	SCF/hr

Waste Water Treatment

Equipment	*Description*	*Usage (Production)*		*Section Total*	
Section 500				1,112.4	lb organics
D-500	Waste Water Treatment for S-508	1,112.4	lb organics		
Total Waste Water Treatment Requirement				1,112.4	lb organics/hr

6.0 Equipment List and Unit Descriptions

Preliminary estimations of equipment costs are computed according to the Individual Factors Method of Guthrie (1969, 1974), which are outlined in *Product and Process Design Principles: Synthesis, Analysis and Design, 3rd Edition* (Seider, Seader, Lewin, & Widagdo, 2009). The equipment pricing guidelines in the text are indexed to the Chemical Engineering (CE) Plant Index for 2006 (CE=500), and thus must be updated to current levels to accurately reflect prices in April 2009. According to the March 2009 issue of the *Chemical Engineering* journal, which publishes CE index estimates on a monthly basis, the CE Index as of December 2008 is 548.4 (Chemical Engineering, 2009).

$$Cost = Base\ Cost \left(\frac{I}{I_{base}}\right)$$

To find the base module cost (C_{BM}), the f.o.b. costs (C_p), which are computed using Guthrie's method, are multiplied by the Bare Module Factor (BMF) for the equipment type in question.

As a rule of thumb for selecting the materials of construction for each piece of equipment, the cheapest option, carbon steel, is used for all equipment involving cooling water or pressurized steam. Maleic acid and succinic acid are weak organic acids, GBL is a lactone, BDO is an alcohol, and THF is an ether, all of which are damaging to carbon steel. Hydrogen is also known to corrode carbon steel. Thus, stainless steel is selected for equipment with these compounds as major components in the feed streams.

This section consists of three segments:

1. **Summary Cost Sheet**: this outlines key sizing and costing data, f.o.b. costs, bare module costs, and utility requirements are provided for each piece of equipment. It is organized by process flowsheet sections 100-600.
2. **Written descriptions**: for each piece of equipment; they discuss its specifications, design methodologies, important approximations, and usage. It is in paragraph form and is organized alphanumerically, by equipment ID.
3. **Specification Sheets:** for each piece of equipment; they include detailed sizing and costing information and stream information for all incoming and outgoing streams. It is organized alphanumerically, by equipment ID.

For detailed calculations of equipment size and cost, refer to Appendix A.2 on Page 188.

6.1 Summary Cost Sheets

6.1.1 Section 100

Key Sizing Data and Costs Summary

Section 100: Preparation of Reactants and Reactor			Bare Module Factor	Total Installation Cost (CE=548.4)

Heat Exchanger, X-100			3.17	$ 71,000
Heat Duty	2,786,743	Btu/hr		
ΔT	97.200	°F (Cold Side)		
Overall HT Coefficient (U)	150.000	Btu/hr-ft2 -F		
Heat Transfer Area	130.783	ft2		
Steam Required	*2,900.999*	*lb/hr (50 psig)*		
F.o.b. Cost (C_p)	$ 22,400			

Pump, P-100			3.30	$ 291,100
Brake Power	206.012	Hp		
Pressure Change	2,040.000	psi		
Flow Rate	725.200	ft3/hr		
Pump Efficiency	0.522			
Electricity Required	*153.623*	*kW*		
F.o.b. Cost (C_p)	$ 88,200			

2-Stage Compressor + Intercooler, C-100			2.15	$ 7,776,300
Total Brake Power	1,644.127	Hp		
Total Pressure Change	1,790.000	psi		
Flow Rate	2,142.880	lb/hr		
Efficiency	0.720			
Cooling Water Required	*57,348.283*	*lb/hr*		
Electricity Required	*1,315.834*	*kW*		
F.o.b. Cost (C_p)	$ 3,616,900			

Reactor, R-100			4.16	$ 3,195,300
Vessel Diameter	5.361	ft		
Vessel Height	102.308	ft		
Vessel Wall Thickness	5.074	in		
Vessel Weight	401,915.933	lb		
Heat Duty	0.000	Btu/hr		
Operating Pressure	2,000.000	psig		
Operating Temperature	482.000	°F		
Flow Rate	55,405.368	lb/hr		
F.o.b. Cost (C_p)	$ 768,100			

Total Cooling Water Requirement	57,348.283	lb/hr		
Total Electricity Requirement	1,469.46	kW		
Total 50 psig Steam Requirement	2,900.999	lb/hr		
Total F.o.b. Cost for Section 100			$	4,495,600
Total Installed Cost for Section 100			**$**	**11,333,700**

6.1.2 Section 200:

Key Sizing Data and Costs Summary

Section 200: Hydrogen Recycle			Bare Module Factor	Total Installation Cost (CE=548.4)
Heat Exchanger, X-200			3.17	$ 850,200
Heat Duty	-49,017,997	Btu/hr		
ΔT	-376.397	°F (Hot Side)		
Overall HT Coefficient (U)	60.000	Btu/hr-ft2 -F		
Heat Transfer Area	12,440.899	ft2		
BFW Required	*43,274.387*	*lb/hr (50 psig)*		
F.o.b. Cost (C_p)	$ 268,200			
Flash, F-200			4.16	$ 322,400
Vessel Diameter	2.643	ft		
Vessel Height	7.929	ft		
Vessel Wall Thickness	2.445	in		
Vessel Weight	9,141.180	lb		
Heat Duty	0.000	Btu/hr		
Operating Pressure	1,995.000	psig		
Operating Temperature	104.000	°F		
Flow Rate	55,405.368	lb/hr		
F.o.b. Cost (C_p)	$ 77,500			
Hydrogen Separation Membrane, M-200			2.32	$ 226,100
Total Area	9,745.229	ft2		
Retentate Pressure Drop	10.000	psi		
Permeate Pressure Drop	300.000	psi		
F.o.b. Cost (C_p)	$ 97,450			
Compressor, C-200			2.15	$ 3,461,900
Total Brake Power	716.879	Hp		
Total Pressure Change	345.000	psi		
Flow Rate	11,771.762	lb/hr		
Efficiency	0.720			
Electricity Required	*574.39*	*kW*		
F.o.b. Cost (C_p)	$ 1,610,200			
Heat Exchanger, X-201			3.17	$ 311,600
Heat Duty	17,038,956	Btu/hr		
ΔT	423.207	°F (Cold Side)		
Overall HT Coefficient (U)	102.500	Btu/hr-ft2 -F		
Heat Transfer Area	4,028.974	ft2		
F.o.b. Cost (C_p)	$ 98,300			

Pump, P-200				3.30	$	22,800
Brake Power		26.582	Hp			
Pressure Change		3.000	psi			
Flow Rate		1,186.613	ft3/hr			
Pump Efficiency		0.584				
Electricity Required		*22.406*	*kW*			
F.o.b. Cost (C_p)	$	6,900				

Fired Heater, H-200				2.20	$	1,542,200
Heat Duty		17,038,956	Btu/hr			
ΔT		496.207	°F			
Flow Rate (Dowtherm A)		68,093.367	lb/hr			
Natural Gas Required		*3,805.863*	*SCF/hr*			
F.o.b. Cost (C_p)	$	701,000				

Total Boiler Feed Water Requirement	43,274.387	lb/hr		
Total Electricity Requirement	596.79	kW		
Total Natural Gas Requirement	3,805.863	SCF/hr		
Total F.o.b. Cost for Section 200			$	2,859,600
Total Installed Cost for Section 200			**$**	**9,596,900**

6.1.3 Section 300

Key Sizing Data and Costs Summary

Section 300: Liquid Intermediate Recycle			Bare Module Factor	Total Installation Cost (CE=548.4)
Flash, F-300			4.16	$ 277,500
Vessel Diameter	3.617	ft		
Vessel Height	10.851	ft		
Vessel Wall Thickness	0.996	in		
Vessel Weight	6,624.954	lb		
Heat Duty	0.000	Btu/hr		
Operating Pressure	585.300	psig		
Operating Temperature	104.009	°F		
Flow Rate	42,052.700	lb/hr		
F.o.b. Cost (C_p)	$ 66,700			
Column, D-300			4.16	$ 1,007,600
Actual Number of Stages	24			
Mass Reflux Ratio	0.600			
Operating Pressure	5.300	psig		
Stage Pressure Drop	0.083	psig		
Vessel Diameter	6.269	ft		
Vessel Height	62.000	ft		
Vessel Wall Thickness	0.375	in		
Vessel Weight	20,700.155	lb		
F.o.b. Cost (C_p)	$ 242,200			
Condenser, X-300			3.17	$ 373,100
Heat Duty	-45,344,534	Btu/hr		
ΔT	-53.653	°F (Hot Side)		
Overall HT Coefficient (U)	100.000	Btu/hr-ft2 -F		
Heat Transfer Area	5,047.551	ft2		
Cooling Water Required	*1,517,566.040*	*lb/hr*		
F.o.b. Cost (C_p)	$ 117,700			
Reflux Accumulator, A-300			3.05	$ 138,200
Vessel Diameter	6.039	ft		
Vessel Length	12.077	ft		
Vessel Wall Thickness	0.313	in		
Vessel Weight	4,189.867	lb		
Heat Duty	0.000	Btu/hr		
Operating Pressure	5.300	psig		
Operating Temperature	168.527	°F		
Flow Rate	59,680.411	lb/hr		
F.o.b. Cost (C_p)	$ 45,300			

Reflux Pump, P-301				3.30	$	113,500
Brake Power		197.399	Hp			
Pressure Change		24.762	psi			
Flow Rate		1,037.694	ft3/hr			
Pump Efficiency		0.568				
Electricity Required		*160.455*	*kW*			
F.o.b. Cost (C_p)	$	34,400				

Reboiler Pump, P-302				3.30	$	32,300
Brake Power		24.133	Hp			
Pressure Change		3.000	psi			
Flow Rate		1,049.797	ft3/hr			
Pump Efficiency		0.569				
Electricity Required		*20.386*	*kW*			
F.o.b. Cost (C_p)	$	9,800				

Thermosyphon Reboiler, X-301				3.17	$	624,500
Heat Duty		47,247,168	Btu/hr			
ΔT		20.702	°F (Cold Side)			
Overall HT Coefficient (U)		100.000	Btu/hr-ft2 -F			
Heat Transfer Area		9,055.189	ft2			
Steam Required (50 psig)		*51,829.341*	*lb/hr (50 psig)*			
F.o.b. Cost (C_p)	$	197,000				

Pump, P-300				3.30	$	63,000
Brake Power		35.341	Hp			
Pressure Change		2,032.696	psi			
Flow Rate		70.680	ft3/hr			
Pump Efficiency		0.296				
Electricity Required		*26.354*	*kW*			
F.o.b. Cost (C_p)	$	19,100				

Total Cooling Water Requirement	1,517,566.040	lb/hr		
Total Electricity Requirement	207.20	kW		
Total 50 psig Steam Requirement	51,829.341	lb/hr		
Total F.o.b. Cost for Section 300			$	732,200
Total Installed Cost for Section 300			**$**	**2,629,700**

6.1.4 Section 400

Key Sizing Data and Costs Summary

Section 400: THF Recovery from Incineration Streams			Bare Module Factor	Total Installation Cost (CE=548.4)
Flash, F-400			4.16	$ 32,000
Vessel Diameter	0.781	ft		
Vessel Height	2.344	ft		
Vessel Wall Thickness	0.250	in		
Vessel Weight	77.849	lb		
Heat Duty	0.000	Btu/hr		
Operating Pressure	150.000	psig		
Operating Temperature	105.249	°F		
Flow Rate	1,580.905	lb/hr		
F.o.b. Cost (C_p)	$ 7,700			
Heat Exchanger, X-400			3.17	$ 85,900
Heat Duty	-132,532	Btu/hr		
ΔT	-78.155	°F (Hot Side)		
Overall HT Coefficient (U)	20.000	Btu/hr-ft2 -F		
Heat Transfer Area	362.561	ft2		
F.o.b. Cost (C_p)	$ 27,100			
Pump, P-400			3.30	$ 22,100
Brake Power	0.396	Hp		
Pressure Change	3.000	psi		
Flow Rate	30.243	ft3/hr		
Pump Efficiency	1.000			
Electricity Required	*0.384*	*kW*		
F.o.b. Cost (C_p)	$ 6,700			
Refrigerator, H-400			1.00	$ 274,200
Heat Duty	-132,532	Btu/hr		
ΔT	-85.155	°F		
Flow Rate (Ethylene Glycol/Water)	2,047.051	lb/hr		
Refrigeration Duty (-30 °F)	*11.044*	*ton-day/hr*		
F.o.b. Cost (C_p)	$ 274,200			

Flash, F-401				4.16	$	18,700
Vessel Diameter		0.370	ft			
Vessel Height		1.109	ft			
Vessel Wall Thickness		0.250	in			
Vessel Weight		17.920	lb			
Heat Duty		0.000	Btu/hr			
Operating Pressure		150.000	psig			
Operating Temperature		0.000	°F			
Flow Rate		656.587	lb/hr			
F.o.b. Cost (C_p)	$	4,500				

Total Refrigeration Duty (-30°F)	11.044	ton-day/hr		
Total Electricity Requirement	0.38	kW		
Total F.o.b. Cost for Section 400			$	320,200
Total Installed Cost for Section 400			**$**	**432,900**

6.1.5 Section 500

Key Sizing Data and Costs Summary

Section 500: Pressure-Swing Distillation			Bare Module Factor	Total Installation Cost (CE=548.4)
Column, D-500			4.16	$ 1,159,000
Actual Number of Stages	40			
Mass Reflux Ratio	0.904			
Operating Pressure	0.300	psig		
Stage Pressure Drop	0.051	psig		
Vessel Diameter	4.566	ft		
Vessel Height	94.000	ft		
Vessel Wall Thickness	0.438	in		
Vessel Weight	25,709.152	lb		
F.o.b. Cost (C_p)	$ 278,600			
Condenser, X-500			3.17	$ 233,000
Heat Duty	-10,973,901	Btu/hr		
ΔT	-0.037	°F (Hot Side)		
Overall HT Coefficient (U)	100.000	Btu/hr-ft2 -F		
Heat Transfer Area	2,713.426	ft2		
Cooling Water Required	*367,268.511*	*lb/hr*		
F.o.b. Cost (C_p)	$ 73,500			
Reflux Accumulator, A-500			3.05	$ 146,100
Vessel Diameter	5.856	ft		
Vessel Length	11.712	ft		
Vessel Wall Thickness	0.375	in		
Vessel Weight	4,732.830	lb		
Heat Duty	0.000	Btu/hr		
Operating Pressure	0.300	psig		
Operating Temperature	147.258	°F		
Flow Rate	50,536.243	lb/hr		
F.o.b. Cost (C_p)	$ 47,900			
Reflux Pump, P-500			3.30	$ 139,900
Brake Power	258.659	Hp		
Pressure Change	34.862	psi		
Flow Rate	946.269	ft3/hr		
Pump Efficiency	0.557			
Electricity Required	*209.500*	*kW*		
F.o.b. Cost (C_p)	$ 42,400			

Reboiler Pump, P-501				3.30	$	30,000
Brake Power		18.892	Hp			
Pressure Change		3.000	psi			
Flow Rate		763.374	ft3/hr			
Pump Efficiency		0.529				
Electricity Required		*16.051*	*kW*			
F.o.b. Cost (C_p)	$	9,100				

Thermosyphon Reboiler, X-501				3.17	$	142,300
Heat Duty		11,195,257	Btu/hr			
ΔT		10.034	°F (Cold Side)			
Overall HT Coefficient (U)		100.000	Btu/hr-ft2 -F			
Heat Transfer Area		1,219.432	ft2			
Steam Required (50 psig)		*12,281.007*	*lb/hr (50 psig)*			
F.o.b. Cost (C_p)	$	44,900				

Pump, P-502				3.30	$	27,400
Brake Power		8.063	Hp			
Pressure Change		105.000	psi			
Flow Rate		496.880	ft3/hr			
Pump Efficiency		0.471				
Electricity Required		*6.012*	*kW*			
F.o.b. Cost (C_p)	$	8,300				

Column, D-501				4.16	$	413,500
Actual Number of Stages		18				
Mass Reflux Ratio		0.855				
Operating Pressure		100.300	psig			
Stage Pressure Drop		0.105	psig			
Vessel Diameter		3.356	ft			
Vessel Height		50.000	ft			
Vessel Wall Thickness		0.174	in			
Vessel Weight		4,045.677	lb			
F.o.b. Cost (C_p)	$	99,400				

Condenser, X-502				3.17	$	84,300
Heat Duty		-5,727,472	Btu/hr			
ΔT		-1.046	°F (Hot Side)			
Overall HT Coefficient (U)		100.000	Btu/hr-ft2 -F			
Heat Transfer Area		337.721	ft2			
Cooling Water Required		*191,683.892*	*lb/hr*			
F.o.b. Cost (C_p)	$	26,600				

Reflux Accumulator, A-501				3.05	$	104,300
Vessel Diameter		4.853	ft			
Vessel Length		9.706	ft			
Vessel Wall Thickness		0.252	in			
Vessel Weight		2,182.275	lb			
Heat Duty		0.000	Btu/hr			
Operating Pressure		100.300	psig			
Operating Temperature		274.480	°F			
Flow Rate		26,036.243	lb/hr			
F.o.b. Cost (C_p)	$	34,200				

Reflux Pump, P-503				3.30	$	58,400
Brake Power		81.867	Hp			
Pressure Change		16.787	psi			
Flow Rate		538.546	ft3/hr			
Pump Efficiency		0.482				
Electricity Required		*67.468*	*kW*			
F.o.b. Cost (C_p)	$	17,700				

Reboiler Pump, P-504				3.30	$	35,300
Brake Power		30.738	Hp			
Pressure Change		3.000	psi			
Flow Rate		1,422.363	ft3/hr			
Pump Efficiency		0.606				
Electricity Required		*25.825*	*kW*			
F.o.b. Cost (C_p)	$	10,700				

Thermosyphon Reboiler, X-503				3.17	$	136,600
ΔT		0.342	°F (Cold Side)			
Heat Duty		7,640,278	Btu/hr			
Overall HT Coefficient (U)		100.000	Btu/hr-ft2 -F			
Heat Transfer Area		1,105.752	ft2			
Steam Required (150 psig)		*8,916.639*	*lb/hr (150 psig)*			
F.o.b. Cost (C_p)	$	43,100				

Total Cooling Water Requirement	558,952.403	lb/hr		
Total Electricity Requirement	324.86	kW		
Total 50 psig Steam Requirement	12,281.007	lb/hr		
Total 150 psig Steam Requirement	8,916.639	lb/hr		
Total F.o.b. Cost for Section 500			$	736,400
Total Installed Cost for Section 500			**$**	**2,710,100**

6.1.6 Section 600

Key Sizing Data and Costs Summary

Section 600: Product Production and Storage			Bare Module Factor	Total Installation Cost (CE=548.4)
Heat Exchanger, X-600			3.17	$ 90,000
Heat Duty	-1,199,440	Btu/hr		
ΔT	-67.331	°F (Hot Side)		
Overall HT Coefficient (U)	100.000	Btu/hr-ft2 -F		
Heat Transfer Area	417.442	ft2		
Cooling Water Required	*34,705.034*	*lb/hr*		
F.o.b. Cost (C_p)	$ 28,400			
Storage Tanks, T-600			4.16	$ 2,942,800
Holdup	48	hours		
Volume	83,325.426	gal		
Design Temperature	90.000	°F		
Design Pressure	3.000	psig		
Type	2 Floating Roof Tanks (CE 2006=500)			
F.o.b. Cost (C_p)	$ 707,400			
Total Cooling Water Requirement	34,705.034	lb/hr		
Total F.o.b. Cost for Section 600				$ 735,800
Total Installed Cost for Section 600				**$ 3,032,800**

6.1.7 Supplementary Chemical and Catalyst Costs

Supplementary Chemical and Catalyst Costs

					Total Installation Cost (CE=548.4)
Catalyst, R-100				$	875,600
Mass Required		20,833	lb		
% Pd		0.5%			
% Re		0.5%			
Annual Regeneration Cost	$	130,900	per year		
F.o.b. Cost (C_p)	$	875,600			
Dowtherm A Thermal Fluid				$	53,100
Mass Required		11,349.000	lb		
Unit Price		4.680	per lb		
F.o.b. Cost (C_p)	$	53,110			
Ethylene Glycol Thermal Fluid				$	110
% Ethylene Glycol		50.000%			
Mass Ethylene Glycol Required		170.600	lb		
Mass Water Required		170.600	lb		
Ethylene Glycol Unit Price		0.650	per lb		
Process Water Unit Price		0.002	per gal		
F.o.b. Cost (C_p)	$	110			

6.2 Equipment Design Descriptions

6.2.1 Horizontal Pressure Vessels

A-300: Reflux Accumulator

A-300 is the reflux accumulator for column D-300. It collects 1038 ft^3/hr of condensed liquid from the column overhead condenser and stores it for an average holdup time of 5 minutes before it is split into the distillate stream and reflux stream. The vessel operates half-full. The operating pressure is 5.3 psig and operating temperature is 169°F. The vessel is 6.0 ft in diameter, 12.1 ft in length, and is constructed from Stainless Steel 304 in order to prevent corrosion from the organic solvents in the overhead. The estimated purchase cost (CE 2008= 548.4) is $45,300, and the total purchase and installation cost is $138,200. The reflux accumulator was modeled using Professor Fabiano's Flash Sizing spreadsheet and ASPEN Plus 2006 using the NRTL-RK property setting. (See the specification sheet on Page 77 and design calculations on Page 189 in the Appendix)

A-500: Reflux Accumulator

A-500 is the reflux accumulator for column D-500. It collects 946 ft^3/hr of condensed liquid from the column overhead condenser and stores it for a holdup time of 5 minutes before it is sent into the distillate and reflux streams. The vessel operates half-full. The operating pressure is 0.3 psig and operating temperature is 147°F. The vessel is 5.8 ft in diameter, 11.7 ft in length, and is constructed from Stainless Steel 304 in order to prevent corrosion from the organic solvents in the overhead. The estimated purchase cost (CE 2008= 548.4) is $47,900 and the total purchase and installation cost is $146,100. The reflux accumulator was modeled using Professor Fabiano's Flash Sizing spreadsheet and ASPEN Plus 2006 using the NRTL-RK property setting. (See the specification sheet on Page 78 and design calculations on Page 189 in the Appendix)

A-501: Reflux Accumulator

A-501 is the reflux accumulator for column D-501. It collects 539 ft^3/hr of condensed liquid from the column overhead condenser and stores it for a holdup of 5 minutes before it is split into the distillate stream and reflux stream. The vessel operates half-full. The operating pressure is 100.3 psig and operating temperature is 274°F. The vessel is 4.9 ft in diameter, 9.7 ft in length, and is constructed from Stainless Steel 304 in order to prevent corrosion from the organic solvents in the overhead. The estimated purchase cost (CE 2008= 548.4) is $34,200 and the total purchase and installation cost is $104,300. The reflux accumulator was modeled using Professor Fabiano's Flash Sizing spreadsheet and ASPEN Plus 2006 using the NRTL-RK property setting. (See the specification sheet on Page 79 and design calculations on Page 190 in the Appendix)

6.2.2 Compressors

C-100: Two-Stage Reciprocating Compressor with Intercooler

C-100 is used to compress the hydrogen make-up supplied to the reactor to 2040 psig in order to ensure that the reactor pressure stays at 2000 psig. The extra 40 psi is supplied to give the hydrogen enough pressure to overcome the liquid head present at the bottom of the reactor. To achieve a pressure increase of 1,790 psi, the compressor requires two stages and an intercooler to keep the compression ratios within an acceptable range. The maximum single-stage compression ratio is 3.75 for a diatomic gas (Seider, Seader, Lewin, & Widagdo, 2009), and accordingly, bringing the pressure from 250 psig to 2040 psig requires two stages. The first stage compression raises the pressure to 723 psig and the temperature of the hydrogen stream to 334 °F, requiring an intercooler after the first stage to bring the temperature down to 104°F with cooling water. The second compressor raises the pressure to 2040 psig and the temperature to 390 °F, but no intercooler is required after the second stage because the elevated temperature of the hydrogen maintains the adiabatic aspect of the reactor.

Reciprocating compressors are selected for both stages, since they are more efficient than screw compressors, and the process does not involve the high flow rates and large pressure changes that centrifugal compressors are designed for (Seider, Seader, Lewin, & Widagdo, 2009). Both compressors utilize electric motors, which are the most common drivers in compressors (Seider, Seader, Lewin, & Widagdo, 2009). The compressor compresses 2,143 lb/hr of hydrogen, requires a total brake power of 1,644 Hp, and uses approximately 1,316 kW of electricity. It is constructed from Stainless Steel 304 in order to prevent corrosion due to the hydrogen.

The intercooler is a shell-and-tube heat exchanger that cools the pressurized hydrogen to 104°F on the tube side using 57,348 lb/hr of cooling water on the shell side. The heat duty of the exchanger is -1,713,554 Btu/hr. The overall heat transfer coefficient for the cooling water/high pressure hydrogen heat transfer was assumed to be 60 Btu/hr-ft^2-°F, which was selected with guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). For economic reasons, the hot hydrogen stream is placed on the tube-side, which is constructed using Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $3,616,900, and the total purchase and installation cost is $7,776,300. The compressor was modeled with ASPEN Plus 2006 using the Polytropic ASME calculation method and PSRK property setting. (See the specification sheets on Page 80 and design calculations on Pages 190 and 191 in the Appendix)

C-200: One-Stage Reciprocating Compressor

C-200 is used to compress the hydrogen recycle stream supplied to the reactor to 2040 psig in order to ensure that the reactor pressure stays at 2000 psig. The extra 40 psi is supplied in order to give the hydrogen enough pressure to overcome the liquid head present at the bottom of the reactor. To achieve a pressure increase of 345 psi in the 11,772 lb/hr stream, the compressor requires a total brake power of 717 Hp and uses approximately 574 kW of electricity. Only a single stage is needed, since the compression ratio is well below the maximum of 3.75. It is constructed from Stainless Steel 304 in order to prevent hydrogen corrosion. The estimated purchase cost (CE 2008= 548.4) is $1,610,200, and the total purchase and installation cost is $3,461,900. The compressor was modeled with ASPEN Plus 2006 using the Polytropic ASME calculation method and PSRK property setting. (See the specification sheet on Page 82 and design calculations on Page 191 in the Appendix)

6.2.3 Distillation Columns

D-300: Distillation Column

D-300 is used to separate the heavy liquid intermediates BDO and GBL that are carried out in the vapor effluent from the reactor so that they may be recycled back into the reactor. The intermediates leave the column at relatively high purity from the bottoms (4,479 lb/hr) and the remaining THF, water, and other organics leave through the distillate (37,300 lb/hr). The column has 24 stages (2 ft between trays) and uses Koch Flexitray sieve plates, which are selected due to their widespread use in chemical production processes. When pricing the trays using Guthrie's method outlined in *Product and Process Design Principles, 3rd Edition*, tray factors for sieve trays are used. After including a standard 10 ft sump and 4 ft disengagement height, the total tower height is 62 ft and the diameter is 6.3 ft. It operates at a mass reflux ratio of 0.60, has an overhead pressure of 5.30 psig, and exhibits a pressure drop of 2 psi throughout the column. It is constructed from Stainless Steel 304 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) is $242,200, and the total purchase and installation cost is $1,007,600. The column was modeled with ASPEN Plus 2006 using the NRTL-RK property setting. (See the specification sheet on Page 83 and design calculations on Page 192 in the Appendix)

D-500: Distillation Column

D-500 is the first, atmospheric column in the pressure-swing distillation train, and it is used to break the water-THF azeotrope that is present in the product stream. The distillate (26,536 lb/hr) contains the azeotrope at 95.1 mole% THF, and the bottoms (26.277 lb/hr) contains 95.8% by weight water and is sent to a waste water treatment center, which is assumed to be a viable option given the proximity of this plant to other large chemical plants. The main feeds, liquid distillate from D-300 and D-501, enter the column at the 20th stage. The liquid effluent from F-401 enters in stage 16 and the liquid effluent from F-400 enters in stage 2. Feed stages are selected to ensure that the feed concentrations of THF are close to the tray concentrations at which they enter. The column has 40 stages (2 ft between trays) and uses Koch Flexitray sieve plates, which are selected due to their widespread use in chemical production processes. When pricing the trays using Guthrie's method outlined in *Product and Process Design Principles, 3rd Edition*, tray factors for sieve trays are used. After including a standard 10 ft sump and 4 ft disengagement height, the total tower height is 94 ft and the diameter is 4.6 ft. It operates at a mass reflux ratio of 0.90, has an overhead pressure of 0.30 psig, and exhibits a pressure drop of 2 psi throughout the column. It is constructed from Stainless Steel 304 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) is $278,600 and the total purchase and installation cost is $1,159,000. The column was modeled with ASPEN Plus 2006 using the NRTL-RK property setting. (See the specification sheet on Page 84 and design calculations on Page 194 in the Appendix)

D-501: Distillation Column

D-501 is the second, high-pressure column in the pressure-swing distillation train, and it is used to break the water-THF azeotrope that is present in the reactor effluent stream. The distillate from D-500 is fed into the 9th stage of the column, which is the middle tray. The distillate (14,036 lb/hr) contains the azeotrope at 90.7% by weight THF and is sent back to D-500. The bottoms stream (12,500 lb/hr) contains 99.97% by weight THF and is the product stream. The column has 18 stages (2 ft between trays) and uses Koch Flexitray sieve plates, which are selected due to their widespread use in chemical production processes. When pricing the trays using Guthrie's method outlined in *Product and Process Design Principles, 3rd Edition*, tray factors for sieve trays are used. After including a standard 10 ft sump and 4 ft disengagement height, the total tower height is 50 ft and the diameter is 3.4 ft in diameter. It operates at a mass reflux ratio of 0.86, has an overhead pressure of 100.30 psig, and exhibits a pressure drop of 2 psi throughout the column. It is constructed from Stainless Steel 304 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) is $99,400 and the total purchase and installation cost is $413,500. The column was modeled with ASPEN Plus 2006 using the NRTL-RK property setting. (See the specification sheet on Page 85 and design calculations on Page 195 in the Appendix)

6.2.4 Heaters/Coolers

H-200: Fired Heater for Dowtherm A Heating Fluid

H-200 is used to heat Dowtherm A heating fluid from 164°F to 660°F after it is used to heat the hydrogen recycle stream entering the reactor. The required 660°F is out of the range of the highest pressure steam available, 700 psig steam, which is available at its saturation temperature of 505.5°F. A Dowtherm heating unit was selected due to explosion concerns that arose when the design originally used a furnace to directly heat the hydrogen stream. Dowtherm A is an extremely safe, nonflammable intermediate heating fluid. The fluid has a relatively long lifetime, and adds a small cost for its purchase and annual maintenance fees.

For design purposes, the design team assumed a 10 minute cycle through the Dowtherm A heating loop, which results in a purchase of 11,349 lb of Dowtherm A fluid. A sales representative at Dow Chemicals provided a quote of $4.68/lb of Dowtherm A, which yields an estimated cost of $53,100 for the fluid. H-200 has a heat duty of 17,038,956 Btu/hr and uses a combination of pipeline natural gas and the incineration stream created in Section 400 of the process, which contains mostly hydrogen, butane, propane, and methane. The net requirement of natural gas for the fired heater is 3,806 SCF/hr. The estimated purchase cost (CE 2008= 548.4) is $701,000 and the total purchase and installation cost is $1,542,200. The heater was modeled with ASPEN Plus 2006 using the PSRK property setting. (See the specification sheet on Page 90 and design calculations on Page 201 in the Appendix)

H-400: Air-Cooled Refrigerator for 50% Ethylene Glycol/Water Coolant

H-400 is used to refrigerate 50% ethylene glycol and water coolant from 63°F to -22°F after the mixture has cooled the two incineration streams in Section 400 so that condensed THF may be recovered. Although the operation of a refrigerator is costly, the incineration streams are small at a combined flow of 657 lb/hr and the unit allows for the recovery of 325 lb/hr of THF. The refrigerator has a total heat duty of -132,532 Btu/hr and requires 11.0 ton-day/hr of refrigeration duty to cool 2,047 lb/hr of coolant.

For design purposes, the design team assumed a 10 minute cycle through the refrigeration cooling loop, which results in a purchase of 170.6 lb of ethylene glycol and 170.6 lb of process water to form the required volume of 50% ethylene glycol coolant. According to the ICIS website, the market price of ethylene glycol is $0.65/lb, which results in a total purchase cost of $110 for ethylene glycol. The cost of the water is negligible. The estimated total purchase and installation cost of the refrigerator (CE 2008= 548.4) is $274,200. The cooler was modeled with ASPEN Plus 2006 using the PSRK property setting. (See the specification sheet on Page 91 and design calculations on Page 201 in the Appendix)

6.2.5 Vertical Pressure Vessels

F-200: High Pressure, Adiabatic Flash Vessel

F-200 is used to recover un-reacted hydrogen from the vapor effluent from the reactor so that it may be recycled back to the reactor. The hydrogen recycle stream allows for a greater overall conversion in the reactor. The hydrogen recovered in the vapor phase (13,353 lb/hr) is significant, since it is used as a carrier to move the THF product into the vapor phase and out of the reactor. The liquid phase (42,053 lb/hr) contains the remaining condensable components and is fed into F-300 for further separation. The operating pressure is 1995 psig and operating temperature is 104°F. The vessel is 2.6 ft in diameter, 7.9 ft tall, and is constructed from Stainless Steel 304 in order to prevent corrosion from the hydrogen and organic solvents. The estimated purchase cost (CE 2008= 548.4) is $77,500 and the total purchase and installation cost is $322,400. The flash vessel was modeled using Professor Fabiano’s Flash Sizing spreadsheet and ASPEN Plus 2006, using the PSRK property setting. (See the specification sheet on Page 86 and design calculations on Page 197 in the Appendix)

F-300: Moderate Pressure, Adiabatic Flash Vessel

F-300 is used to remove most of the remaining hydrogen and other non-condensables from the liquid phase output from F-200 by reducing the pressure from 1995 psig to 585.3 psig. Doing so will stabilize the downstream distillation columns. The vapor phase (272 lb/hr) contains hydrogen and a significant amount of THF and is sent to a THF recovery train before it is incinerated to recover heat value. This stream was not considered valuable enough to send through the hydrogen recycle loop because it is at a much lower pressure, and it was deemed uneconomical to re-compress the small amount of hydrogen back to 2040 psig. The liquid phase (41,780 lb/hr) contains the remaining condensable components and is fed into D-300 for further separation. The operating pressure is 585.3 psig and operating temperature is 78°F; these conditions were selected via trial and error, since they yielded the required amount of hydrogen separation. The vessel is 3.6 ft in diameter, 10.9 ft tall, and is constructed from Stainless Steel 304 in order to prevent corrosion from the hydrogen and organic solvents. The estimated purchase cost (CE 2008= 548.4) is $66,700 and the total purchase and installation cost is $277,500. The flash vessel was modeled using Professor Fabiano’s Flash Sizing spreadsheet and ASPEN Plus 2006, using the NRTL-RK property setting. (See the specification sheet on Page 87 and design calculations on Page 198 in the Appendix)

F-400: Low Pressure, Adiabatic Flash Vessel

F-400 is used to recover a significant amount of THF from M-200 by reducing the pressure from 1995 psig to 150 psig. The vapor phase (384 lb/hr) contains hydrogen, alkanes, and a significant amount of THF and is sent to a THF recovery train before it is incinerated to recover heat value. The liquid phase (1,197 lb/hr) contains 1,143 lb/hr of THF and other liquid impurities and is fed into D-500 for further separation. The operating pressure is 150 psig and operating temperature is 110°F; these conditions were selected via trial and error since they yielded the best hydrogen and alkane removal from the liquid without losing too much THF in the vapor. The vessel is 0.8 ft in diameter, 2.3 ft tall, and is constructed from Stainless Steel 304 in order to prevent corrosion from the hydrogen and organic solvents. The estimated purchase cost (CE 2008= 548.4) is $7,700 and the total purchase and installation cost is $32,000. The flash vessel was modeled using Professor Fabiano’s Flash Sizing spreadsheet and ASPEN Plus 2006, using the NRTL-RK property setting. (See the specification sheet on Page 88 and design calculations on Page 199 in the Appendix)

F-401: Low Pressure, Adiabatic Flash Vessel

F-401 is used to recover a significant amount of THF from the two vapor streams from F-300 and F-400 before they are incinerated and after they are cooled via refrigeration in X-400. The vapor phase (300 lb/hr) contains hydrogen, alkanes, and a small amount of THF (13.5 lb/hr), and this stream is incinerated in the furnace, H-200, where it supplements the natural gas used to fire the Dowtherm A heater. The liquid phase (357 lb/hr) contains 325 lb/hr THF and other impurities; it is fed into D-500 for further separation. The operating pressure is 150 psig and operating temperature is 0°F; these values were selected in order to maximize THF recovery while balancing refrigeration costs. The vessel is 0.4 ft in diameter, 1.1 ft tall, and is constructed from Stainless Steel 304 in order to prevent corrosion from the hydrogen and organic solvents. The estimated purchase cost (CE 2008= 548.4) is $4,500 and the total purchase and installation cost is $18,700. The flash vessel was modeled using Professor Fabiano’s Flash Sizing spreadsheet and ASPEN Plus 2006, using the NRTL-RK property setting. (See the specification sheet on Page 89 and design calculations on Page 200 in the Appendix)

6.2.6 Membranes

M-200: Hydrogen Separation Membrane

M-200 is a size-exclusion hydrogen membrane provided by Air Products PRISM® Membranes which separates hydrogen from the F-200 vapor effluent. Hydrogen serves as both a reactant and agitator in the chemical reactor, and thus it is desirable to recover as much of it as possible (Robbins, Hydrogen Recycle, 2009). In addition, the alkanes must be separated from the hydrogen to avoid a continuous buildup of compounds in the reactor. Gas permeation essentially separates components based upon their molecular weight, so it functions as a size filtration unit (Seader & Henley, Separation Process Principles, 2005, pp. 525-527). Smaller compounds such as hydrogen and water will be able to readily permeate through the membrane, whereas larger components such as propane, butane, their respective alkanols, and THF will not. Thus, the desired split fractions of the permeate that were provided to PRISM® Membranes are: hydrogen (0.99), water (0.99), THF (0.125), methane (0.2), n-butane (0.125), and propane (0.125). As can be seen, most of the hydrogen and water will permeate through the membrane, whereas a much smaller fraction of the larger compounds are allowed through (Robbins, Hydrogen Recycle, 2009). The membrane is constructed from polysulfonate polymer, since it does not deform at high pressures, allowing for constant permeance throughout the membrane.

A shell-and-tube countercurrent membrane is recommended by literature to achieve optimal separation (Seader & Henley, Separation Process Principles, 2005). In this way, the permeate can be released from the shell, while the retentate remains in the tubes. A spiral configuration has been historically used to separate the hydrogen permeate from methane in the process of fuel reformation, so this is the design used for this process as well (Seader & Henley, Separation Process Principles, 2005). The membrane's thickness is approximately 1000 Å, or 10^{-5} cm, so the hydrogen can readily filter out. The area of the membrane is 9,745 ft^2 and exhibits a pressure drop of 300 psi in the permeate and 10 psi in the retentate. The membrane is modeled in Microsoft Excel following guidance from Air Products PRISM® Membrane engineer Adam Histed and Project Advisor Professor Seider. The estimated purchase cost (CE 2008= 548.4) is $97,500 and the total purchase and installation cost is $226,200. (See the specification sheet on Page 92 and design calculations on Page 202 in the Appendix)

6.2.7 Pumps

P-100: Reciprocating Pump

P-100 is used to increase the pressure of the maleic acid feed to 2040 psig in order to ensure that the reactor pressure stays at 2000 psig. The extra 40 psi is supplied in order to give the hydrogen enough pressure to overcome the liquid head present at the bottom of the reactor. To achieve a pressure increase of 2040 psi in the 37,016 lb/hr stream, the pump requires a total brake power of 206 Hp and uses 154 kW of electricity. A reciprocating pump is selected because the large pressure increase of 2040 psig implies a developed head of 5,755 ft, which is out of the range of a centrifugal pump. It is constructed from a Ni-Al-Bronze alloy, which is the cheapest material that can withstand weak organic acid corrosion. The estimated purchase cost (CE 2008= 548.4) is $88,200 and the total purchase and installation cost is $291,100. The pump was modeled with ASPEN Plus 2006, using the PSRK property setting. (See the specification sheet on Page 93 and design calculations on Page 203 in the Appendix)

P-200: Centrifugal Pump

P-200 is used to maintain circulation within the Dowtherm A heating loop so that the thermal fluid may cycle between the fired heater and process heat exchanger. It is assumed that the Dowtherm A, which is on the shell side of X-201, experiences a 3 psi pressure drop, which is restored by P-200. To achieve a pressure increase of 3 psi in the 68,093 lb/hr stream, the pump requires a total brake power of 26.6 Hp and uses 22.4 kW of electricity. A centrifugal pump is selected because the small pressure increase of 3 psi implies a developed head of 7.5 ft, which is within the range of a centrifugal pump. It is constructed from Carbon Steel, since Dowtherm A does not have extremely corrosive properties. The estimated purchase cost (CE 2008= 548.4) is $6,900 and the total purchase and installation cost is $22,800. The pump was modeled with Microsoft Excel, knowing the desired pressure drop and flow rate of the stream. (See the specification sheet on Page 94 and design calculations on Page 203 in the Appendix)

P-300: Reciprocating Pump

P-300 is used to increase the pressure of the liquid intermediate recycle stream to 2040 psig in order to ensure that the reactor pressure stays at 2000 psig. The extra 40 psi is supplied in order to give the hydrogen enough pressure to overcome the liquid head present at the bottom of the reactor. To achieve a pressure increase of 2033 psi in the 4,479 lb/hr stream, the pump requires a total brake power of 35.3 Hp and uses 26.4 kW of electricity. A reciprocating pump is selected because the large pressure increase of 2033 psig implies a developed head of 4,619 ft, which is out of the range of a centrifugal pump. It is constructed from a Ni-Al-Bronze alloy, which is the cheapest material that can withstand weak organic solvent corrosion. The estimated purchase cost (CE 2008= 548.4) is $19,100 and the total purchase and installation cost is $63,000. The pump was modeled with ASPEN Plus 2006, using the NRTL-RK property setting. (See the specification sheet on Page 95 and design calculations on Page 204 in the Appendix)

P-301: Centrifugal Reflux Pump

P-301 is used to pump the liquid reflux from the reflux accumulator back into the top tray of D-300. Adhering to guidance provided by our industrial consultants and Professor Fabiano, the required pressure increase is set as 24.8 psi, which is the pressure required to pump the liquid from the ground level to the top of the column. To achieve a pressure increase of 24.8 psi in the 22,380 lb/hr stream, the pump requires a total brake power of 197.4 Hp and uses 160.5 kW of electricity. A centrifugal pump is selected because the small pressure increase implies a developed head of 62 ft, which is within the range of a centrifugal pump. It is constructed from Stainless Steel 304 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) is $34,400 and the total purchase and installation cost is $113,500. The pump was modeled with Microsoft Excel, knowing the desired pressure drop and flow rate of the stream. (See the specification sheet on Page 96 and design calculations on Page 205 in the Appendix)

P-302: Centrifugal Reboiler Pump

P-302 is used to pump the liquid boilup from the last stage of the column back into the bottom tray of D-300. Adhering to guidance provided by our industrial consultants and Professor Fabiano, the required pressure increase is set as 3 psi, which is slightly higher than the pressure drop across the column. To achieve a pressure increase of 3 psi in the 22,380 lb/hr stream, the pump requires a total brake power of 24.1 Hp and uses 20.4 kW of electricity. A centrifugal pump is selected because the small pressure increase of 3 psi implies a developed head of 7.5 ft, which is within the range of a centrifugal pump. It is constructed from Stainless Steel 304 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) is $9,800 and the total purchase and installation cost is $32,300. The pump was modeled with Microsoft Excel, knowing the desired pressure drop and flow rate of the stream. (See the specification sheet on Page 97 and design calculations on Page 205 in the Appendix)

P-400: Centrifugal Pump

P-400 is used to maintain circulation within the coolant heating loop so that the thermal fluid may cycle between the refrigerator and process heat exchanger. It is assumed that the 50% ethylene glycol and water coolant, which is on the shell side of X-400, experiences a 3 psi pressure drop, which is restored by P-400. To achieve a pressure increase of 3 psi in the 2,047 lb/hr stream, the pump requires a total brake power of 0.40 Hp and uses 0.38 kW of electricity. A centrifugal pump is selected because the small pressure increase of 3 psi implies a developed head of 6.4 ft, which is within the range of a centrifugal pump. It is constructed from Carbon Steel, since Dowtherm A does not have extremely corrosive properties. The estimated purchase cost (CE 2008= 548.4) is $6,700 and the total purchase and installation cost is $22,200. The pump was modeled with Microsoft Excel, knowing the desired pressure drop and flow rate of the stream. (See the specification sheet on Page 98 and design calculations on Page 207 in the Appendix)

P-500: Centrifugal Reflux Pump

P-500 is used to pump the liquid reflux from the reflux accumulator back into the top tray of D-500. Adhering to guidance provided by our industrial consultants and Professor Fabiano, the required pressure increase is set as 34.9 psi, which is the pressure required to pump the liquid from the ground level to the top of the column. To achieve a pressure increase of 34.9 psi in the 24,000 lb/hr stream, the pump requires a total brake power of 258.7 Hp and uses 209.5 kW of electricity. A centrifugal pump is selected because the small pressure increase implies a developed head of 94 ft, which is within the range of a centrifugal pump. It is constructed from Stainless Steel 304 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) is $42,400 and the total purchase and installation cost is $139,900. The pump was modeled with Microsoft Excel, knowing the desired pressure drop and flow rate of the stream. (See the specification sheet on Page 99 and design calculations on Page 208 in the Appendix)

P-501: Centrifugal Reboiler Pump

P-501 is used to pump the liquid boilup from the last stage of the column back into the bottom tray of D-500. Adhering to guidance provided by our industrial consultants and Professor Fabiano, the required pressure increase is set as 3 psi, which is slightly higher than the pressure drop across the column. To achieve a pressure increase of 3 psi in the 42,192 lb/hr stream, the pump requires a total brake power of 18.9 Hp and uses 16.1 kW of electricity. A centrifugal pump is selected because the small pressure increase of 3 psi implies a developed head of 7.8 ft, which is within the range of a centrifugal pump. It is constructed from Stainless Steel 304 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) is $9,100 and the total purchase and installation cost is $30,000. The pump was modeled with Microsoft Excel, knowing the desired pressure drop and flow rate of the stream. (See the specification sheet on Page 100 and design calculations on Page 208 in the Appendix)

P-502: Centrifugal Pump

P-502 is used to increase the pressure of the liquid distillate from the first pressure-swing column to the pressure, 100.3 psig, present in the second column in order to ensure that the stream does not disrupt the pressure profile within the column. To achieve a pressure increase of 105 psi in the 26,536 lb/hr stream, the pump requires a total brake power of 8.1 Hp and uses 6.0 kW of electricity. A centrifugal pump is selected because the moderate pressure increase of 105 psi implies a developed head of 283.1 ft, which is within the range of a centrifugal pump. It is constructed from Stainless Steel 304 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) is $8,300 and the total purchase and installation cost is $27,400. The pump was modeled with ASPEN Plus 2006, using the NRTL-RK property setting. (See the specification sheet on Page 101 and design calculations on Page 210 in the Appendix)

P-503: Centrifugal Reflux Pump

P-503 is used to pump the liquid reflux from the reflux accumulator back into the top tray of D-501. Adhering to guidance provided by our industrial consultants and Professor Fabiano, the required pressure increase is set as 16.8 psi, which is the pressure required to pump the liquid from the ground level to the top of the column. To achieve a pressure increase of 16.8 psi in the 12,000 lb/hr stream, the pump requires a total brake power of 81.9 Hp and uses 67.5 kW of electricity. A centrifugal pump is selected because the small pressure increase implies a developed head of 50 ft, which is within the range of a centrifugal pump. It is constructed from Stainless Steel 304 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) is $17,700 and the total purchase and installation cost is $58,400. The pump was modeled with Microsoft Excel, knowing the desired pressure drop and flow rate of the stream. (See the specification sheet on Page 102 and design calculations on Page 211 in the Appendix)

P-504 Centrifugal Reboiler Pump

P-504 is used to pump the liquid boilup from the last stage of the column back into the bottom tray of D-501. Adhering to guidance provided by our industrial consultants and Professor Fabiano, the required pressure increase is set as 3 psi, which is slightly higher than the pressure drop across the column. To achieve a pressure increase of 3 psi in the 64,489 lb/hr stream, the pump requires a total brake power of 30.7 Hp and uses 25.8 kW of electricity. A centrifugal pump is selected because the small pressure increase of psi implies a developed head of 9.5 ft, which is within the range of a centrifugal pump. It is constructed from Stainless Steel 304 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) is $10,700 and the total purchase and installation cost is $35,300. The pump was modeled with Microsoft Excel, knowing the desired pressure drop and flow rate of the stream. (See the specification sheet on Page 100 and design calculations on Page 208 in the Appendix)

6.2.8 Reactors

R-100: Back-Mix Tank Reactor

R-100 is an adiabatic, back-mix tank reactor that operates at 480°F and 2000 psig. A 40 psi head develops at the bottom of the tank as a result of the liquid height, and thus all feeds must be pumped or compressed to 2040 psig before entering the reactor. Temperature control within the reactor is managed by adjusting the maleic acid feed temperature. Agitation is provided by the large excess of hydrogen gas from the hydrogen makeup stream from the compressor and the hydrogen recycle stream, which is fed into the bottom and bubble up through the reactor. The vapor product is carried out with the hydrogen out of the top of the reactor. To achieve a target space-time yield (STY) of 600 lbs THF/hr-lb catalyst, the reactor must contain 20833 lbs of catalyst on carbon support, which is approximately the same density of the liquid contents of the reactor. Assuming a catalyst density of 10 lb/ft^3, a reasonable assumption for hydrogenation reactors, the volume of the liquid in the reactor is approximately 2083 ft^3. Thus, the liquid height is 92.3 ft and combined with a disengagement height of 10 ft, where liquid entrained in the vapor product can fall back into the reactor, yields a reactor height of 102.3 ft and diameter of 5.4 ft. The large height to diameter aspect ratio was recommended by Mr. Wayne Robbins, the project industry consultant. The reactor is constructed from a thick layer of carbon steel to withstand the 2000 psig reaction pressure, and is coated inside with hydrogen-resistant stainless steel. This is more cost-effective than creating the entire vessel from hydrogen-resistant material, which would be extremely costly and unnecessary. The estimated purchase cost (CE 2008= 548.4) is $768,100 and the total purchase and installation cost is $3,195,300. The reactor was modeled with ASPEN Plus 2006 using the RSTOIC block and the PSRK property setting. (See the specification sheet on Page 104 and design calculations on Page 213 in the Appendix)

In the process, there is a single reactor in which several reactions occur simultaneously to produce THF from maleic acid. The reactions are essentially a series of hydrogenations in which bonds are broken in the reacting maleic acid and chemical intermediates. Since hydrogen gas does not readily react with the compounds, a palladium-rhenium coated carbon support system is utilized. The carbon support maximizes the available surface area for the reaction to occur and the palladium and rhenium metals provide active sites for the hydrogen to be absorbed. Thus, hydrogen is more readily available to react when maleic acid comes in contact with it.

The catalyst is a 1% palladium-rhenium catalyst on carbon support, and it requires annual regeneration. The initial charge and regeneration services will be provided by BASF Catalysts, Inc., which provided rough estimates for the cost of each. Including freight charges, the initial catalyst charge will cost $875,600 and the annual regeneration costs will be $130,900. (See design calculations on Page 220 and email correspondence with BASF representatives on Pages 343-343)

6.2.9 Storage Tanks

T-600: Floating Head Storage Tanks

Two units of T-600 are used to store 96 hours worth of THF production before it is sent via pipeline to the upstream Lycra® plant to be processed into elastane (spandex). The floating-roof design is selected in order to prevent oxygen from coming in contact with the THF. Failure to prevent oxidation will result in the formation of extremely hazardous peroxides, which increase the risk of explosion upon small physical or thermal shocks. In addition, the floating-roof design prevents vaporization of THF, which occurs readily at atmospheric conditions. Each tank has a volume of 83,325 gallons and is designed to hold THF at near-atmospheric conditions of 90°F and 3 psig. They are constructed out of Stainless Steel 316 in order to prevent corrosion by THF, an ether and powerful organic solvent. The estimated purchase cost (CE 2008= 548.4) for the two tanks is $707,400 and the total purchase and installation cost is $2,942,800. The tanks were modeled with Microsoft Excel, knowing the desired volume and conditions within the tank (See the specification sheet on Page 105 and design calculations on Page 214 in the Appendix)

6.2.10 Heat Exchangers

X-100: Fixed Head Shell and Tube Heat Exchanger

X-100 is a fixed head, shell-and-tube heat exchanger that heats the maleic acid/water feed stream to 201.2°F on the tube side using 2,901 lb/hr of 50 psig steam on the shell side. The heat duty of the exchanger is 2,786,743 Btu/hr and the overall heat transfer coefficient for the condensing steam/low pressure aqueous solution was assumed to be 150 Btu/hr-ft^2-°F, which was selected employing guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 130.8 ft^2. A small pressure drop of 5 psi is observed on the cold side and no drop is observed on the hot side. A fixed head, shell-and-tube heat exchanger was the chosen design because it is economical and is often used in modeling typical chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using organic acid-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $22,400, and the total purchase and installation cost is $71,000. The exchanger was modeled with ASPEN Plus 2006 using the Shortcut method and the RK-SOAVE property setting. (See the specification sheets on Page 106 and design calculations on Page 214 in the Appendix)

X-200: Fixed Head Shell and Tube Heat Exchanger

X-200 is a fixed head, shell-and-tube heat exchanger that cools the vapor reactor effluent stream from 480°F to 104°F on the tube side using 43,274 lb/hr of boiler feed water (BFW) on the shell side. The exchanger recovers much of the heat by producing 50 psig steam, which reduces the amount of pipeline low pressure steam required in other parts of the process. The heat duty of the exchanger is -49,017,997 Btu/hr and the overall heat transfer coefficient for the steam formation/low pressure aqueous solution was assumed to be 60 Btu/hr-ft^2-°F, which was selected employing guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 12,441ft^2. A small pressure drop of 3 psi is observed on the cold side and 3 psi on the hot side. A fixed head, shell-and-tube heat exchanger was the chosen design because it is economical and is often used in modeling typical chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using organic solvent-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $268,200 and the total purchase and installation cost is $850,200. The exchanger was modeled with ASPEN Plus 2006 using the Shortcut method and the PSRK property setting. (See the specification sheets on Page 107 and design calculations on Page 215 in the Appendix)

X-201: Fixed Head Shell and Tube Heat Exchanger

X-201 is a fixed head, shell-and-tube heat exchanger that heats the hydrogen recycle stream from 149°F to 572°F on the tube side using 68,093 lb/hr of Dowtherm A heating fluid on the shell side. The heat duty of the exchanger is 17,038,956 Btu/hr and the overall heat transfer coefficient for high pressure hydrogen/thermal fluid was assumed to be 102.5 Btu/hr-ft^2-°F, which was selected employing guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 4,029 ft^2. A small pressure drop of 3 psi is observed on the hot side and no drop is observed on the cold side. A fixed head, shell-and-tube heat exchanger was the chosen design because it is economical and is often used in modeling typical chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using hydrogen corrosion-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $98,300 and the total purchase and installation cost is $311,600. The exchanger was modeled with ASPEN Plus 2006 and Microsoft Excel using the Shortcut method. (See the specification sheets on Page 108 and design calculations on Page 215 in the Appendix)

X-300: Condenser (Fixed Head Shell and Tube Heat Exchanger)

X-300 is a fixed head, shell-and-tube heat exchanger that condenses the vapor overhead of D-300 from 222°F to 169°F on the tube side using 1,517,566 lb/hr of cooling water on the shell side. The heat duty of the exchanger is -45,344,534 Btu/hr, but it is difficult to recover this heat value since the hot stream comes in at 222°F, and thus it is hard to produce high pressure steam. The only other option is to send this hot stream past a cold stream elsewhere in the process, such as the maleic acid preheating, but condensers are typically modeled as self-contained heat exchangers within the tower for simplicity. The overall heat transfer coefficient for the organic solvent/cooling water system was assumed to be 100 Btu/hr-ft^2-°F, which was selected with guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 5,048 ft^2. A small pressure drop of 10 psi is observed on the cold side and no drop is observed on the hot side. A fixed head, shell-and-tube heat exchanger was the chosen design because it is economical and is often used in modeling typical chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using organic solvent-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $117,700 and the total purchase and installation cost is $373,100. The exchanger was modeled with ASPEN Plus 2006 using the Shortcut method and the NRTL-RK property setting. (See the specification sheets on Page 109 and design calculations on Page 216 in the Appendix)

X-301: Thermosyphon Reboiler

X-301 is a fixed head, thermosyphon reboiler that vaporizes the liquid boilup of D-300 from 234°F to 255°F on the tube side using 51,829 lb/hr of 50 psig steam on the shell side. The heat duty of the exchanger is 47,247,168 Btu/hr. The overall heat transfer coefficient for the organic solvent/condensing steam system was assumed to be 100 Btu/hr-ft^2-°F, which was selected employing guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 9,055 ft^2. A small pressure drop of 5 psi is observed on the cold side and no drop is observed on the hot side. A thermosyphon exchanger was the chosen design because it is often used in column reboilers in chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using organic solvent-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $197,000 and the total purchase and installation cost is $624,500. The exchanger was modeled with ASPEN Plus 2006 using the Shortcut method and the NRTL-RK property setting. (See the specification sheets on Page 110 and design calculations on Page 216 in the Appendix)

X-400: Fixed Head Shell and Tube Heat Exchanger

X-400 is a fixed head, shell-and-tube heat exchanger that cools the incineration streams from 78°F and 90°F to 0°F on the tube side using 2,047 lb/hr of 50% ethylene glycol and water coolant on the shell side. The heat duty of the exchanger is -132,532 Btu/hr and the overall heat transfer coefficient for low pressure hydrogen/thermal fluid was assumed to be 20 Btu/hr-ft^2-°F, which was selected employing guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 363 ft^2. A small pressure drop of 3 psi is observed on the cold side and no drop is observed on the hot side. A fixed head, shell-and-tube heat exchanger was the chosen design because it is economical and is often used in modeling typical chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using organic solvent-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $27,100 and the total purchase and installation cost is $85,900. The exchanger was modeled with ASPEN Plus 2006 and Microsoft Excel using the Shortcut method. (See the specification sheets on Page 111 and design calculations on Page 217 in the Appendix)

X-500: Condenser (Fixed Head Shell and Tube Heat Exchanger)

X-500 is a fixed head, shell-and-tube heat exchanger that condenses the vapor overhead of D-500 at 147°F on the tube side using 367,269 lb/hr of cooling water on the shell side. The heat duty of the exchanger is -10,973,901 Btu/hr. The overall heat transfer coefficient for the organic solvent/cooling water system was assumed to be 100 Btu/hr-ft^2-°F, which was selected with guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 2,713 ft^2. A small pressure drop of 10 psi is observed on the cold side and no drop is observed on the hot side. A fixed head, shell-and-tube heat exchanger was the chosen design because it is economical and is often used in modeling typical chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using organic solvent-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $73,500 and the total purchase and installation cost is $233,000. The exchanger was modeled with ASPEN Plus 2006 using the Shortcut method and the NRTL-RK property setting. (See the specification sheets on Page 112 and design calculations on Page 217 in the Appendix)

X-501: Thermosyphon Reboiler

X-501 is a fixed head, thermosyphon reboiler that vaporizes the liquid boilup of D-500 from 200°F to 211°F on the tube side using 12,281 lb/hr of 50 psig steam on the shell side. The heat duty of the exchanger is 47,247,168 Btu/hr. The overall heat transfer coefficient for the organic solvent/condensing steam system was assumed to be 100 Btu/hr-ft^2-°F, which was selected employing guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 1,219 ft^2. A small pressure drop of 5 psi is observed on the cold side and no drop is observed on the hot side. A thermosyphon exchanger was the chosen design because it is often used in column reboilers in chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using organic solvent-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $44,900 and the total purchase and installation cost is $142,300. The exchanger was modeled with ASPEN Plus 2006 using the Shortcut method and the NRTL-RK property setting. (See the specification sheets on Page 113 and design calculations on Page 218 in the Appendix)

X-502: Condenser (Fixed Head Shell and Tube Heat Exchanger)

X-502 is a fixed head, shell-and-tube heat exchanger that condenses the vapor overhead of D-501 at 275°F on the tube side using 191,684 lb/hr of cooling water on the shell side. The heat duty of the exchanger is -5,727,472 Btu/hr. The overall heat transfer coefficient for the organic solvent/cooling water system was assumed to be 100 Btu/hr-ft^2-°F, which was selected employing guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 338 ft^2. A small pressure drop of 10 psi is observed on the cold side and no drop is observed on the hot side. A fixed head, shell-and-tube heat exchanger was the chosen design because it is economical and is often used in modeling typical chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using organic solvent-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $26,600 and the total purchase and installation cost is $84,300. The exchanger was modeled with ASPEN Plus 2006 using the Shortcut method and the NRTL-RK property setting. (See the specification sheets on Page 114 and design calculations on Page 218 in the Appendix)

X-503: Thermosyphon Reboiler

X-503 is a fixed head, thermosyphon reboiler that vaporizes the liquid boilup of D-500 at 298°F on the tube side using 8,917 lb/hr of 150 psig steam on the shell side. The heat duty of the exchanger is 7,640,278 Btu/hr. The overall heat transfer coefficient for the organic solvent/condensing steam system was assumed to be 100 Btu/hr-ft^2-°F, which was selected employing guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 1,106 ft^2. A small pressure drop of 5 psi is observed on the cold side and no drop is observed on the hot side. A thermosyphon exchanger was the chosen design because it is often used in column reboilers in chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using organic solvent-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $43,100 and the total purchase and installation cost is $136,600. The exchanger was modeled with ASPEN Plus 2006 using the Shortcut method and the NRTL-RK property setting. (See the specification sheets on Page 115 and design calculations on Page 219 in the Appendix)

X-600: Fixed Head Shell and Tube Heat Exchanger

X-600 is a fixed head, shell-and-tube heat exchanger that cools the vapor reactor effluent stream from 171°F to 104°F on the tube side using 34,705 lb/hr of cooling water on the shell side. The heat duty of the exchanger is -1,199,440 Btu/hr, which was deemed too insignificant for heat recovery. The overall heat transfer coefficient for the organic solvent/cooling water system was assumed to be 100 Btu/hr-ft^2-°F, which was selected employing guidance from the industrial consultants and Table 11-3 in Perry's Handbook (Perry, 1999). These values yield an estimated area for heat transfer of 417 ft^2. A small pressure drop of 10 psi is observed on the cold side and 1.4 psi on the hot side. A fixed head, shell-and-tube heat exchanger was the chosen design because it is economical and is often used in modeling typical chemical engineering processes. For economic reasons, the process stream is placed on the tube-side, which is constructed using organic solvent-resistant Stainless Steel 304, so that the shell may be constructed of the carbon steel. The estimated purchase cost (CE 2008= 548.4) is $28,400 and the total purchase and installation cost is $90,000. The exchanger was modeled with ASPEN Plus 2006 using the Shortcut method and the NRTL-RK property setting on the hot side and RK-SOAVE on the cold side. (See the specification sheets on Page 116 and design calculations on Page 219 in the Appendix)

6.3 Equipment Specification Sheets

HORIZONTAL PRESSURE VESSEL

Identification:	**Item**	**Reflux Accumulator**			Date:	4/6/2009
	Item #	A-300				
	# Required	1				
Function:	Reflux accumulator for distillation column D-300					
Operation:	Continuous					
Materials:		*S-303*	*S-304*	*S-306*		
		Feed	Reflux	Distillate		
	Composition (lb/hr)					
	MALEIC	-	-	-		
	HYDROGEN	-	-	-		
	SUCCINIC	-	-	-		
	GBL	135.51	50.82	84.69		
	BDO	0.04	0.02	0.03		
	THF	17,660.70	6,622.76	11,037.94		
	METHANE	-	-	-		
	NBUTANE	-	-	-		
	WATER	40,262.19	15,098.32	25,163.87		
	PROPANE	-	-	-		
	NBUTANOL	1,239.73	464.90	774.83		
	PROPANOL	382.23	143.34	238.90		
	Total	59,680.41	22,380.15	37,300.26		
	Vapor Fraction	0.00	0.00	0.00		
	Temperature (°F)	168.53	168.53	168.53		
Design Data:	Diameter		6.039	ft		
	Length		12.077	ft		
	Thickness		0.313	in		
	Weight		4,189.87	lb		
	Material of Construction		Stainless Steel 304			
	Design Temperature		170.00	°F		
	Design Pressure		5.300	psig		
Purchase Cost:	Vessel					$38,430
	Platforms and Ladders					$2,890
	Total (CE 2006=500)					$41,320
	Total (CE 2008=548.4)					**$45,300**

HORIZONTAL PRESSURE VESSEL

Identification:	**Item**	**Reflux Accumulator**	Date:	4/6/2009
	Item #	A-500		
	# Required	1		
Function:	Reflux accumulator for distillation column D-500			
Operation:	Continuous			

Materials:		*S-501*	*S-502*	*S-504*
		Feed	Reflux	Distillate
	Composition (lb/hr)			
	MALEIC	-	-	-
	HYDROGEN	-	-	-
	SUCCINIC	-	-	-
	GBL	0.09	0.04	0.05
	BDO	-	-	-
	THF	48,042.56	22,815.73	25,226.83
	METHANE	-	-	-
	NBUTANE	-	-	-
	WATER	2,485.15	1,180.21	1,304.94
	PROPANE	-	-	-
	NBUTANOL	1.56	0.74	0.82
	PROPANOL	6.89	3.27	3.62
	Total	50,536.24	24,000.00	26,536.24
	Vapor Fraction	0.00	0.00	0.00
	Temperature (°F)	147.26	147.26	147.26

Design Data:	Diameter	5.856	ft
	Length	11.712	ft
	Thickness	0.375	in
	Weight	4,732.83	lb
	Material of Construction	Stainless Steel 304	
	Design Temperature	170.00	°F
	Design Pressure	0.300	psig

Purchase Cost:	Vessel	$40,820
	Platforms and Ladders	$2,870
	Total (CE 2006=500)	$43,690
	Total (CE 2008=548.4)	**$47,900**

HORIZONTAL PRESSURE VESSEL

Identification:	**Item**	**Reflux Accumulator**	Date:	4/6/2009
	Item #	A-501		
	# Required	1		
Function:	Reflux accumulator for distillation column D-501			
Operation:	Continuous			

Materials:

	S-512 Feed	*S-513* Reflux	*S-515* Distillate
Composition (lb/hr)			
MALEIC	-	-	-
HYDROGEN	-	-	-
SUCCINIC	-	-	-
GBL	0.08	0.04	0.04
BDO	-	-	-
THF	23,614.72	10,883.93	12,730.79
METHANE	-	-	-
NBUTANE	-	-	-
WATER	2,419.85	1,115.30	1,304.55
PROPANE	-	-	-
NBUTANOL	0.04	0.02	0.02
PROPANOL	1.54	0.71	0.83
Total	26,036.24	12,000.00	14,036.24
Vapor Fraction	0.00	0.00	0.00
Temperature (°F)	274.48	274.48	274.48

Design Data:	Diameter	4.853	ft
	Length	9.706	ft
	Thickness	0.252	in
	Weight	2,182.28	lb
	Material of Construction	Stainless Steel 304	
	Design Temperature	300.00	°F
	Design Pressure	100.300	psig

Purchase Cost:	Vessel	$28,440
	Platforms and Ladders	$2,760
	Total (CE 2006=500)	$31,200
	Total (CE 2008=548.4)	**$34,200**

RECIPROCATING COMPRESSOR, LESS INTERCOOLER

Identification:	**Item**	**Reciprocating Compressor**	Date:	4/6/2009
	Item #	C-100		
	# Required	1		
Function:	Compress make-up hydrogen to reactor pressure			
Operation:	Continuous			

Materials:		*S-103* Inlet	*S-104* Outlet
	Composition (lb/hr)		
	MALEIC	-	-
	HYDROGEN	2,142.88	2,142.88
	SUCCINIC	-	-
	GBL	-	-
	BDO	-	-
	THF	-	-
	METHANE	-	-
	NBUTANE	-	-
	WATER	-	-
	PROPANE	-	-
	NBUTANOL	-	-
	PROPANOL	-	-
	Total	2,142.88	2,142.88
	Vapor Fraction	1.00	1.00
	Temperature (°F)	68.00	389.67

Design Data:	Number of Stages	2	
	Stage 1 Brake Power	783.207	
	Stage 1 Motor Efficiency	0.932	Hp
	Stage 1 ΔP	472.779	psi
	Stage 1 Pressure Ratio	2.786	
	Stage 2 Brake Power	860.920	Hp
	Stage 2 Motor Efficiency	0.93	
	Stage 2 ΔP	1,317.221	psi
	Stage 2 Pressure Ratio	2.786	
	Compressor Efficiency	0.72	
	Material of Construction	Stainless Steel	
	Design Temperature	400.00	°F
	Design Pressure	2,040.000	psig

Purchase Cost:	Stage 1 Compressor	$1,574,830
	Stage 2 Compressor	$1,697,620
	Total (CE 2006=500)	$3,272,450
	Total (CE 2008=548.4)	**$3,589,200**
Utilities:	Electricity	

COMPRESSOR INTERCOOLER

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date:	4/6/2009
	Item #	C-100		
	# Required	1		
Function:	Intercooler for 2-stage compression of hydrogen make-up			
Operation:	Continuous			

Materials:

	U-102 Cold Inlet	*U-103* Cold Outlet	*S-103'* Hot Inlet	*S-103''* Hot Outlet
Composition (lb/hr)				
MALEIC	-	-	-	-
HYDROGEN	-	-	2,142.88	2,142.88
SUCCINIC	-	-	-	-
GBL	-	-	-	-
BDO	-	-	-	-
THF	-	-	-	-
METHANE	-	-	-	-
NBUTANE	-	-	-	-
WATER	57,348.28	57,348.28	-	-
PROPANE	-	-	-	-
NBUTANOL	-	-	-	-
PROPANOL	-	-	-	-
Total	57,348.28	57,348.28	2,142.88	2,142.88
Vapor Fraction	0.00	0.00	1.00	1.00
Temperature (°F)	90.00	120.00	334.32	104.00

Design Data:	Area for Heat Transfer	388.987	ft^2
	Duty	-1,713,554	Btu/hr
	Overall HT Coefficient	60.000	Btu/hr-ft^2 -F
	Average LMTD	73.419	°F
	ΔT	-230.318	°F (Hot Side)
	Hot Side ΔP	-1.000	psi
	Cold Side ΔP	-5.000	psi
	Shell Material of Construction	Carbon Steel	
	Tube Material of Construction	Stainless Steel	
	Design Temperature	350.00	°F
	Design Pressure	65.000	psig

Purchase Cost:	Fixed Head Heat Exchanger (CE 2006= 500)	$25,280
	Fixed Head Heat Exchanger (CE 2008=548.4)	**$27,700**
Utilities:	Cooling water	

RECIPROCATING COMPRESSOR

Identification:	**Item**	**Reciprocating Compressor**	Date:	4/6/2009
	Item #	C-200		
	# Required	1		
Function:	Compress recycle hydrogen to reactor pressure			
Operation:	Continuous			

Materials:

	S-204 Inlet	*S-205* Outlet
Composition (lb/hr)		
MALEIC	-	-
HYDROGEN	11,454.41	11,454.41
SUCCINIC	-	-
GBL	-	-
BDO	-	-
THF	181.90	181.90
METHANE	17.19	17.19
NBUTANE	13.44	13.44
WATER	103.05	103.05
PROPANE	1.77	1.77
NBUTANOL	-	-
PROPANOL	-	-
Total	11,771.76	11,771.76
Vapor Fraction	1.00	1.00
Temperature (°F)	105.25	148.79

Design Data:	Brake Power	716.879	Hp
	Compressor Efficiency	0.72	
	Motor Efficiency	0.931	
	ΔP	345.000	psi
	Pressure Ratio	2.786	
	Material of Construction	Stainless Steel	
	Design Temperature	160.00	°F
	Design Pressure	2,040.000	psig

Purchase Cost:	Compressor (CE 2006=500)	$1,468,070
	Compressor (CE 2008=548.4)	**$1,610,200**
Utilities:	Electricity	

DISTILLATION COLUMN

Identification:	**Item**	**Distillation Column**	Date:	4/6/2009
	Item #	D-300		
	# Required	1		

Function:	Separate gamma-butyrolactone and 1,4-butanediol from tetrahydrofuran/water mixture
Operation:	Continuous

Materials:		*S-301*	*S-306*	*S-311*
		Feed	Distillate	Bottoms
	Composition (lb/hr)			
	MALEIC	5.09	-	5.09
	HYDROGEN	-	-	-
	SUCCINIC	39.23	-	39.23
	GBL	3,838.19	84.69	3,753.50
	BDO	232.99	0.03	232.97
	THF	11,037.94	11,037.94	-
	METHANE	-	-	-
	NBUTANE	-	-	-
	WATER	25,611.73	25,163.87	447.86
	PROPANE	-	-	-
	NBUTANOL	774.83	774.83	-
	PROPANOL	238.90	238.90	-
	Total	41,778.90	37,300.26	4,478.65
	Vapor Fraction	0.00	0.00	0.00
	Temperature (°F)	108.77	168.53	255.19

Design Data:	Actual Number of Stages	24	
	Mass Reflux Ratio	0.600	
	Feed Stage(s)	12	
	Overhead Pressure	5.300	psig
	Stage Pressure Drop	0.083	psig
	Tray Type	Koch Flexitray	
	Mass Flow of Vapor	56,098.77	lb/hr
	Column Inside Diameter	6.269	ft
	Height	62.00	ft
	Column Thickness	0.375	in
	Weight	20,700.15	lb
	Material of Construction	Stainless Steel 304	
	Design Temperature	290.00	°F
	Design Pressure	5.300	psig

Purchase Cost:	Distillation column	$145,650
	Trays	$48,860
	Platforms and Ladders	$26,300
	Total (CE 2006=500)	$220,810
	Total (CE 2008=548.4)	**$242,200**

DISTILLATION COLUMN

Identification:	**Item**	**Distillation Column**	Date:	4/6/2009
	Item #	D-500		
	# Required	1		
Function:	Remove waste water and output a THF/water azeotrope at atmospheric conditions			
Operation:	Continuous			

Materials:	*S-306* Feed (D-300)	*S-400* Feed (F-400)	*S-404* Feed (F-401)	*S-515* Feed (D-501)	*S-504* Distillate	*S-508* Bottoms
Composition (lb/hr)						
MALEIC	-	-	-	-	-	-
HYDROGEN	-	-	-	-	-	-
SUCCINIC	-	-	-	-	-	-
GBL	84.69	8.02	0.02	0.04	0.05	92.73
BDO	0.03	-	-	-	-	0.03
THF	11,037.94	1,143.24	325.39	12,720.64	25,226.83	0.39
METHANE	-	-	-	-	-	-
NBUTANE	-	-	-	-	-	-
WATER	25,163.87	0.99	0.54	1,304.63	1,304.94	25,165.09
PROPANE	-	-	-	-	-	-
NBUTANOL	774.83	5.13	1.26	0.02	0.82	780.43
PROPANOL	238.90	2.33	0.25	0.96	3.62	238.82
Total	37,300.26	1,159.72	327.45	14,026.30	26,536.24	26,277.48
Feed Stage	20	2	16	20		
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00
Temperature (°F)	168.53	89.99	0.00	274.48	147.26	210.82

Design Data:	Actual Number of Stages	40	
	Mass Reflux Ratio	0.904	
	Overhead Pressure	0.300	psig
	Stage Pressure Drop	0.051	psig
	Tray Type	Koch Flexitray	
	Mass Flow of Vapor	50,536.24	lb/hr
	Column Inside Diameter	4.566	ft
	Height	94.00	ft
	Column Thickness	0.438	in
	Weight	25,709.15	lb
	Material of Construction	Stainless Steel 304	
	Design Temperature	230.00	°F
	Design Pressure	0.300	psig

Purchase Cost:	Distillation column	$167,460
	Trays	$56,540
	Platforms and Ladders	$30,040
	Total (CE 2006=500)	$254,040
	Total (CE 2008=548.4)	**$278,600**

DISTILLATION COLUMN

Identification:	**Item**	**Distillation Column**	Date:	4/6/2009
	Item #	D-501		
	# Required	1		
Function:	Produce 99.97% pure THF and send THF/water azeotrope at elevated pressure to D-500			
Operation:	Continuous			

Materials:		*S-510*	*S-515*	*S-518*
		Feed	Distillate	Bottoms
	Composition (lb/hr)			
	MALEIC	-	-	-
	HYDROGEN	-	-	-
	SUCCINIC	-	-	-
	GBL	0.05	0.04	-
	BDO	-	-	-
	THF	25,226.83	12,730.79	12,496.03
	METHANE	-	-	-
	NBUTANE	-	-	-
	WATER	1,304.94	1,304.55	0.38
	PROPANE	-	-	-
	NBUTANOL	0.82	0.02	0.80
	PROPANOL	3.62	0.83	2.79
	Total	26,536.24	14,036.24	12,500.00
	Vapor Fraction	0.00	0.00	0.00
	Temperature (°F)	148.43	274.48	298.48

Design Data:	Actual Number of Stages	18	
	Mass Reflux Ratio	0.855	
	Feed Stage(s)	9	
	Overhead Pressure	100.300	psig
	Stage Pressure Drop	0.105	psig
	Tray Type	Koch Flexitray	
	Mass Flow of Vapor	26,036.24	lb/hr
	Column Inside Diameter	3.356	ft
	Height	50.00	ft
	Column Thickness	0.174	in
	Weight	4,045.68	lb
	Material of Construction	Stainless Steel 304	
	Design Temperature	320.00	°F
	Design Pressure	100.300	psig

Purchase Cost:	Distillation column	$54,550
	Trays	$21,220
	Platforms and Ladders	$14,900
	Total (CE 2006=500)	$90,670
	Total (CE 2008=548.4)	**$99,400**

VERTICAL PRESSURE VESSEL

Identification:	**Item**	**Flash Vessel**	Date:	4/6/2009
	Item #	F-200		
	# Required	1		
Function:	Adiabatically separate condensables and non-condensables at 104°F and 1995 psig			
Operation:	Continuous			

Materials:

	S-200 Feed	*S-201* Vapor	*S-202* Liquid
Composition (lb/hr)			
MALEIC	5.09	-	5.09
HYDROGEN	11,622.88	11,570.12	52.76
SUCCINIC	39.23	-	39.23
GBL	3,846.23	8.03	3,838.20
BDO	232.99	-	232.99
THF	12,702.00	1,455.18	11,246.82
METHANE	86.42	85.94	0.48
NBUTANE	116.61	107.54	9.08
WATER	25,716.31	104.09	25,612.22
PROPANE	14.89	14.15	0.73
NBUTANOL	781.23	5.20	776.03
PROPANOL	241.48	2.42	239.06
Total	55,405.37	13,352.67	42,052.70
Vapor Fraction	0.78	1.00	0.00
Temperature (°F)	104.00	104.01	104.01

Design Data:	Diameter	2.643	ft
	Height	7.929	ft
	Thickness	2.445	in
	Weight	9,141.18	lb
	Material of Construction	Stainless Steel 304	
	Design Temperature	115.00	°F
	Design Pressure	2,000.000	psig

Purchase Cost:	Vessel	$67,480
	Platforms and Ladders	$3,210
	Total (CE 2006=500)	$70,690
	Total (CE 2008=548.4)	**$77,500**

VERTICAL PRESSURE VESSEL

Identification:	**Item**	**Flash Vessel**	Date:	4/6/2009
	Item #	F-300		
	# Required	1		

Function: Adiabatically remove hydrogen at 600 psig to stabilize downstream distillation processes

Operation: Continuous

Materials:

	S-202 Feed	*S-300* Vapor	*S-301* Liquid
Composition (lb/hr)			
MALEIC	5.09	-	5.09
HYDROGEN	52.76	52.50	0.27
SUCCINIC	39.23	-	39.23
GBL	3,838.20	0.01	3,838.19
BDO	232.99	-	232.99
THF	11,246.82	208.88	11,037.94
METHANE	0.48	0.45	0.03
NBUTANE	9.08	8.15	0.93
WATER	25,612.22	0.49	25,611.73
PROPANE	0.73	0.63	0.11
NBUTANOL	776.03	1.19	774.83
PROPANOL	239.06	0.16	238.90
Total	42,052.70	272.46	41,780.24
Vapor Fraction	0.00	1.00	0.00
Temperature (°F)	104.01	78.16	78.16

Design Data:	Diameter	3.617	ft
	Height	10.851	ft
	Thickness	0.996	in
	Weight	6,625.0	lb
	Material of Construction	Stainless Steel 304	
	Design Temperature	115.00	°F
	Design Pressure	585.300	psig

Purchase Cost:	Vessel	$55,730
	Platforms and Ladders	$5,050
	Total (CE 2006=500)	$60,780
	Total (CE 2008=548.4)	**$66,700**

VERTICAL PRESSURE VESSEL

Identification:	**Item**	**Flash Vessel**	Date:	4/6/2009
	Item #	F-400		
	# Required	1		
Function:	Adiabatically remove hydrogen at 150 psig to stabilize downstream distillation processes			
Operation:	Continuous			

Materials:		*S-203*	*S-401*	*S-400*
		Feed	Vapor	Liquid
	Composition (lb/hr)			
	MALEIC	-	-	-
	HYDROGEN	115.70	115.40	0.30
	SUCCINIC	-	-	-
	GBL	8.03	-	8.02
	BDO	-	-	0.00
	THF	1,273.29	130.04	1,143.24
	METHANE	68.75	68.13	0.62
	NBUTANE	94.09	59.76	34.33
	WATER	1.04	0.05	0.99
	PROPANE	12.39	10.59	1.80
	NBUTANOL	5.20	0.06	5.13
	PROPANOL	2.42	0.09	2.33
	Total	1,580.91	384.13	1,196.78
	Vapor Fraction	0.74	1.00	0.00
	Temperature (°F)	105.25	89.99	89.99

Design Data:	Diameter	0.781	ft
	Height	2.344	ft
	Thickness	0.250	in
	Weight	77.85	lb
	Material of Construction	Stainless Steel 304	
	Design Temperature	110.00	°F
	Design Pressure	150.000	psig

Purchase Cost:	Vessel	$6,470
	Platforms and Ladders	$550
	Total (CE 2006=500)	$7,020
	Total (CE 2008=548.4)	**$7,700**

VERTICAL PRESSURE VESSEL

Identification:	**Item**	**Flash Vessel**	Date:	4/6/2009
	Item #	F-401		
	# Required	1		
Function:	Adiabatically remove hydrogen at 150 psig and 0°F to recover THF from incineration stream			
Operation:	Continuous			

Materials:

	S-402 Feed	*S-403* Vapor	*S-404* Liquid
Composition (lb/hr)			
MALEIC	-	-	-
HYDROGEN	167.90	167.82	0.08
SUCCINIC	-	-	-
GBL	0.02	-	0.02
BDO	-	-	-
THF	338.92	13.54	325.39
METHANE	68.58	68.38	0.21
NBUTANE	67.90	40.08	27.82
WATER	0.54	-	0.54
PROPANE	11.21	9.82	1.39
NBUTANOL	1.26	-	1.26
PROPANOL	0.25	-	0.25
Total	656.59	299.64	356.94
Vapor Fraction	0.95	1.00	0.00
Temperature (°F)	0.00	0.00	0.00

Design Data:	Diameter	0.370	ft
	Height	1.109	ft
	Thickness	0.250	in
	Weight	17.92	lb
	Material of Construction	Stainless Steel 304	
	Design Temperature	0.000	°F
	Design Pressure	150.000	psig

Purchase Cost:	Vessel	$3,870
	Platforms and Ladders	$190
	Total (CE 2006=500)	$4,060
	Total (CE 2008=548.4)	**$4,500**

FIRED HEATER (DOWTHERM A)

Identification:	**Item**	**Fired Heater for Dowtherm A**	Date:	4/6/2009
	Item #	H-200		
	# Required	1		
Function:	Heats Dowtherm A thermal fluid to heat hydrogen recycle stream			
Operation:	Continuous			

Materials:

	HF-202 Inlet	*HF-200* Outlet
Composition (lb/hr)		
MALEIC	-	-
HYDROGEN	-	-
SUCCINIC	-	-
GBL	-	-
BDO	-	-
THF	-	-
METHANE	-	-
NBUTANE	-	-
WATER	-	-
PROPANE	-	-
NBUTANOL	-	-
PROPANOL	-	-
Dowtherm-A	68,093.37	68,093.37
Total	68,093.37	68,093.37
Vapor Fraction	0.00	0.00
Temperature (°F)	163.79	660.00

Design Data:	Duty	17,038,956	Btu/hr
	ΔT	496.21	°F
	Design Temperature	690.00	°F
	Design Pressure	3.000	psig

Purchase Cost:	Fired Heater (Dowtherm A) (CE 2006= 500)	$639,160
	Fired Heater (Dowtherm A) (CE 2008=548.4)	**$701,000**
Utilities:	Natural gas fuel and incineration credits	

REFRIDGERATION UNIT

Identification:	**Item**	**Mechanical Refrigeration Unit**	Date:	4/6/2009
	Item #	H-400		
	# Required	1		
Function:	Cools 50% ethylene glycol to cool incineration streams to recover THF			
Operation:	Continuous			

Materials:		*HF-402* Inlet	*HF-400* Outlet
	Composition (lb/hr)		
	MALEIC	-	-
	HYDROGEN	-	-
	SUCCINIC	-	-
	GBL	-	-
	BDO	-	-
	THF	-	-
	METHANE	-	-
	NBUTANE	-	-
	WATER	-	-
	PROPANE	-	-
	NBUTANOL	-	-
	PROPANOL	-	-
	50% Ethylene Glycol	2,047.05	2,047.05
	Total	2,047.05	2,047.05
	Vapor Fraction	0.00	0.00
	Temperature (°F)	63.16	-22.00

Design Data:	Duty	-132,532	Btu/hr	
	ΔT	-85.16	°F	
	Design Temperature	70.00	°F	
	Design Pressure	3.000	psig	
Purchase Cost:	Refrigeration Unit (CE 2004= 400)			$200,000
	Refrigeration Unit (CE 2008=548.4)			**$274,200**
Utilities:	Electricity			

HYDROGEN SEPARATION MEMBRANE

Identification:	**Item**	**Hydrogen Separation Membrane**	Date:	4/6/2009
	Item #	M-200		
	# Required	1		
Function:	Utilizes size exclusion to remove hydrogen into the permeate so that it can be recycled			
Operation:	Continuous			

Materials:		*S-201* Feed	*S-203* Retentate	*S-204* Permeate
	Composition (lb/hr)			
	MALEIC	-	-	-
	HYDROGEN	11,570.12	115.70	11,454.41
	SUCCINIC	-	-	-
	GBL	8.03	8.03	-
	BDO	-	-	-
	THF	1,455.18	1,273.29	181.90
	METHANE	85.94	68.75	17.19
	NBUTANE	107.54	94.09	13.44
	WATER	104.09	1.04	103.05
	PROPANE	14.15	12.39	1.77
	NBUTANOL	5.20	5.20	-
	PROPANOL	2.42	2.42	-
	Total	13,352.67	1,580.91	11,771.76
	Vapor Fraction	1.00	0.74	1.00
	Temperature (°F)	104.01	105.25	105.25

Design Data:	Area	9,745.229	ft^2
	Required H_2 Split Fraction	0.990	
	Material of Construction	Polysulfonate Polymer	
	Design Temperature	104.00	°F
	Design Pressure	2,000.000	psig
Purchase Cost:	**Total (CE 2008=548.4)**		**$97,500**

RECIPROCATING PUMP

Identification:	**Item**	**Reciprocating Pump**		Date: 4/6/2009
	Item #	P-100		
	# Required	1		
Function:	Increase pressure of maleic acid feed to reactor			
Operation:	Continuous			

Materials:

	S-101 Inlet	*S-102* Outlet
Composition (lb/hr)		
MALEIC	22,209.45	22,209.45
HYDROGEN	-	-
SUCCINIC	-	-
GBL	-	-
BDO	-	-
THF	-	-
METHANE	-	-
NBUTANE	-	-
WATER	14,806.30	14,806.30
PROPANE	-	-
NBUTANOL	-	-
PROPANOL	-	-
Total	37,015.76	37,015.76
Vapor Fraction	0.00	0.00
Temperature (°F)	201.20	218.84

Design Data:

Flow Rate	725.200	ft3/hr
Head Developed	5,755.242	ft
NPSH Available	12.869	ft-lbf/lb
Brake Horsepower	206.012	Hp
Shaft RPM	3,600.00	
Pressure Change	2,040.00	psi
Pump Efficiency	0.522	
Material of Construction	Ni-Al-Bronze	
Design Temperature	210.00	°F
Design Pressure	2,040.000	psig

Purchase Cost:

Reciprocating Pump and Motor (CE 2006=500)	$80,410
Reciprocating Pump and Motor (CE 2008=548.4)	**$88,200**

Utilities: Electricity

RADIAL CENTRIFUGAL PUMP

Identification:	**Item**	**Radial Centrifugal Pump**		Date: 4/6/2009
	Item #	P-200		
	# Required	1		
Function:	Pump the Dowtherm A heating fluid to heat the hydrogen recycle			
Operation:	Continuous			
Materials:		*HF-201*	*HF-202*	
		Inlet	Outlet	
	Composition (lb/hr)			
	MALEIC	-	-	
	HYDROGEN	-	-	
	SUCCINIC	-	-	
	GBL	-	-	
	BDO	-	-	
	THF	-	-	
	METHANE	-	-	
	NBUTANE	-	-	
	WATER	-	-	
	PROPANE	-	-	
	NBUTANOL	-	-	
	Dowtherm-A	68,093.37	68,093.37	
	Total	68,093.37	68,093.37	
	Vapor Fraction	0.00	0.00	
	Temperature (°F)	163.79	163.79	
Design Data:	Flow Rate		1,186.613	ft3/hr
	Head Developed		7.528	ft
	NPSH Available		-	ft-lbf/lb
	Brake Horsepower		26.582	Hp
	Shaft RPM		3,600.00	
	Pressure Change		3.000	psi
	Pump Efficiency		0.584	
	Material of Construction		Carbon Steel	
	Design Temperature		170.00	°F
	Design Pressure		3.000	psig
Purchase Cost:	Motor			$3,390
	Pump			$2,910
	Total (CE 2006=500)			$6,300
	Total (CE 2008=548.4)			**$6,900**
Utilities:	Electricity			

RECIPROCATING PUMP

Identification:	**Item**	**Reciprocating Pump**	Date: 4/6/2009
	Item #	P-300	
	# Required	1	
Function:	Increase pressure of liquid intermediate recycle to the reactor		
Operation:	Continuous		

Materials:

	S-311 Inlet	*S-312* Outlet
Composition (lb/hr)		
MALEIC	5.09	5.09
HYDROGEN	-	-
SUCCINIC	39.23	39.23
GBL	3,753.50	3,753.50
BDO	232.97	232.97
THF	-	-
METHANE	-	-
NBUTANE	-	-
WATER	447.86	447.86
PROPANE	-	-
NBUTANOL	-	-
PROPANOL	-	-
Total	4,478.65	4,478.65
Vapor Fraction	0.00	0.00
Temperature (°F)	255.19	286.77

Design Data:

Flow Rate	70.680	ft3/hr
Head Developed	4,619.379	ft
NPSH Available	-	ft-lbf/lb
Brake Horsepower	35.341	Hp
Shaft RPM	3,600.00	
Pressure Change	2,032.70	psi
Pump Efficiency	0.296	
Material of Construction	Ni-Al-Bronze	
Design Temperature	300.00	°F
Design Pressure	2,040.000	psig

Purchase Cost:

Reciprocating Pump and Motor	$17,430
Reciprocating Pump and Motor (CE 2008=548.4)	**$19,100**

Utilities: Electricity

REFLUX PUMP

Identification:	**Item**	**Radial Centrifugal Pump**	Date:	4/6/2009
	Item #	P-301		
	# Required	1		
Function:	Pump the liquid reflux in the distillation column D-300			
Operation:	Continuous			

Materials:

	S-304	*S-305*
	Inlet	Outlet
Composition (lb/hr)		
MALEIC	-	-
HYDROGEN	-	-
SUCCINIC	-	-
GBL	50.82	50.82
BDO	0.02	0.02
THF	6,622.76	6,622.76
METHANE	-	-
NBUTANE	-	-
WATER	15,098.32	15,098.32
PROPANE	-	-
NBUTANOL	464.90	464.90
PROPANOL	143.34	143.34
Total	22,380.15	22,380.15
Vapor Fraction	0.00	0.00
Temperature (°F)	168.53	168.53

Design Data:

Flow Rate	1,037.694	ft3/hr
Head Developed	62.000	ft
NPSH Available	-	ft-lbf/lb
Brake Horsepower	197.399	Hp
Shaft RPM	3,600.00	
Pressure Change	24.762	psi
Pump Efficiency	0.568	
Material of Construction	Stainless Steel	
Design Temperature	170.00	°F
Design Pressure	30.000	psig

Purchase Cost:

Motor	$25,160
Pump	$6,190
Total (CE 2006=500)	$31,350
Total (CE 2008=548.4)	**$34,400**

Utilities: Electricity

REBOILER PUMP

Identification:	**Item**	**Radial Centrifugal Pump**	Date:	4/6/2009
	Item #	P-302		
	# Required	1		
Function:	Pump the liquid boilup in the distillation column D-300			
Operation:	Continuous			

Materials:		*S-307*	*S-308*	
		Inlet	Outlet	
	Composition (lb/hr)			
	MALEIC	68.81	68.81	
	HYDROGEN	-	-	
	SUCCINIC	530.67	530.67	
	GBL	50,769.16	50,769.2	
	BDO	3,151.05	3,151.05	
	THF	0.00	0.00	
	METHANE	-	-	
	NBUTANE	-	-	
	WATER	6,057.74	6,057.74	
	PROPANE	-	-	
	NBUTANOL	0.00	0.00	
	PROPANOL	0.00	0.00	
	Total	60,577.42	60,577.42	
	Vapor Fraction	0.00	0.00	
	Temperature (°F)	234.49	234.49	
Design Data:	Flow Rate		1,049.797	ft3/hr
	Head Developed		7.486	ft
	NPSH Available		-	ft-lbf/lb
	Brake Horsepower		24.133	Hp
	Shaft RPM		3,600.00	
	Pressure Change		3.000	psi
	Pump Efficiency		0.569	
	Material of Construction		Stainless Steel	
	Design Temperature		280.00	°F
	Design Pressure		7.300	psig

Purchase Cost:	Motor	$3,110
	Pump	$5,800
	Total (CE 2006=500)	$8,910
	Total (CE 2008=548.4)	**$9,800**
Utilities:	Electricity	

RADIAL CENTRIFUGAL PUMP

Identification:	**Item**	**Radial Centrifugal Pump**	Date:	4/6/2009
	Item #	P-400		
	# Required	1		
Function:	Pump the ethylene-glycol coolant to lower the temperature of the incineration streams			
Operation:	Continuous			

Materials:

	HF-401 Inlet	*HF-402* Outlet
Composition (lb/hr)		
MALEIC	-	-
HYDROGEN	-	-
SUCCINIC	-	-
GBL	-	-
BDO	-	-
THF	-	-
METHANE	-	-
NBUTANE	-	-
WATER	-	-
PROPANE	-	-
NBUTANOL	-	-
50% Ethylene Glycol	2,047.05	2,047.05
Total	2,047.05	2,047.05
Vapor Fraction	0.00	0.00
Temperature (°F)	63.16	63.16

Design Data:

Flow Rate	30.243	ft3/hr
Head Developed	6.382	ft
NPSH Available	-	ft-lbf/lb
Brake Horsepower	0.396	Hp
Shaft RPM	3,600.00	
Pressure Change	3.000	psi
Pump Efficiency	1.000	
Material of Construction	Carbon Steel	
Design Temperature	70.00	°F
Design Pressure	3.000	psig

Purchase Cost:

Motor	$570
Pump	$5,560
Total (CE 2006=500)	$6,130
Total (CE 2008=548.4)	**$6,700**

Utilities: Electricity

REFLUX PUMP

Identification:	**Item**	**Radial Centrifugal Pump**	Date:	4/6/2009
	Item #	P-500		
	# Required	1		
Function:	Pump the liquid reflux in the distillation column D-500			
Operation:	Continuous			

Materials:		*S-502*	*S-503*
		Inlet	Outlet
	Composition (lb/hr)		
	MALEIC	-	-
	HYDROGEN	-	-
	SUCCINIC	-	-
	GBL	0.04	0.04
	BDO	-	-
	THF	22,815.73	22,815.73
	METHANE	-	-
	NBUTANE	-	-
	WATER	1,180.21	1,180.21
	PROPANE	-	-
	NBUTANOL	0.74	0.74
	PROPANOL	3.27	3.27
	Total	24,000.00	24,000.00
	Vapor Fraction	0.00	0.00
	Temperature (°F)	147.26	147.26

Design Data:	Flow Rate	946.269	ft3/hr
	Head Developed	94.000	ft
	NPSH Available	-	ft-lbf/lb
	Brake Horsepower	258.659	Hp
	Shaft RPM	3,600.00	
	Pressure Change	34.862	psi
	Pump Efficiency	0.557	
	Material of Construction	Stainless Steel	
	Design Temperature	170.00	°F
	Design Pressure	40.000	psig

Purchase Cost:	Motor	$32,400
	Pump	$6,280
	Total (CE 2006=500)	$38,680
	Total (CE 2008=548.4)	**$42,400**
Utilities:	Electricity	

REBOILER PUMP

Identification:	**Item**	**Radial Centrifugal Pump**	Date:	4/6/2009
	Item #	P-501		
	# Required	1		
Function:	Pump the liquid boilup in the distillation column D-500			
Operation:	Continuous			

Materials:

	S-505	*S-506*
	Inlet	Outlet
Composition (lb/hr)		
MALEIC	-	-
HYDROGEN	-	-
SUCCINIC	-	-
GBL	148.90	148.9
BDO	0.05	0.05
THF	0.62	0.62
METHANE	-	-
NBUTANE	-	-
WATER	40,406.27	40,406.27
PROPANE	-	-
NBUTANOL	1,253.09	1,253.09
PROPANOL	383.46	383.46
Total	42,192.39	42,192.39
Vapor Fraction	0.00	0.00
Temperature (°F)	200.78	200.78

Design Data:

Flow Rate	763.374	ft3/hr
Head Developed	7.816	ft
NPSH Available	-	ft-lbf/lb
Brake Horsepower	18.892	Hp
Shaft RPM	3,600.00	
Pressure Change	3.000	psi
Pump Efficiency	0.529	
Material of Construction	Stainless Steel	
Design Temperature	215.00	°F
Design Pressure	2.300	psig

Purchase Cost:

Motor	$2,520
Pump	$5,810
Total (CE 2006=500)	$8,330
Total (CE 2008=548.4)	**$9,100**

Utilities: Electricity

RADIAL CENTRIFUGAL PUMP

Identification:	**Item**	**Radial Centrifugal Pump**		Date: 4/6/2009
	Item #	P-502		
	# Required	1		
Function:	Increase pressure of distillate from atmospheric pressure-swing distillation column			
Operation:	Continuous			
Materials:		*S-504*	*S-510*	
		Inlet	Outlet	
	Composition (lb/hr)			
	MALEIC	-	-	
	HYDROGEN	-	-	
	SUCCINIC	-	-	
	GBL	0.05	0.05	
	BDO	-	-	
	THF	25,226.83	25,226.83	
	METHANE	-	-	
	NBUTANE	-	-	
	WATER	1,304.94	1,304.94	
	PROPANE	-	-	
	NBUTANOL	0.82	0.82	
	PROPANOL	3.62	3.62	
	Total	26,536.24	26,536.24	
	Vapor Fraction	0.00	0.00	
	Temperature (°F)	147.26	148.43	
Design Data:	Flow Rate		496.880	ft3/hr
	Head Developed		283.115	ft
	NPSH Available		-	ft-lbf/lb
	Brake Horsepower		8.063	Hp
	Shaft RPM		3,600.00	
	Pressure Change		105.00	psi
	Pump Efficiency		0.471	
	Material of Construction		Stainless Steel	
	Design Temperature		150.00	°F
	Design Pressure		105.300	psig
Purchase Cost:	Motor			$1,350
	Pump			$6,210
	Total (CE 2006=500)			$7,560
	Total (CE 2008=548.4)			**$8,300**
Utilities:	Electricity			

REFLUX PUMP

Identification:	**Item**	**Radial Centrifugal Pump**	Date:	4/6/2009
	Item #	P-503		
	# Required	1		
Function:	Pump the liquid reflux in the distillation column D-501			
Operation:	Continuous			

Materials:		*S-513*	*S-514*
		Inlet	Outlet
	Composition (lb/hr)		
	MALEIC	-	-
	HYDROGEN	-	-
	SUCCINIC	-	-
	GBL	0.04	0.04
	BDO	-	-
	THF	10,883.93	10,883.93
	METHANE	-	-
	NBUTANE	-	-
	WATER	1,115.30	1,115.30
	PROPANE	-	-
	NBUTANOL	0.02	0.02
	PROPANOL	0.71	0.71
	Total	12,000.00	12,000.00
	Vapor Fraction	0.00	0.00
	Temperature (°F)	274.48	274.48

Design Data:	Flow Rate	538.546	ft3/hr
	Head Developed	50.000	ft
	NPSH Available	-	ft-lbf/lb
	Brake Horsepower	81.867	Hp
	Shaft RPM	3,600.00	
	Pressure Change	16.787	psi
	Pump Efficiency	0.482	
	Material of Construction	Stainless Steel	
	Design Temperature	300.00	°F
	Design Pressure	120.000	psig

Purchase Cost:	Motor	$10,290
	Pump	$5,840
	Total (CE 2006=500)	$16,130
	Total (CE 2008=548.4)	**$17,700**
Utilities:	Electricity	

REBOILER PUMP

Identification:	**Item**	**Radial Centrifugal Pump**		Date: 4/6/2009
	Item #	P-504		
	# Required	1		
Function:	Pump the liquid boilup in the distillation column D-501			
Operation:	Continuous			
Materials:		*S-516*	*S-517*	
		Inlet	Outlet	
	Composition (lb/hr)			
	MALEIC	-	-	
	HYDROGEN	-	-	
	SUCCINIC	-	-	
	GBL	0.00	0.0	
	BDO	0.00	0.00	
	THF	64,468.15	64,468.15	
	METHANE	-	-	
	NBUTANE	-	-	
	WATER	1.97	1.97	
	PROPANE	-	-	
	NBUTANOL	4.11	4.11	
	PROPANOL	14.38	14.38	
	Total	64,488.61	64,488.61	
	Vapor Fraction	0.00	0.00	
	Temperature (°F)	298.13	298.13	
Design Data:	Flow Rate		1,422.363	ft3/hr
	Head Developed		9.528	ft
	NPSH Available		-	ft-lbf/lb
	Brake Horsepower		30.738	Hp
	Shaft RPM		3,600.00	
	Pressure Change		3.000	psi
	Pump Efficiency		0.606	
	Material of Construction		Stainless Steel	
	Design Temperature		310.00	°F
	Design Pressure		102.300	psig
Purchase Cost:	Motor			$3,870
	Pump			$5,870
	Total (CE 2006=500)			$9,740
	Total (CE 2008=548.4)			**$10,700**
Utilities:	Electricity			

VERTICAL PRESSURE VESSEL

Identification:	**Item**	**Reactor**	Date:	4/6/2009
	Item #	R-100		
	# Required	1		
Function:	Adiabatically produce THF-rich vapor product from maleic and hydrogen feeds			
Operation:	Continuous			

Materials:		*S-102* Maleic Feed	*S-104* H2 Makeup	*S-206* H2 Recycle	*S-312* GBL-BDO	*S-105* Product
	Composition (lb/hr)					
	MALEIC	22,209.45	-	-	5.09	5.09
	HYDROGEN	-	2,142.88	11,454.41	-	11,622.88
	SUCCINIC	-	-	-	39.23	39.23
	GBL	-	-	-	3,753.50	3,846.23
	BDO	-	-	-	232.97	232.99
	THF	-	-	181.90	-	12,702.00
	METHANE	-	-	17.19	-	86.42
	NBUTANE	-	-	13.44	-	116.61
	WATER	14,806.30	-	103.05	447.86	25,716.31
	PROPANE	-	-	1.77	-	14.89
	NBUTANOL	-	-	-	-	781.23
	PROPANOL	-	-	-	-	241.48
	Total	37,015.76	2,142.88	11,771.76	4,478.65	55,405.37
	Vapor Fraction	0.00	1.00	1.00	0.00	1.00
	Temperature (°F)	218.84	389.67	572.00	286.77	480.40

Design Data:	Diameter	5.361	ft
	Height	102.308	ft
	Thickness	5.074	in
	Weight	401,915.9	lb
	Material of Construction	Coated Carbon Steel	
	Design Temperature	572.00	°F
	Design Pressure	2,040.000	psig

Purchase Cost:	Vessel	$667,350
	Platforms and Ladders	$33,000
	Total (CE 2006=500)	$700,350
	Total (CE 2008=548.4)	**$768,100**

STORAGE TANK

Identification:	**Item**	**THF Storage Tank**	Date:	4/6/2009
	Item #	T-600		
	# Required	2		
Function:	Store holdup volume of 48 hours of THF production			
Operation:	Storage			
Materials:		S-601 THF Product		
	Composition (lb/hr)			
	MALEIC	-		
	HYDROGEN	-		
	SUCCINIC	-		
	GBL	-		
	BDO	-		
	THF	12,496.03		
	METHANE	-		
	NBUTANE	-		
	WATER	0.38		
	PROPANE	-		
	NBUTANOL	0.80		
	PROPANOL	2.79		
	Total	12,500.00		
	Vapor Fraction	0.00		
	Temperature (°F)	104.00		
Design Data:	Volume	83,325.43	gal	
	Material of Construction	Stainless Steel 316		
	Design Temperature	90.00	°F	
	Design Pressure	3.000	psig	
Purchase Cost:	2 Floating Roof Tanks (CE 2006=500)			$644,970
	2 Floating Roof Tanks (CE 2008=548.4)			**$707,400**

HEAT EXCHANGER

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date:	4/6/2009
	Item #	X-100		
	# Required	1		
Function:	Preheat the maleic feed before it enters the reactor			
Operation:	Continuous			

Materials:

	S-100 Cold Inlet	*S-101* Cold Outlet	*U-100* Hot Inlet	*U-101* Hot Outlet
Composition (lb/hr)				
MALEIC	22,209.45	22,209.45	-	-
HYDROGEN	-	-	-	-
SUCCINIC	-	-	-	-
GBL	-	-	-	-
BDO	-	-	-	-
THF	-	-	-	-
METHANE	-	-	-	-
NBUTANE	-	-	-	-
WATER	14,806.30	14,806.30	2,901.00	2,901.00
PROPANE	-	-	-	-
NBUTANOL	-	-	-	-
PROPANOL	-	-	-	-
Total	37,015.76	37,015.76	2,901.00	2,901.00
Vapor Fraction	0.00	0.00	1.00	0.00
Temperature (°F)	104.00	201.20	300.15	300.15

Design Data:	Area for Heat Transfer	130.783	ft^2
	Duty	2,786,743	Btu/hr
	Overall HT Coefficient	150.000	Btu/hr-ft^2 -F
	Average LMTD	142.054	°F
	ΔT	97.20	°F (Cold Side)
	Hot Side ΔP	0.000	psi
	Cold Side ΔP	-5.000	psi
	Shell Material of Construction	Carbon Steel	
	Tube Material of Construction	Stainless Steel	
	Design Temperature	320.00	°F
	Design Pressure	50.000	psig

Purchase Cost:	Fixed Head Heat Exchanger (CE 2006= 500)	$20,410
	Fixed Head Heat Exchanger (CE 2008=548.4)	**$22,400**
Utilities:	Steam at 50 psig	

HEAT EXCHANGER

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date:	4/6/2009
	Item #	X-200		
	# Required	1		

Function:	Cool reactor effluent to flash temperature while simultaneously producing 50 psig steam
Operation:	Continuous

Materials:

	U-200	*U-201*	*S-105*	*S-200*
	Cold Inlet	Cold Outlet	Hot Inlet	Hot Outlet
Composition (lb/hr)				
MALEIC	-	-	5.09	5.09
HYDROGEN	-	-	11,622.88	11,622.88
SUCCINIC	-	-	39.23	39.23
GBL	-	-	3,846.23	3,846.23
BDO	-	-	232.99	232.99
THF	-	-	12,702.00	12,702.00
METHANE	-	-	86.42	86.42
NBUTANE	-	-	116.61	116.61
WATER	43,274.39	43,274.39	25,716.31	25,716.31
PROPANE	-	-	14.89	14.89
NBUTANOL	-	-	781.23	781.23
PROPANOL	-	-	241.48	241.48
Total	43,274.39	43,274.39	55,405.37	55,405.37
Vapor Fraction	0.00	1.00	1.00	0.78
Temperature (°F)	90.00	297.72	480.40	104.00

Design Data:

Area for Heat Transfer	12,440.899	ft^2
Duty	-49,017,997	Btu/hr
Overall HT Coefficient	60.000	$Btu/hr\text{-}ft^2\text{ -}F$
Average LMTD	65.668	°F
ΔT	-376	°F (Hot Side)
Hot Side ΔP	-2.000	psi
Cold Side ΔP	-3.000	psi
Shell Material of Construction	Carbon Steel	
Tube Material of Construction	Stainless Steel	
Design Temperature	482.00	°F
Design Pressure	50.000	psig

Purchase Cost:

Fixed Head Heat Exchanger (CE 2006= 500)	$244,570
Fixed Head Heat Exchanger (CE 2008=548.4)	**$268,200**

Utilities: Boiler Feed Water at 50 psig

HEAT EXCHANGER

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date:	4/6/2009
	Item #	X-201		
	# Required	1		
Function:	Preheat the hydrogen recycle before it enters the reactor			
Operation:	Continuous			

Materials:

	S-205 Cold Inlet	*S-206* Cold Outlet	*HF-200* Hot Inlet	*HF-201* Hot Outlet
Composition (lb/hr)				
MALEIC	-	-	-	-
HYDROGEN	11,454.41	11,454.41	-	-
SUCCINIC	-	-	-	-
GBL	-	-	-	-
BDO	-	-	-	-
THF	181.90	181.90	-	-
METHANE	17.19	17.19	-	-
NBUTANE	13.44	13.44	-	-
WATER	103.05	103.05	-	-
PROPANE	1.77	1.77	-	-
NBUTANOL	-	-	-	-
PROPANOL	-	-	-	-
Dowtherm-A			68,093.37	68,093.37
Total	11,771.76	11,771.76	68,093.37	68,093.37
Vapor Fraction	1.00	1.00	0.00	0.00
Temperature (°F)	148.79	572.00	660.00	163.79

Design Data:	Area for Heat Transfer	4,028.974	ft^2
	Duty	17,038,956	Btu/hr
	Overall HT Coefficient	102.500	Btu/hr-ft^2 -F
	Average LMTD	41.260	°F
	ΔT	423.21	°F (Cold Side)
	Hot Side ΔP	-3.000	psi
	Cold Side ΔP	0.000	psi
	Shell Material of Construction	Carbon Steel	
	Tube Material of Construction	Stainless Steel	
	Design Temperature	690.00	°F
	Design Pressure	2,040.000	psig

Purchase Cost:	Fixed Head Heat Exchanger (CE 2006= 500)	$89,630
	Fixed Head Heat Exchanger (CE 2008=548.4)	**$98,300**

CONDENSER (FIXED HEAD HX)

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date:	4/6/2009
	Item #	X-300		
	# Required	1		
Function:	Condenser for distillation column D-300			
Operation:	Continuous			

Materials:

	U-300 Cold Inlet	*U-301* Cold Outlet	*S-302* Hot Inlet	*S-303* Hot Outlet
Composition (lb/hr)				
MALEIC	-	-	-	-
HYDROGEN	-	-	-	-
SUCCINIC	-	-	-	-
GBL	-	-	135.51	135.51
BDO	-	-	0.04	0.04
THF	-	-	17,660.70	17,660.70
METHANE	-	-	-	-
NBUTANE	-	-	-	-
WATER	1,517,566	1,517,566	40,262.19	40,262.19
PROPANE	-	-	-	-
NBUTANOL	-	-	1,239.73	1,239.73
PROPANOL	-	-	382.23	382.23
Total	1,517,566	1,517,566	59,680.41	59,680.41
Vapor Fraction	0.00	0.00	1.00	0.00
Temperature (°F)	90.00	120.00	222.18	168.53

Design Data:	Area for Heat Transfer	5,047.551	ft^2
	Duty	-45,344,534	Btu/hr
	Overall HT Coefficient	100.000	Btu/hr-ft^2 -F
	Average LMTD	89.835	°F
	ΔT	-53.653	°F (Hot Side)
	Hot Side ΔP	0.000	psi
	Cold Side ΔP	-10.000	psi
	Shell Material of Construction	Carbon Steel	
	Tube Material of Construction	Stainless Steel	
	Design Temperature	240.00	°F
	Design Pressure	65.000	psig

Purchase Cost:	Fixed Head Heat Exchanger (CE 2006= 500)	$107,320
	Fixed Head Heat Exchanger (CE 2008=548.4)	**$117,700**
Utilities:	Cooling water	

THERMOSYPHON REBOILER

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date: 4/6/2009
	Item #	X-301	
	# Required	1	
Function:	Reboiler for distillation column D-300		
Operation:	Continuous		

Materials:

	S-309 Cold Inlet	*S-310* Cold Outlet	*U-302* Hot Inlet	*U-303* Hot Outlet
Composition (lb/hr)				
MALEIC	63.72	63.72	-	-
HYDROGEN	-	-		
SUCCINIC	491.44	491.44		
GBL	47,015.66	47,015.66		
BDO	2,918.08	2,918.08		
THF	0.00	0.00		
METHANE	-	-		
NBUTANE	-	-		
WATER	5,609.87	5,609.87	51,829.34	51,829.34
PROPANE	-	-		
NBUTANOL	0.00	0.00		
PROPANOL	0.00	0.00		
Total	56,098.8	56,098.8	51,829.34	51,829.34
Vapor Fraction	0.00	1.00	1.00	0.00
Temperature (°F)	234.49	255.19	297.70	297.70

Design Data:

Area for Heat Transfer	9,055.189	ft^2
Duty	47,247,168	Btu/hr
Overall HT Coefficient	100.000	Btu/hr-ft^2 -F
Average LMTD	52.177	°F
ΔT	20.70	°F (Cold Side)
Hot Side ΔP	0.000	psi
Cold Side ΔP	-5.000	psi
Shell Material of Construction	Carbon Steel	
Tube Material of Construction	Stainless Steel	
Design Temperature	300.00	°F
Design Pressure	50.000	psig

Purchase Cost:

Fixed Head Heat Exchanger (CE 2006= 500)	$179,610
Fixed Head Heat Exchanger (CE 2008=548.4)	**$197,000**

Utilities: Steam at 50 psig

HEAT EXCHANGER

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date:	4/6/2009
	Item #	X-400		
	# Required	1		
Function:	Condense THF out of the incineration streams using refrigerated coolant			
Operation:	Continuous			

Materials:

	HF-400	*HF-401*	*S-300*	*S-401*	*S-402*
	Cold Inlet	Cold Outlet	Hot Inlet 1	Hot Inlet 2	Hot Outlet
Composition (lb/hr)					
MALEIC	-	-	-	-	-
HYDROGEN	-	-	52.50	115.40	167.90
SUCCINIC	-	-	-	-	-
GBL	-	-	0.01	-	0.01
BDO	-	-	-	-	-
THF	-	-	208.88	130.04	338.92
METHANE	-	-	0.45	68.13	68.58
NBUTANE	-	-	8.15	59.76	67.90
WATER	-	-	0.49	0.05	0.54
PROPANE	-	-	0.63	10.59	11.21
NBUTANOL	-	-	1.19	0.06	1.26
PROPANOL	-	-	0.16	0.09	0.25
50% Ethylene Glycol	2,047.05	2,047.05	-		-
Total	2,047.05	2,047.05	272.46	384.13	656.58
Vapor Fraction	0.00	0.00	1.00	1.00	0.95
Temperature (°F)	-22.00	63.16	78.16	89.99	0.00

Design Data:

Area for Heat Transfer	362.561	ft^2
Duty	-132,532	Btu/hr
Overall HT Coefficient	20.000	Btu/hr-ft^2 -F
Average LMTD	18.277	°F
ΔT	-78.155	°F (Hot Side)
Hot Side ΔP	0.000	psi
Cold Side ΔP	-3.000	psi
Shell Material of Construction	Carbon Steel	
Tube Material of Construction	Stainless Steel	
Design Temperature	70.00	°F
Design Pressure	150.000	psig

Purchase Cost:

Fixed Head Heat Exchanger (CE 2006= 500)	$24,750
Fixed Head Heat Exchanger (CE 2008=548.4)	**$27,100**

CONDENSER (FIXED HEAD HX)

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date:	4/6/2009
	Item #	X-500		
	# Required	1		
Function:	Condenser for distillation column D-500			
Operation:	Continuous			

Materials:

	U-500 Cold Inlet	*U-501* Cold Outlet	*S-500* Hot Inlet	*S-501* Hot Outlet
Composition (lb/hr)				
MALEIC	-	-	-	-
HYDROGEN	-	-	-	-
SUCCINIC	-	-	-	-
GBL	-	-	0.09	0.09
BDO	-	-	-	-
THF	-	-	48,042.56	48,042.56
METHANE	-	-	-	-
NBUTANE	-	-	-	-
WATER	367,268.5	367,268.5	2,485.15	2,485.15
PROPANE	-	-	-	-
NBUTANOL	-	-	1.56	1.56
PROPANOL	-	-	6.89	6.89
Total	367,268.5	367,268.5	50,536.24	50,536.24
Vapor Fraction	0.00	0.00	1.00	0.00
Temperature (°F)	90.00	120.00	147.29	147.26

Design Data:	Area for Heat Transfer	2,713.426	ft^2
	Duty	-10,973,901	Btu/hr
	Overall HT Coefficient	100.000	Btu/hr-ft^2 -F
	Average LMTD	40.443	°F
	ΔT	-0.037	°F (Hot Side)
	Hot Side ΔP	0.000	psi
	Cold Side ΔP	-10.000	psi
	Shell Material of Construction	Carbon Steel	
	Tube Material of Construction	Stainless Steel	
	Design Temperature	160.00	°F
	Design Pressure	65.000	psig

Purchase Cost:	Fixed Head Heat Exchanger (CE 2006= 500)	$66,970
	Fixed Head Heat Exchanger (CE 2008=548.4)	**$73,500**
Utilities:	Cooling water	

THERMOSYPHON REBOILER

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date:	4/6/2009
	Item #	X-501		
	# Required	1		
Function:	Reboiler for distillation column D-500			
Operation:	Continuous			

Materials:		*S-507*	*S-509*	*U-502*	*U-503*
		Cold Inlet	Cold Outlet	Hot Inlet	Hot Outlet
	Composition (lb/hr)				
	MALEIC	-	-	-	-
	HYDROGEN	-	-	-	-
	SUCCINIC	-	-	-	-
	GBL	56.16	56.16	-	-
	BDO	0.02	0.02	-	-
	THF	0.24	0.24	-	-
	METHANE	-	-	-	-
	NBUTANE	-	-	-	-
	WATER	15,241.19	15,241.19	12,281.01	12,281.01
	PROPANE	-	-	-	-
	NBUTANOL	472.66	472.66	-	-
	PROPANOL	144.64	144.64	-	-
	Total	15,914.9	15,914.9	12,281.01	12,281.01
	Vapor Fraction	0.00	1.00	1.00	0.00
	Temperature (°F)	200.78	210.82	297.70	297.70

Design Data:	Area for Heat Transfer	1,219.432	ft^2
	Duty	11,195,257	Btu/hr
	Overall HT Coefficient	100.000	Btu/hr-ft^2 -F
	Average LMTD	91.807	°F
	ΔT	10.03	°F (Cold Side)
	Hot Side ΔP	0.000	psi
	Cold Side ΔP	-5.000	psi
	Shell Material of Construction	Carbon Steel	
	Tube Material of Construction	Stainless Steel	
	Design Temperature	300.00	°F
	Design Pressure	50.000	psig

Purchase Cost:	Fixed Head Heat Exchanger (CE 2006= 500)	$40,900
	Fixed Head Heat Exchanger (CE 2008=548.4)	**$44,900**
Utilities:	Steam at 50 psig	

CONDENSER (FIXED HEAD HX)

Identification:	**Item**	**Fixed Head Heat Exchanger**		Date:	4/6/2009
	Item #	X-502			
	# Required	1			
Function:	Condenser for distillation column D-501				
Operation:	Continuous				
Materials:		*U-504*	*U-505*	*S-511*	*S-512*
		Cold Inlet	Cold Outlet	Hot Inlet	Hot Outlet
	Composition (lb/hr)				
	MALEIC	-	-	-	-
	HYDROGEN	-	-	-	-
	SUCCINIC	-	-	-	-
	GBL	-	-	0.08	0.08
	BDO	-	-	-	-
	THF	-	-	23,614.72	23,614.72
	METHANE	-	-	-	-
	NBUTANE	-	-	-	-
	WATER	191,683.9	191,683.9	2,419.85	2,419.85
	PROPANE	-	-	-	-
	NBUTANOL	-	-	0.04	0.04
	PROPANOL	-	-	1.54	1.54
	Total	191,683.9	191,683.9	26,036.24	26,036.24
	Vapor Fraction	0.00	0.00	1.00	0.00
	Temperature (°F)	90.00	120.00	275.53	274.48
Design Data:	Area for Heat Transfer		337.721	ft^2	
	Duty		-5,727,472	Btu/hr	
	Overall HT Coefficient		100.000	Btu/hr-ft^2 -F	
	Average LMTD		169.592	°F	
	ΔT		-1.046	°F (Hot Side)	
	Hot Side ΔP		0.000	psi	
	Cold Side ΔP		-10.000	psi	
	Shell Material of Construction		Carbon Steel		
	Tube Material of Construction		Stainless Steel		
	Design Temperature		300.00	°F	
	Design Pressure		100.300	psig	
Purchase Cost:	Fixed Head Heat Exchanger (CE 2006= 500)				$24,260
	Fixed Head Heat Exchanger (CE 2008=548.4)				**$26,600**
Utilities:	Cooling water				

THERMOSYPHON REBOILER

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date:	4/6/2009
	Item #	X-503		
	# Required	1		
Function:	Reboiler for distillation column D-501			
Operation:	Continuous			

Materials:		*S-519*	*S-520*	*U-506*	*U-507*
		Cold Inlet	Cold Outlet	Hot Inlet	Hot Outlet
	Composition (lb/hr)				
	MALEIC	-	-	-	-
	HYDROGEN	-	-	-	-
	SUCCINIC	-	-	-	-
	GBL	-	-	-	-
	BDO	-	-	-	-
	THF	51,972.12	51,972.12	-	-
	METHANE	-	-	-	-
	NBUTANE	-	-	-	-
	WATER	1.59	1.59	8,916.64	8,916.64
	PROPANE	-	-	-	-
	NBUTANOL	3.31	3.31	-	-
	PROPANOL	11.59	11.59	-	-
	Total	51,988.6	51,988.6	8,916.64	8,916.64
	Vapor Fraction	0.00	1.00	1.00	0.00
	Temperature (°F)	298.13	298.48	365.90	365.90

Design Data:	Area for Heat Transfer	1,105.752	ft^2
	Duty	7,640,278	Btu/hr
	Overall HT Coefficient	100.000	Btu/hr-ft^2 -F
	Average LMTD	69.096	°F
	ΔT	0.34	°F (Cold Side)
	Hot Side ΔP	0.000	psi
	Cold Side ΔP	-5.000	psi
	Shell Material of Construction	Carbon Steel	
	Tube Material of Construction	Stainless Steel	
	Design Temperature	380.00	°F
	Design Pressure	150.000	psig

Purchase Cost:	Fixed Head Heat Exchanger (CE 2006= 500)	$39,280
	Fixed Head Heat Exchanger (CE 2008=548.4)	**$43,100**
Utilities:	Steam at 150 psig	

HEAT EXCHANGER

Identification:	**Item**	**Fixed Head Heat Exchanger**	Date:	4/6/2009
	Item #	X-600		
	# Required	1		

Function:	Cool THF product to near-storage temperature
Operation:	Continuous

Materials:		*U-600* Cold Inlet	*U-601* Cold Outlet	*S-600* Hot Inlet	*S-601* Hot Outlet
	Composition (lb/hr)				
	MALEIC	-	-	-	-
	HYDROGEN	-	-	-	-
	SUCCINIC	-	-	-	-
	GBL	-	-	-	-
	BDO	-	-	-	-
	THF	-	-	12,496.03	12,496.03
	METHANE	-	-	-	-
	NBUTANE	-	-	-	-
	WATER	34,705.03	34,705.03	0.38	0.38
	PROPANE	-	-	-	-
	NBUTANOL	-	-	0.80	0.80
	PROPANOL	-	-	2.79	2.79
	Total	34,705.03	34,705.03	12,500.00	12,500.00
	Vapor Fraction	0.00	0.00	0.38	0.00
	Temperature (°F)	90.00	120.00	171.33	104.00

Design Data:	Area for Heat Transfer	417.442	ft^2
	Duty	-1,199,440	Btu/hr
	Overall HT Coefficient	100.000	Btu/hr-ft^2 -F
	Average LMTD	28.733	°F
	ΔT	-67.331	°F (Hot Side)
	Hot Side ΔP	-1.400	psi
	Cold Side ΔP	-10.000	psi
	Shell Material of Construction	Carbon Steel	
	Tube Material of Construction	Stainless Steel	
	Design Temperature	190.00	°F
	Design Pressure	65.000	psig

Purchase Cost:	Fixed Head Heat Exchanger (CE 2006= 500)	$25,850
	Fixed Head Heat Exchanger (CE 2008=548.4)	**$28,400**

Utilities:	Cooling water

7.0 Fixed Capital Investment Summary and Operating Cost

To estimate the fixed capital investment for the proposed plant construction, rough estimates for Total Bare Module Investment (TBM), Total Direct Permanent Investment (DPI), Total Depreciable Capital (TDC), Total Permanent Investment (TPI), and Total Capital Investment (TCI) are provided in the table below.

FIXED CAPITAL INVESTMENT SUMMARY		
Total Bare Module Costs (CE 2008=548.4)		
Fabricated Equipment	$	9,428,700
Process Machinery	$	14,558,400
Spares	$	-
Storage Tanks	$	2,942,800
Initial Catalyst Charge	$	875,600
Computers and Software	$	-
Total Bare Module Investment (TBM)	**$**	**27,806,000**
Cost of Site Preparation	$	1,390,300
Cost of Service Facilities	$	1,390,300
Allocated Costs for Utility Plants/Related Facilities	$	-
Total Direct Permanent Investment (DPI)	**$**	**30,587,000**
Cost of Contingencies and Contractor's Fee	$	5,505,700
Total Depreciable capital (TDC)	**$**	**36,093,000**
Cost of Land	$	721,900
Cost of Royalties	$	-
Cost of Plant Startup	$	3,609,300
Total Permanent Investment (TPI)	**$**	**40,424,000**
Working Capital	$	6,324,000
Total Capital Investment (TCI)	**$**	**46,748,000**

For the economic analysis, the cost of site preparation and the cost of service facilities were both assumed to be 5.0% of TBM, since the plant is not a grassroots plant and will be built next to existing facilities. The allocated costs were set at 0.0% because no related facilities or utility plants will be constructed on site for this plant. The cost of contingencies and contractor’s fee was assumed to be 18.0% of DPI. The costs of land and plant startup were assumed to be 2.0% and 10.0%, respectively, of TDC. Per guidance from the industrial consultants, the cost of royalties was set to 0% because no outside research or development is used in the construction or operation of the plant. Working capital is computed assuming 4 days of inventory (from two 48 hour storage tanks) and 10 days of accounts receivable. The analysis also does include accounts payable or cash reserves held, according to advice from Professor Seider, our project advisor. Since the project is built to support a downstream Lycra® plant and operates using maleic acid feed from an upstream plant, the expected time to payment and thus, working capital is reduced significantly. The framework for this estimation is provided in Table 22.9 in *Product and Process Design Principles, 3rd Edition* by Seider et. al. (Seider, Seader, Lewin, & Widagdo, 2009)

8.0 Other Important Considerations

8.1 Environmental and Safety Concerns:

THF is a highly flammable organic solvent that forms peroxides when it comes into contact with oxygen. Therefore, care must be taken during THF storage and shipment to avoid contact with air. Consequently, to minimize THF emissions, today's designs now use an internal floating roof design. Outside or detached storage is preferred, and inside storage should be in a standard flammable liquids storage area or room. Containers of THF should be protected from physical damage and be stored well away from oxidizers, heat, sparks, and open flames. Drums must be equipped with self-closing valves and flame arrestors. Only non-sparking tools may be used to handle THF, and to prevent static sparks, containers should be grounded and bonded for transfers.

The peroxides formed by THF can cause severe problems after purification. Peroxides are high boilers and can become concentrated in the bottom of the distillation columns. If they become concentrated to a sufficient level they can pose a considerable risk of explosion as they are shock-sensitive. Such explosions have occurred numerous times in laboratories due to the improper storage of THF (Gosselin, Smith, & Hodge, 1984). To prevent the formation of peroxides, a stabilizer, butylated hydroxyl-toluene (BHT), is added to the THF product before its shipment. Although this is not needed if the storage facility or tanks are within pipeline distance, it is necessary if the THF is being shipped by a truck or another vehicle.

Tetrahydrofuran is a central nervous system depressant for humans. Based on effects seen in animals, it may also cause irritation of the mucous membranes and upper respiratory tract along with liver and kidney damage. There are no reports of chronic effects in humans (Hathaway, Proctor, & Hughes, 1991, p. 537). However, investigators exposed to unknown concentrations while testing THF's pharmacological properties developed severe occipital headaches (Gosselin, Smith, & Hodge, 1984, p. 408). Researchers engaged in the experimental spinning of synthetic fibers showed a marked decrease in white blood cell count that is believed to have been caused by exposure to THF, which was used as a solvent. Thus, care must be taken to limit employee exposure to THF. Methods that are effective in controlling worker exposures to THF, depending on the feasibility of implementation are:

1. Process enclosure
2. Local exhaust ventilation
3. General dilution ventilation
4. Personal protective equipment.

8.2 Catalyst Regeneration

Each year, the catalyst must be removed from the reactor and sent to a catalyst regeneration service provider. Significant fouling can build up on the catalyst over the course of a year, reducing its efficacy and thus, slowing down the reaction rate. The design team looked into several catalyst regeneration companies and decided that BASF Catalysts, Inc. located in New Jersey is the best choice for Pd-Re catalyst regeneration. The cost of this regeneration process is estimated to be $130,900 per year, which is 15% of the original catalyst cost. (See Page 220 for computation of catalyst regeneration costs and Pages 343-343 for correspondence with BASF Catalysts representatives)

8.3 Startup Considerations

A number of additional measures must be addressed during the startup phase. The first pertains to the supply of raw materials, or more specifically, the supply of maleic acid. Although the maleic acid source is produced by an internal upstream production facility, its regular supply is not guaranteed. The upstream facility will be required to shut down for regular periods due to maintenance, and it is very important to ensure that the change in supply of maleic acid during such periods does not severely affect the THF production. This can be accomplished by synchronizing the THF facility's shutdowns with those of the upstream plant, or by filling storage tanks with maleic acid to ensure an uninterrupted supply. Clearly, the latter option will be far more costly and will accrue additional transportation and storage costs. Secondly, the reactor must be charged with the Pd-Re on carbon support catalyst prior to operation. The raw materials must then be fed in the right proportions before hydrogen is bubbled through to initiate the reaction. Likewise, the fired heater (H-200) and the refrigerator (H-400) will have to be charged with their respective Dowtherm A and Ethylene Glycol recycle systems. Lastly, the unit D-300, which makes use of pressurized steam created by the process, will have to utilize pressurized steam from the market until the process reaches steady state. H-200, which uses the incineration stream created by D-401, will also need to draw upon the natural gas utility in full until the system reaches steady state.

9.0 Economic Analysis

A thorough economic analysis was carried out using the conditions and inputs described in the preceding sections. The "Profitability Analysis Version 1" spreadsheet provided with *Product and Process Design Principles, 2nd Edition* was used for the analysis. The input summary, net present value (NPV) calculations and other important results are included in the following pages.

The analysis resulted in a cumulative net present value (NPV) of $54,340,000 over the duration of the plant's life and an investor's rate of return (IRR) of 32.7 %. The return on investment (ROI) based on the third production year was computed to be 45.9%, which not only demonstrates the economic feasibility of the project, but also its considerable attractiveness. However, a word of caution is in order; the initial total permanent investment required is quite significant at $40,424,000, and the profitability of the project is subject to a variety of external factors. The impact of some of these factors will be evaluated through sensitivity analyses in Section 10.

Input Summary

General Information

Process Title: **THF Production**
Product: **THF**
Plant Site Location: **Gulf Coast**
Site Factor: **1.00**
Operating Hours per Year: **8,000**
Operating Days per Year: **333**
Operating Factor: **0.9132**

Chronology

	Year	Action	Distribution of Total Permanent Investment	Distribution of Total Working Capital	Production Capacity (% of Design Capacity)	Percentage of Total Capital Investment for Depreciation
Start Year	2009	Design	50.0%	50.0%	0.0%	
	2010	Construction	50.0%	50.0%	0.0%	
	2011	Production			45.0%	20.0%
	2012	Production			67.5%	32.0%
	2013	Production			90.0%	19.2%
	2014	Production			90.0%	11.5%
	2015	Production			90.0%	11.5%
	2016	Production			90.0%	5.8%
	2017	Production			90.0%	
	2018	Production			90.0%	
	2019	Production			90.0%	
	2020	Production			90.0%	
	2021	Production			90.0%	
	2022	Production			90.0%	
	2023	Production			90.0%	
	2024	Production			90.0%	
End Year	2025	Production			90.0%	

Product Information

The Process will yield:

⇨ **12,500** lb of THF per hour.
⇨ **300,000** lb of THF per day.
⇨ **100,000,000** lb of THF per year.

The Price per lb of THF is: **$ 1.55**

Raw Materials

Raw Material	Unit of Measure	Ratio to Product	Cost of Raw Material
Hydrogen	lb	0.1714 lb per lb of THF	$0.7500 per lb
Maleic Acid	lb	1.7760 lb per lb of THF	$0.4536 per lb

Equipments Costs

Fabricated Equipment	Purchase Cost	Bare Module Factor	Bare Module Cost
F-200	$ 77,500	4.16	$ 322,400
F-400	$ 7,700	4.16	$ 32,032
F-300	$ 66,700	4.16	$ 277,472
F-401	$ 4,500	4.16	$ 18,720
R-100	$ 768,100	4.16	$ 3,195,296
D-300	$ 242,200	4.16	$ 1,007,552
D-500	$ 278,600	4.16	$ 1,158,976
D-501	$ 99,440	4.16	$ 413,670
X-100	$ 22,400	3.17	$ 71,008
Condenser(X-300,X-500,X-502)	$ 217,800	3.17	$ 690,426
Reboilers(X-301,X-501,X-503)	$ 285,000	3.17	$ 903,450
X-201	$ 98,300	3.17	$ 311,611
X-200	$ 268,200	3.17	$ 850,194
X-400	$ 27,100	3.17	$ 85,907
X-600	$ 28,400	3.17	$ 90,028

Process Machinery		**Purchase Cost**	**Bare Module Factor**	**Bare Module Cost**
	P-100	$ 88,200	3.3	$ 291,060
	P-300	$ 19,100	3.3	$ 63,030
	P-502	$ 8,300	3.3	$ 27,390
	All Distillation Pumps	$ 124,100	3.3	$ 409,530
	Accumulators(A-300,A-500,A-501)	$ 127,400	3.05	$ 388,570
	M-200	$ 97,450	2.32	$ 226,084
	C-100	$ 3,616,900	2.15	$ 7,776,335
	C-200	$ 1,610,200	2.15	$ 3,461,930
	P-200	$ 6,900	3.3	$ 22,770
	P-400	$ 6,700	3.3	$ 22,110
	H-200	$ 701,000	2.2	$ 1,542,200
	H-400	$ 274,200	1	$ 274,200
	Dowtherm A	$ 53,110	1	$ 53,110
	Ethylene Glycol	$ 110	1	$ 110

Storage		**Purchase Cost**	**Bare Module Factor**	**Bare Module Cost**
	T-600	$ 353,701	4.16	$ 1,471,398
	T-600	$ 353,701	4.16	$ 1,471,398
Catalyst		**Purchase Cost**	**Bare Module Factor**	**Bare Module Cost**
	Carbon Support Catalyst	$ 875,600	1	$ 875,600

Total Permanent Investment

Cost of Site Preparations: **5.0% of Total Bare Module Costs**
Cost of Service Facilities: **5.0% of Total Bare Module Costs**
Allocated Costs for utility plants and related facilities: **$0**
Cost of Contingencies and Contractor Fees: **18.0% of Direct Permanent Investment**
Cost of Land: **2.0% of Total Depreciable Capital**
Cost of Royalties: **$0**
Cost of Plant Start-Up: **10.0% of Total Depreciable Capital**

Working Capital

THF	⇨	Inventory: **4 Days**	⇨	1,200,000.00 lb
Hydrogen	⇨	Inventory: **Days**	⇨	0.00 lb
Maleic Acid	⇨	Inventory: **Days**	⇨	0.00 lb
Accounts Receivable	⇨	**10 Days**		
Cash Reservces	⇨	**None**		
Accounts Payable	⇨	**None**		

Utilities

Utility	**Unit of Measure**	**Ratio to Product**	**Cost of Utility**
High Pressure Steam	lb	0.7133 lb per lb of THF	$0.0053 per lb
Low Pressure Steam	lb	1.8990 lb per lb of THF	$0.0033 per lb
Cooling Water	gal	20.7767 gal per lb of THF	$0.0001 per gal
Natural Gas	SCF	0.3045 SCF per lb of THF	$0.0035 per SCF
Electricity	kW-hr	0.2079 kW-hr per lb of THF	$0.0658 per kW-hr
Boiler Feed Water (BFW)	gal	0.4146 gal per lb of THF	$0.0020 per gal
Refrigeration (-30F)	ton-day	0.0009 ton-day per lb of THF	$2.6328 per ton-day
Waste Water Treatment	lb removed	0.0890 lb removed per lb of THF	$0.1646 per lb removed
Catalyst Regeneration	lb	1.0000 lb per lb of THF	$10.4707 per lb

Other Variable Costs

General Expenses

Selling / Transfer Expenses: **1.00% of Sales**
Direct Research: **1.50% of Sales**
Allocated Research: **1.00% of Sales**
Administrative Expense: **2.00% of Sales**
Management Incentive Compensation: **1.25% of Sales**

Fixed Costs

Operations

Operators per Shift: **7** (Assuming 5 Shifts)
Direct Wages and Benefits: **$35.00 per Operator Hour**
Direct Salaries and Benefits: **15.00% of Direct Wages and Benefits**
Operating Supplies and Services: **6.00% of Direct Wages and Benefits**
Technical Assistance to Manufacturing: **$60,000.00 per year, for each Operator per Shift**
Control Laboratory: **$65,000.00 per year, for each Operator per Shift**

Maintenance

Wages and Benefits: **4.50% of Total Depreciable Capital**
Salaries and Benefits: **25.00% of Maintenance Wages and Benefits**
Materials and Services: **100.00% of Maintenance Wages and Benefits**
Maintenance Overhead: **5.00% of Maintenance Wages and Benefits**

Operating Overhead

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

Property Taxes and Insurance

Property Taxes and Insurance: **2.00% of Total Depreciable Capital**

Straight Line Depreciation

Direct Plant: **8.00% of Total Depreciable Capital, less1.18 times the Allocated Costs for Utility Plants and Related Facilities**
Allocated Plant: **6.00% of 1.18 times the Allocated Costs for Utility Plants and Related Facilities**

Depletion Allowance

Annual Depletion Allowance: **$0.00**

Investment Summary

April, 2009

THF Production

		TOTAL
Bare Module Costs		
Fabricated Equipment		
F-200	$322,400	
F-400	$32,000	
F-300	$277,500	
F-401	$18,700	
R-100	$3,195,300	
D-300	$1,007,600	
D-500	$1,159,000	
D-501	$413,700	
X-100	$71,000	
Condenser(X-300,X-500,X-502)	$690,400	
Reboilers(X-301,X-501,X-503)	$903,500	
X-201	$311,600	
X-200	$850,200	
X-400	$85,900	
X-600	$90,000	
Total Fabricated Equipment:	**$9,428,700**	
Process Machinery		
P-100	$291,100	
P-300	$63,000	
P-502	$27,400	
All Distillation Pumps	$409,500	
Accumulators(A-300,A-500,A-501)	$388,600	
M-200	$226,100	
C-100	$7,776,300	
C-200	$3,461,900	
P-200	$22,800	
P-400	$22,100	
H-200	$1,542,200	
H-400	$274,200	
Dowtherm A	$53,100	
Ethylene Glycol	$100	
Total Process Machinery:	**$14,558,400**	
Storage		
T-600	$1,471,400	
T-600	$1,471,400	
Total Storage:	**$2,942,800**	
Catalysts		
Carbon Support Catalyst	$875,600	
Total Catalysts:	**$875,600**	
Total Bare Module Costs:		**$27,806,000**
Direct Permanent Investment		
Cost of Site Preparation:	$1,390,300	
Cost of Service Facilities:	$1,390,300	
Allocated Costs for utility plants and related facilities:	$0	
Direct Permanent Investment:		**$30,587,000**

Total Depreciable Capital				
Cost of Contigencies and Contractor Fees:		$5,505,700		
			Total Depreciable Capital:	**$36,093,000**
Total Permanent Investment				
Cost of Land:		$721,900		
Cost of Royalties:		$0		
Cost of Plant Start-Up:		$3,609,300		
			Total Permanent Investment:	**$40,424,000**
Working Capital				
Inventory				
THF	⇨ 1,080,000 lb		$1,674,000	
		Total Inventory:	**$1,674,000**	
Accounts Receivable:			$4,650,000	
Cash Reservces:			$0	
Accounts Payable:			$0	
		Total Working Capital:	$6,324,000	
TOTAL CAPITAL INVESTMENT				**$46,748,000**

Variable Cost Summary

THF Production

April, 2009

	Per lb THF		TOTAL
Raw Materials			
Hydrogen	$0.13 per lb of THF	$12,855,000	
Maleic Acid	$0.81 per lb of THF	$80,559,400	
Total Raw Materials:	**$0.93 per lb of THF**	**$93,414,400**	**$93,414,400**
Utilties			
High Pressure Steam	$0.00 per lb of THF	$375,600	
Low Pressure Steam	$0.01 per lb of THF	$624,900	
Cooling Water	$0.00 per lb of THF	$170,900	
Natural Gas	$0.00 per lb of THF	$106,900	
Electricity	$0.01 per lb of THF	$1,368,400	
Boiler Feed Water (BFW)	$0.00 per lb of THF	$81,900	
Refrigeration (-30F)	$0.00 per lb of THF	$232,600	
Waste Water Treatment	$0.01 per lb of THF	$1,464,400	
Catalyst Regeneration	$0.00 per lb of THF	$130,900	
Total Raw Materials:	**$0.05 per lb of THF**	**$4,556,500**	**$97,970,900**
General Expenses			
Selling / Transfer:	$0.02 per lb of THF	$1,550,000	
Direct Research:	$0.02 per lb of THF	$2,325,000	
Allocated Research:	$0.02 per lb of THF	$1,550,000	
Administrative Expense:	$0.03 per lb of THF	$3,100,000	
Management Incentives:	$0.02 per lb of THF	$1,937,500	
Total Byproducts:	**$0.10 per lb of THF**	**$10,462,500**	**$108,433,400**
TOTAL	**$1.08 per lb of THF**	**$108,433,300**	**$108,433,300**

Fixed Cost Summary

April, 2009

THF Production

			TOTAL
Operations			
	Direct Wages and Benefits:	$2,548,000	
	Direct Salaries and Benefits:	$382,200	
	Operating Supplies and Services:	$152,880	
	Technical Assistance to Manufacturing:	$420,000	
	Control Laboratory:	$455,000	
	Total Operations:	**$3,958,080**	**$3,958,080**
Maintenance			
	Wages and Benefits:	$1,624,185	
	Salaries and Benefits:	$406,046	
	Materials and Services:	$1,624,185	
	Maintenance Overhead:	$81,209	
	Total Maintenance:	**$3,735,625**	**$7,693,705**
Operating Overhead			
	General Plant Overhead:	$352,191	
	Mechanical Department Services:	$119,050	
	Employee Relations Department:	$292,665	
	Business Services:	$367,072	
	Total Operating Overhead:	**$1,130,978**	**$8,824,683**
Property Insurance and Taxes			
	Total Property Insurance and Taxes:	**$721,860**	**$9,546,543**
TOTAL			**$9,546,543**

Cash Flow Summary

April, 2009

THF Production

Year	Percentage of Design Capacity	Sales	Capital Costs	Working Capital	Variable Costs	Fixed Costs	Depreciation Allowance	Depletion Allowance	Taxable Income	Income Tax Costs	Net Earnings	Annual Cash Flow	Cumulative Net Present Value at 15.0%
2009	0.0%	Design	-$20,212,000	-$3,162,000								-$23,374,000	-$23,374,000
2010	0.0%	Construction	-$20,212,000	-$3,162,000								-$23,374,000	-$43,699,200
2011	45.0%	$69,750,000			-$48,795,000	-$9,546,500	-$7,218,600	$0	$4,189,900	-$1,550,300	$2,639,600	$9,858,200	-$36,245,000
2012	67.5%	$104,625,000			-$73,192,500	-$9,546,500	-$11,549,800	$0	$10,336,200	-$3,824,400	$6,511,800	$18,061,600	-$24,369,200
2013	90.0%	$139,500,000			-$97,590,000	-$9,546,500	-$6,929,900	$0	$25,433,600	-$9,410,400	$16,023,200	$22,953,100	-$11,245,700
2014	90.0%	$139,500,000			-$97,590,000	-$9,546,500	-$4,157,900	$0	$28,205,600	-$10,436,100	$17,769,500	$21,927,400	-$343,900
2015	90.0%	$139,500,000			-$97,590,000	-$9,546,500	-$4,157,900	$0	$28,205,600	-$10,436,100	$17,769,500	$21,927,400	$9,135,900
2016	90.0%	$139,500,000			-$97,590,000	-$9,546,500	-$2,079,000	$0	$30,284,500	-$11,205,300	$19,079,200	$21,158,200	$17,090,100
2017	90.0%	$139,500,000			-$97,590,000	-$9,546,500		$0	$32,363,500	-$11,974,500	$20,389,000	$20,389,000	$23,755,300
2018	90.0%	$139,500,000			-$97,590,000	-$9,546,500		$0	$32,363,500	-$11,974,500	$20,389,000	$20,389,000	$29,551,100
2019	90.0%	$139,500,000			-$97,590,000	-$9,546,500		$0	$32,363,500	-$11,974,500	$20,389,000	$20,389,000	$34,590,900
2020	90.0%	$139,500,000			-$97,590,000	-$9,546,500		$0	$32,363,500	-$11,974,500	$20,389,000	$20,389,000	$38,973,400
2021	90.0%	$139,500,000			-$97,590,000	-$9,546,500		$0	$32,363,500	-$11,974,500	$20,389,000	$20,389,000	$42,784,200
2022	90.0%	$139,500,000			-$97,590,000	-$9,546,500		$0	$32,363,500	-$11,974,500	$20,389,000	$20,389,000	$46,098,000
2023	90.0%	$139,500,000			-$97,590,000	-$9,546,500		$0	$32,363,500	-$11,974,500	$20,389,000	$20,389,000	$48,979,600
2024	90.0%	$139,500,000			-$97,590,000	-$9,546,500		$0	$32,363,500	-$11,974,500	$20,389,000	$20,389,000	$51,485,300
2025	90.0%	$139,500,000		$6,324,000	-$97,590,000	-$9,546,500		$0	$32,363,500	-$11,974,500	$20,389,000	$26,713,000	$54,340,000

Profitability Measures

THF Production

April, 2009

The Investor's Rate of Return (IRR) for this Project is: **32.70%**

The Net Present Value (NPV) at 15% for this Project is: **$54,340,000**

ROI Analysis (Third Production Year)

Annual Sales:	$139,500,000
Annual Costs:	-$107,136,500
Depreciation:	-$2,887,400
Income Tax:	-$10,906,200
Net Earnings:	$21,457,300
Total Capital Investment:	$46,748,000
ROI:	**45.9%**

April, 2009

IRR Analysis - Single Variable

THF Production

Product Prices

Product Prices	$1.32	$1.36	$1.40	$1.43	$1.47	$1.51	$1.55	$1.59	$1.63	$1.67	$1.71	$1.74	$1.78
IRR	14.70%	18.35%	21.65%	24.69%	27.52%	30.18%	32.70%	35.11%	37.41%	39.63%	41.76%	43.82%	45.81%

Variable Cost

Variable Cost	$92,168,300	$94,879,100	$97,590,000	$100,300,800	$103,011,600	$105,722,500	$108,433,300	$111,144,100	$113,855,000	$116,565,800	$119,276,600	$121,987,500	$124,698,300
IRR	43.30%	41.64%	39.94%	38.20%	36.42%	34.59%	32.70%	30.76%	28.74%	26.65%	24.46%	22.17%	19.74%

Fixed Cost

Fixed Cost	$8,114,600	$8,353,200	$8,591,900	$8,830,600	$9,069,200	$9,307,900	$9,546,500	$9,785,200	$10,023,900	$10,262,500	$10,501,200	$10,739,900	$10,978,500
IRR	34.05%	33.83%	33.61%	33.38%	33.16%	32.93%	32.70%	32.48%	32.25%	32.02%	31.79%	31.57%	31.34%

Initial Investment (TPI)

Inititial Investment	$34,360,400.0	$35,371,000	$36,381,600	$37,392,200	$38,402,800	$39,413,400	$40,424,000	$41,434,600	$42,445,200	$43,455,800	$44,466,400	$45,477,000	$46,487,600
IRR	36.63%	35.91%	35.23%	34.56%	33.92%	33.30%	32.70%	32.13%	31.57%	31.03%	30.50%	30.00%	29.50%

IRR Analysis - Two Variable

April, 2009

THF Production

Product Prices vs Variable Costs

Product Prices

	$92,168,300	$94,879,100	$97,590,000	$100,300,800	$103,011,600	$105,722,500	$108,433,300	$111,144,100	$113,855,000	$116,565,800	$119,276,600	$121,987,500	$124,698,300
$ 1.32	28.03%	25.86%	23.59%	21.19%	18.65%	15.92%	12.95%	9.65%	5.87%	1.31%	-4.73%	Out of Range	Out of Range
$ 1.36	30.90%	28.85%	26.72%	24.50%	22.17%	19.69%	17.06%	14.21%	11.07%	7.53%	3.37%	-1.86%	Out of Range
$ 1.40	33.61%	31.67%	29.66%	27.57%	25.39%	23.11%	20.71%	18.15%	15.40%	12.41%	9.07%	5.23%	0.56%
$ 1.43	36.19%	34.33%	32.42%	30.44%	28.39%	26.26%	24.03%	21.69%	19.21%	16.55%	13.68%	10.51%	6.92%
$ 1.47	38.66%	36.87%	35.04%	33.16%	31.21%	29.20%	27.11%	24.92%	22.64%	20.22%	17.66%	14.89%	11.87%
$ 1.51	41.02%	39.30%	37.54%	35.74%	33.88%	31.96%	29.98%	27.93%	25.80%	23.56%	21.21%	18.72%	16.05%
$ 1.55	43.30%	41.64%	39.94%	38.20%	36.42%	34.59%	32.70%	30.76%	28.74%	26.65%	24.46%	22.17%	19.74%
$ 1.59	45.49%	43.88%	42.24%	40.57%	38.85%	37.09%	35.29%	33.43%	31.51%	29.53%	27.48%	25.33%	23.09%
$ 1.63	47.61%	46.05%	44.46%	42.84%	41.18%	39.49%	37.75%	35.97%	34.14%	32.25%	30.30%	28.29%	26.19%
$ 1.67	49.67%	48.15%	46.61%	45.04%	43.43%	41.79%	40.12%	38.40%	36.64%	34.84%	32.98%	31.06%	29.08%
$ 1.71	51.67%	50.19%	48.69%	47.16%	45.60%	44.01%	42.39%	40.74%	39.04%	37.31%	35.52%	33.69%	31.81%
$ 1.74	53.61%	52.17%	50.70%	49.21%	47.70%	46.16%	44.59%	42.98%	41.35%	39.67%	37.96%	36.20%	34.39%
$ 1.78	55.50%	54.09%	52.66%	51.21%	49.73%	48.23%	46.71%	45.15%	43.57%	41.95%	40.29%	38.60%	36.86%

Product Prices vs Initial Investment

Product Prices

	$34,360,400	$35,371,000	$36,381,600	$37,392,200	$38,402,800	$39,413,400	$40,424,000	$41,434,600	$42,445,200	$43,455,800	$44,466,400	$45,477,000	$46,487,600
$ 1.32	17.32%	16.84%	16.38%	15.94%	15.51%	15.10%	14.70%	14.32%	13.94%	13.58%	13.23%	12.89%	12.56%
$ 1.36	21.22%	20.70%	20.19%	19.71%	19.24%	18.79%	18.35%	17.93%	17.52%	17.13%	16.74%	16.37%	16.01%
$ 1.40	24.76%	24.19%	23.64%	23.12%	22.61%	22.12%	21.65%	21.19%	20.75%	20.32%	19.91%	19.51%	19.12%
$ 1.43	28.01%	27.41%	26.82%	26.26%	25.72%	25.19%	24.69%	24.20%	23.72%	23.27%	22.82%	22.39%	21.97%
$ 1.47	31.05%	30.41%	29.79%	29.19%	28.61%	28.05%	27.52%	27.00%	26.49%	26.01%	25.53%	25.08%	24.63%
$ 1.51	33.92%	33.24%	32.58%	31.95%	31.34%	30.75%	30.18%	29.63%	29.10%	28.58%	28.09%	27.60%	27.13%
$ 1.55	36.63%	35.91%	35.23%	34.56%	33.92%	33.30%	32.70%	32.13%	31.57%	31.03%	30.50%	30.00%	29.50%
$ 1.59	39.22%	38.47%	37.75%	37.05%	36.38%	35.73%	35.11%	34.51%	33.92%	33.36%	32.81%	32.28%	31.76%
$ 1.63	41.70%	40.91%	40.16%	39.44%	38.74%	38.06%	37.41%	36.78%	36.17%	35.58%	35.01%	34.46%	33.92%
$ 1.67	44.07%	43.26%	42.48%	41.73%	41.00%	40.30%	39.63%	38.97%	38.34%	37.73%	37.13%	36.56%	36.00%
$ 1.71	46.36%	45.52%	44.72%	43.94%	43.18%	42.46%	41.76%	41.08%	40.42%	39.79%	39.17%	38.58%	38.00%
$ 1.74	48.57%	47.71%	46.87%	46.07%	45.29%	44.54%	43.82%	43.12%	42.44%	41.78%	41.15%	40.53%	39.93%
$ 1.78	50.71%	49.82%	48.96%	48.13%	47.33%	46.56%	45.81%	45.09%	44.39%	43.71%	43.06%	42.42%	41.80%

Variable vs. Fixed Costs

Variable Costs

	$8,114,600	$8,353,200	$8,591,900	$8,830,600	$9,069,200	$9,307,900	$9,546,500	$9,785,200	$10,023,900	$10,262,500	$10,501,200	$10,739,900	$10,978,500
$ 92,168,300	44.50%	44.30%	44.10%	43.90%	43.70%	43.50%	43.30%	43.09%	42.89%	42.69%	42.49%	42.28%	42.08%
$ 94,879,100	42.86%	42.66%	42.46%	42.25%	42.05%	41.84%	41.64%	41.43%	41.23%	41.02%	40.81%	40.61%	40.40%
$ 97,590,000	41.19%	40.98%	40.77%	40.56%	40.36%	40.15%	39.94%	39.73%	39.52%	39.31%	39.10%	38.89%	38.68%
$ 100,300,800	39.47%	39.26%	39.05%	38.84%	38.63%	38.42%	38.20%	37.99%	37.78%	37.56%	37.35%	37.14%	36.92%
$ 103,011,600	37.71%	37.50%	37.28%	37.07%	36.85%	36.64%	36.42%	36.20%	35.99%	35.77%	35.55%	35.33%	35.12%
$ 105,722,500	35.91%	35.69%	35.47%	35.25%	35.03%	34.81%	34.59%	34.37%	34.15%	33.92%	33.70%	33.48%	33.26%
$ 108,433,300	34.05%	33.83%	33.61%	33.38%	33.16%	32.93%	32.70%	32.48%	32.25%	32.02%	31.79%	31.57%	31.34%
$ 111,144,100	32.14%	31.91%	31.68%	31.45%	31.22%	30.99%	30.76%	30.52%	30.29%	30.06%	29.82%	29.59%	29.35%
$ 113,855,000	30.16%	29.93%	29.69%	29.45%	29.22%	28.98%	28.74%	28.50%	28.26%	28.02%	27.78%	27.54%	27.30%
$ 116,565,800	28.11%	27.87%	27.63%	27.38%	27.14%	26.89%	26.65%	26.40%	26.15%	25.90%	25.65%	25.40%	25.15%
$ 119,276,600	25.98%	25.73%	25.47%	25.22%	24.97%	24.71%	24.46%	24.20%	23.95%	23.69%	23.43%	23.17%	22.91%
$ 121,987,500	23.74%	23.48%	23.22%	22.96%	22.70%	22.43%	22.17%	21.90%	21.63%	21.36%	21.09%	20.82%	20.55%
$ 124,698,300	21.40%	21.12%	20.85%	20.57%	20.30%	20.02%	19.74%	19.46%	19.18%	18.90%	18.62%	18.33%	18.04%

10.0 Sensitivity Analysis

The economic analysis presented in Section 9.0 can be affected by numerous factors including, but not limited to: changes in THF prices or raw material availability, changes in utility prices, wage increases, more stringent environmental regulations, and new labor laws. All of these factors could have a significant impact on the economic validity of the proposed project. Consequently, it is necessary to analyze the impact that these variables can have on the plant's profitability and the viability of the process. Such an analysis will help establish the bounds of error in our current estimates and will help determine whether our proposal is viable. The analysis can also help us estimate the impact of unforeseeable factors on cash flows and profitability.

For the purposes of this report, the impact of changes in the various variables are evaluated through sensitivity analyses. The relative magnitude of change in the measures of profitability, such as the NPV, IRR, and ROI will be studied for a given change in a variable.

10.1 Non-probabilistic Sensitivity

The various factors that could have an impact on the financial future of the THF plant are numerous and range from the obvious to the unforeseen. It is impossible to try to identify and analyze every individual factor; instead, a better approach is to identify the major sources of uncertainty that are present and to evaluate their impact. Some of the major sources of uncertainty for typical chemical plants are given below:

1) **The demand for the product**: The demand of the product is a function of various factors such as the general state of the economy, the demand elasticities of the downstream users, and technological advancements. Significant increases in demand for the product could considerably improve the profitability, whereas decreases in demand could have very detrimental effects. Therefore, management should perform a thorough evaluation of the product's scope and product market before any investment decision is considered. The THF produced in the proposed plant will be used in another in-house plant, which keeps the demand for THF steady. The possibility exists that demand for the final product, Lycra® (spandex), may decrease, but then the excess THF could be sold on the open market. Having this plant produce the raw material for an in-house plant considerably reduces the risk associated with changing demand.
2) **The length of the study period used for the analysis**: For the economic analysis to be accurate, the conditions and prices that are assumed must remain constant throughout the course of the

study period. However, as the time scale increases, this is less likely to be true. Hence, analyses with shorter durations tend to be more accurate. Since the THF plant has a considerably long lifetime, the accuracy of the analysis can be questioned.

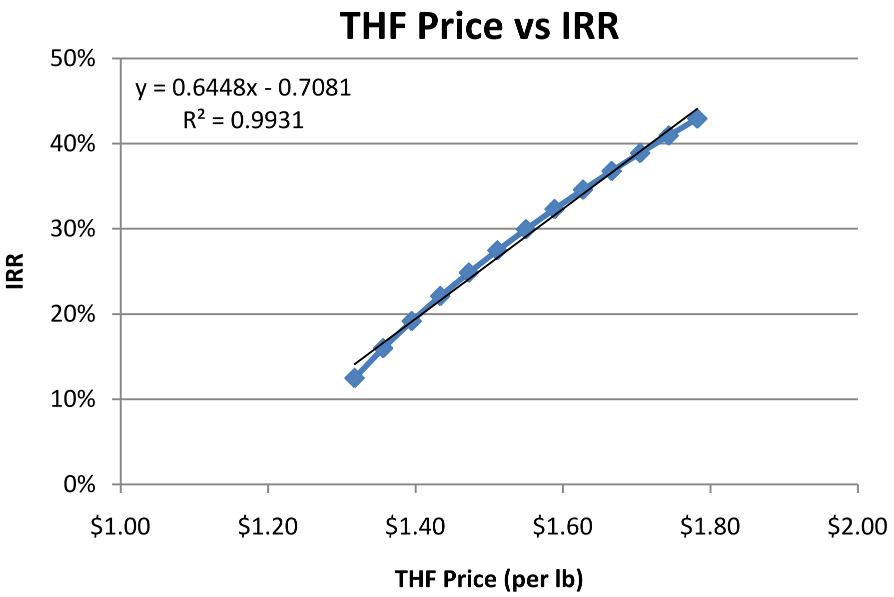
10.2 Probabilistic Analysis of Natural Disasters

Regardless of how well the plant is built or how carefully it is inspected and maintained, there always exists the possibility that the plant could suffer severe damage from natural disasters such as hurricanes or flooding. Hurricanes Katrina and Rita demonstrated the considerable destructive power of Mother Nature, and The American Geophysical Union predicts that the frequency of intense hurricanes and severe rainfall will continue increasing considerably in the next several decades (AGU, 2006). Any project under consideration must assess the possibility of such natural disasters.

Methods of accounting for such natural disasters can range from the simple to the exceedingly complex. An exhaustive probabilistic model was developed by Jagger, Elsner, & Niu (2001) and could be used to conduct a detailed analysis into the probability of hurricane occurances. For less rigourous studies, the writers recommend that the annual probability of moderate hurricanes in the Gulf Coast region is about 15% (Jagger, Elsner, & Niu, 2001). According to this study, a moderate hurricane can be expected about once every seven years. Chemical plants are typically able to withstand the onslaught of moderate hurricanes. Occasionally, a severe hurricane such as Katrina can cause significant damage, and while the probability of a severe hurricane occuring is low, a conservative analysis may want to take it into account.

10.3 Project Sensitivity to THF Prices

One of the two most likely economic variables to change is the market price of THF, and it is therefore necessary to evaluate the impact this change will have on the profitability. The graph below indicates how changes in THF prices will affect the IRR, with all other variables remaining unchanged.

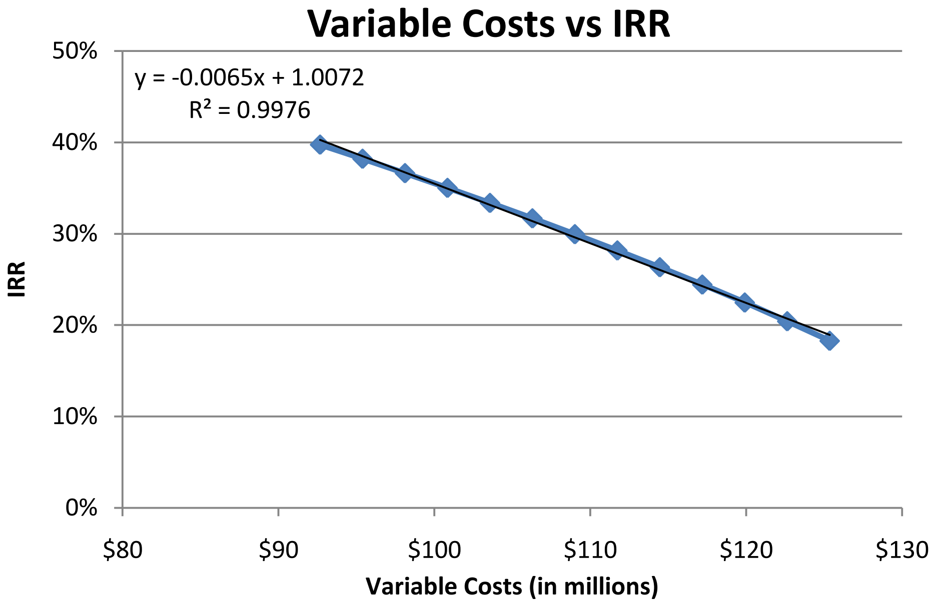


As can be seen by the graph, the IRR and THF price share a strong linear relationship. A change in the price of THF from $1.32 to $1.78 causes the IRR to rise from 12.50% to 42.94%. A 35% increase in the price of THF causes the IRR to nearly quadruple, signifying that small changes in THF prices can cause large variations in the IRR. This can be considered a mixed blessing since a large drop in the price of THF could quickly make this venture unprofitable. However, if the price of THF rises, then the venture will generate substantial returns.

The break-even price of THF is the market price of THF at which the venture has an NPV of zero. At a 15% cost of capital, this price was determined to be $1.20/lb. Currently the price of THF on the market is $1.55/lb and for the venture to be unprofitable, the price would have to fall by 22%, which is unlikely considering the diversified uses of THF.

10.4 Project Sensitivity to Variable Costs

The other most likely factor to change is the variable costs. The variable costs include the price of raw materials and utilities, both of which are susceptible to change in the future. Variable costs are most likely to vary over several years and since they are quite sizeable, they can have a considerable impact on the IRR as the graph below demonstrates.



According to the graph, a 10% increase in the variable costs can decrease the IRR by about 17%, which confirms our expectation that the variable costs are a significant determinant of the IRR. The above analysis referred to variable costs as a whole, but as was mentioned earlier, variable costs have several components. The effects of these factors are evaluated individually in Section 10.6.

10.5 Analysis of Transfer Price

This plant will be supplying THF to another internal downstream plant, and thus the price received for THF will not be the market price of $1.55/lb used in the preceding analysis. Thus, running the analysis using the transfer price of $1.39/lb will demonstrate the economic benefit of having an internal THF production plant. The previous profitability was assessed based on the assumption that in the absence of this THF plant, the downstream plant would be forced to buy THF at the market price.

Given that the plant is deemed profitable using market prices, its construction will clearly boost the profitability of the parent company. The transfer price of THF would then be negotiated between the THF plant and the downstream plant, so that savings may be distributed among the two plants and both would operate at a positive NPV. To compute the total savings of the parent company, this analysis will investigate the transfer price that sets the NPV of the THF plant equal to zero.

To get an NPV of zero the transfer price would have to be $1.335/lb of THF. In this case the ROI would be 19.3% and the IRR would be 15.62%. This analysis shows that the given transfer price is too high since the NPV is not zero. The corresponding values for ROI and IRR are 28.2% and 21.24%. Refer to the following cash flow summary, profitability measures summary, and IRR analysis.

If this plant is built with the specifications set forth in the analysis and with a transfer price of $1.39/lb of THF, then the downstream plant would save $16.0 million per year. If the price of $1.34/lb of THF is used then the savings would be $21.0 million per year.

Cash Flow Summary

April, 2009

THF Production

Year	Percentage of Design Capacity	Sales	Capital Costs	Working Capital	Variable Costs	Fixed Costs	Depreciation Allowance	Depletion Allowance	Taxable Income	Income Tax Costs	Net Earnings	Annual Cash Flow	Cumulative Net Present Value at 15.0%
2009	0.0%	Design	-$20,212,000	-$2,835,600								-$23,047,600	-$23,047,600
2010	0.0%	Construction	-$20,212,000	-$2,835,600								-$23,047,600	-$43,089,000
2011	45.0%	$62,550,000			-$48,309,000	-$9,546,500	-$7,218,600	$0	-$2,524,100	$933,900	-$1,590,200	$5,628,400	-$38,833,100
2012	67.5%	$93,825,000			-$72,463,500	-$9,546,500	-$11,549,800	$0	$265,200	-$98,100	$167,100	$11,716,900	-$31,129,000
2013	90.0%	$125,100,000			-$96,618,000	-$9,546,500	-$6,929,900	$0	$12,005,600	-$4,442,100	$7,563,500	$14,493,400	-$22,842,400
2014	90.0%	$125,100,000			-$96,618,000	-$9,546,500	-$4,157,900	$0	$14,777,600	-$5,467,700	$9,309,900	$13,467,800	-$16,146,500
2015	90.0%	$125,100,000			-$96,618,000	-$9,546,500	-$4,157,900	$0	$14,777,600	-$5,467,700	$9,309,900	$13,467,800	-$10,324,000
2016	90.0%	$125,100,000			-$96,618,000	-$9,546,500	-$2,079,000	$0	$16,856,500	-$6,236,900	$10,619,600	$12,698,600	-$5,550,100
2017	90.0%	$125,100,000			-$96,618,000	-$9,546,500		$0	$18,935,500	-$7,006,100	$11,929,400	$11,929,400	-$1,650,400
2018	90.0%	$125,100,000			-$96,618,000	-$9,546,500		$0	$18,935,500	-$7,006,100	$11,929,400	$11,929,400	$1,740,700
2019	90.0%	$125,100,000			-$96,618,000	-$9,546,500		$0	$18,935,500	-$7,006,100	$11,929,400	$11,929,400	$4,689,500
2020	90.0%	$125,100,000			-$96,618,000	-$9,546,500		$0	$18,935,500	-$7,006,100	$11,929,400	$11,929,400	$7,253,600
2021	90.0%	$125,100,000			-$96,618,000	-$9,546,500		$0	$18,935,500	-$7,006,100	$11,929,400	$11,929,400	$9,483,300
2022	90.0%	$125,100,000			-$96,618,000	-$9,546,500		$0	$18,935,500	-$7,006,100	$11,929,400	$11,929,400	$11,422,200
2023	90.0%	$125,100,000			-$96,618,000	-$9,546,500		$0	$18,935,500	-$7,006,100	$11,929,400	$11,929,400	$13,108,200
2024	90.0%	$125,100,000			-$96,618,000	-$9,546,500		$0	$18,935,500	-$7,006,100	$11,929,400	$11,929,400	$14,574,300
2025	90.0%	$125,100,000		$5,671,200	-$96,618,000	-$9,546,500		$0	$18,935,500	-$7,006,100	$11,929,400	$17,600,600	$16,455,200

Profitability Measures

THF Production

April, 2009

The Investor's Rate of Return (IRR) for this Project is: **21.24%**

The Net Present Value (NPV) at 15% for this Project is: **$16,455,200**

ROI Analysis (Third Production Year)

Annual Sales:	$125,100,000
Annual Costs:	-$106,164,500
Depreciation:	-$2,887,400
Income Tax:	-$5,937,800
Net Earnings:	$12,997,700
Total Capital Investment:	$46,095,200
ROI:	**28.2%**

IRR Analysis - Single Variable

THF Production

April, 2009

Product Prices

Product Prices	$1.18	$1.22	$1.25	$1.29	$1.32	$1.36	$1.39	$1.42	$1.46	$1.49	$1.53	$1.56	$1.60
IRR	-5.64%	1.82%	7.09%	11.34%	15.00%	18.26%	21.24%	24.00%	26.59%	29.03%	31.35%	33.57%	35.70%

Variable Cost

Variable Cost	$91,250,300	$93,934,100	$96,618,000	$99,301,800	$101,985,600	$104,669,500	$107,353,300	$110,037,100	$112,721,000	$115,404,800	$118,088,600	$120,772,500	$123,456,300
IRR	33.92%	32.00%	30.02%	27.97%	25.83%	23.59%	21.24%	18.75%	16.07%	13.17%	9.96%	6.31%	1.95%

Fixed Cost

Fixed Cost	$8,114,600	$8,353,200	$8,591,900	$8,830,600	$9,069,200	$9,307,900	$9,546,500	$9,785,200	$10,023,900	$10,262,500	$10,501,200	$10,739,900	$10,978,500
IRR	22.87%	22.60%	22.33%	22.06%	21.79%	21.52%	21.24%	20.97%	20.69%	20.41%	20.13%	19.85%	19.57%

Initial Investment (TPI)

Inititial Investment	$34,360,400.0	$35,371,000	$36,381,600	$37,392,200	$38,402,800	$39,413,400	$40,424,000	$41,434,600	$42,445,200	$43,455,800	$44,466,400	$45,477,000	$46,487,600
IRR	24.32%	23.76%	23.22%	22.70%	22.19%	21.71%	21.24%	20.79%	20.35%	19.93%	19.52%	19.12%	18.73%

10.6 Variables for Further Sensitivity Analyses

As discussed earlier in the report, the project has considerable uncertainties associated with it that range from financial uncertainties to unpredictable natural disasters. The two major sensitivities have already been discussed: project profitability in response to changes in total variable costs and to THF prices. This section will attempt to list and qualitatively explain some of the other major sources of uncertainties that could arise. Refer to Sections 10.7 to 10.11 for a quantitative analysis of each variable.

Demand for Lycra

Considering that the THF produced in this plant will be used as raw material for the production of Lycra®, a change in the Lycra® demand could significantly affect the viability of this project. Over the past few years the demand for Lycra® has exploded due to its incorporation in a variety of consumer clothes. Furthermore, it seems that consumers may actually prefer a Lycra blend over other types of clothing materials as a recent study unveiled when it discovered that consumers would pay a 20% premium for a wool-Lycra skirt than for a 100% wool skirt (Allan, 2007). Indications from previous years suggest that Lycra demand will continue to grow substantially. However, the current global recession could hinder such growth, since consumer spending has been hit particularly hard as people refrain from buying goods to conserve capital.

A significant reduction in the demand for Lycra could result in a reduction in the downstream Lycra® plant production, which in turn would decrease the demand for THF. There are two possible avenues that could be taken from this point onwards; one is to reduce the production of THF to meet the requirements of the Lycra® plant, and the other is to keep production the same and to sell the excess on the open market. Both of these options would significantly affect the profitability of our venture.

In the case of reducing production, the plant would have excess capacity and would be forgoing profits from the sale of THF. However, the sale of the excess THF could also reduce profitability since sale to outside customers would require additional transportation costs. Furthermore, the current tanks can only hold 4 days worth of THF product and it is likely that the company would need to construct larger tanks to store the excess THF while management finds new buyers and arranges transportation. In addition, the THF may need to be sold at a discount to market prices to entice prospective buyers away from their current suppliers.

Raw Materials

The two raw materials that will be used for the THF production are pipeline hydrogen and internally-manufactured maleic acid. The maleic acid is sold to the THF production plant at a transfer price that is lower than current market prices. However, the maleic acid plant is subject to the same weather and maintenance delays as the THF plant, and a disruption in its activities would force the downstream plant to buy maleic acid at a higher price, reducing its profitability. The supply of hydrogen could be affected by disruptions in the pipeline, or its price could change as a result of demand and supply forces.

Utility Requirements

Utilities are a significant component of the variable cost, totaling over $5 million. The wide range of utilities used (waste water treatment, electricity, boiler feed water, and pressurized steam) increases the facility’s vulnerability to price changes. Low pressure steam, waste water treatment, and electricity are currently the three largest utility costs, each costing over $1 million per year. Changes in the price of such utilities can have a significant impact on the ROI.

Labor Costs

Employee wages and benefits, along with contracted help and technical assistance occupy a considerable portion of the variable costs as well, and it is worthwhile to gauge the impact of changes in these variables. According to the US Bureau of Labor Statistics, over the past three years the nominal wage rate has increased by about 8%, but the real wage rate (having adjusted for inflation) has remained relatively constant (Bureau of Labor Statistics, 2009). In light of the current economic downturn and the relative abundance of labor, wage rates are not expected to make a significant increase in the near future. In addition, the proposed THF production facility is a continuous process with minimal transportation and storage work, and is thus not a very labor-intensive plant.

Inflation

National inflation rates are relevant for the comparable financial attractiveness of the THF product and consequently their effect should be determined. In the latter half of 2008, inflation was constantly low or negative. Although it has been 0.3% and 0.4% respectively in the first two months of 2009, (Bureau of Labor Statistics, 2009) it is not expected to rise considerably after the recession.

Natural Disasters

History has demonstrated that the Gulf Coast is particularly susceptible to hurricanes and natural disasters. As a result, although all of the process machinery and vessels are capable of withstanding high winds, many days of shutdown at other plants have historically resulted due to natural disasters. This may not be due solely due to damage to the plant, but could also be the result of damaged roads or flooding that prevents employees from reaching the plant.

10.7 Analysis of Lycra Demand

It was stated in Section 10.6 that a drop in the Lycra® demand could either force the plant to reduce the production of THF or to try selling it on the open market. The case of the reduced production of THF will be analyzed first. The following analysis assumes that the current global economic downturn reduces the THF required by the Lycra plant by 10%. In such a situation, the ROI decreases from 45.9% to 40.8% and the IRR decreases from 32.7% to 29.7%, which are not considerable drops. It would be very improbable that the demand for Lycra would fall by more than 10% due to its somewhat inelastic demand in undergarment products, so this case demonstrates a worst case scenario in this regard. The profitability is helped by the reduction in variable costs (due to the production of less product).

Variable Cost Summary

THF Production

April, 2009

		Per lb THF		TOTAL
Raw Materials				
	Hydrogen	$0.13 per lb of THF	$11,569,500	
	Maleic Acid	$0.81 per lb of THF	$72,503,400	
	Total Raw Materials:	**$0.93 per lb of THF**	**$84,072,900**	**$84,072,900**
Utilties				
	High Pressure Steam	$0.00 per lb of THF	$338,100	
	Low Pressure Steam	$0.01 per lb of THF	$562,500	
	Cooling Water	$0.00 per lb of THF	$153,800	
	Natural Gas	$0.00 per lb of THF	$96,200	
	Electricity	$0.01 per lb of THF	$1,231,500	
	Boiler Feed Water (BFW)	$0.00 per lb of THF	$73,700	
	Refrigeration (-30F)	$0.00 per lb of THF	$209,400	
	Waste Water Treatment	$0.01 per lb of THF	$1,317,900	
	Catalyst Regeneration	$0.00 per lb of THF	$117,800	
	Total Raw Materials:	**$0.05 per lb of THF**	**$4,100,800**	**$88,173,700**
General Expenses				
	Selling / Transfer:	$0.02 per lb of THF	$1,395,000	
	Direct Research:	$0.02 per lb of THF	$2,092,500	
	Allocated Research:	$0.02 per lb of THF	$1,395,000	
	Administrative Expense:	$0.03 per lb of THF	$2,790,000	
	Management Incentives:	$0.02 per lb of THF	$1,743,800	
	Total Byproducts:	**$0.10 per lb of THF**	**$9,416,300**	**$97,590,000**
TOTAL		**$1.08 per lb of THF**	**$97,590,000**	**$97,590,000**

Profitability Measures

THF Production

April, 2009

The Investor's Rate of Return (IRR) for this Project is: **29.66%**

The Net Present Value (NPV) at 15% for this Project is: **$42,870,700**

ROI Analysis (Third Production Year)

Annual Sales:	$125,550,000
Annual Costs:	-$97,377,500
Depreciation:	-$2,887,400
Income Tax:	-$9,355,500
Net Earnings:	$18,817,000
Total Capital Investment:	$46,115,600
ROI:	**40.8%**

Cash Flow Summary

April, 2009

THF Production

Year	Percentage of Design Capacity	Sales	Capital Costs	Working Capital	Variable Costs	Fixed Costs	Depreciation Allowance	Depletion Allowance	Taxable Income	Income Tax Costs	Net Earnings	Annual Cash Flow	Cumulative Net Present Value at 15.0%
2009	0.0%	Design	-$20,212,000	-$2,845,800								-$23,057,800	-$23,057,800
2010	0.0%	Construction	-$20,212,000	-$2,845,800								-$23,057,800	-$43,108,100
2011	45.0%	$62,775,000			-$43,915,500	-$9,546,500	-$7,218,600	$0	$2,094,400	-$774,900	$1,319,500	$8,538,100	-$36,652,100
2012	67.5%	$94,162,500			-$65,873,300	-$9,546,500	-$11,549,800	$0	$7,192,900	-$2,661,400	$4,531,500	$16,081,300	-$26,078,400
2013	90.0%	$125,550,000			-$87,831,000	-$9,546,500	-$6,929,900	$0	$21,242,600	-$7,859,800	$13,382,800	$20,312,700	-$14,464,500
2014	90.0%	$125,550,000			-$87,831,000	-$9,546,500	-$4,157,900	$0	$24,014,600	-$8,885,400	$15,129,200	$19,287,100	-$4,875,400
2015	90.0%	$125,550,000			-$87,831,000	-$9,546,500	-$4,157,900	$0	$24,014,600	-$8,885,400	$15,129,200	$19,287,100	$3,462,900
2016	90.0%	$125,550,000			-$87,831,000	-$9,546,500	-$2,079,000	$0	$26,093,500	-$9,654,600	$16,438,900	$18,517,900	$10,424,500
2017	90.0%	$125,550,000			-$87,831,000	-$9,546,500		$0	$28,172,500	-$10,423,800	$17,748,700	$17,748,700	$16,226,600
2018	90.0%	$125,550,000			-$87,831,000	-$9,546,500		$0	$28,172,500	-$10,423,800	$17,748,700	$17,748,700	$21,271,900
2019	90.0%	$125,550,000			-$87,831,000	-$9,546,500		$0	$28,172,500	-$10,423,800	$17,748,700	$17,748,700	$25,659,100
2020	90.0%	$125,550,000			-$87,831,000	-$9,546,500		$0	$28,172,500	-$10,423,800	$17,748,700	$17,748,700	$29,474,100
2021	90.0%	$125,550,000			-$87,831,000	-$9,546,500		$0	$28,172,500	-$10,423,800	$17,748,700	$17,748,700	$32,791,500
2022	90.0%	$125,550,000			-$87,831,000	-$9,546,500		$0	$28,172,500	-$10,423,800	$17,748,700	$17,748,700	$35,676,200
2023	90.0%	$125,550,000			-$87,831,000	-$9,546,500		$0	$28,172,500	-$10,423,800	$17,748,700	$17,748,700	$38,184,600
2024	90.0%	$125,550,000			-$87,831,000	-$9,546,500		$0	$28,172,500	-$10,423,800	$17,748,700	$17,748,700	$40,365,800
2025	90.0%	$125,550,000		$5,691,600	-$87,831,000	-$9,546,500		$0	$28,172,500	-$10,423,800	$17,748,700	$23,440,300	$42,870,700

The alternative solution would be to sell the excess THF on the open market. However, this may require it to be sold at a slight discount to market prices in order to quickly attract buyers, which is not included in the analysis. It would also raise transportation and selling costs from 1% of sales to 3% of sales and would require the construction of more storage tanks to hold the excess THF product (10 days worth).

Running the analysis with additional storage tanks and increased selling costs lowered the ROI to 36.4% and the IRR to 27.01, which is a sharper decrease than was achieved with the previous analysis. Furthermore, the cumulative NPV is also significantly lower than that over the base case provided in Section 9. If there was a decrease in the demand of THF from the downstream plant, then this plant would be better served by cutting its production than by trying to sell THF on the open market.

Variable Cost Summary

April, 2009

THF Production

	Per lb THF		TOTAL
Raw Materials			
Hydrogen	$0.13 per lb of THF	$12,855,000	
Maleic Acid	$0.81 per lb of THF	$80,559,400	
Total Raw Materials:	**$0.93 per lb of THF**	**$93,414,400**	**$93,414,400**
Utilties			
High Pressure Steam	$0.00 per lb of THF	$375,600	
Low Pressure Steam	$0.01 per lb of THF	$624,900	
Cooling Water	$0.00 per lb of THF	$170,900	
Natural Gas	$0.00 per lb of THF	$106,900	
Electricity	$0.01 per lb of THF	$1,368,400	
Boiler Feed Water (BFW)	$0.00 per lb of THF	$81,900	
Refrigeration (-30F)	$0.00 per lb of THF	$232,600	
Waste Water Treatment	$0.01 per lb of THF	$1,464,400	
Catalyst Regeneration	$0.00 per lb of THF	$130,900	
Total Raw Materials:	**$0.05 per lb of THF**	**$4,556,500**	**$97,970,900**
General Expenses			
Selling / Transfer:	$0.05 per lb of THF	$4,650,000	
Direct Research:	$0.02 per lb of THF	$2,325,000	
Allocated Research:	$0.02 per lb of THF	$1,550,000	
Administrative Expense:	$0.03 per lb of THF	$3,100,000	
Management Incentives:	$0.02 per lb of THF	$1,937,500	
Total Byproducts:	**$0.14 per lb of THF**	**$13,562,500**	**$111,533,400**
TOTAL	**$1.12 per lb of THF**	**$111,533,300**	**$111,533,300**

Profitability Measures

April, 2009

THF Production

The Investor's Rate of Return (IRR) for this Project is: **27.01%**

The Net Present Value (NPV) at 15% for this Project is: **$39,127,400**

ROI Analysis (Third Production Year)

Annual Sales:	$139,500,000
Annual Costs:	-$110,707,600
Depreciation:	-$3,345,800
Income Tax:	-$9,415,200
Net Earnings:	$19,377,200
Total Capital Investment:	$53,165,000
ROI:	**36.4%**

Cash Flow Summary

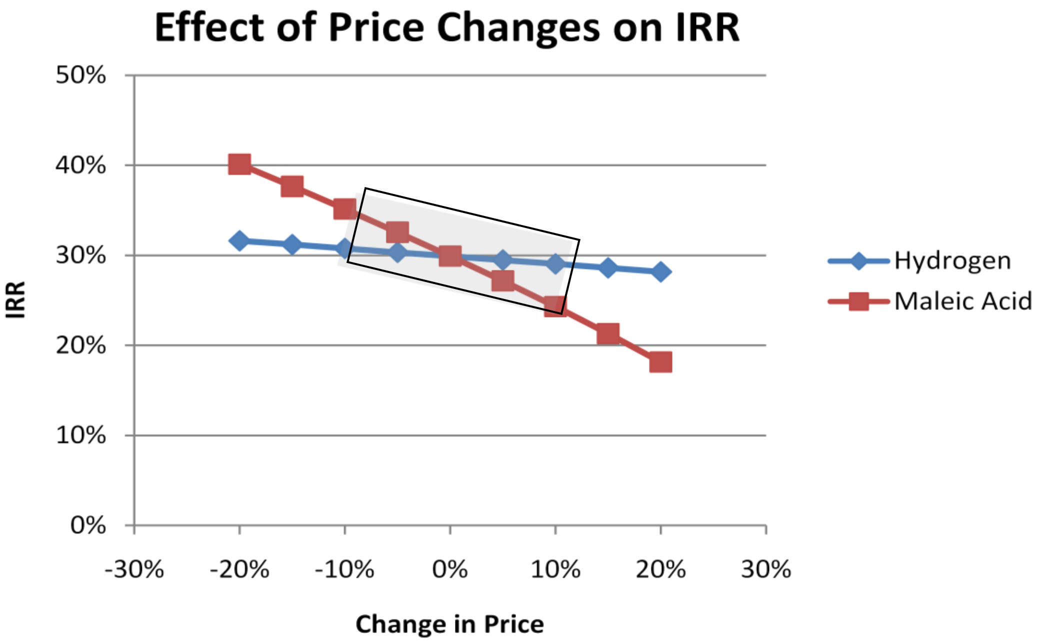
April, 2009

THF Production

Year	Percentage of Design Capacity	Sales	Capital Costs	Working Capital	Variable Costs	Fixed Costs	Depreciation Allowance	Depletion Allowance	Taxable Income	Income Tax Costs	Net Earnings	Annual Cash Flow	Cumulative Net Present Value at 15.0%
2009	0.0%	Design	-$23,420,500	-$3,162,000								-$26,582,500	-$26,582,500
2010	0.0%	Construction	-$23,420,500	-$3,162,000								-$26,582,500	-$49,697,700
2011	45.0%	$69,750,000			-$50,190,000	-$10,327,600	-$8,364,400	$0	$868,000	-$321,200	$546,800	$8,911,200	-$42,959,600
2012	67.5%	$104,625,000			-$75,285,000	-$10,327,600	-$13,383,000	$0	$5,629,400	-$2,082,900	$3,546,500	$16,929,500	-$31,828,200
2013	90.0%	$139,500,000			-$100,380,000	-$10,327,600	-$8,029,800	$0	$20,762,600	-$7,682,200	$13,080,400	$21,110,200	-$19,758,400
2014	90.0%	$139,500,000			-$100,380,000	-$10,327,600	-$4,817,900	$0	$23,974,500	-$8,870,600	$15,103,900	$19,921,800	-$9,853,700
2015	90.0%	$139,500,000			-$100,380,000	-$10,327,600	-$4,817,900	$0	$23,974,500	-$8,870,600	$15,103,900	$19,921,800	-$1,241,000
2016	90.0%	$139,500,000			-$100,380,000	-$10,327,600	-$2,408,900	$0	$26,383,500	-$9,761,900	$16,621,600	$19,030,500	$5,913,300
2017	90.0%	$139,500,000			-$100,380,000	-$10,327,600		$0	$28,792,400	-$10,653,200	$18,139,200	$18,139,200	$11,843,000
2018	90.0%	$139,500,000			-$100,380,000	-$10,327,600		$0	$28,792,400	-$10,653,200	$18,139,200	$18,139,200	$16,999,300
2019	90.0%	$139,500,000			-$100,380,000	-$10,327,600		$0	$28,792,400	-$10,653,200	$18,139,200	$18,139,200	$21,483,000
2020	90.0%	$139,500,000			-$100,380,000	-$10,327,600		$0	$28,792,400	-$10,653,200	$18,139,200	$18,139,200	$25,381,900
2021	90.0%	$139,500,000			-$100,380,000	-$10,327,600		$0	$28,792,400	-$10,653,200	$18,139,200	$18,139,200	$28,772,200
2022	90.0%	$139,500,000			-$100,380,000	-$10,327,600		$0	$28,792,400	-$10,653,200	$18,139,200	$18,139,200	$31,720,300
2023	90.0%	$139,500,000			-$100,380,000	-$10,327,600		$0	$28,792,400	-$10,653,200	$18,139,200	$18,139,200	$34,283,900
2024	90.0%	$139,500,000			-$100,380,000	-$10,327,600		$0	$28,792,400	-$10,653,200	$18,139,200	$18,139,200	$36,513,100
2025	90.0%	$139,500,000		$6,324,000	-$100,380,000	-$10,327,600		$0	$28,792,400	-$10,653,200	$18,139,200	$24,463,200	$39,127,400

10.8 Analysis of Raw Materials

Hydrogen and maleic acid are the only raw materials to the plant, and the impact of their price changes on the feasibility of the project must be evaluated. The prices of maleic acid and hydrogen were varied in 5% intervals and the effect on the IRR was noted to produce the graph below.



The results demonstrate that even large changes in the price of hydrogen have a small effect on the IRR. However, the impact of maleic acid price changes is far more significant. A 5% increase in the price of maleic acid decreases the IRR by 5%. This substantiates the function of the upstream maleic acid plant, which provides it at a transfer price of $0.45/lb on an anhydrous basis instead of the market price of $0.60/lb (ICIS, 2009). The availability of maleic acid at such a discount provides a substantial boost to the IRR. However, as seen in the graph above, changes in the price of raw materials or other costs of maleic acid production could change its transfer price, which would directly have an effect on this project's IRR. Since the maleic acid is being produced by an internal plant, its price is not expected to fluctuate widely, and the most likely range of variations that is for maleic acid and hydrogen prices is depicted by the boxed area in the graph (-10% to 10%).

However, there is the possibility that due to unforeseen circumstances such as industrial accidents, production at the maleic acid plant could be disrupted. In such a situation, the THF plant would be forced to buy maleic acid at the market price. Thus, it is also useful to conduct this analysis with the market prices of maleic acid to determine the benefit of having an upstream plant. For the proceeding analysis, the market price of maleic acid of $0.60/lb was used.

Immediately noticeable is the sharp increase in the variable costs to $134.4 million, which is due to the increased maleic acid price. The ROI plummets from 45.9% to 14.4% and the IRR drops from 32.7% to 9.4%. Such a drastic decrease in profitability underscores the importance of having the internal upstream maleic acid plant.

In addition, production using maleic acid purchased on the open market would be unfavorable, as shown by a negative NPV. Nonetheless, other plants that do not have an internal source of maleic acid still manage to return profits. This could potentially be the result of various competitive advantages they have in terms of reactor design, chemical conversion, plant design, research and development, and heat integration. Due to the scope and nature of this project, alternative designs were not modeled, but the design team suggests further research into these areas in the future.

Variable Cost Summary

April, 2009

THF Production

		Per lb THF		TOTAL
Raw Materials				
	Hydrogen	$0.13 per lb of THF	$12,855,000	
	Maleic Acid	$1.07 per lb of THF	$106,560,000	
	Total Raw Materials:	**$1.19 per lb of THF**	**$119,415,000**	**$119,415,000**
Utilties				
	High Pressure Steam	$0.00 per lb of THF	$375,600	
	Low Pressure Steam	$0.01 per lb of THF	$624,900	
	Cooling Water	$0.00 per lb of THF	$170,900	
	Natural Gas	$0.00 per lb of THF	$106,900	
	Electricity	$0.01 per lb of THF	$1,368,400	
	Boiler Feed Water (BFW)	$0.00 per lb of THF	$81,900	
	Refrigeration (-30F)	$0.00 per lb of THF	$232,600	
	Waste Water Treatment	$0.01 per lb of THF	$1,464,400	
	Catalyst Regeneration	$0.00 per lb of THF	$130,900	
	Total Raw Materials:	**$0.05 per lb of THF**	**$4,556,500**	**$123,971,500**
General Expenses				
	Selling / Transfer:	$0.02 per lb of THF	$1,550,000	
	Direct Research:	$0.02 per lb of THF	$2,325,000	
	Allocated Research:	$0.02 per lb of THF	$1,550,000	
	Administrative Expense:	$0.03 per lb of THF	$3,100,000	
	Management Incentives:	$0.02 per lb of THF	$1,937,500	
	Total Byproducts:	**$0.10 per lb of THF**	**$10,462,500**	**$134,434,000**
TOTAL		**$1.34 per lb of THF**	**$134,434,000**	**$134,434,000**

Profitability Measures

April, 2009

THF Production

The Investor's Rate of Return (IRR) for this Project is: **9.36%**

The Net Present Value (NPV) at 15% for this Project is: **-$12,623,200**

ROI Analysis (Third Production Year)

Annual Sales:	$139,500,000
Annual Costs:	-$130,537,100
Depreciation:	-$2,887,400
Income Tax:	-$2,247,900
Net Earnings:	$6,715,000
Total Capital Investment:	$46,748,000
ROI:	**14.4%**

Cash Flow Summary

April, 2009

THF Production

Year	Percentage of Design Capacity	Sales	Capital Costs	Working Capital	Variable Costs	Fixed Costs	Depreciation Allowance	Depletion Allowance	Taxable Income	Income Tax Costs	Net Earnings	Annual Cash Flow	Cumulative Net Present Value at 15.0%
2009	0.0%	Design	-$20,212,000	-$3,162,000								-$23,374,000	-$23,374,000
2010	0.0%	Construction	-$20,212,000	-$3,162,000								-$23,374,000	-$43,699,200
2011	45.0%	$69,750,000			-$60,495,300	-$9,546,500	-$7,218,600	$0	-$7,510,400	$2,778,800	-$4,731,600	$2,487,000	-$41,818,700
2012	67.5%	$104,625,000			-$90,743,000	-$9,546,500	-$11,549,800	$0	-$7,214,300	$2,669,300	-$4,545,000	$7,004,800	-$37,212,900
2013	90.0%	$139,500,000			-$120,990,600	-$9,546,500	-$6,929,900	$0	$2,033,000	-$752,200	$1,280,800	$8,210,700	-$32,518,400
2014	90.0%	$139,500,000			-$120,990,600	-$9,546,500	-$4,157,900	$0	$4,805,000	-$1,777,900	$3,027,100	$7,185,000	-$28,946,200
2015	90.0%	$139,500,000			-$120,990,600	-$9,546,500	-$4,157,900	$0	$4,805,000	-$1,777,900	$3,027,100	$7,185,000	-$25,839,900
2016	90.0%	$139,500,000			-$120,990,600	-$9,546,500	-$2,079,000	$0	$6,883,900	-$2,547,000	$4,336,900	$6,415,900	-$23,427,900
2017	90.0%	$139,500,000			-$120,990,600	-$9,546,500		$0	$8,962,900	-$3,316,300	$5,646,600	$5,646,600	-$21,582,000
2018	90.0%	$139,500,000			-$120,990,600	-$9,546,500		$0	$8,962,900	-$3,316,300	$5,646,600	$5,646,600	-$19,976,900
2019	90.0%	$139,500,000			-$120,990,600	-$9,546,500		$0	$8,962,900	-$3,316,300	$5,646,600	$5,646,600	-$18,581,100
2020	90.0%	$139,500,000			-$120,990,600	-$9,546,500		$0	$8,962,900	-$3,316,300	$5,646,600	$5,646,600	-$17,367,400
2021	90.0%	$139,500,000			-$120,990,600	-$9,546,500		$0	$8,962,900	-$3,316,300	$5,646,600	$5,646,600	-$16,312,000
2022	90.0%	$139,500,000			-$120,990,600	-$9,546,500		$0	$8,962,900	-$3,316,300	$5,646,600	$5,646,600	-$15,394,300
2023	90.0%	$139,500,000			-$120,990,600	-$9,546,500		$0	$8,962,900	-$3,316,300	$5,646,600	$5,646,600	-$14,596,300
2024	90.0%	$139,500,000			-$120,990,600	-$9,546,500		$0	$8,962,900	-$3,316,300	$5,646,600	$5,646,600	-$13,902,400
2025	90.0%	$139,500,000		$6,324,000	-$120,990,600	-$9,546,500		$0	$8,962,900	-$3,316,300	$5,646,600	$11,970,600	-$12,623,200

10.9 Analysis of Utilities

All of the combined utilities constitute about $5 million of the $108.9 million of the annual variable costs. However, changes in their prices could have a substantial impact on our profitability, as determined by the analysis carried out below.

Given the widespread availability of cooling water, boiler feed water, pressurized steam, and electricity in the Gulf Coast, a 10% increase in the price of utilities is taken as the upper bound for utility price changes. This change had a negligible impact on the ROI, lowering it from 45.9% to 45.4%. The IRR also exhibited a minute change, dropping from 32.7% to 32.4%. Consequently, the profitability of this production facility is not a strong function of utility usage.

Variable Cost Summary

THF Production

April, 2009

		Per lb THF		TOTAL
Raw Materials				
	Hydrogen	$0.13 per lb of THF	$12,855,000	
	Maleic Acid	$0.81 per lb of THF	$80,559,400	
	Total Raw Materials:	**$0.93 per lb of THF**	**$93,414,400**	**$93,414,400**
Utilties				
	High Pressure Steam	$0.00 per lb of THF	$412,700	
	Low Pressure Steam	$0.01 per lb of THF	$687,400	
	Cooling Water	$0.00 per lb of THF	$188,000	
	Natural Gas	$0.00 per lb of THF	$117,600	
	Electricity	$0.02 per lb of THF	$1,505,200	
	Boiler Feed Water (BFW)	$0.00 per lb of THF	$90,100	
	Refrigeration (-30F)	$0.00 per lb of THF	$255,900	
	Waste Water Treatment	$0.02 per lb of THF	$1,610,800	
	Catalyst Regeneration	$0.00 per lb of THF	$130,900	
	Total Raw Materials:	**$0.05 per lb of THF**	**$4,998,600**	**$98,413,000**
General Expenses				
	Selling / Transfer:	$0.02 per lb of THF	$1,550,000	
	Direct Research:	$0.02 per lb of THF	$2,325,000	
	Allocated Research:	$0.02 per lb of THF	$1,550,000	
	Administrative Expense:	$0.03 per lb of THF	$3,100,000	
	Management Incentives:	$0.02 per lb of THF	$1,937,500	
	Total Byproducts:	**$0.10 per lb of THF**	**$10,462,500**	**$108,875,500**
TOTAL		**$1.09 per lb of THF**	**$108,875,400**	**$108,875,400**

Profitability Measures

THF Production

April, 2009

The Investor's Rate of Return (IRR) for this Project is: **32.39%**

The Net Present Value (NPV) at 15% for this Project is: **$53,201,500**

ROI Analysis (Third Production Year)

Annual Sales:	$139,500,000
Annual Costs:	-$107,534,400
Depreciation:	-$2,887,400
Income Tax:	-$10,758,900
Net Earnings:	$21,206,700
Total Capital Investment:	$46,748,000
ROI:	**45.4%**

Cash Flow Summary

April, 2009

THF Production

Year	Percentage of Design Capacity	Sales	Capital Costs	Working Capital	Variable Costs	Fixed Costs	Depreciation Allowance	Depletion Allowance	Taxable Income	Income Tax Costs	Net Earnings	Annual Cash Flow	Cumulative Net Present Value at 15.0%
2009	0.0%	Design	-$20,212,000	-$3,162,000								-$23,374,000	-$23,374,000
2010	0.0%	Construction	-$20,212,000	-$3,162,000								-$23,374,000	-$43,699,200
2011	45.0%	$69,750,000			-$48,993,900	-$9,546,500	-$7,218,600	$0	$3,991,000	-$1,476,700	$2,514,300	$9,732,900	-$36,339,700
2012	67.5%	$104,625,000			-$73,490,900	-$9,546,500	-$11,549,800	$0	$10,037,800	-$3,714,000	$6,323,800	$17,873,600	-$24,587,500
2013	90.0%	$139,500,000			-$97,987,900	-$9,546,500	-$6,929,900	$0	$25,035,700	-$9,263,200	$15,772,500	$22,702,400	-$11,607,300
2014	90.0%	$139,500,000			-$97,987,900	-$9,546,500	-$4,157,900	$0	$27,807,700	-$10,288,800	$17,518,900	$21,676,800	-$830,100
2015	90.0%	$139,500,000			-$97,987,900	-$9,546,500	-$4,157,900	$0	$27,807,700	-$10,288,800	$17,518,900	$21,676,800	$8,541,400
2016	90.0%	$139,500,000			-$97,987,900	-$9,546,500	-$2,079,000	$0	$29,886,600	-$11,058,000	$18,828,600	$20,907,600	$16,401,300
2017	90.0%	$139,500,000			-$97,987,900	-$9,546,500		$0	$31,965,600	-$11,827,300	$20,138,300	$20,138,300	$22,984,500
2018	90.0%	$139,500,000			-$97,987,900	-$9,546,500		$0	$31,965,600	-$11,827,300	$20,138,300	$20,138,300	$28,709,100
2019	90.0%	$139,500,000			-$97,987,900	-$9,546,500		$0	$31,965,600	-$11,827,300	$20,138,300	$20,138,300	$33,687,000
2020	90.0%	$139,500,000			-$97,987,900	-$9,546,500		$0	$31,965,600	-$11,827,300	$20,138,300	$20,138,300	$38,015,600
2021	90.0%	$139,500,000			-$97,987,900	-$9,546,500		$0	$31,965,600	-$11,827,300	$20,138,300	$20,138,300	$41,779,600
2022	90.0%	$139,500,000			-$97,987,900	-$9,546,500		$0	$31,965,600	-$11,827,300	$20,138,300	$20,138,300	$45,052,600
2023	90.0%	$139,500,000			-$97,987,900	-$9,546,500		$0	$31,965,600	-$11,827,300	$20,138,300	$20,138,300	$47,898,700
2024	90.0%	$139,500,000			-$97,987,900	-$9,546,500		$0	$31,965,600	-$11,827,300	$20,138,300	$20,138,300	$50,373,600
2025	90.0%	$139,500,000		$6,324,000	-$97,987,900	-$9,546,500		$0	$31,965,600	-$11,827,300	$20,138,300	$26,462,300	$53,201,500

April, 2009

IRR Analysis - Single Variable

THF Production

Product Prices

Product Prices	$1.32	$1.36	$1.40	$1.43	$1.47	$1.51	$1.55	$1.59	$1.63	$1.67	$1.71	$1.74	$1.78
IRR	14.22%	17.92%	21.25%	24.32%	27.17%	29.85%	32.39%	34.81%	37.12%	39.35%	41.49%	43.55%	45.56%

Variable Cost

Variable Cost	$92,544,100	$95,266,000	$97,987,900	$100,709,700	$103,431,600	$106,153,500	$108,875,400	$111,597,300	$114,319,200	$117,041,100	$119,762,900	$122,484,800	$125,206,700
IRR	43.07%	41.40%	39.69%	37.94%	36.14%	34.29%	32.39%	30.42%	28.39%	26.27%	24.06%	21.73%	19.27%

Fixed Cost

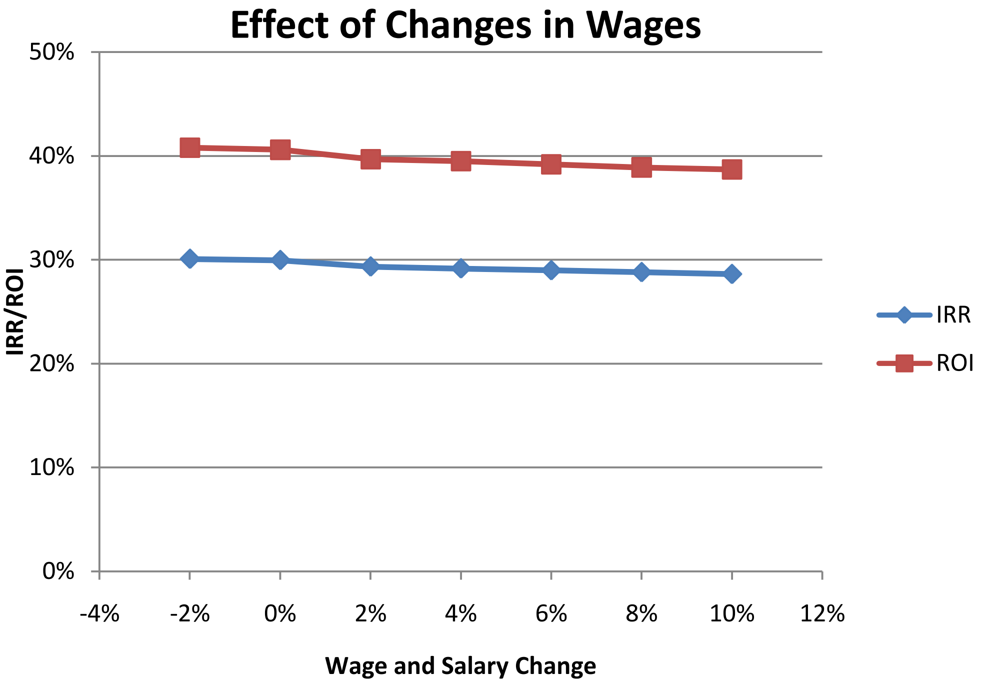
Fixed Cost	$8,114,600	$8,353,200	$8,591,900	$8,830,600	$9,069,200	$9,307,900	$9,546,500	$9,785,200	$10,023,900	$10,262,500	$10,501,200	$10,739,900	$10,978,500
IRR	33.75%	33.52%	33.30%	33.07%	32.84%	32.62%	32.39%	32.16%	31.93%	31.71%	31.48%	31.25%	31.02%

Initial Investment (TPI)

Initital Investment	$34,360,400.0	$35,371,000	$36,381,600	$37,392,200	$38,402,800	$39,413,400	$40,424,000	$41,434,600	$42,445,200	$43,455,800	$44,466,400	$45,477,000	$46,487,600
IRR	36.29%	35.58%	34.90%	34.24%	33.60%	32.98%	32.39%	31.82%	31.26%	30.72%	30.20%	29.70%	29.21%

10.10 Analysis of Labor Costs

As was mentioned in Section 10.6, labor costs are not expected to jump significantly in the current economic climate. However, for the sake of completeness, its effects on ROI and IRR were analyzed. As is shown in the graph below, labor costs have a very negligible impact on profitability. Even a 10% increase in all labor costs would only serve to decrease the IRR by about 1.3%.



10.11 Analysis of Inflation

The design team conducted an analysis to account for inflationary and deflationary effects using an inflation range of -0.45% to 2.30%. This created IRR values between 32.1% and 35.6%. In accordance with historical trends over the past 2 years and data from the US Bureau for Labor Statistics, it is estimated that the average inflation rate over the next decade is likely to be around 2.0% per year. The analysis below was conducted with inflation set at 2.0%, which resulted in an IRR of 35.2% and a ROI of 49.5%. This increase in profitability is observed because the plant was already profitable in the base case (no inflation), and an increase in both costs and revenues magnified its profitability.

Variable Cost Summary

April, 2009

THF Production

		Per lb THF		TOTAL
Raw Materials				
	Hydrogen	$0.13 per lb of THF	$12,855,000	
	Maleic Acid	$0.81 per lb of THF	$80,559,400	
	Total Raw Materials:	**$0.93 per lb of THF**	**$93,414,400**	**$93,414,400**
Utilties				
	High Pressure Steam	$0.00 per lb of THF	$375,600	
	Low Pressure Steam	$0.01 per lb of THF	$624,900	
	Cooling Water	$0.00 per lb of THF	$170,900	
	Natural Gas	$0.00 per lb of THF	$106,900	
	Electricity	$0.01 per lb of THF	$1,368,400	
	Boiler Feed Water (BFW)	$0.00 per lb of THF	$81,900	
	Refrigeration (-30F)	$0.00 per lb of THF	$232,600	
	Waste Water Treatment	$0.01 per lb of THF	$1,464,400	
	Catalyst Regeneration	$0.00 per lb of THF	$130,900	
	Total Raw Materials:	**$0.05 per lb of THF**	**$4,556,500**	**$97,970,900**
General Expenses				
	Selling / Transfer:	$0.02 per lb of THF	$1,550,000	
	Direct Research:	$0.02 per lb of THF	$2,325,000	
	Allocated Research:	$0.02 per lb of THF	$1,550,000	
	Administrative Expense:	$0.03 per lb of THF	$3,100,000	
	Management Incentives:	$0.02 per lb of THF	$1,937,500	
	Total Byproducts:	**$0.10 per lb of THF**	**$10,462,500**	**$108,433,400**
TOTAL		**$1.08 per lb of THF**	**$108,433,300**	**$108,433,300**

Profitability Measures

April, 2009

THF Production

The Investor's Rate of Return (IRR) for this Project is: **35.18%**

The Net Present Value (NPV) at 15% for this Project is: **$68,322,600**

ROI Analysis (Third Production Year)

Annual Sales:	$150,999,300
Annual Costs:	-$115,968,000
Depreciation:	-$2,887,400
Income Tax:	-$11,893,200
Net Earnings:	$23,138,100
Total Capital Investment:	$46,748,000
ROI:	**49.5%**

Cash Flow Summary

April, 2009

THF Production

Year	Percentage of Design Capacity	Sales	Capital Costs	Working Capital	Variable Costs	Fixed Costs	Depreciation Allowance	Depletion Allowance	Taxable Income	Income Tax Costs	Net Earnings	Annual Cash Flow	Cumulative Net Present Value at 15.0%
2009	0.0%	Design	-$20,212,000	-$3,162,000								-$23,374,000	-$23,374,000
2010	0.0%	Construction	-$20,616,200	-$3,162,000								-$23,778,200	-$44,050,700
2011	45.0%	$72,567,900			-$50,766,300	-$9,932,200	-$7,218,600	$0	$4,650,800	-$1,720,800	$2,930,000	$10,148,600	-$36,376,900
2012	67.5%	$111,028,900			-$77,672,400	-$10,130,900	-$11,549,800	$0	$11,675,800	-$4,320,000	$7,355,800	$18,905,600	-$23,946,200
2013	90.0%	$150,999,300			-$105,634,500	-$10,333,500	-$6,929,900	$0	$28,101,400	-$10,397,500	$17,703,900	$24,633,800	-$9,861,700
2014	90.0%	$154,019,300			-$107,747,200	-$10,540,200	-$4,157,900	$0	$31,574,000	-$11,682,400	$19,891,600	$24,049,500	$2,095,200
2015	90.0%	$157,099,700			-$109,902,200	-$10,751,000	-$4,157,900	$0	$32,288,600	-$11,946,800	$20,341,800	$24,499,700	$12,687,100
2016	90.0%	$160,241,700			-$112,100,200	-$10,966,000	-$2,079,000	$0	$35,096,500	-$12,985,700	$22,110,800	$24,189,800	$21,780,900
2017	90.0%	$163,446,500			-$114,342,200	-$11,185,300		$0	$37,919,000	-$14,030,000	$23,889,000	$23,889,000	$29,590,300
2018	90.0%	$166,715,400			-$116,629,000	-$11,409,000		$0	$38,677,400	-$14,310,600	$24,366,800	$24,366,800	$36,516,900
2019	90.0%	$170,049,700			-$118,961,600	-$11,637,200		$0	$39,450,900	-$14,596,800	$24,854,100	$24,854,100	$42,660,500
2020	90.0%	$173,450,700			-$121,340,900	-$11,869,900		$0	$40,239,900	-$14,888,800	$25,351,100	$25,351,100	$48,109,500
2021	90.0%	$176,919,700			-$123,767,700	-$12,107,300		$0	$41,044,700	-$15,186,500	$25,858,200	$25,858,200	$52,942,600
2022	90.0%	$180,458,100			-$126,243,000	-$12,349,500		$0	$41,865,600	-$15,490,300	$26,375,300	$26,375,300	$57,229,300
2023	90.0%	$184,067,300			-$128,767,900	-$12,596,500		$0	$42,702,900	-$15,800,100	$26,902,800	$26,902,800	$61,031,400
2024	90.0%	$187,748,600			-$131,343,300	-$12,848,400		$0	$43,556,900	-$16,116,100	$27,440,800	$27,440,800	$64,403,700
2025	90.0%	$191,503,600		$8,681,500	-$133,970,100	-$13,105,400		$0	$44,428,100	-$16,438,400	$27,989,700	$36,671,200	$68,322,600

April, 2009

IRR Analysis - Two Variable

THF Production

Product Prices vs Inflation

		1.70%	1.75%	1.80%	1.85%	1.90%	1.95%	2.00%	2.05%	2.10%	2.15%	2.20%	2.25%	2.30%
Product Prices	$ 1.32	16.47%	16.52%	16.58%	16.63%	16.68%	16.73%	16.79%	16.84%	16.89%	16.94%	17.00%	17.05%	17.10%
	$ 1.36	20.19%	20.25%	20.30%	20.35%	20.41%	20.46%	20.52%	20.57%	20.63%	20.68%	20.73%	20.79%	20.84%
	$ 1.40	23.55%	23.61%	23.66%	23.72%	23.77%	23.83%	23.89%	23.94%	24.00%	24.05%	24.11%	24.17%	24.22%
	$ 1.43	26.64%	26.70%	26.76%	26.82%	26.87%	26.93%	26.99%	27.05%	27.10%	27.16%	27.22%	27.28%	27.33%
	$ 1.47	29.52%	29.58%	29.64%	29.70%	29.76%	29.82%	29.88%	29.94%	30.00%	30.06%	30.12%	30.18%	30.24%
	$ 1.51	32.24%	32.30%	32.36%	32.42%	32.48%	32.54%	32.60%	32.66%	32.72%	32.78%	32.84%	32.90%	32.97%
	$ 1.55	34.81%	34.87%	34.93%	34.99%	35.06%	35.12%	35.18%	35.24%	35.31%	35.37%	35.43%	35.49%	35.55%
	$ 1.59	37.26%	37.32%	37.39%	37.45%	37.51%	37.58%	37.64%	37.70%	37.77%	37.83%	37.89%	37.96%	38.02%
	$ 1.63	39.61%	39.67%	39.74%	39.80%	39.86%	39.93%	39.99%	40.06%	40.12%	40.19%	40.25%	40.32%	40.38%
	$ 1.67	41.86%	41.93%	41.99%	42.06%	42.12%	42.19%	42.26%	42.32%	42.39%	42.45%	42.52%	42.58%	42.65%
	$ 1.71	44.03%	44.10%	44.17%	44.23%	44.30%	44.37%	44.43%	44.50%	44.57%	44.64%	44.70%	44.77%	44.84%
	$ 1.74	46.13%	46.20%	46.27%	46.33%	46.40%	46.47%	46.54%	46.61%	46.68%	46.74%	46.81%	46.88%	46.95%
	$ 1.78	48.16%	48.23%	48.30%	48.37%	48.44%	48.51%	48.58%	48.65%	48.72%	48.78%	48.85%	48.92%	48.99%

Variable Costs vs. Inflation

		1.70%	1.75%	1.80%	1.85%	1.90%	1.95%	2.00%	2.05%	2.10%	2.15%	2.20%	2.25%	2.30%
Variable Costs	$ 92,168,300	45.59%	45.66%	45.73%	45.80%	45.86%	45.93%	46.00%	46.07%	46.14%	46.20%	46.27%	46.34%	46.41%
	$ 94,879,100	43.90%	43.97%	44.04%	44.11%	44.17%	44.24%	44.31%	44.37%	44.44%	44.51%	44.57%	44.64%	44.71%
	$ 97,590,000	42.18%	42.24%	42.31%	42.38%	42.44%	42.51%	42.57%	42.64%	42.70%	42.77%	42.84%	42.90%	42.97%
	$ 100,300,800	40.41%	40.47%	40.54%	40.60%	40.67%	40.73%	40.80%	40.86%	40.93%	40.99%	41.06%	41.12%	41.19%
	$ 103,011,600	38.59%	38.66%	38.72%	38.79%	38.85%	38.91%	38.98%	39.04%	39.11%	39.17%	39.23%	39.30%	39.36%
	$ 105,722,500	36.73%	36.79%	36.86%	36.92%	36.98%	37.04%	37.11%	37.17%	37.23%	37.30%	37.36%	37.42%	37.49%
	$ 108,433,300	34.81%	34.87%	34.93%	34.99%	35.06%	35.12%	35.18%	35.24%	35.31%	35.37%	35.43%	35.49%	35.55%
	$ 111,144,100	32.83%	32.89%	32.95%	33.01%	33.07%	33.13%	33.19%	33.25%	33.31%	33.38%	33.44%	33.50%	33.56%
	$ 113,855,000	30.77%	30.83%	30.89%	30.95%	31.01%	31.07%	31.13%	31.19%	31.25%	31.31%	31.37%	31.43%	31.49%
	$ 116,565,800	28.64%	28.70%	28.76%	28.82%	28.88%	28.93%	28.99%	29.05%	29.11%	29.17%	29.23%	29.29%	29.35%
	$ 119,276,600	26.41%	26.47%	26.53%	26.59%	26.65%	26.70%	26.76%	26.82%	26.88%	26.93%	26.99%	27.05%	27.11%
	$ 121,987,500	24.08%	24.14%	24.19%	24.25%	24.31%	24.36%	24.42%	24.47%	24.53%	24.59%	24.64%	24.70%	24.76%
	$ 124,698,300	21.61%	21.67%	21.72%	21.78%	21.83%	21.89%	21.94%	22.00%	22.05%	22.11%	22.16%	22.22%	22.27%

Initial Investment vs Inflation

		1.70%	1.75%	1.80%	1.85%	1.90%	1.95%	2.00%	2.05%	2.10%	2.15%	2.20%	2.25%	2.30%
Initial Investment (TPI)	$ 34,360,400	38.79%	38.85%	38.91%	38.98%	39.04%	39.10%	39.17%	39.23%	39.29%	39.36%	39.42%	39.49%	39.55%
	$ 35,371,000	38.06%	38.12%	38.19%	38.25%	38.31%	38.38%	38.44%	38.50%	38.57%	38.63%	38.69%	38.76%	38.82%
	$ 36,381,600	37.36%	37.42%	37.49%	37.55%	37.61%	37.68%	37.74%	37.80%	37.87%	37.93%	37.99%	38.06%	38.12%
	$ 37,392,200	36.69%	36.75%	36.81%	36.88%	36.94%	37.00%	37.07%	37.13%	37.19%	37.25%	37.32%	37.38%	37.44%
	$ 38,402,800	36.04%	36.10%	36.16%	36.23%	36.29%	36.35%	36.41%	36.48%	36.54%	36.60%	36.67%	36.73%	36.79%
	$ 39,413,400	35.41%	35.48%	35.54%	35.60%	35.66%	35.72%	35.79%	35.85%	35.91%	35.97%	36.04%	36.10%	36.16%
	$ 40,424,000	34.81%	34.87%	34.93%	34.99%	35.06%	35.12%	35.18%	35.24%	35.31%	35.37%	35.43%	35.49%	35.55%
	$ 41,434,600	34.22%	34.29%	34.35%	34.41%	34.47%	34.53%	34.60%	34.66%	34.72%	34.78%	34.84%	34.90%	34.97%
	$ 42,445,200	33.66%	33.72%	33.78%	33.84%	33.90%	33.97%	34.03%	34.09%	34.15%	34.21%	34.27%	34.34%	34.40%
	$ 43,455,800	33.11%	33.17%	33.23%	33.30%	33.36%	33.42%	33.48%	33.54%	33.60%	33.66%	33.73%	33.79%	33.85%
	$ 44,466,400	32.58%	32.64%	32.70%	32.76%	32.83%	32.89%	32.95%	33.01%	33.07%	33.13%	33.19%	33.25%	33.32%
	$ 45,477,000	32.07%	32.13%	32.19%	32.25%	32.31%	32.37%	32.43%	32.49%	32.56%	32.62%	32.68%	32.74%	32.80%
	$ 46,487,600	31.57%	31.63%	31.69%	31.75%	31.81%	31.87%	31.93%	31.99%	32.06%	32.12%	32.18%	32.24%	32.30%

10.12 Worst Case Scenario 1 – High Initial Investment

Regardless of how carefully the equipment and process machinery was selected and constructed, it is likely that the actual initial investment cost may exceed the estimated amount. This could be the result of problems surfacing during construction, the emergence of specifications and considerations not accounted for during the design phase, or simply inaccurate estimation and calculations. To consider the worst case scenario in this regard the additional initial investment required to bring the NPV to 0 was determined. This occurred at a value of $33 million, making the total initial investment $94.7 million. At this point, the IRR was 15.1% and the ROI was 20.1%. It is difficult to imagine such a large additional initial investment occurring outside of the amount accounted for in the contingencies, but it offers a worst case scenario and demonstrates at what value of initial investment the NPV will be zero.

Cash Flow Summary

April, 2009

THF Production

Year	Percentage of Design Capacity	Sales	Capital Costs	Working Capital	Variable Costs	Fixed Costs	Depreciation Allowance	Depletion Allowance	Taxable Income	Income Tax Costs	Net Earnings	Annual Cash Flow	Cumulative Net Present Value at 15.0%
2009	0.0%	Design	-$44,199,000	-$3,162,000								-$47,361,000	-$47,361,000
2010	0.0%	Construction	-$44,199,000	-$3,162,000								-$47,361,000	-$88,544,500
2011	45.0%	$69,750,000			-$48,795,000	-$15,385,900	-$15,785,400	$0	-$10,216,300	$3,780,000	-$6,436,300	$9,349,100	-$81,475,200
2012	67.5%	$104,625,000			-$73,192,500	-$15,385,900	-$25,256,600	$0	-$9,210,000	$3,407,700	-$5,802,300	$19,454,300	-$68,683,700
2013	90.0%	$139,500,000			-$97,590,000	-$15,385,900	-$15,154,000	$0	$11,370,100	-$4,206,900	$7,163,200	$22,317,200	-$55,923,800
2014	90.0%	$139,500,000			-$97,590,000	-$15,385,900	-$9,092,400	$0	$17,431,700	-$6,449,700	$10,982,000	$20,074,400	-$45,943,300
2015	90.0%	$139,500,000			-$97,590,000	-$15,385,900	-$9,092,400	$0	$17,431,700	-$6,449,700	$10,982,000	$20,074,400	-$37,264,600
2016	90.0%	$139,500,000			-$97,590,000	-$15,385,900	-$4,546,200	$0	$21,977,900	-$8,131,800	$13,846,100	$18,392,300	-$30,350,300
2017	90.0%	$139,500,000			-$97,590,000	-$15,385,900		$0	$26,524,100	-$9,813,900	$16,710,200	$16,710,200	-$24,887,700
2018	90.0%	$139,500,000			-$97,590,000	-$15,385,900		$0	$26,524,100	-$9,813,900	$16,710,200	$16,710,200	-$20,137,600
2019	90.0%	$139,500,000			-$97,590,000	-$15,385,900		$0	$26,524,100	-$9,813,900	$16,710,200	$16,710,200	-$16,007,100
2020	90.0%	$139,500,000			-$97,590,000	-$15,385,900		$0	$26,524,100	-$9,813,900	$16,710,200	$16,710,200	-$12,415,400
2021	90.0%	$139,500,000			-$97,590,000	-$15,385,900		$0	$26,524,100	-$9,813,900	$16,710,200	$16,710,200	-$9,292,100
2022	90.0%	$139,500,000			-$97,590,000	-$15,385,900		$0	$26,524,100	-$9,813,900	$16,710,200	$16,710,200	-$6,576,200
2023	90.0%	$139,500,000			-$97,590,000	-$15,385,900		$0	$26,524,100	-$9,813,900	$16,710,200	$16,710,200	-$4,214,600
2024	90.0%	$139,500,000			-$97,590,000	-$15,385,900		$0	$26,524,100	-$9,813,900	$16,710,200	$16,710,200	-$2,161,000
2025	90.0%	$139,500,000		$6,324,000	-$97,590,000	-$15,385,900		$0	$26,524,100	-$9,813,900	$16,710,200	$23,034,200	$300,500

Profitability Measures

April, 2009

THF Production

The Investor's Rate of Return (IRR) for this Project is: **15.06%**

The Net Present Value (NPV) at 15% for this Project is: **$300,500**

ROI Analysis (Third Production Year)

Annual Sales:	$139,500,000
Annual Costs:	-$112,975,900
Depreciation:	-$6,314,200
Income Tax:	-$7,477,700
Net Earnings:	$19,046,400
Total Capital Investment:	$94,722,000
ROI:	**20.1%**

IRR Analysis - Two Variable

April, 2009

THF Production

Product Prices vs Initial Investment

Product Prices

	$75,138,300	$77,348,300	$79,558,200	$81,768,200	$83,978,100	$86,188,100	$88,398,000	$90,608,000	$92,817,900	$95,027,900	$97,237,800	$99,447,800	$101,657,700
$ 1.32	1.46%	1.11%	0.77%	0.44%	0.13%	-0.18%	-0.47%	-0.76%	-1.03%	-1.30%	-1.56%	-1.81%	-2.05%
$ 1.36	5.22%	4.83%	4.46%	4.10%	3.75%	3.42%	3.09%	2.78%	2.48%	2.19%	1.90%	1.63%	1.36%
$ 1.40	8.36%	7.94%	7.54%	7.15%	6.77%	6.41%	6.06%	5.73%	5.40%	5.09%	4.78%	4.48%	4.20%
$ 1.43	11.11%	10.66%	10.23%	9.81%	9.41%	9.02%	8.65%	8.29%	7.94%	7.61%	7.28%	6.97%	6.66%
$ 1.47	13.58%	13.10%	12.64%	12.20%	11.78%	11.37%	10.97%	10.59%	10.22%	9.87%	9.52%	9.19%	8.86%
$ 1.51	15.85%	15.34%	14.86%	14.39%	13.94%	13.51%	13.09%	12.69%	12.30%	11.93%	11.56%	11.21%	10.87%
$ 1.55	17.95%	17.42%	16.91%	16.42%	15.95%	15.50%	15.06%	14.64%	14.23%	13.84%	13.46%	13.09%	12.73%
$ 1.59	19.93%	19.37%	18.84%	18.33%	17.84%	17.36%	16.91%	16.46%	16.04%	15.63%	15.23%	14.84%	14.47%
$ 1.63	21.80%	21.22%	20.66%	20.13%	19.62%	19.12%	18.65%	18.19%	17.74%	17.31%	16.90%	16.50%	16.11%
$ 1.67	23.57%	22.97%	22.40%	21.84%	21.31%	20.79%	20.30%	19.82%	19.36%	18.92%	18.49%	18.07%	17.66%
$ 1.71	25.27%	24.65%	24.05%	23.48%	22.92%	22.39%	21.88%	21.39%	20.91%	20.45%	20.00%	19.57%	19.15%
$ 1.74	26.90%	26.26%	25.64%	25.05%	24.48%	23.93%	23.40%	22.88%	22.39%	21.91%	21.45%	21.01%	20.57%
$ 1.78	28.48%	27.81%	27.17%	26.56%	25.97%	25.40%	24.86%	24.33%	23.82%	23.33%	22.85%	22.39%	21.94%

Variable Costs vs. Initial Investment

Variable Costs

	$75,138,300	$77,348,300	$79,558,200	$81,768,200	$83,978,100	$86,188,100	$88,398,000	$90,608,000	$92,817,900	$95,027,900	$97,237,800	$99,447,800	$101,657,700
$ 92,168,300	26.30%	25.66%	25.04%	24.45%	23.88%	23.33%	22.81%	22.30%	21.81%	21.33%	20.87%	20.43%	20.00%
$ 94,879,100	25.02%	24.40%	23.80%	23.22%	22.67%	22.13%	21.62%	21.13%	20.65%	20.19%	19.74%	19.31%	18.89%
$ 97,590,000	23.70%	23.10%	22.51%	21.95%	21.42%	20.90%	20.40%	19.92%	19.45%	19.01%	18.57%	18.15%	17.74%
$ 100,300,800	22.34%	21.75%	21.19%	20.65%	20.13%	19.62%	19.14%	18.67%	18.22%	17.79%	17.36%	16.96%	16.56%
$ 103,011,600	20.93%	20.36%	19.82%	19.29%	18.79%	18.30%	17.83%	17.38%	16.94%	16.52%	16.11%	15.72%	15.34%
$ 105,722,500	19.47%	18.92%	18.40%	17.89%	17.40%	16.93%	16.48%	16.04%	15.62%	15.21%	14.81%	14.43%	14.06%
$ 108,433,300	17.95%	17.42%	16.91%	16.42%	15.95%	15.50%	15.06%	14.64%	14.23%	13.84%	13.46%	13.09%	12.73%
$ 111,144,100	16.36%	15.85%	15.36%	14.89%	14.44%	14.00%	13.58%	13.17%	12.78%	12.40%	12.03%	11.68%	11.33%
$ 113,855,000	14.69%	14.20%	13.73%	13.28%	12.84%	12.42%	12.02%	11.63%	11.25%	10.89%	10.53%	10.19%	9.86%
$ 116,565,800	12.92%	12.45%	12.00%	11.57%	11.15%	10.75%	10.36%	9.99%	9.63%	9.28%	8.94%	8.61%	8.29%
$ 119,276,600	11.03%	10.58%	10.16%	9.74%	9.35%	8.96%	8.59%	8.24%	7.89%	7.56%	7.23%	6.92%	6.62%
$ 121,987,500	8.99%	8.57%	8.16%	7.77%	7.39%	7.03%	6.68%	6.34%	6.01%	5.69%	5.39%	5.09%	4.80%
$ 124,698,300	6.76%	6.36%	5.98%	5.61%	5.25%	4.91%	4.58%	4.26%	3.95%	3.65%	3.36%	3.08%	2.80%

Fixed Costs vs Initial Investment

Fixed Costs

	$75,138,300	$77,348,300	$79,558,200	$81,768,200	$83,978,100	$86,188,100	$88,398,000	$90,608,000	$92,817,900	$95,027,900	$97,237,800	$99,447,800	$101,657,700
$ 13,078,000	19.59%	19.04%	18.51%	17.99%	17.50%	17.03%	16.57%	16.13%	15.70%	15.29%	14.89%	14.51%	14.13%
$ 13,462,700	19.32%	18.77%	18.24%	17.73%	17.25%	16.77%	16.32%	15.88%	15.46%	15.05%	14.66%	14.27%	13.90%
$ 13,847,300	19.05%	18.51%	17.98%	17.48%	16.99%	16.52%	16.07%	15.64%	15.22%	14.81%	14.42%	14.04%	13.67%
$ 14,231,900	18.78%	18.24%	17.72%	17.21%	16.73%	16.27%	15.82%	15.39%	14.97%	14.57%	14.18%	13.80%	13.44%
$ 14,616,600	18.51%	17.97%	17.45%	16.95%	16.47%	16.01%	15.57%	15.14%	14.73%	14.33%	13.94%	13.57%	13.20%
$ 15,001,200	18.23%	17.70%	17.18%	16.69%	16.21%	15.76%	15.32%	14.89%	14.48%	14.08%	13.70%	13.33%	12.97%
$ 15,385,900	17.95%	17.42%	16.91%	16.42%	15.95%	15.50%	15.06%	14.64%	14.23%	13.84%	13.46%	13.09%	12.73%
$ 15,770,500	17.67%	17.15%	16.64%	16.16%	15.69%	15.24%	14.81%	14.39%	13.98%	13.59%	13.21%	12.85%	12.49%
$ 16,155,200	17.39%	16.87%	16.37%	15.89%	15.43%	14.98%	14.55%	14.13%	13.73%	13.34%	12.97%	12.60%	12.25%
$ 16,539,800	17.11%	16.59%	16.10%	15.62%	15.16%	14.72%	14.29%	13.88%	13.48%	13.09%	12.72%	12.36%	12.01%
$ 16,924,500	16.83%	16.32%	15.82%	15.35%	14.89%	14.45%	14.03%	13.62%	13.22%	12.84%	12.47%	12.11%	11.77%
$ 17,309,100	16.54%	16.03%	15.55%	15.08%	14.62%	14.19%	13.77%	13.36%	12.97%	12.59%	12.22%	11.86%	11.52%
$ 17,693,800	16.26%	15.75%	15.27%	14.80%	14.35%	13.92%	13.50%	13.10%	12.71%	12.33%	11.97%	11.62%	11.27%

10.13 Worst Case Scenario 2 – High Costs

The next worst case scenario analysis considers the case of a sharp rise in all costs. First, all variable costs (except for raw materials) were doubled. This resulted in a substantial drop in ROI and IRR to 23.0% and 18.45%, respectively. The NPV was still positive at $12,000, indicating that the endeavor would still be profitable even if all variable costs except raw materials doubled.

The next step consisted of doubling all fixed costs, keeping property taxes, insurance, and depreciation constant, in addition to the variable costs doubled in the first analysis. Under such conditions, the project was discovered to be infeasible; the ROI plunged to 13.4% and the NPV became negative $13.6 million. Whereas doubling the variable costs in the first part of the analysis only increased annual costs by about $16 million, doubling the fixed costs increased annual costs by an additional $8.8 million. The results of this analysis are shown below.

This analysis demonstrates that it would take a substantially large increase in costs, assuming no subsequent increase in the price of THF, for this venture to become unprofitable. Thus, the project is robust against changes in all types of costs, other than the internally-supplied maleic acid cost.

Variable Cost Summary

April, 2009

THF Production

		Per lb THF		TOTAL
Raw Materials				
	Hydrogen	$0.13 per lb of THF	$12,855,000	
	Maleic Acid	$0.81 per lb of THF	$80,559,400	
	Total Raw Materials:	**$0.93 per lb of THF**	**$93,414,400**	**$93,414,400**
Utilties				
	High Pressure Steam	$0.01 per lb of THF	$751,200	
	Low Pressure Steam	$0.04 per lb of THF	$3,528,500	
	Cooling Water	$0.00 per lb of THF	$342,300	
	Natural Gas	$0.00 per lb of THF	$213,800	
	Electricity	$0.02 per lb of THF	$2,330,400	
	Boiler Feed Water (BFW)	$0.00 per lb of THF	$165,900	
	Refrigeration (-30F)	$0.00 per lb of THF	$465,200	
	Waste Water Treatment	$0.03 per lb of THF	$2,928,700	
	Total Raw Materials:	**$0.20 per lb of THF**	**$10,726,000**	**$104,140,400**
General Expenses				
	Selling / Transfer:	$0.03 per lb of THF	$3,100,000	
	Direct Research:	$0.05 per lb of THF	$4,650,000	
	Allocated Research:	$0.03 per lb of THF	$3,100,000	
	Administrative Expense:	$0.06 per lb of THF	$6,200,000	
	Management Incentives:	$0.04 per lb of THF	$3,875,000	
	Total Byproducts:	**$0.21 per lb of THF**	**$20,925,000**	**$125,065,400**
TOTAL		**$1.34 per lb of THF**	**$125,065,400**	**$125,065,400**

Fixed Cost Summary

April, 2009

THF Production

			TOTAL
Operations			
	Direct Wages and Benefits:	$2,548,000	
	Direct Salaries and Benefits:	$382,200	
	Operating Supplies and Services:	$152,880	
	Technical Assistance to Manufacturing:	$420,000	
	Control Laboratory:	$455,000	
	Total Operations:	**$3,958,080**	**$3,958,080**
Maintenance			
	Wages and Benefits:	$1,607,670	
	Salaries and Benefits:	$401,918	
	Materials and Services:	$1,607,670	
	Maintenance Overhead:	$80,384	
	Total Maintenance:	**$3,697,642**	**$7,655,722**
Operating Overhead			
	General Plant Overhead:	$350,725	
	Mechanical Department Services:	$118,555	
	Employee Relations Department:	$291,447	
	Business Services:	$365,544	
	Total Operating Overhead:	**$1,126,271**	**$8,781,993**
	Additional Costs:	$8,782,500	**$17,564,493**
Property Insurance and Taxes			
	Total Property Insurance and Taxes:	**$714,520**	**$18,279,013**
TOTAL			**$18,279,013**

Profitability Measures

April, 2009

THF Production

The Investor's Rate of Return (IRR) for this Project is: **10.60%**

The Net Present Value (NPV) at 15% for this Project is: **-$13,599,300**

ROI Analysis (Third Production Year)

Annual Sales:	$139,500,000
Annual Costs:	-$129,959,600
Depreciation:	-$2,858,100
Income Tax:	-$2,472,500
Net Earnings:	$7,067,900
Total Capital Investment:	$52,571,700
ROI:	**13.4%**

April, 2009

IRR Analysis - Single Variable

THF Production

Product Prices

Product Prices	$1.32	$1.36	$1.40	$1.43	$1.47	$1.51	$1.55	$1.59	$1.63	$1.67	$1.71	$1.74	$1.78
IRR	-	-	-	-	2.62%	7.00%	10.60%	13.74%	16.59%	19.22%	21.69%	24.02%	26.24%

Variable Cost

Variable Cost	$113,770,700	$117,116,900	$120,463,100	$123,809,300	$127,155,500	$130,501,700	$133,847,900	$137,194,100	$140,540,300	$143,886,500	$147,232,700	$150,578,900	$153,925,100
IRR	26.61%	24.31%	21.90%	19.37%	16.68%	13.78%	10.60%	6.98%	2.61%	-	-	-	-

Fixed Cost

Fixed Cost	$8,072,000	$8,309,400	$8,546,900	$8,784,300	$9,021,700	$9,259,100	$9,496,500	$9,733,900	$9,971,300	$10,208,800	$10,446,200	$10,683,600	$10,921,000
IRR	12.29%	12.02%	11.74%	11.45%	11.17%	10.89%	10.60%	10.31%	10.02%	9.72%	9.43%	9.13%	8.83%

Initial Investment (TPI)

Initital Investment	$34,011,100.0	$35,011,400	$36,011,700	$37,012,000	$38,012,400	$39,012,700	$40,013,000	$41,013,300	$42,013,700	$43,014,000	$44,014,300	$45,014,600	$46,015,000
IRR	12.14%	11.86%	11.59%	11.33%	11.08%	10.84%	10.60%	10.37%	10.15%	9.93%	9.72%	9.52%	9.32%

IRR Analysis - Two Variable

April, 2009

THF Production

Product Prices vs Variable Costs

Variable Costs

Product Prices	$113,770,700	$117,116,900	$120,463,100	$123,809,300	$127,155,500	$130,501,700	$133,847,900	$137,194,100	$140,540,300	$143,886,500	$147,232,700	$150,578,900	$153,925,100
$ 1.32	7.34%	2.94%	-	-	-	-	-	-	-	-	-	-	-
$ 1.36	11.48%	7.93%	3.70%	-	-	-	-	-	-	-	-	-	-
$ 1.40	15.05%	11.96%	8.49%	4.41%	-0.88%	-	-	-	-	-	-	-	-
$ 1.43	18.26%	15.47%	12.43%	9.04%	5.10%	0.08%	-	-	-	-	-	-	-
$ 1.47	21.23%	18.64%	15.88%	12.89%	9.58%	5.75%	0.98%	-	-	-	-	-	-
$ 1.51	24.00%	21.56%	19.00%	16.28%	13.34%	10.09%	6.38%	1.82%	-	-	-	-	-
$ 1.55	26.61%	24.31%	21.90%	19.37%	16.68%	13.78%	10.60%	6.98%	2.61%	-	-	-	-
$ 1.59	29.10%	26.90%	24.61%	22.23%	19.72%	17.06%	14.21%	11.09%	7.57%	3.36%	-	-	-
$ 1.63	31.47%	29.37%	27.18%	24.92%	22.56%	20.07%	17.45%	14.64%	11.57%	8.13%	4.07%	-1.18%	-
$ 1.67	33.75%	31.72%	29.63%	27.47%	25.22%	22.88%	20.42%	17.83%	15.05%	12.04%	8.68%	4.75%	-0.22%
$ 1.71	35.95%	33.99%	31.97%	29.89%	27.75%	25.52%	23.20%	20.76%	18.20%	15.46%	12.50%	9.21%	5.41%
$ 1.74	38.06%	36.17%	34.22%	32.22%	30.15%	28.02%	25.81%	23.51%	21.10%	18.56%	15.86%	12.94%	9.72%
$ 1.78	40.11%	38.27%	36.39%	34.45%	32.46%	30.41%	28.30%	26.10%	23.82%	21.43%	18.92%	16.26%	13.38%

Product Prices vs Fixed Costs

Fixed Costs

Product Prices	$8,072,000	$8,309,400	$8,546,900	$8,784,300	$9,021,700	$9,259,100	$9,496,500	$9,733,900	$9,971,300	$10,208,800	$10,446,200	$10,683,600	$10,921,000
$ 1.32	-	-	-	-	-	-	-	-	-	-	-	-	-
$ 1.36	-	-	-	-	-	-	-	-	-	-	-	-	-
$ 1.40	-	-	-	-	-	-	-	-	-	-	-	-	-
$ 1.43	-0.18%	-0.68%	-1.19%	-	-	-	-	-	-	-	-	-	-
$ 1.47	4.94%	4.57%	4.20%	3.81%	3.42%	3.03%	2.62%	2.21%	1.78%	1.35%	0.90%	0.45%	-0.02%
$ 1.51	8.92%	8.61%	8.29%	7.97%	7.65%	7.33%	7.00%	6.67%	6.33%	5.99%	5.65%	5.30%	4.94%
$ 1.55	12.29%	12.02%	11.74%	11.45%	11.17%	10.89%	10.60%	10.31%	10.02%	9.72%	9.43%	9.13%	8.83%
$ 1.59	15.30%	15.04%	14.79%	14.53%	14.27%	14.01%	13.74%	13.48%	13.22%	12.95%	12.68%	12.41%	12.14%
$ 1.63	18.05%	17.81%	17.57%	17.32%	17.08%	16.84%	16.59%	16.35%	16.10%	15.85%	15.60%	15.35%	15.10%
$ 1.67	20.61%	20.38%	20.15%	19.92%	19.69%	19.46%	19.22%	18.99%	18.76%	18.52%	18.29%	18.05%	17.81%
$ 1.71	23.02%	22.80%	22.58%	22.36%	22.13%	21.91%	21.69%	21.47%	21.24%	21.02%	20.79%	20.57%	20.34%
$ 1.74	25.30%	25.09%	24.88%	24.66%	24.45%	24.24%	24.02%	23.81%	23.59%	23.37%	23.16%	22.94%	22.72%
$ 1.78	27.49%	27.28%	27.07%	26.86%	26.66%	26.45%	26.24%	26.03%	25.82%	25.61%	25.40%	25.19%	24.98%

10.14 Worst Case Scenario 3 – Natural Disasters

In this section, an attempt is made to model the impact of a disastrous hurricane on the plant. While the likelihood of such an occurrence is small, Hurricane Katrina demonstrated the large-scale destruction that can be caused and thus, weather effects should be taken into account for a complete analysis.

In order to model the impact the effect of a hurricane the design team considered the following assumptions.

1) The plant will suffer significant damage and will need an additional capital infusion to reconstruct process machinery. This value will be taken as $20 million, or about one-third of the direct permanent investment.
2) As a result of the damage caused to the plant, suppliers, and nearby infrastructure, the plant will not be able to operate at full capacity for 4 years.
3) To account for the disruption and shortages in the supply of utilities, the prices of all utilities will be doubled.
4) Similarly, to account for the disruption in the supply of raw materials, the cost of hydrogen will be increased to $0.85/lb and the price of maleic acid will be increased to $0.46/lb.

Such a worst case scenario created an IRR value of 13.4%, an ROI of 12.1% and an NPV of negative $6.3 million.

Cash Flow Summary

April, 2009

THF Production

Year	Percentage of Design Capacity	Sales	Capital Costs	Working Capital	Variable Costs	Fixed Costs	Depreciation Allowance	Depletion Allowance	Taxable Income	Income Tax Costs	Net Earnings	Annual Cash Flow	Cumulative Net Present Value at 15.0%
2009	0.0%	Design	-$34,749,500	-$3,162,000								-$37,911,500	-$37,911,500
2010	0.0%	Construction	-$34,749,500	-$3,162,000								-$37,911,500	-$70,878,000
2011	45.0%	$69,750,000			-$52,068,600	-$13,085,500	-$12,410,600	$0	-$7,814,700	$2,891,400	-$4,923,300	$7,487,300	-$65,216,500
2012	54.0%	$83,700,000			-$62,482,300	-$13,085,500	-$19,857,000	$0	-$11,724,800	$4,338,200	-$7,386,600	$12,470,400	-$57,017,000
2013	63.0%	$97,650,000			-$72,896,000	-$13,085,500	-$11,914,200	$0	-$245,700	$90,900	-$154,800	$11,759,400	-$50,293,500
2014	72.0%	$111,600,000			-$83,309,800	-$13,085,500	-$7,148,500	$0	$8,056,200	-$2,980,800	$5,075,400	$12,223,900	-$44,216,100
2015	81.0%	$125,550,000			-$93,723,500	-$13,085,500	-$7,148,500	$0	$11,592,500	-$4,289,200	$7,303,300	$14,451,800	-$37,968,200
2016	90.0%	$139,500,000			-$104,137,200	-$13,085,500	-$3,574,300	$0	$18,703,000	-$6,920,100	$11,782,900	$15,357,200	-$32,194,900
2017	90.0%	$139,500,000			-$104,137,200	-$13,085,500		$0	$22,277,300	-$8,242,600	$14,034,700	$14,034,700	-$27,606,900
2018	90.0%	$139,500,000			-$104,137,200	-$13,085,500		$0	$22,277,300	-$8,242,600	$14,034,700	$14,034,700	-$23,617,400
2019	90.0%	$139,500,000			-$104,137,200	-$13,085,500		$0	$22,277,300	-$8,242,600	$14,034,700	$14,034,700	-$20,148,200
2020	90.0%	$139,500,000			-$104,137,200	-$13,085,500		$0	$22,277,300	-$8,242,600	$14,034,700	$14,034,700	-$17,131,500
2021	90.0%	$139,500,000			-$104,137,200	-$13,085,500		$0	$22,277,300	-$8,242,600	$14,034,700	$14,034,700	-$14,508,300
2022	90.0%	$139,500,000			-$104,137,200	-$13,085,500		$0	$22,277,300	-$8,242,600	$14,034,700	$14,034,700	-$12,227,300
2023	90.0%	$139,500,000			-$104,137,200	-$13,085,500		$0	$22,277,300	-$8,242,600	$14,034,700	$14,034,700	-$10,243,800
2024	90.0%	$139,500,000			-$104,137,200	-$13,085,500		$0	$22,277,300	-$8,242,600	$14,034,700	$14,034,700	-$8,519,000
2025	90.0%	$139,500,000		$6,324,000	-$104,137,200	-$13,085,500		$0	$22,277,300	-$8,242,600	$14,034,700	$20,358,700	-$6,343,400

Profitability Measures

April, 2009

THF Production

The Investor's Rate of Return (IRR) for this Project is: **13.42%**

The Net Present Value (NPV) at 15% for this Project is: **-$6,343,400**

ROI Analysis (Third Production Year)

Annual Sales:	$97,650,000
Annual Costs:	-$85,981,500
Depreciation:	-$4,964,200
Income Tax:	-$2,480,600
Net Earnings:	$9,187,900
Total Capital Investment:	$75,823,000
ROI:	**12.1%**

April, 2009

IRR Analysis - Single Variable

THF Production

Product Prices

Product Prices	$1.32	$1.36	$1.40	$1.43	$1.47	$1.51	$1.55	$1.59	$1.63	$1.67	$1.71	$1.74	$1.78
IRR	-6.60%	-1.21%	2.75%	5.97%	8.74%	11.19%	13.42%	15.48%	17.39%	19.19%	20.90%	22.53%	24.09%

Variable Cost

Variable Cost	$98,351,800	$101,244,500	$104,137,200	$107,029,900	$109,922,600	$112,815,300	$115,708,000	$118,600,700	$121,493,400	$124,386,100	$127,278,800	$130,171,500	$133,064,200
IRR	22.41%	21.06%	19.67%	18.21%	16.70%	15.10%	13.42%	11.63%	9.71%	7.62%	5.32%	2.71%	-0.34%

Fixed Cost

Fixed Cost	$11,122,700	$11,449,800	$11,777,000	$12,104,100	$12,431,300	$12,758,400	$13,085,500	$13,412,700	$13,739,800	$14,067,000	$14,394,100	$14,721,200	$15,048,400
IRR	14.99%	14.73%	14.47%	14.21%	13.95%	13.69%	13.42%	13.16%	12.89%	12.62%	12.35%	12.08%	11.80%

Initial Investment (TPI)

Inititial Investment	$59,074,200.0	$60,811,600	$62,549,100	$64,286,600	$66,024,100	$67,761,500	$69,499,000	$71,236,500	$72,974,000	$74,711,400	$76,448,900	$78,186,400	$79,923,900
IRR	15.94%	15.48%	15.04%	14.61%	14.20%	13.81%	13.42%	13.05%	12.69%	12.35%	12.01%	11.68%	11.37%

10.15 Additional Considerations

Plant Idling Time

The proposed plant is designed to work at a maximum production capacity of 100 million pounds of THF per year. The plant has been designed in such a way that it allows 35 days of idling time per year that can be used for maintenance, so that the plant can avoid a future drop in THF output. However, it is desirable to understand the effect that the operation to idling time ratio will have in the attractiveness of our project.

Government's Corporate Policy

To help alleviate the current economic recession, the government has offered various incentives and stimulus packages to corporations. Most of these have been confined to financial firms, but there could be various other changes in the future that would affect the viability of this plant. For instance, a reduction in the corporate income tax rate and the addition of items to the corporate tax deduction list could help increase profitability.

11.0 Conclusion and Recommendations

It is clear from the process design and the economic analysis that the implementation of this project, though requiring a significant initial total permanent investment of $40 million, will be very profitable. The current design easily achieves the targeted production level of 100 million lbs of 99.95% pure THF per year and results in an ROI of 45.9% and an IRR of 32.7%. These measures, along with the highly positive NPV, speak very favorably for the viability of the project. Such high profit margins make additional research and development costs for increased efficiency possible.

Raw materials, particularly maleic acid, occupy a very significant proportion of the total variable costs, and therefore, reducing these costs should be a key goal for future design improvements. The price of raw materials for this project is substantially reduced due to the presence of the internal upstream plant, which generates maleic acid. This provides the plant with a significant competitive advantage and helps to boost profitability, enabling it to better withstand sudden price shocks in utilities, wages, and other costs, as was shown in the sensitivity analysis.

The overall economic and sensitivity analysis showed this undertaking to be very profitable under all reasonable scenarios, and even some worst case scenarios. Furthermore, the economic sensitivity studies revealed that the project was most susceptible to changes in the price of maleic acid, and not particularly sensitive to changes in utility costs or wage rates. This could be a strong incentive to build additional tanks to store maleic acid for times when supplies are scarce.

In these uncertain economic times, the projects that will be successful will be those that have a high degree of flexibility and are able to withstand changes in demand and costs. This process is robust against all variable and fixed costs, except for maleic acid, which is manufactured internally.

12.0 Acknowledgments:

We would like to express our gratitude to Mr. Wayne Robbins, an extremely knowledgeable veteran of process design and retired Senior Engineer from DuPont, for recommending the project and for his time and patience. As our industrial consultant project advisor, he aided us enthusiastically and tirelessly for the last fourteen weeks and provided invaluable insight on reactor kinetics, pressure-swing distillation and other separation modeling, and materials of construction for our specialized vessels. Most laudably, he sat with us for hours, going through the process model step-by-step to ensure convergence and feasibility of all of the blocks. We would also like to thank Mr. Adam Brostow, Principal Process Engineer from Air Products, for putting us in contact with very helpful people at his firm who helped us immensely with our membrane model and sizing.

We would especially like to thank Dr. Warren Seider, our faculty consultant, and Professor Leonard Fabiano. In addition to teaching us the fundamentals of process design last semester, Dr. Seider was also an indispensible source of modeling suggestions, and he taught us numerous aspects of chemical production and process design. We would also like to thank Professor Fabiano for teaching us how to size and price heat exchangers, flash vessels, and distillation towers and for tirelessly answering our questions on any aspect of our project.

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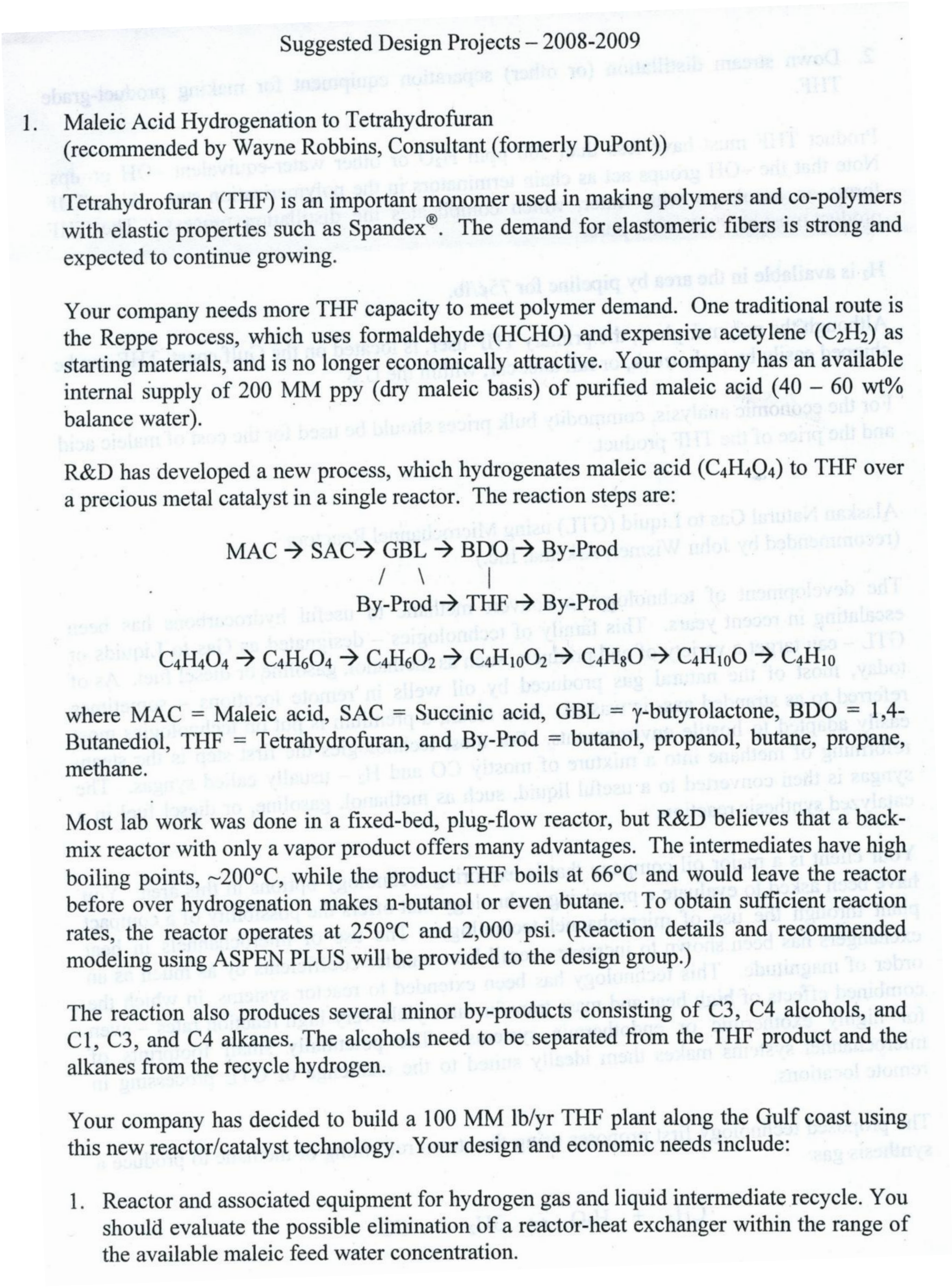
Appendix

The following appendices contain all relevant material, references, calculations, simulation results, and correspondence utilized in the production of this design report.

A.1 Problem Statement



Suggested Design Projects – 2008-2009

1. Maleic Acid Hydrogenation to Tetrahydrofuran
(recommended by Wayne Robbins, Consultant (formerly DuPont))

Tetrahydrofuran (THF) is an important monomer used in making polymers and co-polymers with elastic properties such as Spandex®. The demand for elastomeric fibers is strong and expected to continue growing.

Your company needs more THF capacity to meet polymer demand. One traditional route is the Reppe process, which uses formaldehyde (HCHO) and expensive acetylene (C_2H_2) as starting materials, and is no longer economically attractive. Your company has an available internal supply of 200 MM ppy (dry maleic basis) of purified maleic acid (40 – 60 wt% balance water).

R&D has developed a new process, which hydrogenates maleic acid ($C_4H_4O_4$) to THF over a precious metal catalyst in a single reactor. The reaction steps are:

MAC → SAC → GBL → BDO → By-Prod
/ \ |
By-Prod → THF → By-Prod

$$C_4H_4O_4 \rightarrow C_4H_6O_4 \rightarrow C_4H_6O_2 \rightarrow C_4H_{10}O_2 \rightarrow C_4H_8O \rightarrow C_4H_{10}O \rightarrow C_4H_{10}$$

where MAC = Maleic acid, SAC = Succinic acid, GBL = γ-butyrolactone, BDO = 1,4-Butanediol, THF = Tetrahydrofuran, and By-Prod = butanol, propanol, butane, propane, methane.

Most lab work was done in a fixed-bed, plug-flow reactor, but R&D believes that a back-mix reactor with only a vapor product offers many advantages. The intermediates have high boiling points, ~200°C, while the product THF boils at 66°C and would leave the reactor before over hydrogenation makes n-butanol or even butane. To obtain sufficient reaction rates, the reactor operates at 250°C and 2,000 psi. (Reaction details and recommended modeling using ASPEN PLUS will be provided to the design group.)

The reaction also produces several minor by-products consisting of C3, C4 alcohols, and C1, C3, and C4 alkanes. The alcohols need to be separated from the THF product and the alkanes from the recycle hydrogen.

Your company has decided to build a 100 MM lb/yr THF plant along the Gulf coast using this new reactor/catalyst technology. Your design and economic needs include:

1. Reactor and associated equipment for hydrogen gas and liquid intermediate recycle. You should evaluate the possible elimination of a reactor-heat exchanger within the range of the available maleic feed water concentration.

2. Down stream distillation (or other) separation equipment for making product-grade THF.

Product THF must have less than 300 ppm H_2O or other water-equivalent –OH groups. Note that the –OH groups act as chain terminators in the polymerization step. Also, THF forms an azeotrope with water, which complicates the distillation process. The THF product must be 99.95 wt% pure.

H_2 is available in the area by pipeline for 75¢/lb.

Although the polymer plant, the primary THF user, is located on the Gulf coast, THF can be shipped easily by tank, truck, or rail tank car, within the U.S.

For the economic analysis, commodity bulk prices should be used for the cost of maleic acid and the price of the THF product.

Maleic Hydrogenation to Tetrahydrofuran (W. T. Robbins)

Reaction Details

The hydrogenation of maleic acid to tetrahydrofuran using a Pd/Re/C catalyst was studied in a series of lab reactor experiments in a tubular, isothermal reactor. Reaction rate constants were fitted to the lab data with the following results.

Abbreviations

The following abbreviations are used:

MAC = Maleic acid (C4H4O4, MW=116)
SAC = Succinic acid (C4H6O4, MW=118)
GBL = γ-butyrolactone (C4H6O2, MW=86)
BDO = 1,4-butanediol (C4H10O2, MW=90)
THF = Tetrahydrofuran (C4H8O, MW=72)
ROH = n-butanol and n-propanol
ByPr = ROH + alkanes (n-butane, n-propane, methane)

Reactions

The following seven reactions are postulated as routes to the various intermediates and products:

```
               1         2         6
MAC/SAC → GBL → BDO → ByPr
                 /    \ 3     5 |
               4 ↓    ——→THF → ByPr
               ByPr                 7
```

MAC and SAC are combined since experimental results show that MAC quickly reacts to SAC at all conditions tested.

Poynting Correction

The rate Ks are corrected for H2 partial pressure (total pressure – VP water) with the water vapor corrected for the non-condensable gas effect using the Poynting factor. As an example, at 250˚C and 2000 PSIG system pressure the H2 partial pressure is:

2015 – 577*1.24 = 1297 PSIA

Adsorption Term – Ka

The effect of acid adsorption on the catalyst was noted in the experimental work and also reported in published articles, which attribute the Ka to SAC adsorption on the catalyst.
Data at 5, 10 and 20 Wt% MAC feed shows the dominance of the Ka term. In effect, the hydrogenation rate does not increase with acid concentration in the 5 to 20 Wt% acid feed range. In fitting the experimental data, the Ka effect was included as an exponent on the MAC feed concentration.

H2 Limitation

The rates are nearly independent of the organic concentration. This observation indicates that rates are limited by H2 mass transfer, replacement of reacted H2 on the catalyst or an adsorption term involving one or more of the organics. The question was not resolved.

Reactant Concentrations/Rates

The following rate constant equations apply to the standard Pd/Re/C catalyst. The rate constants from the individual runs were fitted by a multiple linear regression analysis of the equation:

$\mathrm{Ln}\ K = a/T^{\circ}K + b*\mathrm{Ln}(H_2) + c*\mathrm{Ln}(Cat) + d*\mathrm{Ln}(\%MAC)$

Where: H2 = H2 partial pressure, PSI
Cat = weight of catalyst, g
%MAC = Wt% MAC in feed

Although b, c and d were allowed to vary for all reactions the typical values were b=~1, c=~1 and d=~-1. Rates increased linearly with H2 and catalyst and were inversely proportional to wt% MAC feed.

For the model, the H2 and catalyst exponents were set at 1. The actual exponents are close to 1 and probably within the range of experimental data.

MAC/SAC (K0)

The rate equation for the MAC/SAC → GBL hydrogenation is:

$\mathrm{Ln}(K0/H_2/Cat) = -11.911 - 5983*(1/T^{\circ}K - 1/523.15)$

The acid hydrogenation rate is more sensitive to temperature at higher acid feeds. The maleic hydrogenation rate is very fast and it is believed that K0 is actually the SAC rate. For modeling purposes it is recommended that the MAC → SAC rate be set at 10x K0 to avoid stiff equations in the model. All MAC goes to SAC then to GBL.

The acid reactions appear to be 100% selective to GBL and no by-products are seen.

GBL (K1)

The rate equation for GBL → BDO + THF + ByPr is:

$\mathrm{Ln}(K1/H_2/Cat) = -12.159 - 5408*(1/T^{\circ}K - 523.15)$

The GBL reaction rate closely parallels but is slightly less than the acid rate, another indication that Ka terms and H2 availability on the catalyst surface are significant.

GBL can react to either THF directly or to THF via BDO. It is also the primary source of by-products. Therefore it was necessary to breakdown the GBL (K1) into its four separate reactions.

$\mathrm{Ln}(k1b/H_2/Cat) = -13.214 - 3185*(1/T^{\circ}K - 1/523.15)$

Ln(k1t/H2/Cat) = -12.658 – 8894*(1/T˚K – 1/523.15)

Ln(k1bu/H2/Cat) = -14.832 – 6998*(1/T˚K – 1/523.15)

Ln(k1pr/H2/Cat) = -15.646 – 13189*(1/T˚K – 1/523.15)

The GBL to BDO rate is least sensitive to temperature. At the same time, both THF and ROH rates increase rapidly with temperature, especially the by-product rate. Between 150 and 275˚C the by-product increases from ~4% to ~18% of the BDO reacted.

BDO (K2)

The rate equations for BDO going to THF and by-products are:

Ln(k2t/H2/Cat) = - 12.827 – 8584*(1/T˚K – 1/523.15)

Ln(k2bu/H2/Cat) = - 15.380 – 7725*(1/T˚K – 1/523.15)

Ln(k2pr/H2/Cat) = -16.193 - 13912*(1/T˚K – 1/523.15)

THF (K3)

The rate equations for THF going to by-products are:

Ln(k3bu/H2/Cat) = - 14.837 - 8301*(1/T˚K – 1/523.15)

Ln(k3pr/H2/Cat) = -16.326 - 14558*(1/T˚K – 1/523.15)

By-product splits

For modeling purposes the following by-product splits are recommended:

For k2bu or k3bu to n-butanol or n-butane (85% alcohol, 15% alkane)

For k2pr or k3pr to n-propanol or n-propane + methane (90% alcohol, 10% alkanes)

The reactions may be modeled by using a Ka term or by adjusting the individual Ks for the feed MAC concentration. If Ka term is used the recommended equation is:

$$\text{Rate} = \frac{\text{Kr*(SAC … THF)}}{\text{1+100*(mole frac total org)}}$$

General Comments

The catalyst density is very close to water and it is readily mixed by even mild H2 sparging. No mechanical agitation is required.

Reaction rates are slow and a large reactor is required. Space-time yield (STY) is defined as Lbs/Hr THF/1000 Lbs catalyst. In a plug-flow reactor the maximum THF STY occurs just before the acid feed is reacted away and typical values are 400 to 500. The values do not vary with acid feed for reasons discussed above.

The reactor must be an ASPEN Block that does simultaneous reaction kinetics and VLE calculations. In previous work a RADFRAC Block was modified to do this. More recent versions of ASPEN may have other Blocks available.

Catalyst must be regenerated annually. The Pd/Re are recovered and applied to a new batch of carbon support. It is not necessary to purchase new Pd/Re each year.

A.2 Equipment Sizing Calculations

A-300: HORIZONTAL PRESSURE VESSEL

Estimation of Vessel Diameter

L/D=	2		Aspect Ratio
τ =	0.083333333	hr	Residence Time
Frac=	0.5		Fraction of drum full

$$\boxed{D = \left[\frac{4 v \tau}{\pi}\right]^{1/3}}$$

v=	1037.69442	ft3/hr	Volumetric Flow Rate into Drum

D = 6.039 ft

Estimation of Vessel Size

$$\boxed{W = \pi (D_i + t_s)(L + 0.8 D_i) t_s \rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2 P_d}}$$

Diameter (D_i)=	6.039	ft	--->	72.464288	in
Length (L)=	12.077381	ft	--->	144.92858	in
Volume (V)=	345.90	ft^3			

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_0 =	5.3	psig	
P_d =	8.485031782	psig	
S =	15000	psia	maximum allowable stress for 482 F
E =	1.00		weld efficiency

At low P, check for min wall thickness= MIN

t_s = 0.3125 inches

Material Used :	Stainless Steel 304	
Density of Material:	0.2890183	lb/in^3

W = 4189.866998 lb

Purchase Cost of Reflux Accumulator

$$\boxed{C_V = \exp(8.9552 - 0.2330 \ln W + 0.04333(\ln W)^2)}$$

C_v = $22,607.39 Cost of Empty Horizontal Vessels for 1000<W<920,000 lb including nozzles, manholes, and supports

$$\boxed{C_{PL} = 2005(D_i)^{0.20294}}$$

C_{PL} = $2,888.01 Cost of platforms and ladders

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material= Stainless Steel 304

F_m = 1.7

C_P = $41,320.57

A-500: HORIZONTAL PRESSURE VESSEL

Estimation of Vessel Diameter

L/D=	2		Aspect Ratio
τ =	0.083333333	hr	Residence Time
Frac=	0.5		Fraction of drum full

$$\boxed{D = \left[\frac{4 v \tau}{\pi}\right]^{1/3}}$$

v=	946.269272	ft3/hr	Volumetric Flow Rate into Drum

D = 5.856 ft

Estimation of Vessel Size

$$\boxed{W = \pi (D_i + t_s)(L + 0.8 D_i) t_s \rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2 P_d}}$$

Diameter (D_i)=	5.856	ft	--->	70.270404	in
Length (L)=	11.711734	ft	--->	140.54081	in
Volume (V)=	315.42	ft^3			

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_0 =	0.3	psig	
P_d =	0.609771847	psig	
S =	15000	psia	maximum allowable stress for 482 F
E =	1.00		weld efficiency

At low P, check for min wall thickness= MIN

t_s = 0.375 inches

Material Used :	Stainless Steel 304	
Density of Material:	0.2890183	lb/in^3

W = 4732.830255 lb

Purchase Cost of Reflux Accumulator

$$\boxed{C_V = \exp(8.9552 - 0.2330 \ln W + 0.04333(\ln W)^2)}$$

C_v = $24,013.16 Cost of Empty Horizontal Vessels for 1000<W<920,000 lb including nozzles, manholes, and supports

$$\boxed{C_{PL} = 2005(D_i)^{0.20294}}$$

C_{PL} = $2,870.05 Cost of platforms and ladders

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material= Stainless Steel 304

F_m = 1.7

C_P = $43,692.42

A-501: HORIZONTAL PRESSURE VESSEL

Estimation of Vessel Diameter

L/D=	2		Aspect Ratio
τ =	0.083333333	hr	Residence Time
Frac=	0.5		Fraction of drum full

$$\boxed{D = \left[\frac{4v\tau}{\pi}\right]^{1/3}}$$

v=	538.546401	ft3/hr	Volumetric Flow Rate into Drum

D = 4.853 ft

Estimation of Vessel Size

$$\boxed{W = \pi(D_i + t_s)(L + 0.8D_i)t_s\rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2P_d}}$$

Diameter (D_i)=	4.853	ft	--->	58.233815	in
Length (L)=	9.7056359	ft	--->	116.46763	in
Volume (V)=	179.52	ft^3			

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_0 =	100.3	psig	
P_d =	129.1655213	psig	
S =	15000	psia	maximum allowable stress for 482 F
E =	1.00		weld efficiency

At low P, check for min wall thickness= CORRELATION

t_s = 0.252028841 inches

Material Used : Stainless Steel 304

Density of Material: 0.2890183 lb/in3

W = 2182.275376 lb

Purchase Cost of Reflux Accumulator

$$\boxed{C_V = \exp(8.9552 - 0.2330\ln W + 0.04333(\ln W)^2)}$$

C_v = $16,730.42 — Cost of Empty Horizontal Vessels for 1000<W<920,000 lb including nozzles, manholes, and supports

$$\boxed{C_{PL} = 2005(D_i)^{0.20294}}$$

C_{PL} = $2,762.68 — Cost of platforms and ladders

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material= Stainless Steel 304

F_m = 1.7

C_P = $31,204.39

C-100: RECIPROCATING COMPRESSOR, LESS INTERCOOLER

Purchase Cost of Compressor Stage 1

$$\boxed{\eta_M = 0.80 + 0.0319\ln P_B - 0.00182(\ln P_B)^2}$$

P_B=	783.207356	Hp	Brake Power
η_M=	0.931752804		Motor Efficiency

$$\boxed{P_C = \frac{P_B}{\eta_M}}$$

P_C=	840.5741877	Hp	Consumed Power

$$\boxed{C_B = \exp(7.9661 + 0.80\ln(P_C))}$$

C_B= $ 629,932.64

$$\boxed{C_P = F_D F_M C_B}$$

F_D=	1.00	Driver Factor
Material=	Stainless Steel	
F_M=	2.50	Materials Factor

C_P= $ 1,574,831.60

F_D	
Electric motor	1.00
Steam turbine	1.15
Gas turbine	1.25

F_M	
Carbon steel	1.00
Stainless Steel	2.50
Nickel Alloy	5.00

Purchase Cost of Compressor Stage 2

$$\boxed{\eta_M = 0.80 + 0.0319\ln P_B - 0.00182(\ln P_B)^2}$$

P_B=	860.919632	Hp	Brake Power
η_M=	0.932459782		Motor Efficiency

$$\boxed{P_C = \frac{P_B}{\eta_M}}$$

P_C=	923.2780316	Hp	Consumed Power

$$\boxed{C_B = \exp(7.9661 + 0.80\ln(P_C))}$$

C_B= $ 679,046.12

$$\boxed{C_P = F_D F_M C_B}$$

F_D=	1.00	Driver Factor
Material=	Stainless Steel	
F_M=	2.50	Materials Factor

C_P= $ 1,697,615.31

F_D	
Electric motor	1.00
Steam turbine	1.15
Gas turbine	1.25

F_M	
Carbon steel	1.00
Stainless Steel	2.50
Nickel Alloy	5.00

Total Purchase Cost of Compressor, less Intercooler

Stage 1=	$ 1,574,831.60
Stage 2=	$ 1,697,615.31

C_P= $ 3,272,446.91

C-100: COMPRESSOR INTERCOOLER

Estimation of Intercooler Size

U=	60	$Btu/hr\text{-}ft^2$ -F
Q=	-1713553.9	Btu/hr

$$\boxed{A = \frac{Q}{U\,\Delta T_{LM}}}$$

$T_{C,i}$=	90	F
$T_{C,o}$=	120	F
$T_{H,i}$=	334.317868	F
$T_{H,o}$=	104	F

$$\boxed{\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1/\Delta T2)}}$$

ΔT1=	214.317868	F
ΔT2=	14	F
ΔT_{LM}=	**73.41945887**	F
A=	**388.9872264**	**ft^2**

Purchase Cost of Intercooler (Fixed Head)

Type= Fixed Head

$$\boxed{C_P = F_P F_M F_L C_B}$$

$$\boxed{C_B = \exp(11.0545 - 0.9228\ln A + 0.09861(\ln A)^2\}}$$

$$\boxed{F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2}$$

For P>100 psig, else F_P=1

P=	65 psig	
Material=	Carbon Steel/Stainless Steel	
C_B=	$ 8,589.49	
F_P=	1	Pressure Factor
F_M=	2.943140518	Materials Factor- Table 22.25
F_L=	1	Tube Length Factor

C_P= $ 25,280.06

C-200: RECIPROCATING COMPRESSOR

Purchase Cost of Compressor

$$\boxed{\eta_M = 0.80 + 0.0319\ln P_B - 0.00182(\ln P_B)^2}$$

P_B=	716.87872 Hp	Brake Power
η_M=	0.931062019	Motor Efficiency

$$\boxed{P_C = \frac{P_B}{\eta_M}}$$

P_C=	769.9580752 Hp	Consumed Power

$$\boxed{C_B = \exp(7.9661 + 0.80\ln(P_C))}$$

C_B= $ 587,228.24

$$\boxed{C_P = F_D F_M C_B}$$

F_D=	1.00	Driver Factor
Material=	Stainless Steel	
F_M=	2.50	Materials Factor

C_P= $ 1,468,070.61

F_D	
Electric motor	1.00
Steam turbine	1.15
Gas turbine	1.25

F_M	
Carbon steel	1.00
Stainless Steel	2.50
Nickel Alloy	5.00

D-300 DISTILLATION COLUMN

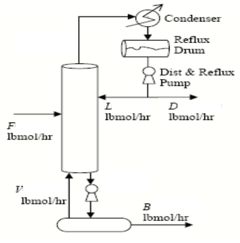
Estimation of Droplet Velocity U:

$$\boxed{U = 0.85U_f}$$

$$\boxed{Uf = \sqrt{\frac{\rho_L - \rho_V}{\rho_V}}C}$$

$$\boxed{C = C_{SB}F_{ST}F_F F_{HA}}$$

$$\boxed{F_{LG} = \frac{L}{V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2}}$$



Spacing=	2 ft	
L=	60577.4211 lb/hr	Reflux Rate
G=	56098.7741 lb/hr	Vapor Flow Rate from Top Tray
σ=	54.2833892 dyne/cm	Stage 9 Liquid Surface Tension
ρ_L=	57.7039301 lb/ft^3	Stage 9 Liquid Density
ρ_V=	0.06027024 lb/ft^3	Stage 9 Vapor Density
F_{LG}=	0.034898453	Fair Correlation Liquid/Gas Factor
C_{SB}=	**0.29** ft/s	From Fair Correlation (Fig 14.4 of Seider)
F_{ST}=	**1.221032973**	Surface Tension Factor
F_F=	**1**	Foaming Factor (=1 for non-foaming)
F_{HA}=	**1**	Hole Area Factor (=1 for valve/bubble cap)
C=	**0.354099562**	
Uf=	10.95089722 ft/s	
U=	**9.308262635 ft/s**	

Estimation of Column Diameter, D

$$\boxed{D = 2\sqrt{\frac{v}{0.9\pi U}}}$$

v=	258.5520284 ft^3/s	Stage 9 Vapor Volumetric Flow Rate
D=	**6.268641955 ft**	

Purchase Cost of Column:

$$\boxed{L = N_T x_T + x_D + x_S}$$

N_T=	24	Number of Trays
xT=	2 ft	Tray Spacing
xD=	4 ft	Disengagement Height
xS=	10 ft	Sump
L=	62 ft	Height of Column

$$\boxed{W = \pi(D_i + ts)(L + 0.8Di)t_s\rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2P_d}}$$

D_i=	6.268641955 ft	Internal Diameter
V=	1913.500151 ft^3	Volume of Column

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_O=	5.3 psig	
P_d =	8.485031782 psig	
S =	15000 psi	Maximum Allowable Stress for 482 F
E =	1.00	Weld Efficiency

At low P, check for min wall thickness= MIN

t_s =	**0.375 inches**	Wall Thickness

Material Used : Stainless Steel 304

Density of Material: 0.289018337 lb/in^3

W=	**20700.15482** lb	Weight

$$\boxed{C_v = \exp\{7.2756 + 0.18255[\ln W] + 0.02297[\ln W]^2\}}$$

Cv =	**$85,675.42**	Cost of Empty Vertical Vessels including nozzles, manholes, and supports

$$\boxed{C_{PL} = 300.9(D_I)^{0.63316}(L)^{0.80161}}$$

C_{PL} =	**$26,300.24**	Cost of platforms and ladders

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material= Stainless Steel 304

F_m = 1.7

C_p = $171,948.45

Purchase Cost of Trays

$$\boxed{C_T = N_T F_{NT} F_{TT} F_{TM} C_{BT}}$$

$$\boxed{F_{NT} = \frac{2.25}{1.0414^{NT}}}$$

If NT<20, else, $F_{NT}=1$

$$\boxed{C_{BT} = 468\exp(0.1739 D_i)}$$

$$\boxed{F_{TM} = 1.401 + 0.0724 D_i}$$

*For : 316 Stainless Steel

N_T=	24	Number of Trays
F_{NT}=	1	Number of Tray Factor
F_{TT}=	1	Tray Type Factor (for Sieve Trays)
Material=	316 Stainless Steel	
F_{TM}=	1.854849678	Materials Factor
C_{BT}=	1097.635369	Base Cost for Sieve Trays 316 Stainless Steel

C_T = **$48,862.77**

Purchase Cost of Distillation Column

Column	$171,948.45
Trays	$48,862.77

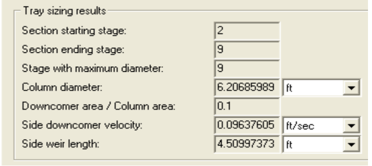
C_P= **$220,811.21**

D-300 TRAY SIZING AND TRAY COUNT

Stage	Temperatur F	Temperatur F	Mass flow l lb/hr	Mass flow v lb/hr	Volume flo cuft/hr	Volume flow v cuft/hr	Molecula	Molecula	Density l lb/cuft	Density v lb/cuft	Viscosity cP	Viscosity vapor to cP
1	168.5268	222.1794	59680.41	59680.41	1037.694	906566.554	23.83	23.83	57.513	0.0658	0.3691	0.0129
2	222.1794	225.2473	17779.81	55080.07	312.1426	911581.589	18.294	21.709	56.961	0.0604	0.2637	0.0129
3	225.2473	226.1094	17981.38	55281.64	315.857	902165.411	18.465	21.772	56.929	0.0613	0.2598	0.013
4	226.1094	227.1415	18317.93	55618.19	321.3423	892213.494	18.827	21.912	57.004	0.0623	0.2598	0.013
5	227.1415	231.3626	54577.79	50099.15	954.5557	950210.01	19.574	18.44	57.176	0.0527	0.2612	0.013
6	231.3626	232.1107	54624.24	50145.6	957.4486	944138.786	19.506	18.375	57.052	0.0531	0.2552	0.013
7	232.1107	232.9067	54813.73	50335.09	960.8921	934534.04	19.566	18.437	57.045	0.0539	0.2543	0.013
8	232.9067	234.4892	55680.05	51201.4	974.8505	925507.833	19.88	18.759	57.117	0.0553	0.2542	0.013
9	234.4892	255.1916	60577.42	56098.77	1049.797	930787.21	21.887	20.806	57.704	0.0603	0.2588	0.0132
10	255.1916	301.3584	4478.647	57945.17	70.67983	805488.533	62.708	26.432	63.365	0.0719	0.4208	0.0136

k-values

Stage	MALEIC	SUCCINIC	**GBL**	BDO	THF	NBUTANE	**WATER**	NBUTA	PROPANOL	α_{12}	η	# Trays
1	6.26E-06	2.28E-06	**0.020448**	0.004598	7.243786		**0.3133**	1.2117	1.5504	15.32	0.32	3.11
2	1.26E-04	4.48E-05	**0.237655**	0.059206	70.69957		**0.8964**	21.753	17.598	3.77	0.49	2.03
3	1.40E-04	4.99E-05	**0.246436**	0.062743	70.33643		**0.9383**	22.382	18.059	3.81	0.49	2.03
4	1.41E-04	5.01E-05	**0.237703**	0.060438	64.19727		**0.9425**	20.737	17.056	3.97	0.49	2.05
5	0.00014	4.96E-05	**0.220874**	0.05566	54.24758		**0.9509**	17.748	15.199	4.31	0.48	2.09
6	0.000166	5.88E-05	**0.241887**	0.063216	58.64742		**1.0156**	19.876	16.668	4.20	0.48	2.07
7	0.000168	5.97E-05	**0.241217**	0.063407	57.8575		**1.0178**	19.737	16.559	4.22	0.48	2.07
8	0.000169	6.00E-05	**0.234454**	0.061598	53.92713		**1.0217**	18.551	15.806	4.36	0.48	2.08
9	0.000163	5.78E-05	**0.196597**	0.049904	36.68595		**1.0486**	12.632	11.923	5.33	0.45	2.20
10	0.000312	0.00011	**0.066336**	0.012987	5.448376		**2.7552**	1.0163	1.8173	41.53	0.24	4.10
										Total Trays=		23.82



Tray sizing results

Section starting stage:	2	
Section ending stage:	9	
Stage with maximum diameter:	9	
Column diameter:	6.20685989	ft
Downcomer area / Column area:	0.1	
Side downcomer velocity:	0.09637605	ft/sec
Side weir length:	4.50997373	ft

D-500: DISTILLATION COLUMN

Purchase Cost of Column:

$$\boxed{L = N_T x_T + x_D + x_S}$$

N_T=	40		Number of Trays
xT=	2	ft	Tray Spacing
xD=	4	ft	Disengagement Height
xS=	10	ft	Sump
L=	94	ft	Height of Column

$$\boxed{W = \pi(D_i + ts)(L + 0.8Di)t_s \rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2P_d}}$$

D_i=	4.56597303	ft	Internal Diameter
V=	1539.162305	ft^3	Volume of Column

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_O=	0.3	psig	
P_d =	0.609771847	psig	
S =	15000	psi	Maximum Allowable Stress for 482 F
E =	1.00		Weld Efficiency

At low P, check for min wall thickness= MIN

t_s =	**0.4375**	**inches**	Wall Thickness

Material Used : Stainless Steel 304

Density of Material: 0.289018337 lb/in^3

W=	**25709.1516**	lb	Weight

$$\boxed{C_v = \exp\{7.2756 + 0.18255[\ln W] + 0.02297[\ln W]^2\}}$$

Cv =	**$98,508.29**	Cost of Empty Vertical Vessels including nozzles, manholes, and supports

$$\boxed{C_{PL} = 300.9(D_I)^{0.63316}(L)^{0.80161}}$$

C_{PL} =	**$30,039.41**	Cost of platforms and ladders

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material= Stainless Steel 304

F_m = 1.7

C_p = $197,503.50

Purchase Cost of Trays

$$\boxed{C_T = N_T F_{NT} F_{TT} F_{TM} C_{BT}}$$

$$\boxed{F_{NT} = \frac{2.25}{1.0414^{NT}}}$$

If NT<20, else, F_{NT}=1

$$\boxed{C_{BT} = 468\exp(0.1739 D_i)}$$

$$\boxed{F_{TM} = 1.401 + 0.0724 D_i}$$

For: 316 Stainless Steel

N_T=	40	Number of Trays
F_{NT}=	1	Number of Tray Factor
F_{TT}=	1	Tray Type Factor
Material=	316 Stainless Steel	
F_{TM}=	1.731576447	Materials Factor for 316 Stainless Steel
C_{BT}=	816.3305461	Base Cost for Sieve Trays

C_T = $56,541.55

Purchase Cost of Distillation Column

Column	$197,503.50
Trays	$56,541.55

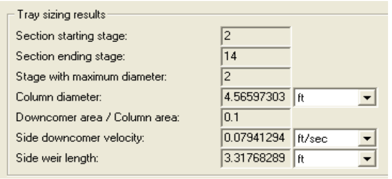
C_P= $254,045.05

D-500 TRAY SIZING AND TRAY COUNT

Stage	Temperatur F	Temperatur F	Mass flow l lb/hr	Mass flow v lb/hr	Volume flo cuft/hr	Volume flow v cuft/hr	Molecula	Molecula	Density l lb/cuft	Density v lb/cuft	Viscosity cP	Viscosity cP
1	147.2576	147.2947	50536.24	50536.24	946.2693	341574.05	62.829	62.829	53.406	0.148	0.3375	0.0099
2	147.2947	147.857	25004.02	50380.54	468.1127	338517.311	62.758	62.611	53.415	0.1488	0.3379	0.0099
3	147.857	148.4705	24625.8	50002.32	460.5317	334611.19	62.117	62.293	53.473	0.1494	0.3385	0.0099
4	148.4705	149.2518	23994.66	49371.18	447.8305	330315.055	61.048	61.769	53.58	0.1495	0.3401	0.01
5	149.2518	150.6536	22756.16	48132.68	422.9663	325023.227	58.95	60.753	53.801	0.1481	0.3442	0.01
6	150.6536	154.8076	20183.65	45232.72	371.5032	320772.734	53.97	58.315	54.33	0.141	0.3549	0.0102
7	155.2509	158.7227	64174.25	37896.76	1125.553	271895.25	30.877	56.907	57.016	0.1394	0.3935	0.0103
8	158.7227	169.1307	5.96E+04	33348.34	1.05E+03	261009.072	29.142	52.635	56.758	0.1278	0.3936	0.0106
9	169.1307	184.8195	5.24E+04	26171.87	9.38E+02	247554.289	26.19	44.347	55.908	0.1057	0.3821	0.0111
10	184.8195	194.575	4.85E+04	22187.85	8.85E+02	245806.939	24.303	38.142	54.761	0.0903	0.3523	0.0113
11	194.575	198.2956	4.73E+04	21069.73	8.75E+02	247535.094	23.672	35.853	54.127	0.0851	0.3328	0.0114
12	198.2956	199.7711	4.71E+04	20820.08	8.74E+02	247087.177	23.512	35.246	53.912	0.0843	0.3255	0.0114
13	199.7711	200.7843	4.70E+04	20711.26	8.72E+02	245593.091	23.446	35.006	53.86	0.0843	0.3225	0.0114
14	200.7843	210.8186	4.22E+04	15914.91	7.63E+02	250458.864	20.986	26.613	55.271	0.0635	0.3109	0.0122
15	210.8186	217.9435	2.63E+04	12193.04	4.62E+02	263109.058	18.604	19.655	56.845	0.0463	0.2834	0.0127

k-values

Stage	MALEIC	SUCCINIC	GBL	BDO	**THF**	**WATER**	NBUTA	PROPANOL	α_{12}	η	# Trays
1	3.25E-06	1.19E-06	0.005273	0.001303	**1.0006**	**0.99785796**	0.1183	0.2643	1.00	0.64	1.56
2	3.25E-06	1.19E-06	0.005268	0.001301	**1.002542**	**0.99262444**	0.1183	0.2642	1.01	0.64	1.56
3	3.25E-06	1.19E-06	0.005298	0.00132	**1.012711**	**0.95114693**	0.119	0.2638	1.06	0.63	1.58
4	3.22E-06	1.18E-06	0.005283	0.001341	**1.031778**	**0.88852507**	0.1202	0.2633	1.16	0.62	1.62
5	3.15E-06	1.16E-06	0.005201	0.001371	**1.075527**	**0.78735316**	0.1233	0.2647	1.37	0.59	1.69
6	3.04E-06	1.12E-06	0.005128	0.001443	**1.20901**	**0.62723576**	0.1362	0.2798	1.93	0.54	1.85
7	3.32E-06	1.22E-06	0.008706	0.002324	**3.268225**	**0.33993025**	0.4393	0.691	9.61	0.36	2.82
8	4.00E-06	1.46E-06	0.011203	0.002607	**3.943636**	**0.35195021**	0.5528	0.8418	11.21	0.34	2.92
9	7.04E-06	2.56E-06	2.11E-02	0.003799	**6.22E+00**	**0.41779925**	0.9832	1.3928	14.88	0.32	3.11
10	1.55E-05	5.60E-06	4.11E-02	0.006551	**1.00E+01**	**0.5666859**	1.8661	2.4471	17.65	0.31	3.18
11	2.44E-05	8.75E-06	5.64E-02	0.008951	**1.26E+01**	**0.68361123**	2.5786	3.2527	18.45	0.32	3.17
12	2.85E-05	1.02E-05	6.22E-02	0.009995	**1.36E+01**	**0.72974021**	2.8667	3.57	18.63	0.32	3.16
13	3.01E-05	1.08E-05	6.43E-02	0.010446	**1.40E+01**	**0.74425137**	2.9844	3.6956	18.82	0.32	3.16
14	3.90E-05	1.40E-05	9.66E-02	0.017029	**2.45E+01**	**0.71577256**	5.671	6.1621	34.21	0.28	3.63
15	8.45E-05	3.02E-05	2.00E-01	0.042974	**6.02E+01**	**0.84596082**	16.408	14.46	71.16	0.24	4.24
									Total Trays=		39.26



Tray sizing results

Section starting stage:	2	
Section ending stage:	14	
Stage with maximum diameter:	2	
Column diameter:	4.56597303	ft
Downcomer area / Column area:	0.1	
Side downcomer velocity:	0.07941294	ft/sec
Side weir length:	3.31768289	ft

D-501: DISTILLATION COLUMN

Purchase Cost of Column:

$$\boxed{L = N_T x_T + x_D + x_S}$$

N_T=	18		Number of Trays
xT=	2	ft	Tray Spacing
xD=	4	ft	Disengagement Height
xS=	10	ft	Sump
L=	50	ft	Height of Column

$$\boxed{W = \pi(D_i + ts)(L + 0.8Di)t_s \rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2P_d}}$$

D_i=	3.35559488	ft	Internal Diameter
V=	442.1798335	ft^3	Volume of Column

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_O=	100.3	psig	
P_d =	129.1655213	psig	
S =	15000	psi	Maximum Allowable Stress for 482 F
E =	1.00		Weld Efficiency

At low P, check for min wall thickness= MIN

t_s =	**0.174271258**	**inches**	Wall Thickness

Material Used : Stainless Steel 304

Density of Material: 0.289018337 lb/in^3

W=	**4045.677267**	lb	Weight

$$\boxed{C_v = \exp\{7.2756 + 0.18255[\ln W] + 0.02297[\ln W]^2\}}$$

Cv =	**$32,087.32**	Cost of Empty Vertical Vessels including nozzles, manholes, and supports

$$\boxed{C_{PL} = 300.9(D_I)^{0.63316}(L)^{0.80161}}$$

C_{PL} =	**$14,901.49**	Cost of platforms and ladders

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material= Stainless Steel 304

F_m = 1.7

C_p = $69,449.93

Purchase Cost of Trays

$$C_T = N_T F_{NT} F_{TT} F_{TM} C_{BT}$$

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

If NT<20, else, $F_{NT}=1$

$$C_{BT} = 468\exp(0.1739 D_i)$$

$$F_{TM} = 1.401 + 0.0724 D_i$$

For: 316 Stainless Steel

N_T=	18	Number of Trays
F_{NT}=	1.084092146	Number of Tray Factor
F_{TT}=	1	Tray Type Factor
Material=	316 Stainless Steel	
F_{TM}=	1.643945069	Materials Factor for 316 Stainless Steel
C_{BT}=	661.3839898	Base Cost for Sieve Trays

C_T = $21,216.79

Purchase Cost of Distillation Column

Column	$69,449.93
Trays	$21,216.79

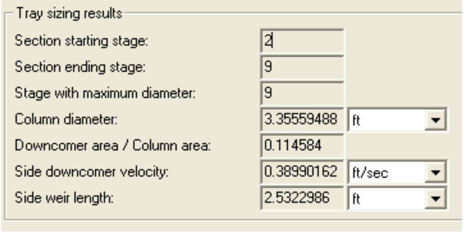
C_P= $90,666.72

D-501 TRAY SIZING AND TRAY COUNT

Stage	Temperatur F	Temperatur F	Mass flow l lb/hr	Mass flow v lb/hr	Volume flo cuft/hr	Volume flow v cuft/hr	Molecula	Molecula	Density l lb/cuft	Density v lb/cuft	Viscosity cP	Viscosity cP
1	274.4802	275.5265	26036.24	26036.24	538.5464	28616.4088	56.374	56.374	48.345	0.9098	0.199	0.0128
2	275.5265	278.0878	13614.57	27650.81	285.5252	29047.8607	61.597	58.83	47.683	0.9519	0.198	0.0127
3	278.0878	280.5934	14919.05	28955.29	316.7336	29417.7069	65.494	60.731	47.103	0.9843	0.1961	0.0127
4	280.5934	282.0355	15620.49	29656.74	334.0562	29615.4023	67.382	61.682	46.76	1.0014	0.1945	0.0126
5	282.0355	290.0157	56742.37	44242.37	1217.533	40683.1193	68.109	67.061	46.604	1.0875	0.1936	0.0125
6	290.0157	295.3215	61202.73	48702.73	1333.326	42664.8575	70.748	70.41	45.902	1.1415	0.1889	0.0124
7	295.3215	297.394	63456.4	50956.4	1393.934	43825.897	71.719	71.627	45.523	1.1627	0.1859	0.0123
8	297.394	298.133	64245.44	51745.44	1415.548	44205.4356	72.001	71.978	45.386	1.1706	0.1848	0.0123
9	298.133	298.4753	64488.61	51988.61	1422.363	44265.397	72.077	72.073	45.339	1.1745	0.1844	0.0123
10	298.4753	298.5016	12500	52075.37	275.822	44329.6166	72.097	72.089	45.319	1.1747	0.1842	0.0123

k-values

Stage	GBL	BDO	**THF**	**WATER**	NBUTANC	PROPANOL	α_{12}	η	# Trays
1	0.15541	0.009092	**0.948736**	**1.125093**	0.295195	0.45247321	1.19	0.70	1.43
2	0.282219	0.008548	**0.880222**	**1.497022**	0.292045	0.47314336	1.70	0.64	1.56
3	0.527133	0.008546	**0.859709**	**2.008015**	0.313757	0.53052826	2.34	0.60	1.68
4	0.787755	0.008792	**0.865335**	**2.408338**	0.337952	0.58358591	2.78	0.57	1.75
5	0.946731	0.008967	**0.871751**	**2.608609**	0.351418	0.61163988	2.99	0.56	1.78
6	2.238767	0.010213	**0.930112**	**3.718407**	0.433295	0.77549439	4.00	0.53	1.90
7	3.528871	0.011167	**0.975641**	**4.401976**	0.488479	0.88172013	4.51	0.51	1.95
8	4.137019	0.011549	**0.993091**	**4.651049**	0.509466	0.92137174	4.68	0.51	1.96
9	4.344841	0.011674	**0.998201**	**4.724306**	0.515967	0.93336876	4.73	0.51	1.97
10	4.418067	0.011721	**0.999588**	**4.745246**	0.51811	0.93709236	4.75	0.51	1.97
							Total Trays=		17.93



Tray sizing results

Section starting stage:	2	
Section ending stage:	9	
Stage with maximum diameter:	9	
Column diameter:	3.35559488	ft
Downcomer area / Column area:	0.114584	
Side downcomer velocity:	0.38990162	ft/sec
Side weir length:	2.5322986	ft

F-200: VERTICAL PRESSURE VESSEL

Estimation of Vessel Size

$$\boxed{W = \pi(D_i + t_s)(L + 0.8D_i)t_s\rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2P_d}}$$

Diameter (D_i)=	2.6430707 ft	--->	31.716849	in
Height (L)=	7.9292354 ft	--->	95.150824	in
Volume (V)=	21.74 ft3			

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_0 =	1995	psig	
P_d =	2116.965005	psig	
S =	15000	psia	maximum allowable stress for 482 F
E =	1.00		weld efficiency

At low P, check for min wall thickness= CORRELATION

t_s = 2.445168779 inches

Material Used : Stainless Steel 304

Density of Material: 0.2890183 lb/in^3

W = 9141.179904 lb

Purchase Cost of Flash Vessel

$$\boxed{C_V = \exp\{7.0132 + 0.18255\ln W + 0.02297(\ln W)^2\}}$$

C_v = $39,691.79 Cost of Empty Vert. Vessels for 4,200<W<1,000,000 lb including nozzles, manholes, and supports

$$\boxed{C_{PL} = 361.8(D_i)^{0.73960}(L)^{0.70684}}$$

C_{PL} = $3,208.28 Cost of platforms and ladders

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material= Stainless Steel 304

F_m = 1.7

C_P = $70,684.33

				FOR F-200			
LBS/HOUR=	55405.368	**INPUT ONLY ONE OF THESE**					
KG/HOUR=							
FLOW=							
VAPOR FRACTION=**INPUT THIS VALUE**	0.7760466		VAPDENSITY=	0.7090555	1	1 FOR LBS/FT3	OR 2 FO KG/CUM
LIQUID FRACTION=	0.2239534		LIQDENSITY=	47.559775			
			VAPDENSITY=	0.7090555	LBS/FT3		
L/D=	3		LIQDENSITY=	47.559775	LBS/FT3		
HOLD-UP TIME,MIN.=	5						
FRACTION OF DRUM FULL FOR HORIZ	0.5						
KFACTOR=	1			**1=DEFAULT=0.27**	0.27		
				2=USER INPUT			
					KFACTOR	FT/SEC	METERS/SEC
VELOCITYALLOWED,FT.SEC=				8.1286424	0.27	2.1947335	0.6689548
VFLOW RATE ,CUF/SEC				16.844452			
LFLOW RATE ,CUF/SEC				0.0724715			
FLOW, LBS/HOUR=					55405.368	LBS/HOUR TOTAL	
AREA REQ'D FOR VAPOR FT2	7.6749422	ACTUAL=	2.741935512	FT2ACTUA	GREATER THAN C18?OK! IF NOT THEN THIS AREA MUS		
VOLUME OF LIQUID HELD,FT3 FOR GIVEN HOLD UP TIME	21.74		0.615650524	meter3			
HEIGHT OF LIQUID IF VERTICAL,FT FOR GIVEN HOLDUP TIME&C18 AREA	7.9292354		2.416830936	meters			
DIAMETER FOR DRUM AT GIVEN HOLD UP, FEET FOR GIVEN %FULL	2.6430707		0.805607963	meters			
LENGTH OF LIQUID IF HORIZONTAL,FT FOR GIVEN HOLD UP TIME, %FULL	7.9292122		2.416823889	meters			
AREA REQ'D FOR LIQUID FT2 AT C9 FULL DRUM, HORIZONTAL	2.7419355		0.835741944	meter2			

F-300: VERTICAL PRESSURE VESSEL

Estimation of Vessel Size

$$\boxed{W = \pi (D_i + t_s)(L + 0.8 D_i) t_s \rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2 P_d}}$$

Diameter (D_i)=	3.6171158	ft	--->	43.405389	inches
Height (L)=	10.851389	ft	--->	130.21667	inches
Volume (V)=	55.72	ft3			

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_0 =	585.3	psig	
P_d =	670.1271099	psig	
S =	15000	psia	maximum allowable stress for 482 F
E =	1		weld efficiency

At low P, check for min wall thickness= CORRELATION

t_s = 0.996276202 inches

Material Used :	Stainless Steel 304	
Density of Material:	0.2890183	lb/in^3

W = 6624.953901 lb

Purchase Cost of Flash Vessel

$$\boxed{C_V = \exp\{7.0132 + 0.18255 \ln W + 0.02297 (\ln W)^2\}}$$

C_v = $32,781.33 Cost of Empty Vertical Vessels for 4,200<W<1,000,000 lb including nozzles, manholes, and supports

$$\boxed{C_{PL} = 361.8 (D_i)^{0.73960} (L)^{0.70684}}$$

C_{PL} = $5,050.75 Cost of platforms and ladders

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material= Stainless Steel 304

F_m = 1.7

C_P = $60,779.02

FOR F-300

LBS/HOUR=	42052.7	INPUT ONLY ONE OF THESE				
KG/HOUR=						
FLOW=						
VAPOR FRACTION=INPUT THIS VALUE	0.0175064	VAPDENSITY=	0.9594657	1	1 FOR LBS/FT3	OR 2 FO KG/CUM
LIQUID FRACTION=	0.9824936	LIQDENSITY=	61.786351			
		VAPDENSITY=	0.9594657 LBS/FT3			
L/D=	3	LIQDENSITY=	61.786351 LBS/FT3			
HOLD-UP TIME,MIN.=	5					
FRACTION OF DRUM FULL FOR HORIZ	0.5					
KFACTOR=	1		1=DEFAULT=0.27	0.27		
			2=USER INPUT			

		KFACTOR	FT/SEC	METERS/SEC
VELOCITYALLOWED,FT.SEC=	7.9621997	0.27	2.1497939	0.6552572
VFLOW RATE ,CUF/SEC	0.213137			
LFLOW RATE ,CUF/SEC	0.1857499			
FLOW, LBS/HOUR=		42052.7 LBS/HOUR TOTAL		

AREA REQ'D FOR VAPOR FT2	0.099143	ACTUAL=	5.135284139	FT2ACTUA GREATER THAN C18?OK! IF NOT THEN THIS AREA MUS
VOLUME OF LIQUID HELD,FT3 FOR GIVEN HOLD UP TIME	55.72		1.577958312	meter3
HEIGHT OF LIQUID IF VERTICAL,FT FOR GIVEN HOLDUP TIME&C18 AREA	10.851389		3.307503414	meters
DIAMETER FOR DRUM AT GIVEN HOLD UP, FEET FOR GIVEN %FULL	3.6171158		1.102496886	meters
LENGTH OF LIQUID IF HORIZONTAL,FT FOR GIVEN HOLD UP TIME, %FULL	10.851347		3.307490657	meters
AREA REQ'D FOR LIQUID FT2 AT C9 FULL DRUM, HORIZONTAL	5.1352841		1.565234606	meter2

F-400: VERTICAL PRESSURE VESSEL

Estimation of Vessel Size

$$\boxed{W = \pi(D_i + t_s)(L + 0.8D_i)t_s\rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2P_d}}$$

Diameter (D_i)=	0.7813261	ft	--->	9.3759131	in
Height (L)=	2.3439765	ft	--->	28.127719	in
Volume (V)=	0.56	ft^3			

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_0 =	150	psig	
P_d =	187.89395	psig	
S =	15000	psia	maximum allowable stress for 482 F
E =	1		weld efficiency

At low P, check for min wall thickness MIN

t_s = 0.25 inches

Material Used :	Stainless Steel 304	
Density of Material:	0.2890183	lb/in^3

W = 77.849197 lb

Purchase Cost of Flash Vessel

$$\boxed{C_V = \exp\{7.0132 + 0.18255 \ln W + 0.02297(\ln W)^2\}}$$

C_v = $3,803.85 Cost of Empty Vertical Vessels for 4,200<W<1,000,000 lb including nozzles, manholes, and supports

$$\boxed{C_{PL} = 361.8(D_i)^{0.73960}(L)^{0.70684}}$$

C_{PL} = $550.43 Cost of platforms and ladders

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material=	Stainless Steel 304
F_m =	1.7

C_P = $7,016.97

					FOR F-400		
LBS/HOUR=	1580.9064	INPUT ONLY ONE OF THESE					
KG/HOUR=							
FLOW=							
VAPOR FRACTION=INPUT THIS VALUE	0.7922803		VAPDENSITY=	0.1655851	1	1 FOR LBS/FT3	OR 2 FO KG/CUM
LIQUID FRACTION=	0.2077197		LIQDENSITY=	48.724234			
			VAPDENSITY=	0.1655851	LBS/FT3		
L/D=	3		LIQDENSITY=	48.724234	LBS/FT3		
HOLD-UP TIME,MIN.=	5						
FRACTION OF DRUM FULL FOR HORIZ	0.5						
KFACTOR=	1		1=DEFAULT=0.27		0.27		
			2=USER INPUT				
					KFACTOR	FT/SEC	METERS/SEC
VELOCITYALLOWED,FT.SEC=				17.124691	0.27	4.6236665	1.4092935
VFLOW RATE ,CUF/SEC				2.101171			
LFLOW RATE ,CUF/SEC				0.0018721			
FLOW, LBS/HOUR=					1580.9064	LBS/HOUR TOTAL	
AREA REQ'D FOR VAPOR FT2	0.4544383	ACTUAL=	0.239609657	FT2ACTUA	GREATER THAN C18?OK! IF NOT THEN THIS AREA MUS		
VOLUME OF LIQUID HELD,FT3	0.56		0.015903887	meter3			
FOR GIVEN HOLD UP TIME							
HEIGHT OF LIQUID IF VERTICAL,FT	2.3439765		0.714444051	meters			
FOR GIVEN HOLDUP TIME&C18 AREA							
DIAMETER FOR DRUM AT GIVEN	0.7813261		0.238148193	meters			
HOLD UP, FEET FOR GIVEN %FULL							
LENGTH OF LIQUID IF HORIZONTAL,FT	2.3439783		0.71444458	meters			
FOR GIVEN HOLD UP TIME, %FULL							
AREA REQ'D FOR LIQUID FT2	0.2396097		0.073033024	meter2			
AT C9 FULL DRUM, HORIZONTAL							

F-401: VERTICAL PRESSURE VESSEL

Estimation of Vessel Size

$$\boxed{W = \pi(D_i + t_s)(L + 0.8D_i)t_s\rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2P_d}}$$

Diameter (D_i)=	0.3695597	ft	--->	4.4347164	in
Height (L)=	1.1086758	ft	--->	13.304109	in
Volume (V)=	0.06	ft3			

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_0 =	150	psig	
P_d =	187.893948	psig	
S =	15000	psia	maximum allowable stress for 482 F
E =	1		weld efficiency

At low P, check for min wall thickness= MIN

t_s = 0.25 inches

Material Used : Stainless Steel 304

Density of Material: 0.2890183 lb/in^3

W = 17.92037138 lb

Purchase Cost of Flash Vessel

$$\boxed{C_V = \exp\{7.0132 + 0.18255 \ln W + 0.02297(\ln W)^2\}}$$

C_v = $2,278.65 Cost of Empty Vert.Vessels for 4,200<W<1,000,000 lb including nozzels, manholes, and supports

$$\boxed{C_{PL} = 361.8(D_i)^{0.73960}(L)^{0.70684}}$$

C_{PL} = $186.38 Cost of platforms and ladders

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material= Stainless Steel 304

F_m = 1.7

C_P = $4,060.08

FOR F-401							
LBS/HOUR=	656.58676	INPUT ONLY ONE OF THESE					
KG/HOUR=							
FLOW=							
VAPOR FRACTION=INPUT THIS VALUE	0.9453132		VAPDENSITY=	0.1121919	1	1 FOR LBS/FT3	OR 2 FO KG/CUM
LIQUID FRACTION=	0.0546868		LIQDENSITY=	50.347737			
			VAPDENSITY=	0.1121919	LBS/FT3		
L/D=	3		LIQDENSITY=	50.347737	LBS/FT3		
HOLD-UP TIME,MIN.=	5						
FRACTION OF DRUM FULL FOR HORIZ	0.5						
KFACTOR=	1			1=DEFAULT=0.27	0.27		
				2=USER INPUT			
					KFACTOR	FT/SEC	METERS/SEC
VELOCITYALLOWED,FT.SEC=				21.160442	0.27	5.7133193	1.7414197
VFLOW RATE ,CUF/SEC				1.5367516			
LFLOW RATE ,CUF/SEC				0.0001981			
FLOW, LBS/HOUR=					656.58676 LBS/HOUR TOTAL		
AREA REQ'D FOR VAPOR FT2	0.268977	ACTUAL=	0.053605441	FT2ACTUA GREATER THAN C18?OK! IF NOT THEN THIS AREA MUST			
VOLUME OF LIQUID HELD,FT3 FOR GIVEN HOLD UP TIME	0.06		0.001682903	meter3			
HEIGHT OF LIQUID IF VERTICAL,FT FOR GIVEN HOLDUP TIME&C18 AREA	1.1086758		0.337924379	meters			
DIAMETER FOR DRUM AT GIVEN HOLD UP, FEET FOR GIVEN %FULL	0.3695597		0.112641796	meters			
LENGTH OF LIQUID IF HORIZONTAL,FT FOR GIVEN HOLD UP TIME, %FULL	1.1086791		0.337925388	meters			
AREA REQ'D FOR LIQUID FT2 AT C9 FULL DRUM, HORIZONTAL	0.0536054		0.016338938	meter2			

H-200: FIRED HEATER (DOWTHERM A)

Purchase Cost of Thermal Fluid Heater

Thermophysical Properties of Dowtherm A Heating Fluid

Temp.	**Thermal Cond.**	**Density**	**Specific Heat**	**Heat Load**
°F	Btu/hr-ft2(°F/ft)	lb/ft3	Btu/lb-°F	Btu/hr
60	0.0805	66.37	0.373	
120	0.0775	64.72	0.396	
163.792788	-	64.691833	0.3963667	449369
180	0.0744	63.03	0.418	1754766.1
240	0.0713	61.3	0.441	1846692.1
300	0.0682	59.51	0.463	1936575.3
360	0.0651	57.65	0.485	2026458.6
420	0.062	55.72	0.507	2116341.8
480	0.059	53.7	0.529	2208267.9
540	0.0559	51.57	0.552	2302236.7
600	0.0528	49.29	0.575	2398248.4
660	0.0497	46.82	0.599	
720	0.0466	44.08	0.627	
780	0.0436	40.93	0.665	
				17038956 **Total Load**

T_{in}= 163.792788 °F

T_{out}= 660 °F

M= 68093.36656 lb/hr

Q= 17038955.9 Btu/hr (X-201 Duty)

$$\boxed{C_P = 12.74Q^{0.65}}$$

Cost for Dowtherm A Fired Heater

C_P= $639,156.73

H-400: REFRIDGERATION UNIT

Purchase Cost of Mechanical Refrigeration Unit

Thermophysical Properties of Dowtherm SR-1 (50% Ethylene Glycol, 50% Water) Coolant

Temp.	**Density**	**Thermal Cc**	**Specific Heat**	**Heat Load**
°F	(lb/ft3)	Btu/hr-ft2(°I	Btu/lb-°F	Btu/hr
-22	68.07	0.1926	0.739	-27395.68
-4	67.93	0.1989	0.748	-84232.05
50	67.34	0.2152	0.776	-20903.79
63.1551182	67.40537379	-	0.7765	
104	66.48	0.2275	0.803	
				-132531.5 **Total Load**

T_{in}= 63.1551182 °F

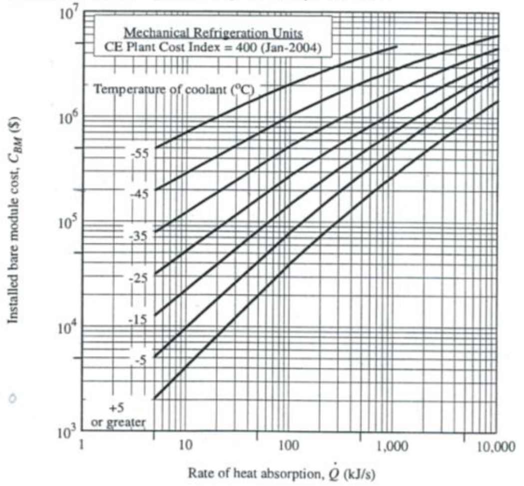
T_{out}= -22 °F

M= 2047.050878 lb/hr

X-400 Duty= -132531.52 Btu/hr

Q= -38.84115438 kJ/s

FIGURE 5.11 Bare module cost for air-cooled mechanical refrigeration units, complete except for the absorptive heat exchanger, which is part of main process module.



C_P= $200,000.00 (=$C_{BM}$ with Bare Module Factor=1)

HYDROGEN SEPARATION MEMBRANE

Estimation of Membrane Area

$$\boxed{\bar{P}_{Mi} = \frac{P_{Mi}}{l_M}}$$

Permeability(P_{Mi})=	250	barrer	--->	0.000000025 cm^3 (STP)-cm/(cm^2-s-cmHg)
Membrane Thickness(l_M)=	1000	Å	--->	0.00001 cm.
Permeance(P'_{Mi})=	0.0025	cm^3(STP)/cm^2-s-cmHg		
Hydrogen Molar Frac in Feed=	0.994			
Hydrogen Molar Flow (Ni)=	5,773	lbmol/hr	--->	1.603611111 lbmol/s
Hydrogen Volume Flow=	4960	ft^3/hr		
Molar Density(ρ_v)=	1.164	lbmol/ft^3	--->	4.1104E-05 lbmol/cm^3

$$\boxed{\bar{N}_i = \rho_V * A_M \frac{P_{Mi}}{l_M}(p_{iF} - p_{iP})}$$

Pressure Step(psi)	Pressure Step(cm Hg)	Area(ft^2)	Number Sections	Total Area(ft^2)	Cost($)
1	5.17	3248.41	300	974522.89	$9,745,228.91
5	25.86	649.68	60	38980.92	$389,809.16
10	51.71	324.84	30	9745.23	$97,452.29
15	77.57	216.56	20	4331.21	$43,312.13
20	103.42	162.42	15	2436.31	$24,363.07
25	129.28	129.94	12	1559.24	$15,592.37
30	155.13	108.28	10	1082.80	$10,828.03
35	180.99	92.81	8.57	795.53	$7,955.29
40	206.84	81.21	7.5	609.08	$6,090.77
45	232.70	72.19	6.67	481.25	$4,812.46
50	258.55	64.97	6	389.81	$3,898.09
55	284.41	59.06	5.45	322.16	$3,221.56
60	310.26	54.14	5	270.70	$2,707.01

Since our system almost exclusively involves hydrogen in the noncondensible stream, gas permeation is utilized to achieve the desired separation from methane, larger alkanes and alkanols, and THF. According to tabulated data, the permeability of hydrogen is 250 barrer at STP (Seader & Henley, Separation Process Principles, 2005, p. 526). According to plasticization pressure graphs, membrane permeability will initially decrease before ultimately increasing as pressure becomes greater (Katz, et al., 1974, p. 241). Though this value is not indicative of our operating conditions of 2009 psia and 40 °C, the plasticization pressure of our membrane can be considered to be negligible because our membrane's fibers are composed of polysulfonate polymer (Histed, 2009).

Further, permeance is defined as the ratio of a substance's permeability to the membrane's thickness (Seader & Henley, Separation Process Principles, 2005, p. 498). In this case, the membrane's suggested thickness is 1000 Å, or 10^{-5} cm, so the permeance is 250 barrer divided by 10^{-5} cm (Histed, 2009).

Using Aspen data from our simulation flowsheet, hydrogen's density was computed by dividing the molar flow rate by the volumetric flow rate to obtain hydrogen's molar density. Additionally, the incoming feed stream's total flowrate (S-201) and each individual component's flowrate were all provided by Aspen. Each component's permeate split fraction was provided by our industry consultant and in turn multiplied by Aspen's flowrate to determine the compositions of the retentate stream (S-203) and the permeate recycle stream (S-204) (Robbins, Split Fractions, 2009)

To compute the area, a variety of pressure drops across a certain section of the membrane were considered. The area was essentially computed by dividing the molar flowrate by the molar density, the permeance, and the corresponding pressure drop per section (Seader & Henley, Separation Process Principles, 2005, p. 527). After analyzing the various membrane areas, it was determined that three membranes connected in series, each with an area of approximately 3250 ft^2, would be optimal based on the physical feasibility of maintaining that section of the plant and also from an economic standpoint. In fact, since each square foot of the membrane costs $10 and the total area amounts to 9745.2 ft^2, the total expenditure for the membrane totals a mere $97,452 (Histed).

P-100: RECIPROCATING PUMP

					Low	High	
Check:	Flow Rate=	725.199626	ft^3/hr	Limits:	---	4010.4166	ft^3/hr
	Head=	5,755.24	ft		---	20000	ft
							OK

Purchase Cost of Reciprocating Pump and Motor

P_B= 206.011781 Hp brake horsepower

$$\boxed{C_B = \exp\{7.8103 + 0.26986 \ln P_B + 0.06718(\ln P_B)^2\}}$$

C_B= $69,921.35

$$\boxed{C_P = F_T F_M C_B}$$

F_T=	1	Type Factor
Material=	Ni-Al-Bronze	
F_M=	1.15	Materials Factor

C_P= $80,409.55

P-200: RADIAL CENTRIFUGAL PUMP

					Low	High
Check:	Flow Rate=	1,186.61	ft^3/hr	Limits:	80.2	40104.2
	Head=	7.5281458	ft		50	3200
	NPSH Available=	---	ft		5	---
						ERROR

Purchase Cost of Electric Motor

$$\boxed{P_B = \frac{QH\rho}{33000\eta_P}} \qquad \boxed{H = \frac{\Delta P}{\rho}}$$

$$\boxed{\eta_P = -0.316 + 0.24015(\ln Q) - 0.01199(\ln Q)^2}$$

Q_i=	1,186.61 ft^3/hr -->	147.94136 gal/min	
H=	7.528145836 ft		
ρ=	57.38464815 lb/ft^3		Average density of Dowtherm A over T range
η_P=	0.584367157		Fractional Efficiency of Pump
P_B=	**26.58233282 Hp**		Brake Horsepower

$$\boxed{\eta_M = 0.80 + 0.0319 \ln P_B - 0.00182(\ln P_B)^2}$$

η_M= 0.885056639 Motor Efficiency

$$\boxed{P_C = \frac{P_B}{\eta_M}}$$

P_C= 30.03461209 Consumed Power

$$\boxed{C_B = \exp\{5.8259 + 0.13141 \ln P_C + 0.053255(\ln P_C)^2 + 0.028628(\ln P_C)^3 - 0.0035549(\ln P_C)^4}$$

C_B= $1,883.04 Base Cost

$$\boxed{C_P = F_T C_B}$$

F_T= 1.8 1.7 for 1800 rpm, 1.8 for 3600 rpm

C_P= $3,389.47 Purchase Cost of Electric Motor

Purchase Cost of Centrifugal Pump

$$\boxed{S = Q(H)^{0.5}}$$

Q=	147.94136	gal/min	Flow Rate
H=	7.528146	ft	Pump Head in ft of Fluid
S=	405.91361		Size Factor

$$\boxed{C_B = \exp\{9.7171 - 0.6019 \ln S + 0.0519(\ln S)^2}$$

C_B=	$2,905.12	Base Cost (valid for S=[400,100000])

$$\boxed{C_P = F_T F_M C_B}$$

F_T=	1	Table 22.20
Material=	Carbon Steel	
F_M=	1	Materials Factor
C_P=	$2,905.12	Purchase Cost of Pump

Purchase Cost of Motor + Pump

C_P=	$6,294.59

P-300: RECIPROCATING PUMP

					Low	High
Check:	Flow Rate=	70.6798313	ft3/hr	Limits:	---	4010.4166
	Head=	4,619.38	ft		---	20000
						OK

Purchase Cost of Reciprocating Pump and Motor

P_B=	35.3407797	Hp	brake horsepower

$$\boxed{C_B = \exp\{7.8103 + 0.26986 \ln P_B + 0.06718(\ln P_B)^2\}}$$

C_B=	$15,156.50

$$\boxed{C_P = F_T F_M C_B}$$

F_T=	1	Type Factor
Material=	Ni-Al-Bronze	
F_M=	1.15	Materials Factor

C_P=	$17,429.97

P-301: RADIAL CENTRIFUGAL PUMP

					Low	High
Check:	Flow Rate=	1,037.69	ft^3/hr	Limits:	80.2	40104.2
	Head=	62	ft		50	3200
	NPSH Available=	---	ft		5	---
						OK

Purchase Cost of Electric Motor

$$P_B = \frac{QH\rho}{33000\eta_P}$$

$$H = \frac{\Delta P}{\rho}$$

$$\eta_P = -0.316 + 0.24015(\ln Q) - 0.01199(\ln Q)^2$$

h=	62	ft	Height of column
ρ=	57.5125117	lb/ft^3	Density of liquid
ΔP=	24.76233143	psi	Required pressure increase

Q_i= 1,037.69 ft^3/hr --> 129.37489 gal/min

H= 62 ft Head developed

η_P=	0.568022281	Fractional Efficiency of Pump
P_B=	**197.3986572 Hp**	Brake Horsepower

$$\eta_M = 0.80 + 0.0319 \ln P_B - 0.00182(\ln P_B)^2$$

η_M=	0.917759524	Motor Efficiency

$$P_C = \frac{P_B}{\eta_M}$$

P_C=	215.0875606 Hp	Consumed Power

$$C_B = \exp\{5.8259 + 0.13141 \ln P_C + 0.053255(\ln P_C)^2 + 0.028628(\ln P_C)^3 - 0.0035549(\ln P_C)^4$$

C_B=	$13,979.27	Base Cost

$$C_P = F_T C_B$$

F_T=	1.8	1.7 for 1800 rpm, 1.8 for 3600 rpm
C_P=	$25,162.69	Purchase Cost of Electric Motor

Purchase Cost of Centrifugal Pump

$$S = Q(H)^{0.5}$$

Q=	129.37489	gal/min	Flow Rate
H=	62.000000	ft	Pump Head in ft of Fluid
S=	1018.69891		Size Factor

$$C_B = \exp\{9.7171 - 0.6019 \ln S + 0.0519(\ln S)^2$$

C_B=	$3,096.38	Base Cost (valid for S=[400,100000])

$$C_P = F_T F_M C_B$$

F_T=	1	Table 22.20
Material=	Stainless Steel	
F_M=	2	Materials Factor
C_P=	$6,192.76	Purchase Cost of Pump

Purchase Cost of Motor + Pump

C_P= $31,355.45

P-302: RADIAL CENTRIFUGAL PUMP

					Low	High
Check:	Flow Rate=	1,049.80	ft^3/hr	Limits:	80.2	40104.2
	Head=	7.4864918	ft		50	3200
	NPSH Available=	---	ft		5	---
						ERROR

Purchase Cost of Electric Motor

$$\boxed{P_B = \frac{QH\rho}{33000\eta_P}} \qquad \boxed{H = \frac{\Delta P}{\rho}}$$

$$\boxed{\eta_P = -0.316 + 0.24015(\ln Q) - 0.01199(\ln Q)^2}$$

Q_i=	1,049.80	ft^3/hr	-->	130.8838 gal/min
H=	7.486491808	ft		
ρ=	57.7039301	lb/ft^3		
η_P=	0.569452637			Fractional Efficiency of Pump
P_B=	**24.13334914**	**Hp**		Brake Horsepower

$$\boxed{\eta_M = 0.80 + 0.0319\ln P_B - 0.00182(\ln P_B)^2}$$

η_M=	0.883110469	Motor Efficiency

$$\boxed{P_C = \frac{P_B}{\eta_M}}$$

P_C=	27.32766735	Consumed Power

$$\boxed{C_B = \exp\{5.8259 + 0.13141\ln P_C + 0.053255(\ln P_C)^2 + 0.028628(\ln P_C)^3 - 0.0035549(\ln P_C)^4}$$

C_B=	$1,726.57	Base Cost

$$\boxed{C_P = F_T C_B}$$

F_T=	1.8	1.7 for 1800 rpm, 1.8 for 3600 rpm
C_P=	$3,107.83	Purchase Cost of Electric Motor

Purchase Cost of Centrifugal Pump

$$\boxed{S = Q(H)^{0.5}}$$

Q=	130.8838049	gal/min	Flow Rate
H=	7.486491808	ft	Pump Head in ft of Fluid
S=	358.1171245		Size Factor

$$\boxed{C_B = \exp\{9.7171 - 0.6019\ln S + 0.0519(\ln S)^2}$$

C_B=	$2,899.65	Base Cost (valid for S=[400,100000])

$$\boxed{C_P = F_T F_M C_B}$$

F_T=	1	Table 22.20
Material=	Stainless Steel	
F_M=	2	Materials Factor
C_P=	$5,799.31	Purchase Cost of Pump

Purchase Cost of Motor + Pump

C_P=	$8,907.14

P-400: RADIAL CENTRIFUGAL PUMP

Check:				Limits:	Low	High
	Flow Rate=	30.24	ft^3/hr		80.2	40104.2
	Head=	6.3823805	ft		50	3200
	NPSH Available=	---	ft		5	---

Purchase Cost of Electric Motor

$$\boxed{P_B = \frac{QH\rho}{33000\eta_P}} \qquad \boxed{H = \frac{\Delta P}{\rho}}$$

$$\boxed{\eta_P = -0.316 + 0.24015(\ln Q) - 0.01199(\ln Q)^2}$$ for 50<Q<5000

Q_i=	30.24 ft^3/hr	--> 3.7705795 gal/min	
H=	6.382380522 ft		
ρ=	67.68634345 lb/ft^3		Average density of coolant over T range
η_P=	1		Fractional Efficiency of Pump, assumed 1
P_B=	**0.395910838 Hp**		Brake Horsepower

$$\boxed{\eta_M = 0.80 + 0.0319\ln P_B - 0.00182(\ln P_B)^2}$$

η_M= 0.768880021 — Motor Efficiency

$$\boxed{P_C = \frac{P_B}{\eta_M}}$$

P_C= 0.514918878 — Consumed Power

$$\boxed{C_B = \exp\{5.8259 + 0.13141\ln P_C + 0.053255(\ln P_C)^2 + 0.028628(\ln P_C)^3 - 0.0035549(\ln P_C)^4}$$

C_B= $315.16 — Base Cost

$$\boxed{C_P = F_T C_B}$$

F_T= 1.8 — 1.7 for 1800 rpm, 1.8 for 3600 rpm

$\boxed{C_P= \$567.29}$ — Purchase Cost of Electric Motor

Purchase Cost of Centrifugal Pump

$$\boxed{S = Q(H)^{0.5}}$$

Q=	3.77058	gal/min	Flow Rate
H=	6.382381	ft	Pump Head in ft of Fluid
S=	9.52576		Size Factor

$$\boxed{C_B = \exp\{9.7171 - 0.6019\ln S + 0.0519(\ln S)^2}$$

C_B= $5,564.13 — Base Cost (valid for S=[400,100000])

$$\boxed{C_P = F_T F_M C_B}$$

F_T=	1	Table 22.20
Material=	Carbon Steel	
F_M=	1	Materials Factor

$\boxed{C_P= \$5,564.13}$ — Purchase Cost of Pump

Purchase Cost of Motor + Pump

$\boxed{C_P= \$6,131.42}$

P-500: RADIAL CENTRIFUGAL PUMP

					Low	High
Check:	Flow Rate=	946.27	ft^3/hr	Limits:	80.2	40104.2
	Head=	94	ft		50	3200
	NPSH Available=	---	ft		5	---
						OK

Purchase Cost of Electric Motor

$$\boxed{P_B = \frac{QH\rho}{33000\eta_P}}$$

$$\boxed{H = \frac{\square P}{\rho}}$$

$$\boxed{\eta_P = -0.316 + 0.24015(\ln Q) - 0.01199(\ln Q)^2}$$

h=	94	ft	Height of column
ρ=	53.4057752	lb/ft^3	Density of liquid
ΔP=	34.86210326	psi	Required presure increase

Q_i= 946.27 ft^3/hr --> 117.97643 gal/min

H= 94 ft

η_P=	0.556530681	Fractional Efficiency of Pump
P_B=	**258.6591006 Hp**	Brake Horsepower

$$\boxed{\eta_M = 0.80 + 0.0319 \ln P_B - 0.00182(\ln P_B)^2}$$

η_M= 0.921048862 Motor Efficiency

$$\boxed{P_C = \frac{P_B}{\eta_M}}$$

P_C= 280.83103 Hp Consumed Power

$$\boxed{C_B = \exp\{5.8259 + 0.13141 \ln P_C + 0.053255(\ln P_C)^2 + 0.028628(\ln P_C)^3 - 0.0035549(\ln P_C)^4}$$

C_B= $17,998.29 Base Cost

$$\boxed{C_P = F_T C_B}$$

F_T= 1.8 1.7 for 1800 rpm, 1.8 for 3600 rpm

C_P= $32,396.92 Purchase Cost of Electric Motor

Purchase Cost of Centrifugal Pump

$$\boxed{S = Q(H)^{0.5}}$$

Q=	117.9764304	gal/min	Flow Rate
H=	94	ft	Pump Head in ft of Fluid
S=	1143.823931		Size Factor

$$\boxed{C_B = \exp\{9.7171 - 0.6019 \ln S + 0.0519(\ln S)^2}$$

C_B= $3,140.84 Base Cost (valid for S=[400,100000])

$$\boxed{C_P = F_T F_M C_B}$$

F_T=	1	Table 22.20
Material=	Stainless Steel	
F_M=	2	Materials Factor

C_P= $6,281.68 Purchase Cost of Pump

Purchase Cost of Motor + Pump

C_P= $38,678.60

P-501: RADIAL CENTRIFUGAL PUMP

					Low	High
Check:	Flow Rate=	763.37	ft^3/hr	Limits:	80.2	40104.2
	Head=	7.8160449	ft		50	3200
	NPSH Available=	---	ft		5	---
						ERROR

Purchase Cost of Electric Motor

$$\boxed{P_B = \frac{QH\rho}{33000\eta_P}} \qquad \boxed{H = \frac{\Delta P}{\rho}}$$

$$\boxed{\eta_P = -0.316 + 0.24015(\ln Q) - 0.01199(\ln Q)^2}$$

Q_i=	763.37	ft^3/hr	-->	95.173912 gal/min
H=	7.816044854	ft		
ρ=	55.2709213	lb/ft^3		
η_P=	0.528979053			Fractional Efficiency of Pump
P_B=	**18.89159997**	**Hp**		Brake Horsepower

$$\boxed{\eta_M = 0.80 + 0.0319\ln P_B - 0.00182(\ln P_B)^2}$$

η_M=	0.878027455	Motor Efficiency

$$\boxed{P_C = \frac{P_B}{\eta_M}}$$

P_C=	21.51595585	Consumed Power

$$\boxed{C_B = \exp\{5.8259 + 0.13141\ln P_C + 0.053255(\ln P_C)^2 + 0.028628(\ln P_C)^3 - 0.0035549(\ln P_C)^4}$$

C_B=	$1,397.97	Base Cost

$$\boxed{C_P = F_T C_B}$$

F_T=	1.8	1.7 for 1800 rpm, 1.8 for 3600 rpm
C_P=	$2,516.35	Purchase Cost of Electric Motor

Purchase Cost of Centrifugal Pump

$$\boxed{S = Q(H)^{0.5}}$$

Q=	95.17391239	gal/min	Flow Rate
H=	7.816044854	ft	Pump Head in ft of Fluid
S=	266.0795173		Size Factor

$$\boxed{C_B = \exp\{9.7171 - 0.6019\ln S + 0.0519(\ln S)^2}$$

C_B=	$2,905.59	Base Cost (valid for S=[400,100000])

$$\boxed{C_P = F_T F_M C_B}$$

F_T=	1	Table 22.20
Material=	Stainless Steel	
F_M=	2	Materials Factor
C_P=	$5,811.18	Purchase Cost of Pump

Purchase Cost of Motor + Pump

C_P=	$8,327.53

P-502: RADIAL CENTRIFUGAL PUMP

					Low	High
Check:	Flow Rate=	496.88	ft3/hr	Limits:	80.2	40104.2
	Head=	283.11545	ft		50	3200
	NPSH Available=	0	ft		5	---
						ERROR

Purchase Cost of Electric Motor

P_B= 8.06279945 Hp brake horsepower

$$\boxed{\eta_M = 0.80 + 0.0319 \ln P_B - 0.00182(\ln P_B)^2}$$

η_M= 0.858654503 motor efficiency

$$\boxed{P_C = \frac{P_B}{\eta_M}}$$

P_C= 9.390039207 consumed power

$$\boxed{C_B = \exp\{5.8259 + 0.13141 \ln P_C + 0.053255(\ln P_C)^2 + 0.028628(\ln P_C)^3 - 0.0035549(\ln P_C)^4}$$

C_B= $749.58 base cost

$$\boxed{C_P = F_T C_B}$$

F_T= 1.8 1.7 for 1800 rpm, 1.8 for 3600 rpm

C_P= $1,349.24 f.o.b. purchase cost for electric motor

Purchase Cost of Centrifugal Pump

$$\boxed{S = Q(H)^{0.5}}$$

Q=	61.94863408	gal/min	flow rate
H=	283.115448	ft	pump head in feet of fluid
S=	1042.349874		size factor

$$\boxed{C_B = \exp\{9.7171 - 0.6019 \ln S + 0.0519(\ln S)^2}$$

C_B= $3,104.80 base cost (valid for S=[400,100000])

$$\boxed{C_P = F_T F_M C_B}$$

F_T=	1	Table 22.20
Material=	Stainless Steel	
F_M=	2	Materials Factor

C_P= $6,209.59 purchase cost of pump

Purchase Cost of Motor + Pump

C_B= $3,854.37

C_P= $7,558.83

P-503: RADIAL CENTRIFUGAL PUMP

					Low	High
Check:	Flow Rate=	538.55	ft^3/hr	Limits:	80.2	40104.2
	Head=	50	ft		50	3200
	NPSH Available=	---	ft		5	---
						ERROR

Purchase Cost of Electric Motor

$$\boxed{P_B = \frac{Q H \rho}{33000 \eta_P}} \qquad \boxed{H = \frac{\Delta P}{\rho}}$$

$$\boxed{\eta_P = -0.316 + 0.24015(\ln Q) - 0.01199(\ln Q)^2}$$

h=	50	ft	Height of column
ρ=	48.3454036	lb/ft^3	Density of Liquid
ΔP=	16.78659847	psi	Required pressure increase

Q_i=	538.55	ft^3/hr	-->	67.143448	gal/min
H=	50	ft			

η_P=	0.481868021		Fractional Efficiency of Pump
P_B=	**81.86651001**	**Hp**	Brake Horsepower

$$\boxed{\eta_M = 0.80 + 0.0319 \ln P_B - 0.00182(\ln P_B)^2}$$

η_M=	0.905205602	Motor Efficiency

$$\boxed{P_C = \frac{P_B}{\eta_M}}$$

P_C=	90.43968552	Hp	Consumed Power

$$\boxed{C_B = \exp\{5.8259 + 0.13141 \ln P_C + 0.053255(\ln P_C)^2 + 0.028628(\ln P_C)^3 - 0.0035549(\ln P_C)^4}$$

C_B=	$5,719.24	Base Cost

$$\boxed{C_P = F_T C_B}$$

F_T=	1.8	1.7 for 1800 rpm, 1.8 for 3600 rpm
C_P=	$10,294.63	Purchase Cost of Electric Motor

Purchase Cost of Centrifugal Pump

$$\boxed{S = Q(H)^{0.5}}$$

Q=	67.14344836	gal/min	Flow Rate
H=	50	ft	Pump Head in ft of Fluid
S=	474.7758765		Size Factor

$$\boxed{C_B = \exp\{9.7171 - 0.6019 \ln S + 0.0519(\ln S)^2}$$

C_B=	$2,918.66	Base Cost (valid for S=[400,100000])

$$\boxed{C_P = F_T F_M C_B}$$

F_T=	1	Table 22.20
Material=	Stainless Steel	
F_M=	2	Materials Factor
C_P=	$5,837.32	Purchase Cost of Pump

Purchase Cost of Motor + Pump

C_P=	$16,131.95

P-504: RADIAL CENTRIFUGAL PUMP

					Low	High
Check:	Flow Rate=	1,422.36	ft^3/hr	Limits:	80.2	40104.2
	Head=	9.5282063	ft		50	3200
	NPSH Available=	---	ft		5	---
						ERROR

Purchase Cost of Electric Motor

$$P_B = \frac{QH\rho}{33000\eta_P}$$

$$H = \frac{\square P}{\rho}$$

$$\eta_P = -0.316 + 0.24015(\ln Q) - 0.01199(\ln Q)^2$$

Q_i=	1,422.36	ft3/hr	--> 177.33358 gal/min
H=	9.528206257	ft	
ρ=	45.3390689	lb/ft3	
η_P=	0.605769485		Fractional Efficiency of Pump
P_B=	**30.73780657**	**Hp**	Brake Horsepower

$$\eta_M = 0.80 + 0.0319\ln P_B - 0.00182(\ln P_B)^2$$

η_M=	0.88791735	Motor Efficiency

$$P_C = \frac{P_B}{\eta_M}$$

P_C=	34.61786907	Consumed Power

$$C_B = \exp\{5.8259 + 0.13141\ln P_C + 0.053255(\ln P_C)^2 + 0.028628(\ln P_C)^3 - 0.0035549(\ln P_C)^4$$

C_B=	$2,152.44	Base Cost

$$C_P = F_T C_B$$

F_T=	1.8	1.7 for 1800 rpm, 1.8 for 3600 rpm
C_P=	$3,874.40	Purchase Cost of Electric Motor

Purchase Cost of Centrifugal Pump

$$S = Q(H)^{0.5}$$

Q=	177.3335764	gal/min	Flow Rate
H=	9.528206257	ft	Pump Head in ft of Fluid
S=	547.3896073		Size Factor

$$C_B = \exp\{9.7171 - 0.6019\ln S + 0.0519(\ln S)^2$$

C_B=	$2,937.49	Base Cost (valid for S=[400,100000])

$$C_P = F_T F_M C_B$$

F_T=	1	Table 22.20
Material=	Stainless Steel	
F_M=	2	Materials Factor
C_P=	$5,874.98	Purchase Cost of Pump

Purchase Cost of Motor + Pump

C_P=	$9,749.38

R-100: REACTOR

Estimation of Reactor Size

Target STY=	600	lb THF/hr-1000 lb cat
Operating Hours=	8000	hr/year
Annual Production Rate=	100000000	lb THF/year
Production Rate=	12500	lb THF/hr
Catalyst Required=	20833.333	lb catalyst
Catalyst Density=	10	lb/ft3
Reactor Liquid Volume=	2083.3333	ft3
ΔP Across Reactor=	40	psi
$\rho_{\text{Reactants}}$=	62.4	lb/ft3
h=	92.307692	ft
Disengagement=	20	ft
Total height=	112.30769	ft
A=	22.569444	ft2
r=	2.6803129	ft

Estimation of Reactor Weight

$$\boxed{W = \pi(D_i + t_s)(L + 0.8D_i)t_s\rho}$$

$$\boxed{t_s = \frac{P_d Di}{2SE - 1.2P_d}}$$

Diameter (D_i)=	5.3606258	ft	--->	64.32751	in
Height (L)=	112.30769	ft	--->	1347.6923	in
Volume (V)=	2534.72	ft3			

$$\boxed{P_d = \exp\{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2}$$

P_0 =	2040	psig	
P_d =	2161.819714	psig	
S =	15000	psia	maximum allowable stress for 482 F
E =	1		weld efficiency

t_s = 5.074268804 in

Main

Material Used : Carbon Steel

Density of Material: 0.284 lb/in^3

W = 439620.4633 lb Weight of Carbon Steel

Coating

$t_{s,inner}$ = 0.25 in

Material Used: Stainless Steel

Density of Material: 0.2890183

W= 20337.94525 lb Weight of Stainless Steel Coating

Purchase Cost of Reactor

$$\boxed{C_V = \exp\{7.0132 + 0.18255 \ln W + 0.02297(\ln W)^2\}}$$

C_v = $596,384.61

$$\boxed{C_{PL} = 361.8(D_i)^{0.73960}(L)^{0.70684}}$$

C_{PL} = $35,245.83

$$\boxed{C_P = F_M C_V + C_{PL}}$$

Material= Carbon Steel with 1/4" Stainless Steel Coating

F_m = 1.2

C_P = $750,907.36

T-600: FLOATING-ROOF STORAGE TANK

Purchase Cost of THF Storage Tank

$$\boxed{C_P = 475 F_M V^{0.51}}$$

Pressure= 3

Holdup= 48 hours

Volume= 83325.4257 gallons

Material= Stainless Steel 316

F_m = 2.1

C_P = $322,484.95

X-100: HEAT EXCHANGER

Estimation of Heat Exchanger Size

U= 150 Btu/hr-ft^2 -F

Q= 2786743.43 Btu/hr

$$\boxed{A = \frac{Q}{U \Delta T_{LM}}}$$

$T_{C,i}$= 104.000003 F

$T_{C,o}$= 201.200002 F

$T_{H,i}$= 300.152258 F

$T_{H,o}$= 300.156288 F

$$\boxed{\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1 / \Delta T2)}}$$

$\Delta T1$= 98.952256 F

$\Delta T2$= 196.156285 F

ΔT_{LM}= **142.0541983** F

A= 130.7831078 ft2

Purchase Cost of Heat Exchanger (Fixed Head)

Type= Fixed Head

$$\boxed{C_P = F_P F_M F_L C_B}$$

$$\boxed{C_B = \exp(11.0545 - 0.9228 \ln A + 0.09861 (\ln A)^2\}}$$

$$\boxed{F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2}$$

For P>100 psig, else F_P=1

P= 50 psig

Material= Carbon Steel/Stainless Steel

C_B= $ 7,327.00

F_P= 1 Pressure Factor

F_M= 2.785503843 Materials Factor- Table 22.25

F_L= 1 Tube Length Factor

C_P= $ 20,409.40

X-200: HEAT EXCHANGER

Estimation of Heat Exchanger Size

U= 60 Btu/hr-ft^2 -F
Q= -49017997.3 Btu/hr

$$\boxed{A = \frac{Q}{U\,\Delta T_{LM}}}$$

$T_{C,i}$= 90 F
$T_{C,o}$= 297.718147 F
$T_{H,i}$= 480.397369 F
$T_{H,o}$= 104 F

$$\boxed{\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1/\Delta T2)}}$$

ΔT1= 182.679222 F
ΔT2= 14 F
ΔT_{LM}= **65.66780983** F

A= 12440.89949 ft2

Purchase Cost of Heat Exchanger (Fixed Head)

Type= Fixed Head

$$\boxed{C_P = F_P F_M F_L C_B}$$

$$\boxed{C_B = \exp\{11.0545 - 0.9228\ln A + 0.09861(\ln A)^2\}}$$

$$\boxed{F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2}$$

For P>100 psig, else F_P=1

P= 50 psig
Material= Carbon Steel/Stainless Steel
C_B= $ 67,521.70
F_P= 1 Pressure Factor
F_M= 3.622107278 Materials Factor- Table 22.25
F_L= 1 Tube Length Factor

C_P= $ 244,570.84

X-201: HEAT EXCHANGER

Estimation of Condenser Size

U= 102.5 Btu/hr-ft^2 -F
Q= 17038955.9 Btu/hr

$$\boxed{A = \frac{Q}{U\,\Delta T_{LM}}}$$

$T_{C,i}$= 148.792788 F
$T_{C,o}$= 572 F
$T_{H,i}$= 660 F
$T_{H,o}$= 163.792788 F

$$\boxed{\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1/\Delta T2)}}$$

ΔT1= 88 F
ΔT2= 15 F
ΔT_{LM}= **41.25956724** F

A= 4028.973816 ft2

Purchase Cost of Condenser (Floating Head HX)

Type= Fixed Head

$$\boxed{C_P = F_P F_M F_L C_B}$$

$$\boxed{C_B = \exp\{11.0545 - 0.9228\ln A + 0.09861(\ln A)^2\}}$$

$$\boxed{F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2}$$

For P>100 psig, else F_P=1

P= 3 psig
Material= Carbon Steel/Stainless Steel
C_B= $ 26,619.73
F_P= 1 Pressure Factor
F_M= 3.366870651 Materials Factor- Table 22.25
F_L= 1 Tube Length Factor

C_P= $ 89,625.18

X-300: CONDENSER (FIXED HEAD HX)

Estimation of Condenser Size

U= 100 Btu/hr-ft^2 -F
Q= -45344534 Btu/hr

$$\boxed{A = \frac{Q}{U \Delta T_{LM}}}$$

$T_{CW,i}$= 90 F
$T_{CW,o}$= 120 F
$T_{H,i}$= 222.179413 F
$T_{H,o}$= 168.526766 F

$$\boxed{\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1 / \Delta T2)}}$$

ΔT1= 102.179413 F
ΔT2= 78.526766 F
ΔT_{LM}= **89.83472797** F

A= 5047.550655 ft^2

Purchase Cost of Condenser (Fixed Head)

Type= Fixed Head

$$\boxed{C_P = F_P F_M F_L C_B}$$

$$\boxed{C_B = \exp(11.0545 - 0.9228 \ln A + 0.09861 (\ln A)^2\}}$$

$$\boxed{F_P = 0.9803 + 0.018 \left(\frac{P}{100}\right) + 0.0017 \left(\frac{P}{100}\right)^2}$$

For P>100 psig, else F_P=1

P= 65 psig
Material= Carbon Steel/Stainless Steel
C_B= $ 31,427.28
F_P= 1 Pressure Factor
F_M= 3.414947291 Materials Factor- Table 22.25
F_L= 1 Tube Length Factor

C_P= $ 107,322.50

X-301: REBOILER (THERMOSYPHON)

Estimation of Reboiler Size

U= 100 Btu/hr-ft^2 -F
Q= 47247168 Btu/hr

$$\boxed{A = \frac{Q}{U \Delta T_{LM}}}$$

$T_{CW,i}$= 234.489191 F
$T_{CW,o}$= 255.191569 F
$T_{H,i}$= 297.7 F
$T_{H,o}$= 297.7 F

$$\boxed{\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1 / \Delta T2)}}$$

ΔT1= 42.508431 F
ΔT2= 63.210809 F
ΔT_{LM}= **52.17689748** F

A= 9055.189229 ft^2 Tube Outside Area

Purchase Cost of Reboiler (Thermosyphon HX)

Type= Thermosyphon Reboiler

$$\boxed{C_P = F_P F_M F_L C_B}$$

$$\boxed{C_B = \exp(11.0545 - 0.9228 \ln A + 0.09861 (\ln A)^2\}}$$

$$\boxed{F_P = 0.9803 + 0.018 \left(\frac{P}{100}\right) + 0.0017 \left(\frac{P}{100}\right)^2}$$

For P>100 psig, else F_P=1

P= 50 psig
Material= Carbon Steel/Stainless Steel
C_B= $ 50,645.14
F_P= 1 Pressure Factor
F_M= 3.546373662 Materials Factor- Table 22.25
F_L= 1 Tube Length Factor

C_P= $ 179,606.58

X-400: HEAT EXCHANGER

Estimation of Condenser Size

U=	20	Btu/hr-ft^2 -F
Q=	-132531.52	Btu/hr

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

$T_{C,i}$=	-22	F
$T_{C,o}$=	63.1551182	F
$T_{H,i}$=	78.1551182	F
$T_{H,o}$=	0	F

$$\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1 / \Delta T2)}$$

ΔT1=	15	F
ΔT2=	22	F
ΔT_{LM}=	**18.27713213**	F
A=	**362.5610381**	**ft2**

Purchase Cost of Condenser (Floating Head HX)

Type= Fixed Head

$$C_P = F_P F_M F_L C_B$$

$$C_B = \exp(11.0545 - 0.9228 \ln A + 0.09861(\ln A)^2\}$$

$$F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2$$

For P>100 psig, else F_P=1

P=	3 psig	
Material=	Carbon Steel/Stainless Steel	
C_B=	$ 8,441.87	
F_P=	1	Pressure Factor
F_M=	2.932277834	Materials Factor- Table 22.25
F_L=	1	Tube Length Factor

C_P= $ 24,753.92

X-500: CONDENSER (FIXED HEAD HX)

Estimation of Condenser Size

U=	100	Btu/hr-ft^2 -F
Q=	-10973901	Btu/hr

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

$T_{CW,i}$=	90	F
$T_{CW,o}$=	120	F
$T_{H,i}$=	147.2947	F
$T_{H,o}$=	147.257571	F

$$\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1 / \Delta T2)}$$

ΔT1=	27.2947	F
ΔT2=	57.257571	F
ΔT_{LM}=	**40.44296411**	F
A=	**2713.426487**	**ft^2**

Purchase Cost of Condenser (Fixed Head)

Type= Fixed Head

$$C_P = F_P F_M F_L C_B$$

$$C_B = \exp(11.0545 - 0.9228 \ln A + 0.09861(\ln A)^2\}$$

$$F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2$$

For P>100 psig, else F_P=1

P=	65 psig	
Material=	Carbon Steel/Stainless Steel	
C_B=	$ 20,382.35	
F_P=	1	Pressure Factor
F_M=	3.285880222	Materials Factor- Table 22.25
F_L=	1	Tube Length Factor

C_P= $ 66,973.95

X-501: REBOILER (THERMOSYPHON)

Estimation of Reboiler Size

U= 100 Btu/hr-ft^2 -F
Q= 11195256.9 Btu/hr

$$\boxed{A = \frac{Q}{U\,\Delta T_{LM}}}$$

$T_{CW,i}$= 200.784331 F
$T_{CW,o}$= 210.81857 F
$T_{H,i}$= 297.7 F
$T_{H,o}$= 297.7 F

$$\boxed{\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1/\Delta T2)}}$$

ΔT1= 86.88143 F
ΔT2= 96.915669 F
ΔT_{LM}= **91.8071751** F

A= 1219.431585 ft^2 Tube Outside Area

Purchase Cost of Reboiler (Thermosyphon HX)

Type= Thermosyphon Reboiler

$$\boxed{C_P = F_P F_M F_L C_B}$$

$$\boxed{C_B = \exp\{11.0545 - 0.9228\ln A + 0.09861(\ln A)^2\}}$$

$$\boxed{F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2}$$

For P>100 psig, else F_P=1

P= 50 psig
Material= Carbon Steel/Stainless Steel
C_B= $ 13,049.24
F_P= 1 Pressure Factor
F_M= 3.13420517 Materials Factor- Table 22.25
F_L= 1 Tube Length Factor

C_P= $ 40,899.01

X-502: CONDENSER (FIXED HEAD HX)

Estimation of Condenser Size

U= 100 Btu/hr-ft^2 -F
Q= -5727471.8 Btu/hr

$$\boxed{A = \frac{Q}{U\,\Delta T_{LM}}}$$

$T_{CW,i}$= 90 F
$T_{CW,o}$= 120 F
$T_{H,i}$= 275.526521 F
$T_{H,o}$= 274.480245 F

$$\boxed{\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1/\Delta T2)}}$$

ΔT1= 155.526521 F
ΔT2= 184.480245 F
ΔT_{LM}= **169.5916532** F

A= 337.7213259 ft^2

Purchase Cost of Condenser (Fixed Head)

Type= Fixed Head

$$\boxed{C_P = F_P F_M F_L C_B}$$

$$\boxed{C_B = \exp\{11.0545 - 0.9228\ln A + 0.09861(\ln A)^2\}}$$

$$\boxed{F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2}$$

For P>100 psig, else F_P=1

P= 65 psig
Material= Carbon Steel/Stainless Steel
C_B= $ 8,303.74
F_P= 1 Pressure Factor
F_M= 2.921419915 Materials Factor- Table 22.25
F_L= 1 Tube Length Factor

C_P= $ 24,258.72

X-503: REBOILER (THERMOSYPHON)

Estimation of Reboiler Size

U= 100 Btu/hr-ft^2 -F
Q= 7640277.99 Btu/hr

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

$T_{CW,i}$= 298.132971 F
$T_{CW,o}$= 298.47527 F
$T_{H,i}$= 367.4 F
$T_{H,o}$= 367.4 F

$$\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1 / \Delta T2)}$$

ΔT1= 68.92473 F
ΔT2= 69.267029 F
ΔT_{LM}= **69.09573819** F

A= 1105.752423 ft^2 Tube Outside Area

Purchase Cost of Reboiler (Thermosyphon HX)

Type= Thermosyphon Reboiler

$$C_P = F_P F_M F_L C_B$$

$$C_B = \exp(11.0545 - 0.9228 \ln A + 0.09861 (\ln A)^2 \}$$

$$F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2$$

For P>100 psig, else F_P=1

P= 150 psig
Material= Carbon Steel/Stainless Steel
C_B= $ 12,463.85
F_P= 1.011125 Pressure Factor
F_M= 3.11670734 Materials Factor- Table 22.25
F_L= 1 Tube Length Factor

C_P= $ 39,278.33

X-600: HEAT EXCHANGER

Estimation of Heat Exchanger Size

U= 100 Btu/hr-ft^2 -F
Q= -1199440.08 Btu/hr

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

$T_{C,i}$= 90 F
$T_{C,o}$= 119.999924 F
$T_{H,i}$= 171.331187 F
$T_{H,o}$= 104 F

$$\Delta T_{LM} = \frac{\Delta T1 - \Delta T2}{\ln(\Delta T1 / \Delta T2)}$$

ΔT1= 51.331263 F
ΔT2= 14 F
ΔT_{LM}= **28.73309534** F

A= 417.4420005 ft2

Purchase Cost of Heat Exchanger (Fixed Head)

Type= Fixed Head

$$C_P = F_P F_M F_L C_B$$

$$C_B = \exp(11.0545 - 0.9228 \ln A + 0.09861 (\ln A)^2 \}$$

$$F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2$$

For P>100 psig, else F_P=1

P= 65 psig
Material= Carbon Steel/Stainless Steel
C_B= $ 8,748.79
F_P= 1 Pressure Factor
F_M= 2.954141429 Materials Factor- Table 22.25
F_L= 1 Tube Length Factor

C_P= $ 25,845.16

CATALYST COST

Estimation of Catalyst Charge and Regeneration Price

Charge Price (As recommended by BASF corporation)

Fabrication Charge	$	70.18	per kg
Rhodium Charge	$	18.65	per kg
Palladium Charge	$	3.63	per kg
Freight Charge	$	0.20	per kg
	$	92.66	per kg

*Note:

Rhodium charge based on 0.5% metal loading per kg and todays market price of $1160 per troy ounce

Palladium charge based on 0.5% metal loading per kg and todays market price of $226 per troy ounce

1% metal on carbon support catalyst requirement specified by project consultant, Wayne Robbins

Regeneration Price (As recommended by BASF corporation)

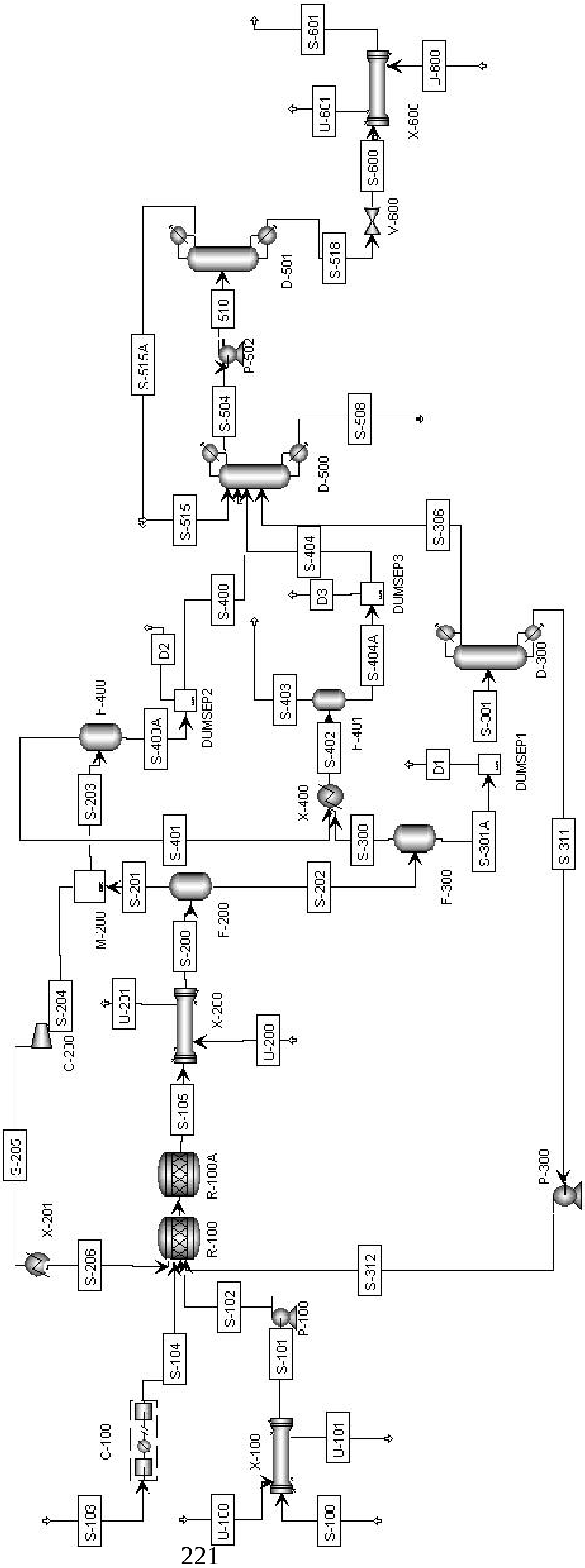
Treatment Charge	$	2.35	per kg
Refining Charge	$	12.00	per troy oz. Pd
	$	58.00	per troy oz. Re
Assay Charge	$	450.00	
Freight Charge	$	0.20	per kg

Cost of Catalyst and Regeneration

Catalyst Requirement	20833.3	lb	=>	9449.8259	kg
0.5% Pd	104.1665	lb	=>	1519.0948	troy ounce
0.5% Re	104.1665	lb	=>	1519.0948	troy ounce

Charge Cost	$875,600.00	
Regeneration Cost	$130,900.00	per year

A.3 ASPEN Simulation Results



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                                                                       TM
AAAAA   SSSSS   PPPPP   EEEEE   NN    N   PPPPP   L       U   U   SSSSS
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AAAAA   SSSSS   PPPPP   EEEEE   N   N N   PPPPP   L       U   U   SSSSS
A   A       S   P       E       N   NN    P       L       U   U       S
A   A   SSSSS   P       EEEEE   N     N   P       LLLLL   UUUUU   SSSSS

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ASPEN TECHNOLOGY, INC.                 U.S.A. 888/996-7100
TEN CANAL PARK                         EUROPE (32) 2/701-9555
CAMBRIDGE, MASSACHUSETTS 02141
617/949-1000

PLATFORM: WIN32                                         APRIL 2, 2009
VERSION: 21.0   Build 52                                THURSDAY
INSTALLATION:                                           6:49:48 P.M.
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                         TABLE OF CONTENTS
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TABLE OF CONTENTS

RUN CONTROL SECTION

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RUN CONTROL INFORMATION
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TYPE OF RUN: NEW

INPUT FILE NAME: _5458ipb.inm

OUTPUT PROBLEM DATA FILE NAME: _5458ipb
LOCATED IN:


PDF SIZE USED FOR INPUT TRANSLATION:
  NUMBER OF FILE RECORDS (PSIZE) =     0
  NUMBER OF IN-CORE RECORDS      =   256
PSIZE NEEDED FOR SIMULATION    =   256

CALLING PROGRAM NAME:          apmain
LOCATED IN:                    C:\PROGRA~1\ASPENT~1\ASPENP~2.5\Engine\xeq

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET
```

```
FLOWSHEET CONNECTIVITY BY STREAMS
---------------------------------

  STREAM     SOURCE     DEST           STREAM     SOURCE     DEST
  S-515      ----       D-500          U-200      ----       X-200
  S-103      ----       C-100          S-100      ----       X-100
  U-100      ----       X-100          U-600      ----       X-600
  S-201      F-200      M-200          S-202      F-200      F-300
  S-306      D-300      D-500          S-311      D-300      P-300
  S-504      D-500      P-502          S-508      D-500      ----
  S-515A     D-501      ----           S-518      D-501      V-600
  S-204      M-200      C-200          S-203      M-200      F-400
  DUMMY      R-100      R-100A         S-105      R-100A     X-200
  S-401      F-400      X-400          S-400A     F-400      DUMSEP2
  S-300      F-300      X-400          S-301A     F-300      DUMSEP1
  D1         DUMSEP1    ----           S-301      DUMSEP1    D-300
  510        P-502      D-501          S-102      P-100      R-100
  S-205      C-200      X-201          S-206      X-201      R-100
  D2         DUMSEP2    ----           S-400      DUMSEP2    D-500
  S-312      P-300      R-100          S-200      X-200      F-200
  U-201      X-200      ----           S-402      X-400      F-401
  S-403      F-401      ----           S-404A     F-401      DUMSEP3
  S-104      C-100      R-100          U-101      X-100      ----
  S-101      X-100      P-100          S-601      X-600      ----
  U-601      X-600      ----           D3         DUMSEP3    ----
  S-404      DUMSEP3    D-500          S-600      V-600      X-600

FLOWSHEET CONNECTIVITY BY BLOCKS
--------------------------------

  BLOCK        INLETS                         OUTLETS
  F-200        S-200                          S-201 S-202
  D-300        S-301                          S-306 S-311
  D-500        S-306 S-400 S-404 S-515        S-504 S-508
  D-501        510                            S-515A S-518
  M-200        S-201                          S-204 S-203
  R-100        S-102 S-104 S-312 S-206        DUMMY
  R-100A       DUMMY                          S-105
  F-400        S-203                          S-401 S-400A
  F-300        S-202                          S-300 S-301A
  DUMSEP1      S-301A                         D1 S-301
  P-502        S-504                          510
  P-100        S-101                          S-102
  C-200        S-204                          S-205
  X-201        S-205                          S-206
  DUMSEP2      S-400A                         D2 S-400
  P-300        S-311                          S-312
  X-200        S-105 U-200                    S-200 U-201
  X-400        S-300 S-401                    S-402
  F-401        S-402                          S-403 S-404A
  C-100        S-103                          S-104
  X-100        U-100 S-100                    U-101 S-101
  X-600        S-600 U-600                    S-601 U-601
  DUMSEP3      S-404A                         D3 S-404
  V-600        S-518                          S-600
```

```
CONVERGENCE STATUS SUMMARY
--------------------------

  DESIGN-SPEC SUMMARY
  ===================


  DESIGN                                                                 CONV
  SPEC      ERROR        TOLERANCE    ERR/TOL       VARIABLE    STAT  BLOCK
  ------    -----        ---------    -------       --------    ----  -----
  DS-1      0.16653E-05  0.10000E-02  0.16653E-02    161.03      #    $OLVER02
  DS-4     -0.76182E-04  0.10000E-02 -0.76182E-01    1926.4      #    $OLVER03
  DS-5       0.0000      0.10000E-03   0.0000        2402.1      #    $OLVER04
  DS-6      0.84131E-05  0.10000E-05   8.4131        2402.1      *    $OLVER05

  TEAR STREAM SUMMARY
  ===================


  STREAM    MAXIMUM                   MAXIMUM     VARIABLE             CONV
  ID        ERROR        TOLERANCE    ERR/TOL     ID              STAT  BLOCK
  ------    -------      ---------    --------    --------        ----  -----
  DUMMY     0.44793E-04  0.63452E-05   7.0593     MASS ENTHALPY    *   $OLVER01

  #  = CONVERGED
  *  = NOT CONVERGED
  LB = AT LOWER BOUNDS
  UB = AT UPPER BOUNDS

DESIGN-SPEC:  DS-1
------------------

  SAMPLED VARIABLES:
    T        : TEMPERATURE IN STREAM S-101 SUBSTREAM MIXED

  SPECIFICATION:
    MAKE T APPROACH 201.200
    WITHIN          0.00100000

  MANIPULATED VARIABLES:
    VARY     : TOTAL MOLEFLOW IN STREAM U-100 SUBSTREAM MIXED
    LOWER LIMIT =          50.0000                   LBMOL/HR
    UPPER LIMIT =       9,000.00                     LBMOL/HR
    FINAL VALUE =         161.030                    LBMOL/HR

  VALUES OF ACCESSED FORTRAN VARIABLES:
    VARIABLE      VALUE AT START      FINAL VALUE     UNITS
                     OF LOOP
    --------      --------------      -----------     -----
    T               267.699            201.200        F

DESIGN-SPEC:  DS-4
------------------

  SAMPLED VARIABLES:
    PRODT    : TEMPERATURE IN STREAM U-601 SUBSTREAM MIXED
```

```
DESIGN-SPEC:  DS-4 (CONTINUED)

  SPECIFICATION:
    MAKE PRODT APPROACH 120.000
    WITHIN          0.00100000

  MANIPULATED VARIABLES:
    VARY     : TOTAL MOLEFLOW IN STREAM U-600 SUBSTREAM MIXED
    LOWER LIMIT =       1,500.00                     LBMOL/HR
    UPPER LIMIT =       2,500.00                     LBMOL/HR
    FINAL VALUE =       1,926.42                     LBMOL/HR

  VALUES OF ACCESSED FORTRAN VARIABLES:
    VARIABLE      VALUE AT START      FINAL VALUE     UNITS
                     OF LOOP
    --------      --------------      -----------     -----
    PRODT           118.897            120.000        F

DESIGN-SPEC:  DS-5
------------------

  SAMPLED VARIABLES:
    BFWVF    : VAPOR FRACTION IN STREAM U-201 SUBSTREAM MIXED

  SPECIFICATION:
    MAKE BFWVF APPROACH 1.00000
    WITHIN          0.000100000

  MANIPULATED VARIABLES:
    VARY     : TOTAL MOLEFLOW IN STREAM U-200 SUBSTREAM MIXED
    LOWER LIMIT =          50.0000                   LBMOL/HR
    UPPER LIMIT =       9,000.00                     LBMOL/HR
    FINAL VALUE =       2,402.09                     LBMOL/HR

  VALUES OF ACCESSED FORTRAN VARIABLES:
    VARIABLE      VALUE AT START      FINAL VALUE     UNITS
                     OF LOOP
    --------      --------------      -----------     -----
    BFWVF          0.924844            1.00000

DESIGN-SPEC:  DS-6
------------------

  SAMPLED VARIABLES:
    TEMP     : TEMPERATURE IN STREAM U-201 SUBSTREAM MIXED

  SPECIFICATION:
    MAKE TEMP APPROACH 297.718
    WITHIN          0.100000-05
```

```
DESIGN-SPEC:  DS-6 (CONTINUED)

  MANIPULATED VARIABLES:
    VARY     : TOTAL MOLEFLOW IN STREAM U-200 SUBSTREAM MIXED
    LOWER LIMIT =       2,200.00                     LBMOL/HR
    UPPER LIMIT =       3,000.00                     LBMOL/HR
    FINAL VALUE =       2,402.09                     LBMOL/HR

  VALUES OF ACCESSED FORTRAN VARIABLES:
    VARIABLE      VALUE AT START      FINAL VALUE     UNITS
                     OF LOOP
    --------      --------------      -----------     -----
    TEMP            297.082            297.718        F

CONVERGENCE BLOCK:  $OLVER01
----------------------------
    Tear Stream  :  DUMMY
    Tolerance used:  0.100D-03
    Trace molefrac:  0.100D-05

    MAXIT=   60 WAIT   1 ITERATIONS BEFORE ACCELERATING
    QMAX =   0.0     QMIN =  -5.0
    METHOD: WEGSTEIN      STATUS: NOT CONVERGED
    TOTAL NUMBER OF ITERATIONS:    60

    ************************************************************************
    *                                                                      *
    *     BLOCK NOT CONVERGED                                              *
    *                                                                      *
    *     EXCEEDED MAXIMUM NUMBER OF ITERATIONS                            *
    *                                                                      *
    ************************************************************************


                         *** FINAL VALUES ***

   VARIABLE                       VALUE           PREV VALUE      ERR/TOL
TOTAL MOLEFLOW   LBMOL/HR     7805.7298      7803.8653         2.3892     *
MALEIC MOLEFLOW  LBMOL/HR      191.3836       191.3836     -2.3308-10
HYDROGENMOLEFLOW LBMOL/HR     6675.4055      6673.5377         2.7988     *
SUCCINICMOLEFLOW LBMOL/HR    5.7145-04      5.7145-04     -3.4445-07
GBL MOLEFLOW     LBMOL/HR       10.9019        10.9018     5.4069-02
BDO MOLEFLOW     LBMOL/HR        0.6422         0.6422        -0.1142
THF MOLEFLOW     LBMOL/HR       34.9989        34.9996        -0.1782
METHANE MOLEFLOW LBMOL/HR        1.2597         1.2597        -0.1633
NBUTANE MOLEFLOW LBMOL/HR        0.4853         0.4852         1.4297     *
WATER MOLEFLOW   LBMOL/HR      888.3702       888.3729     -3.0619-02
PROPANE MOLEFLOW LBMOL/HR    6.5864-02      6.5866-02        -0.3811
NBUTANOLMOLEFLOW LBMOL/HR        2.0534         2.0535        -0.1081
PROPANOLMOLEFLOW LBMOL/HR        0.1626         0.1626        -0.1157
PRESSURE         PSIA         2034.6959      2034.6959          0.0
MASS ENTHALPY    BTU/LB      -2726.0353     -2727.9611         7.0593     *

                         *** ITERATION HISTORY ***
```

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ASPEN PLUS   PLAT: WIN32     VER: 21.0                    04/02/2009  PAGE 6

                              FLOWSHEET SECTION

CONVERGENCE BLOCK:  $OLVER01 (CONTINUED)
```

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ASPEN PLUS   PLAT: WIN32     VER: 21.0                    04/02/2009  PAGE 7

                              FLOWSHEET SECTION

CONVERGENCE BLOCK:  $OLVER01 (CONTINUED)

    TEAR STREAMS:

    ITERATION   MAX-ERR/TOL   STREAM ID   VARIABLE
    ---------   -----------   ---------   --------
         1      0.1000E+07    DUMMY       PRESSURE
         2      0.1000E+05    DUMMY       THF MOLEFLOW
         3       2670.        DUMMY       NBUTANE MOLEFLOW
         4       1552.        DUMMY       PROPANE MOLEFLOW
         5      -3076.        DUMMY       PROPANE MOLEFLOW
         6       1113.        DUMMY       PROPANE MOLEFLOW
         7      -878.9        DUMMY       MASS ENTHALPY
         8       308.5        DUMMY       MASS ENTHALPY
         9       156.5        DUMMY       MASS ENTHALPY
        10       123.7        DUMMY       NBUTANE MOLEFLOW
        11      -388.5        DUMMY       NBUTANE MOLEFLOW
        12      -247.6        DUMMY       PROPANE MOLEFLOW
        13      -570.1        DUMMY       MASS ENTHALPY
        14       210.3        DUMMY       MASS ENTHALPY
        15       106.9        DUMMY       MASS ENTHALPY
        16       60.78        DUMMY       HYDROGENMOLEFLOW
        17      -105.0        DUMMY       NBUTANE MOLEFLOW
        18       88.68        DUMMY       MASS ENTHALPY
        19      -381.1        DUMMY       MASS ENTHALPY
        20       144.9        DUMMY       MASS ENTHALPY
        21       73.71        DUMMY       MASS ENTHALPY
        22       35.77        DUMMY       HYDROGENMOLEFLOW
        23       69.90        DUMMY       MASS ENTHALPY
        24       61.35        DUMMY       MASS ENTHALPY
        25      -258.9        DUMMY       MASS ENTHALPY
        26       100.4        DUMMY       MASS ENTHALPY
        27       51.10        DUMMY       MASS ENTHALPY
        28       22.53        DUMMY       HYDROGENMOLEFLOW
        29       48.79        DUMMY       MASS ENTHALPY
        30       42.61        DUMMY       MASS ENTHALPY
        31      -177.7        DUMMY       MASS ENTHALPY
        32       69.88        DUMMY       MASS ENTHALPY
        33       35.55        DUMMY       MASS ENTHALPY
        34       14.73        DUMMY       HYDROGENMOLEFLOW
        35       34.10        DUMMY       MASS ENTHALPY
        36       29.68        DUMMY       MASS ENTHALPY
        37      -122.7        DUMMY       MASS ENTHALPY
        38       48.71        DUMMY       MASS ENTHALPY
        39       24.78        DUMMY       MASS ENTHALPY
        40       9.861        DUMMY       HYDROGENMOLEFLOW
        41       23.86        DUMMY       MASS ENTHALPY
        42       20.71        DUMMY       MASS ENTHALPY
        43      -85.14        DUMMY       MASS ENTHALPY
        44       34.00        DUMMY       MASS ENTHALPY
        45       17.30        DUMMY       MASS ENTHALPY
        46       6.698        DUMMY       HYDROGENMOLEFLOW
        47       16.69        DUMMY       MASS ENTHALPY
        48       14.46        DUMMY       MASS ENTHALPY
        49      -59.23        DUMMY       MASS ENTHALPY
        50       23.76        DUMMY       MASS ENTHALPY
        51       12.09        DUMMY       MASS ENTHALPY
        52       4.593        DUMMY       HYDROGENMOLEFLOW
        53       11.68        DUMMY       MASS ENTHALPY
        54       10.11        DUMMY       MASS ENTHALPY
```

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 55      -41.29        DUMMY       MASS ENTHALPY
 56       16.61        DUMMY       MASS ENTHALPY
 57       8.448        DUMMY       MASS ENTHALPY
 58       3.171        DUMMY       HYDROGENMOLEFLOW
 59       8.160        DUMMY       MASS ENTHALPY
 60       7.059        DUMMY       MASS ENTHALPY
```

```
                              FLOWSHEET SECTION

CONVERGENCE BLOCK:  $OLVER02
----------------------------
    SPECS: DS-1
    MAXIT=   30 STEP-SIZE=    1.0000    % OF RANGE
                MAX-STEP=       100.    % OF RANGE
                XTOL=       1.000000E-08
    THE NEW ALGORITHM WAS USED WITH BRACKETING=NO
    METHOD: SECANT        STATUS: CONVERGED
    TOTAL NUMBER OF ITERATIONS:    13

                         *** FINAL VALUES ***

   VARIABLE                      VALUE           PREV VALUE      ERR/TOL
TOTAL MOLEFL     LBMOL/HR      161.0299       160.6643      1.6653-03

                         *** ITERATION HISTORY ***

    DESIGN-SPEC ID: DS-1

    ITERATION  VARIABLE         ERROR          ERR/TOL
    ---------  --------         -----          -------
         1      1000.            66.50         0.6650E+05
         2      1090.            97.15         0.9715E+05
         3      805.8            23.35         0.2335E+05
         4      716.1            18.24         0.1824E+05
         5      629.8            15.89         0.1589E+05
         6      254.7            13.93         0.1393E+05
         7      50.00     LB    -66.81        -0.6681E+05
         8      80.66           -48.26        -0.4826E+05
         9      192.1            13.98         0.1398E+05
        10      136.4           -14.74        -0.1474E+05
        11      163.8            1.657          1657.
        12      160.7          -0.2181         -218.1
        13      161.0           0.1665E-05     0.1665E-02

CONVERGENCE BLOCK:  $OLVER03
----------------------------
    SPECS: DS-4
    MAXIT=   30 STEP-SIZE=    1.0000    % OF RANGE
                MAX-STEP=       100.    % OF RANGE
                XTOL=       1.000000E-08
    THE NEW ALGORITHM WAS USED WITH BRACKETING=NO
    METHOD: SECANT        STATUS: CONVERGED
    TOTAL NUMBER OF ITERATIONS:     4

                         *** FINAL VALUES ***

   VARIABLE                      VALUE           PREV VALUE      ERR/TOL
TOTAL MOLEFL     LBMOL/HR     1926.4221      1923.2251     -7.6182-02

                         *** ITERATION HISTORY ***
```

```
CONVERGENCE BLOCK:  $OLVER03 (CONTINUED)

    DESIGN-SPEC ID: DS-4

    ITERATION  VARIABLE         ERROR          ERR/TOL
    ---------  --------         -----          -------
         1      2000.           -1.103         -1103.
         2      2010.           -1.247         -1247.
         3      1923.           0.4976E-01      49.76
         4      1926.          -0.7618E-04    -0.7618E-01

CONVERGENCE BLOCK:  $OLVER04
----------------------------
    SPECS: DS-5
    MAXIT=   30 STEP-SIZE=    1.0000    % OF RANGE
                MAX-STEP=       100.    % OF RANGE
                XTOL=       1.000000E-08
    THE NEW ALGORITHM WAS USED WITH BRACKETING=NO
    METHOD: SECANT        STATUS: CONVERGED
    TOTAL NUMBER OF ITERATIONS:   223
    NUMBER OF ITERATIONS ON LAST OUTER LOOP:     5

                         *** FINAL VALUES ***

   VARIABLE                       VALUE           PREV VALUE      ERR/TOL
TOTAL MOLEFL     LBMOL/HR     2402.0935      2484.0766         0.0

                         *** ITERATION HISTORY ***

    DESIGN-SPEC ID: DS-5

    ITERATION  VARIABLE         ERROR          ERR/TOL
    ---------  --------         -----          -------
         1      2561.          -0.7516E-01     -751.6
         2      2484.          -0.3934E-01     -393.4
         3      2447.          -0.2158E-01     -215.8
         4      2484.          -0.3938E-01     -393.8
         5      2402.            0.000          0.000

CONVERGENCE BLOCK:  $OLVER05
----------------------------
    SPECS: DS-6
```

```
CONVERGENCE BLOCK:  $OLVER05 (CONTINUED)
    MAXIT=   30 STEP-SIZE=    1.0000    % OF RANGE
                MAX-STEP=       100.    % OF RANGE
                XTOL=       1.000000E-08
    THE NEW ALGORITHM WAS USED WITH BRACKETING=NO
    METHOD: SECANT        STATUS: NOT CONVERGED
    TOTAL NUMBER OF ITERATIONS:   605
    NUMBER OF ITERATIONS ON LAST OUTER LOOP:     5

    ***********************************************************************
    *                                                                     *
    *     BLOCK NOT CONVERGED                                             *
    *                                                                     *
    *     DESIGN-SPEC FUNCTION NOT CHANGING                               *
    *                                                                     *
    ***********************************************************************


                         *** FINAL VALUES ***

   VARIABLE                       VALUE           PREV VALUE      ERR/TOL
TOTAL MOLEFL     LBMOL/HR     2402.0935      2402.0935         8.4131     *

                         *** ITERATION HISTORY ***

    DESIGN-SPEC ID: DS-6

    ITERATION  VARIABLE         ERROR          ERR/TOL
    ---------  --------         -----          -------
         1      2403.          -0.6365        -0.6365E+06
         2      2483.           -2.079        -0.2079E+07
         3      2367.            35.37         0.3537E+08
         4      2394.            8.089         0.8089E+07
         5      2402.           0.8413E-05      8.413
```

```
                              FLOWSHEET SECTION

COMPUTATIONAL SEQUENCE
----------------------

SEQUENCE USED WAS:
   ELECTRIC 150PSIG 50PSIG CW1
   $OLVER02 X-100
   (RETURN $OLVER02)
   C-100 P-100
   *$OLVER01 R-100A
   |  $OLVER04
   |  |  *$OLVER05 X-200
   |  |  (RETURN *$OLVER05)
   |  (RETURN $OLVER04)
   |  F-200 M-200 C-200 X-201 F-300 DUMSEP1 D-300 P-300 R-100
   (RETURN *$OLVER01)
   F-400 DUMSEP2 X-400 F-401 DUMSEP3 D-500 P-502 D-501 V-600
   $OLVER03 X-600
   (RETURN $OLVER03)

OVERALL FLOWSHEET BALANCE
-------------------------

                     ***  MASS AND ENERGY BALANCE  ***
                               IN           OUT       GENERATION   RELATIVE DIFF.
  CONVENTIONAL COMPONENTS
          (LBMOL/HR)
     MALEIC             191.340      0.201471E-08  -191.340     -0.207957E-13
     HYDROGEN           1063.00       83.5689      -977.563      0.175709E-02
     SUCCINIC           0.00000      0.515507E-08  0.515849E-08  0.664358E-03
     GBL               0.518980E-03   1.07767       1.07721      0.546968E-04
     BDO               0.252760E-15  0.319721E-03  0.312386E-03 -0.229410E-01
     THF                176.414       350.046       173.632     -0.178150E-05
     METHANE            0.00000       4.31571       4.31569     -0.476714E-05
     NBUTANE            0.00000       1.77503       1.77510      0.390794E-04
     WATER              5383.84       5958.86       575.014     -0.456477E-06
     PROPANE            0.00000      0.297507      0.297505     -0.843704E-05
     NBUTANOL          0.303440E-03   10.5399       10.5396     -0.210624E-05
     PROPANOL          0.159956E-01   4.03419       4.01819     -0.466138E-06
  TOTAL BALANCE
  MOLE(LBMOL/HR)        6814.61       6414.51      -398.233      0.273606E-03
  MASS(LB/HR   )        134065.       134062.                    0.274307E-04
  ENTHALPY(BTU/HR  )   -0.738667E+09 -0.713099E+09              -0.346143E-01
```

```
                           PHYSICAL PROPERTIES SECTION

COMPONENTS
----------

 ID       TYPE  FORMULA        NAME OR ALIAS                       REPORT NAME
  MALEIC   C     C4H4O4-D2      C4H4O4-D2                           MALEIC
  HYDROGEN C     H2             H2                                  HYDROGEN
  SUCCINIC C     C4H6O4-2       C4H6O4-2                            SUCCINIC
  GBL      C     C4H6O2-D2      C4H6O2-D2                           GBL
  BDO      C     C4H10O2-D2     C4H10O2-D2                          BDO
  THF      C     C4H8O-4        C4H8O-4                             THF
  METHANE  C     CH4            CH4                                 METHANE
  NBUTANE  C     C4H10-1        C4H10-1                             NBUTANE
  WATER    C     H2O            H2O                                 WATER
  PROPANE  C     C3H8           C3H8                                PROPANE
  NBUTANOL C     C4H10O-1       C4H10O-1                            NBUTANOL
  PROPANOL C     C3H8O-1        C3H8O-1                             PROPANOL

 LISTID         SUPERCRITICAL COMPONENT LIST
  HC-1           HYDROGEN
```

```
                             U-O-S BLOCK SECTION

BLOCK:  C-100    MODEL: MCOMPR
------------------------------
  INLET STREAMS:    S-103        TO STAGE   1
  OUTLET STREAMS:   S-104      FROM STAGE   2
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                            IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1063.00         1063.00         0.00000
      MASS(LB/HR   )            2142.88         2142.88         0.00000
      ENTHALPY(BTU/HR  )       -58846.3        0.241097E+07    -1.02441

                       ***  INPUT DATA  ***

  POLYTROPIC COMPRESSOR USING ASME METHOD
  NUMBER OF STAGES                                            2
  FINAL PRESSURE, PSIA                                    2,054.70

                 COMPRESSOR SPECIFICATIONS PER STAGE

  STAGE                    MECHANICAL      POLYTROPIC
  NUMBER                   EFFICIENCY      EFFICIENCY


    1                       1.000          0.7200
    2                       1.000          0.7200

                 COOLER SPECIFICATIONS PER STAGE


  STAGE      PRESSURE        COOLER
  NUMBER     DROP            SPECIFICATION
             PSI
    1         0.000          OUTLET TEMPERATURE   104.0      F
    2         0.000          HEAT DUTY            0.000      BTU/HR

                        ***  RESULTS  ***

  FINAL PRESSURE, PSIA                                    2,054.70
  TOTAL WORK REQUIRED, HP                                 1,644.13
  TOTAL COOLING DUTY , BTU/HR                        -1,713,550.
```

```
                             U-O-S BLOCK SECTION

BLOCK:  C-100    MODEL: MCOMPR (CONTINUED)

                          ***  PROFILE  ***

                          COMPRESSOR PROFILE

  STAGE      OUTLET       PRESSURE     OUTLET
  NUMBER     PRESSURE     RATIO        TEMPERATURE
             PSIA                      F

    1        737.5        2.786        334.3
    2        2055.        2.786        389.7

  STAGE      INDICATED      BRAKE
  NUMBER     HORSEPOWER     HORSEPOWER
             HP             HP
    1        783.2          783.2
    2        860.9          860.9

                          COOLER PROFILE

  STAGE      OUTLET          OUTLET       COOLING     VAPOR
  NUMBER     TEMPERATURE     PRESSURE     LOAD        FRACTION
             F               PSIA         BTU/HR

    1         104.0           737.5       -.1714E+07   1.000
    2         389.7           2055.        0.000       1.000

                      ***  ASSOCIATED  UTILITIES  ***

UTILITY USAGE:  ELECTRIC  (ELECTRICITY)
------------------------------
COMPRESSOR STAGE   1    584.0376                       29.2019
COMPRESSOR STAGE   2    641.9877                       32.0994
                   -------------                     -------------
TOTAL:                 1226.0253  KW                   61.3013  $/HR
                   =============
UTILITY USAGE:  CW1       (WATER)
------------------------------
COOLER STAGE       1   5.7348+04                      573.4828
                   -------------                     -------------
TOTAL:                 5.7348+04  LB/HR               573.4828  $/HR
                   =============
```

```
                             U-O-S BLOCK SECTION

BLOCK:  C-200    MODEL: COMPR
-----------------------------
  INLET STREAM:          S-204
  OUTLET STREAM:         S-205
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            5691.68         5691.68         0.00000
      MASS(LB/HR   )            11771.8         11771.8         0.00000
      ENTHALPY(BTU/HR  )        544640.        0.236869E+07   -0.770067

                          ***  INPUT DATA  ***

  POLYTROPIC COMPRESSOR USING ASME METHOD
   OUTLET PRESSURE  PSIA                                    2,054.70
   POLYTROPIC EFFICIENCY                                        0.72000
   MECHANICAL EFFICIENCY                                        1.00000

                          ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                      716.879
   BRAKE      HORSEPOWER REQUIREMENT  HP                      716.879
   NET WORK REQUIRED                  HP                      716.879
   POWER LOSSES                       HP                        0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                      510.851
   CALCULATED OUTLET TEMP  F                                  148.793
   EFFICIENCY (POLYTR/ISENTR) USED                              0.72000
   OUTLET VAPOR FRACTION                                        1.00000
   HEAD DEVELOPED,       FT-LBF/LB                         86,816.4
   MECHANICAL EFFICIENCY USED                                   1.00000
   INLET HEAT CAPACITY RATIO                                    1.41987
   INLET VOLUMETRIC FLOW RATE , CUFT/HR                    21,650.4
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                    19,595.9
   INLET  COMPRESSIBILITY FACTOR                                1.07276
   OUTLET COMPRESSIBILITY FACTOR                                1.08338
   AV. ISENT. VOL. EXPONENT                                     1.53072
   AV. ISENT. TEMP EXPONENT                                     1.40134
   AV. ACTUAL VOL. EXPONENT                                     1.84363
   AV. ACTUAL TEMP EXPONENT                                     1.67775
```

```
                             U-O-S BLOCK SECTION

BLOCK:  C-200    MODEL: COMPR (CONTINUED)

                      ***  ASSOCIATED  UTILITIES  ***

 UTILITY ID FOR ELECTRICITY              ELECTRIC
 RATE OF CONSUMPTION                     534.5764  KW
 COST                                     26.7288  $/HR

BLOCK:  D-300    MODEL: RADFRAC
-------------------------------
   INLETS   - S-301    STAGE   5
   OUTLETS  - S-306    STAGE   1
              S-311    STAGE  10
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG
  HENRY-COMPS ID:        HC-1

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1636.72         1636.72       -0.138921E-15
      MASS(LB/HR   )            41778.9         41778.9        0.687559E-12
      ENTHALPY(BTU/HR  )      -0.198780E+09   -0.196878E+09   -0.957159E-02
```

```
BLOCK:  D-300    MODEL: RADFRAC (CONTINUED)


                        **********************
                        ****  INPUT DATA  ****
                        **********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                                        10
   ALGORITHM OPTION                                       NONIDEAL
   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                  102
   MAXIMUM NO. OF INSIDE LOOP ITERATIONS                   10
   MAXIMUM NUMBER OF FLASH ITERATIONS                      50
   FLASH TOLERANCE                                           0.000100000
   OUTSIDE LOOP CONVERGENCE TOLERANCE                        0.000100000

  ****   COL-SPECS   ****

   MOLAR VAPOR DIST / TOTAL DIST                             0.0
   MOLAR REFLUX RATIO                                        0.60000
   MOLAR BOTTOMS RATE             LBMOL/HR                  75.0000

  ****   THERMOSYPHON REBOILER   ****

   VAPOR FRACTION                                            0.30000

  ****    PROFILES   ****

   P-SPEC          STAGE   1  PRES, PSIA                    20.0000
                           2                                20.0000
```

```
BLOCK:  D-300    MODEL: RADFRAC (CONTINUED)

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

  ***   COMPONENT SPLIT FRACTIONS   ***

                                OUTLET STREAMS
                                --------------
                     S-306       S-311
   COMPONENT:
   MALEIC      .34669E-14   1.0000
   SUCCINIC    .55275E-16   1.0000
   GBL         .22066E-01   .97793
   BDO         .11918E-03   .99988
   THF        1.0000        .16160E-10
   WATER       .98251       .17487E-01
   NBUTANOL   1.0000        .19140E-07
   PROPANOL   1.0000        .22450E-07


  ***    SUMMARY OF KEY RESULTS    ***

   TOP STAGE TEMPERATURE         F                          168.527
   BOTTOM STAGE TEMPERATURE      F                          255.192
   TOP STAGE LIQUID FLOW         LBMOL/HR                   939.178
   BOTTOM STAGE LIQUID FLOW      LBMOL/HR                 7,378.85
   TOP STAGE VAPOR FLOW          LBMOL/HR                     0.0
   BOTTOM STAGE VAPOR FLOW       LBMOL/HR                 2,696.28
   MOLAR REFLUX RATIO                                         0.60000
   MOLAR BOILUP RATIO                                        37.7521
   CONDENSER DUTY (W/O SUBCOOL)  BTU/HR                     -0.453445+08
   REBOILER DUTY                 BTU/HR                      0.472472+08


  ****   MANIPULATED VARIABLES   ****

                                                    BOUNDS           CALCULATED
                                              LOWER         UPPER       VALUE
  MOLAR BOTTOMS RATE         LBMOL/HR        50.000        120.00      71.421

  ****    DESIGN SPECIFICATIONS   ****

NO  SPEC-TYPE     QUALIFIERS              UNIT       SPECIFIED     CALCULATED
                                                       VALUE         VALUE
 1  MASS-FRAC     STREAMS: S-311                      0.10000       0.10000
                  COMPS:   WATER
```

```
                             U-O-S BLOCK SECTION

BLOCK:  D-300    MODEL: RADFRAC (CONTINUED)

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

   DEW POINT                        0.32212E-05  STAGE= 10
   BUBBLE POINT                     0.51626E-05  STAGE= 10
   COMPONENT MASS BALANCE           0.10835E-07  STAGE= 10 COMP=SUCCINIC
   ENERGY BALANCE                   0.60935E-06  STAGE=  1


  ****    PROFILES   ****

  **NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS
           FROM THE STAGE EXCLUDING ANY SIDE PRODUCT.  FOR THE FIRST STAGE,
           THE REPORTED VAPOR FLOW IS THE VAPOR DISTILLATE FLOW.  FOR THE
           LAST STAGE, THE REPORTED LIQUID FLOW IS THE LIQUID BOTTOMS FLOW.

                                                 ENTHALPY
STAGE TEMPERATURE   PRESSURE                     BTU/LBMOL           HEAT DUTY
      F             PSIA            LIQUID       VAPOR          BTU/HR

  1   168.53        20.000      -0.11844E+06  -85090.      -.45345+08
  2   222.18        20.000      -0.12036E+06 -0.10034E+06
  4   226.11        20.500      -0.12078E+06 -0.10137E+06
  5   227.14        20.750      -0.12143E+06 -0.10148E+06
  6   231.36        21.000      -0.12139E+06 -0.10301E+06
  7   232.11        21.250      -0.12142E+06 -0.10304E+06
  8   232.91        21.500      -0.12168E+06 -0.10309E+06
  9   234.49        21.750      -0.12338E+06 -0.10334E+06
 10   255.19        22.000      -0.16074E+06 -0.10487E+06   .47247+08

STAGE     FLOW RATE                  FEED RATE               PRODUCT RATE
           LBMOL/HR                  LBMOL/HR                  LBMOL/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID    VAPOR
  1  939.2      0.000                                     1565.2969
  2  971.9      2504.
  4  972.9      2539.
  5  2788.      2538.      1636.7177
  6  2800.      2717.
  7  2802.      2729.
  8  2801.      2730.
  9  2768.      2729.
 10  71.42      2696.                                       71.4207

   ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE                  FEED RATE               PRODUCT RATE
           LB/HR                     LB/HR                     LB/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID    VAPOR
  1 0.2238E+05  0.000                                     .37300+05
  2 0.1778E+05 0.5968E+05
  4 0.1832E+05 0.5528E+05
```

```
                             U-O-S BLOCK SECTION

BLOCK:  D-300    MODEL: RADFRAC (CONTINUED)

   ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE                  FEED RATE               PRODUCT RATE
           LB/HR                     LB/HR                     LB/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID    VAPOR
  5 0.5458E+05 0.5562E+05  .41779+05
  6 0.5462E+05 0.5010E+05
  7 0.5481E+05 0.5015E+05
  8 0.5568E+05 0.5034E+05
  9 0.6058E+05 0.5120E+05
 10  4479.     0.5610E+05                                4478.6469

                        ****   MOLE-X-PROFILE     ****
  STAGE     MALEIC        SUCCINIC      GBL           BDO           THF
    1     0.0000        0.0000       0.62848E-03   0.19684E-06   0.97794E-01
    2     0.0000        0.0000       0.26445E-02   0.33247E-05   0.13832E-02
    4    0.57234E-08   0.15406E-07   0.10801E-01   0.14310E-03   0.94427E-03
    5    0.15720E-04   0.11916E-03   0.20499E-01   0.98767E-03   0.11184E-02
    6    0.15653E-04   0.11865E-03   0.20632E-01   0.98378E-03   0.19571E-04
    7    0.15646E-04   0.11860E-03   0.21536E-01   0.98217E-03   0.34712E-06
    8    0.15650E-04   0.11863E-03   0.26143E-01   0.99063E-03   0.66052E-08
    9    0.16021E-04   0.12054E-03   0.55203E-01   0.13919E-02   0.18473E-09
   10    0.61364E-03   0.46519E-02   0.61046       0.36194E-01   0.34635E-10

                        ****   MOLE-X-PROFILE     ****
  STAGE     WATER         NBUTANOL      PROPANOL
    1    0.89236       0.66782E-02   0.25396E-02
    2    0.99552       0.30700E-03   0.14431E-03
    4    0.98782       0.20203E-03   0.93814E-04
    5    0.97692       0.23641E-03   0.10541E-03
    6    0.97821       0.12207E-04   0.64904E-05
    7    0.97735       0.63466E-06   0.40222E-06
    8    0.97273       0.35103E-07   0.26110E-07
    9    0.94327       0.28458E-08   0.22444E-08
   10    0.34808       0.28013E-08   0.12495E-08

                        ****   MOLE-Y-PROFILE     ****
  STAGE     MALEIC        SUCCINIC      GBL           BDO           THF
    1     0.0000        0.0000       0.12851E-04   0.90497E-09   0.70841
    2     0.0000        0.0000       0.62848E-03   0.19684E-06   0.97794E-01
    4    0.80652E-12   0.77117E-12   0.25674E-02   0.86485E-05   0.60620E-01
    5    0.21939E-08   0.59054E-08   0.45277E-02   0.54973E-04   0.60670E-01
    6    0.25941E-08   0.69714E-08   0.49905E-02   0.62191E-04   0.11478E-02
    7    0.26352E-08   0.70802E-08   0.51948E-02   0.62276E-04   0.20083E-04
    8    0.26500E-08   0.71186E-08   0.61292E-02   0.61020E-04   0.35620E-06
    9    0.26135E-08   0.69652E-08   0.10853E-01   0.69462E-04   0.67771E-08
   10    0.19116E-06   0.50982E-06   0.40495E-01   0.47005E-03   0.18871E-09
```

```
BLOCK:  D-300    MODEL: RADFRAC (CONTINUED)

                        ****   MOLE-Y-PROFILE     ****
  STAGE     WATER         NBUTANOL      PROPANOL
     1    0.27955       0.80920E-02   0.39374E-02
     2    0.89236       0.66782E-02   0.25396E-02
     4    0.93101       0.41896E-02   0.16001E-02
     5    0.92895       0.41958E-02   0.16021E-02
     6    0.99345       0.24262E-03   0.10818E-03
     7    0.99470       0.12526E-04   0.66602E-05
     8    0.99381       0.65119E-06   0.41271E-06
     9    0.98908       0.35949E-07   0.26761E-07
    10    0.95903       0.28470E-08   0.22708E-08

                        ****   K-VALUES           ****
  STAGE     MALEIC        SUCCINIC      GBL           BDO           THF
     1    0.62606E-05   0.22801E-05   0.20448E-01   0.45976E-02    7.2438
     2    0.12591E-03   0.44787E-04   0.23765       0.59206E-01    70.700
     4    0.14092E-03   0.50057E-04   0.23770       0.60438E-01    64.197
     5    0.13956E-03   0.49559E-04   0.22087       0.55660E-01    54.248
     6    0.16573E-03   0.58756E-04   0.24189       0.63216E-01    58.647
     7    0.16842E-03   0.59699E-04   0.24122       0.63407E-01    57.857
     8    0.16933E-03   0.60008E-04   0.23445       0.61598E-01    53.927
     9    0.16313E-03   0.57784E-04   0.19660       0.49904E-01    36.686
    10    0.31151E-03   0.10959E-03   0.66336E-01   0.12987E-01    5.4484

                        ****   K-VALUES           ****
  STAGE     WATER         NBUTANOL      PROPANOL
     1    0.31327        1.2117        1.5504
     2    0.89638        21.753        17.598
     4    0.94250        20.737        17.056
     5    0.95090        17.748        15.199
     6     1.0156        19.876        16.668
     7     1.0178        19.737        16.559
     8     1.0217        18.551        15.806
     9     1.0486        12.632        11.923
    10     2.7552        1.0163        1.8173

                        ****   MASS-X-PROFILE     ****
  STAGE     MALEIC        SUCCINIC      GBL           BDO           THF
     1     0.0000        0.0000       0.22705E-02   0.74443E-06   0.29592
     2     0.0000        0.0000       0.12445E-01   0.16379E-04   0.54522E-02
     4    0.35286E-07   0.96630E-07   0.49389E-01   0.68499E-03   0.36165E-02
     5    0.93224E-04   0.71890E-03   0.90161E-01   0.45475E-02   0.41200E-02
     6    0.93145E-04   0.71829E-03   0.91057E-01   0.45453E-02   0.72347E-04
     7    0.92823E-04   0.71581E-03   0.94759E-01   0.45240E-02   0.12793E-05
     8    0.91378E-04   0.70467E-03   0.11321       0.44909E-02   0.23958E-07
     9    0.84965E-04   0.65034E-03   0.21713       0.57313E-02   0.60859E-09
    10    0.11359E-02   0.87602E-02   0.83809       0.52017E-01   0.39827E-10
```

```
BLOCK:  D-300    MODEL: RADFRAC (CONTINUED)

                        ****   MASS-X-PROFILE     ****
  STAGE     WATER         NBUTANOL      PROPANOL
     1    0.67463       0.20773E-01   0.64047E-02
     2    0.98037       0.12439E-02   0.47408E-03
     4    0.94521       0.79541E-03   0.29945E-03
     5    0.89914       0.89525E-03   0.32363E-03
     6    0.90345       0.46385E-04   0.19996E-04
     7    0.89990       0.24044E-05   0.12354E-05
     8    0.88150       0.13089E-06   0.78931E-07
     9    0.77640       0.96376E-08   0.61625E-08
    10    0.10000       0.33113E-08   0.11975E-08

                        ****   MASS-Y-PROFILE     ****
  STAGE     MALEIC        SUCCINIC      GBL           BDO           THF
     1     0.0000        0.0000       0.19425E-04   0.14320E-08   0.89687
     2     0.0000        0.0000       0.22705E-02   0.74443E-06   0.29592
     4    0.42998E-11   0.41827E-11   0.10152E-01   0.35799E-04   0.20077
     5    0.11621E-07   0.31825E-07   0.17789E-01   0.22610E-03   0.19965
     6    0.16329E-07   0.44645E-07   0.23299E-01   0.30395E-03   0.44883E-02
     7    0.16646E-07   0.45501E-07   0.24338E-01   0.30543E-03   0.78809E-04
     8    0.16684E-07   0.45595E-07   0.28620E-01   0.29827E-03   0.13931E-05
     9    0.16172E-07   0.43846E-07   0.49807E-01   0.33371E-03   0.26050E-07
    10    0.10664E-05   0.28936E-05   0.16756       0.20361E-02   0.65400E-09

                        ****   MASS-Y-PROFILE     ****
  STAGE     WATER         NBUTANOL      PROPANOL
     1    0.88425E-01   0.10531E-01   0.41545E-02
     2    0.67463       0.20773E-01   0.64047E-02
     4    0.77037       0.14263E-01   0.44165E-02
     5    0.76375       0.14193E-01   0.43939E-02
     6    0.97058       0.97529E-03   0.35256E-03
     7    0.97521       0.50528E-04   0.21782E-04
     8    0.97108       0.26180E-05   0.13452E-05
     9    0.94986       0.14204E-06   0.85731E-07
    10    0.83040       0.10143E-07   0.65589E-08


  **** THERMOSYPHON REBOILER ****

TEMPERATURE   PRESSURE     FLOW RATE     MASS FLOW     VFRAC        HEAT DUTY
    F          PSIA         LBMOL/HR      LB/HR                        BTU/HR
  301.36       22.000       7307.4      0.45823E+06  0.30000      0.47247E+08

                        ****   LIQUID MOLE-FRAC   ****
         MALEIC      SUCCINIC    GBL          BDO          THF          WATER
      .87590E-03  .66436E-02  .81999      .50864E-01  .11340E-10  .12163

                        ****   LIQUID MOLE-FRAC   ****
         NBUTANOL    PROPANOL
      .22423E-08  .73872E-09
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                             U-O-S BLOCK SECTION

BLOCK:  D-300    MODEL: RADFRAC (CONTINUED)

                        ****   VAPOR MOLE-FRAC    ****
         MALEIC      SUCCINIC    GBL         BDO         THF         WATER
      .17076E-05  .45565E-05  .12155      .19642E-02  .88991E-10  .87648

                        ****   VAPOR MOLE-FRAC    ****
         NBUTANOL    PROPANOL
      .41058E-08  .24414E-08



                   ********************************
                   ***** HYDRAULIC PARAMETERS *****
                   ********************************


      *** DEFINITIONS ***

       MARANGONI INDEX = SIGMA - SIGMATO
       FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
       QR = QV*SQRT(RHOV/(RHOL-RHOV))
       F FACTOR = QV*SQRT(RHOV)
         WHERE:
         SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
         SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
         ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
         MV IS THE MASS FLOW OF VAPOR TO THE STAGE
         RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
         RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
         QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE


                    TEMPERATURE
                        F
STAGE       LIQUID FROM       VAPOR TO
   1         168.53            222.18
   2         222.18            225.25
   4         226.11            227.14
   5         227.14            231.36
   6         231.36            232.11
   7         232.11            232.91
   8         232.91            234.49
   9         234.49            255.19
  10         255.19            301.36


           MASS FLOW                VOLUME FLOW         MOLECULAR WEIGHT
             LB/HR                    CUFT/HR
STAGE LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO
   1   59680.      59680.      1037.7     0.90657E+06  23.830      23.830
   2   17780.      55080.      312.14     0.91158E+06  18.294      21.709
   4   18318.      55618.      321.34     0.89221E+06  18.827      21.912
   5   54578.      50099.      954.56     0.95021E+06  19.574      18.440
   6   54624.      50146.      957.45     0.94414E+06  19.506      18.375
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                             U-O-S BLOCK SECTION

BLOCK:  D-300    MODEL: RADFRAC (CONTINUED)


           MASS FLOW                VOLUME FLOW         MOLECULAR WEIGHT
             LB/HR                    CUFT/HR
STAGE LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO
   7   54814.      50335.      960.89     0.93453E+06  19.566      18.437
   8   55680.      51201.      974.85     0.92551E+06  19.880      18.759
   9   60577.      56099.      1049.8     0.93079E+06  21.887      20.806
  10   4478.6      57945.      70.680     0.80549E+06  62.708      26.432


             DENSITY                  VISCOSITY         SURFACE TENSION
             LB/CUFT                     CP                 DYNE/CM
STAGE LIQUID FROM  VAPOR TO     LIQUID FROM  VAPOR TO      LIQUID FROM
   1   57.513      0.65831E-01  0.36909      0.12884E-01    58.296
   2   56.961      0.60423E-01  0.26375      0.12941E-01    56.963
   4   57.004      0.62337E-01  0.25981      0.12959E-01    56.339
   5   57.176      0.52724E-01  0.26124      0.12972E-01    55.942
   6   57.052      0.53113E-01  0.25515      0.12984E-01    55.542
   7   57.045      0.53861E-01  0.25430      0.12995E-01    55.439
   8   57.117      0.55322E-01  0.25422      0.12999E-01    55.231
   9   57.704      0.60270E-01  0.25883      0.13236E-01    54.283
  10   63.365      0.71938E-01  0.42078      0.13610E-01    37.333


      MARANGONI INDEX   FLOW PARAM         QR          REDUCED F-FACTOR
STAGE    DYNE/CM                         CUFT/HR       (LB-CUFT)**.5/HR
   1                    0.33833E-01      30689.          0.23260E+06
   2   -1.3336          0.10513E-01      29706.          0.22408E+06
   4   -.23716          0.10891E-01      29521.          0.22276E+06
   5   -4.7085          0.33081E-01      28868.          0.21819E+06
   6   -.40008          0.33237E-01      28821.          0.21759E+06
   7   -.10300          0.33462E-01      28730.          0.21689E+06
   8   -.20802          0.33844E-01      28818.          0.21769E+06
   9   -.94724          0.34898E-01      30097.          0.22851E+06
  10    2.1050          0.26043E-02      27156.          0.21604E+06
```

```
ASPEN PLUS   PLAT: WIN32     VER: 21.0                   04/02/2009  PAGE 25

                             U-O-S BLOCK SECTION

BLOCK:  D-300    MODEL: RADFRAC (CONTINUED)


                ************************************
                ***** TRAY SIZING CALCULATIONS *****
                ************************************


   *******************
   *** SECTION   1 ***
   *******************

   STARTING STAGE NUMBER                                         2
   ENDING STAGE NUMBER                                           9
   FLOODING CALCULATION METHOD                               B960

   DESIGN PARAMETERS
   -----------------
   PEAK CAPACITY FACTOR                                      1.00000
   SYSTEM FOAMING FACTOR                                     1.00000
   FLOODING FACTOR                                           0.80000
   MINIMUM COLUMN DIAMETER         FT                        1.00000
   MINIMUM DC AREA/COLUMN AREA                               0.100000

   TRAY SPECIFICATIONS
   -------------------
   TRAY TYPE                                                 FLEXI
   NUMBER OF PASSES                                              1
   TRAY SPACING                    FT                        2.00000


           ***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

   STAGE WITH MAXIMUM DIAMETER                                   9
   COLUMN DIAMETER                 FT                        6.20686
   DC AREA/COLUMN AREA                                       0.100000
   DOWNCOMER VELOCITY              FT/SEC                    0.096376
   WEIR LENGTH                     FT                        4.50997


                         **** SIZING PROFILES ****

      STAGE    DIAMETER      TOTAL AREA   ACTIVE AREA   SIDE DC AREA
                 FT            SQFT         SQFT           SQFT
         2       5.7462        25.933       20.746        2.5933
         3       5.7400        25.877       20.701        2.5877
         4       5.7347        25.829       20.663        2.5829
         5       6.0347        28.602       22.882        2.8602
         6       6.0314        28.571       22.857        2.8571
         7       6.0242        28.503       22.802        2.8503
         8       6.0404        28.656       22.925        2.8656
         9       6.2069        30.258       24.206        3.0258

                      ***  ASSOCIATED  UTILITIES  ***

UTILITY USAGE:  CW1       (WATER)
------------------------------
CONDENSER                  1.5176+06                     1.5176+04
                       -------------                     -------------
TOTAL:                     1.5176+06  LB/HR              1.5176+04  $/HR
```

```
                       =============
UTILITY USAGE:  50PSIG    (STEAM)
------------------------------
REBOILER                   5.1829+04                      518.2934
                       -------------                     -------------
TOTAL:                     5.1829+04  LB/HR               518.2934  $/HR
                       =============
```

```
BLOCK:  D-500    MODEL: RADFRAC
------------------------------
   INLETS   - S-306    STAGE   7
              S-400    STAGE   2
              S-404    STAGE   6
              S-515    STAGE   7
   OUTLETS  - S-504    STAGE   1
              S-508    STAGE  15
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1834.82         1834.82        0.371765E-15
      MASS(LB/HR   )           52813.7         52813.7        0.147410E-13
      ENTHALPY(BTU/HR  )      -0.211128E+09   -0.210907E+09   -0.104881E-02



                       **********************
                       ****  INPUT DATA  ****
                       **********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                                         15
   ALGORITHM OPTION                                       NONIDEAL
   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                   75
   MAXIMUM NO. OF INSIDE LOOP ITERATIONS                    10
   MAXIMUM NUMBER OF FLASH ITERATIONS                       50
   FLASH TOLERANCE                                           0.000100000
   OUTSIDE LOOP CONVERGENCE TOLERANCE                        0.000100000
```

```
BLOCK:  D-500    MODEL: RADFRAC (CONTINUED)

  ****   COL-SPECS   ****

   MOLAR VAPOR DIST / TOTAL DIST                                  0.0
   MASS REFLUX RATE              LB/HR                       24,000.0
   MASS BOTTOMS RATE             LB/HR                       26,277.5

  ****   THERMOSYPHON REBOILER   ****

   VAPOR FRACTION                                                 0.30000

  ****    PROFILES   ****

   P-SPEC          STAGE   1  PRES, PSIA                       15.0000
                           2                                   15.0000

   TEMP-EST        STAGE   2  TEMP, F                         145.400
                           5                                  152.600
                           8                                  170.600
                          14                                  212.000

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


  ***   COMPONENT SPLIT FRACTIONS   ***

                            OUTLET STREAMS
                            --------------
                  S-504       S-508
   COMPONENT:
   MALEIC      .34401E-05   1.0000
   SUCCINIC    .12631E-05   1.0000
   GBL         .48544E-03   .99951
   BDO         .50100E-04   .99995
   THF         .99998       .15383E-04
   WATER       .49299E-01   .95070
   NBUTANOL    .10486E-02   .99895
   PROPANOL    .14921E-01   .98508
```

```
                             U-O-S BLOCK SECTION

BLOCK:  D-500    MODEL: RADFRAC (CONTINUED)
  ***    SUMMARY OF KEY RESULTS    ***

   TOP STAGE TEMPERATURE          F                         147.258
   BOTTOM STAGE TEMPERATURE       F                         210.819
   TOP STAGE LIQUID FLOW          LBMOL/HR                  381.992
   BOTTOM STAGE LIQUID FLOW       LBMOL/HR                3,480.26
   TOP STAGE VAPOR FLOW           LBMOL/HR                    0.0
   BOTTOM STAGE VAPOR FLOW        LBMOL/HR                  598.024
   MOLAR REFLUX RATIO                                         0.90442
   MOLAR BOILUP RATIO                                         0.42339
   CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                     -0.109739+08
   REBOILER DUTY                  BTU/HR                      0.111953+08

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

   DEW POINT                       0.57410E-04  STAGE= 10
   BUBBLE POINT                    0.12112E-03  STAGE=  8
   COMPONENT MASS BALANCE          0.27267E-05  STAGE= 13 COMP=THF
   ENERGY BALANCE                  0.37843E-04  STAGE= 10


  ****    PROFILES   ****

  **NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS
           FROM THE STAGE EXCLUDING ANY SIDE PRODUCT.  FOR THE FIRST STAGE,
           THE REPORTED VAPOR FLOW IS THE VAPOR DISTILLATE FLOW.  FOR THE
           LAST STAGE, THE REPORTED LIQUID FLOW IS THE LIQUID BOTTOMS FLOW.

                                          ENTHALPY
STAGE TEMPERATURE   PRESSURE             BTU/LBMOL          HEAT DUTY
      F             PSIA           LIQUID       VAPOR        BTU/HR

  1   147.26        15.000       -95910.      -82254.      -.10974+08
  2   147.29        15.000       -95999.      -82267.
  3   147.86        15.154       -96366.      -82364.
  4   148.47        15.308       -97002.      -82511.
  5   149.25        15.462       -98298.      -82765.
  6   150.65        15.615      -0.10144E+06  -83271.
  7   155.25        15.769      -0.11476E+06  -84603.
  8   158.72        15.923      -0.11632E+06  -85493.
 14   200.78        16.846      -0.12140E+06 -0.10605E+06
 15   210.82        17.000      -0.12064E+06 -0.10447E+06   .11195+08
```

```
                             U-O-S BLOCK SECTION

BLOCK:  D-500    MODEL: RADFRAC (CONTINUED)

STAGE     FLOW RATE                  FEED RATE                PRODUCT RATE
           LBMOL/HR                   LBMOL/HR                  LBMOL/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID    VAPOR
  1  382.0      0.000                                      422.3597
  2  398.4      804.4       16.1111
  3  396.4      804.7
  4  393.0      802.7
  5  386.0      799.3
  6  374.0      792.3        4.5635   96.2032
  7  2078.      679.5      1717.9420
  8  2046.      665.9
 14  2010.      591.7
 15  1412.      598.0                                     1412.4602

   ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE                  FEED RATE                PRODUCT RATE
           LB/HR                      LB/HR                     LB/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID    VAPOR
  1 0.2400E+05  0.000                                     .26536+05
  2 0.2500E+05 0.5054E+05  1159.7228
  3 0.2463E+05 0.5038E+05
  4 0.2399E+05 0.5000E+05
  5 0.2276E+05 0.4937E+05
  6 0.2018E+05 0.4813E+05   327.4463 5778.7980
  7 0.6417E+05 0.3945E+05  .45548+05
  8 0.5963E+05 0.3790E+05
 14 0.4219E+05 0.2071E+05
 15 0.2628E+05 0.1591E+05                                 .26277+05

                        ****   MOLE-X-PROFILE     ****
  STAGE     MALEIC        SUCCINIC      GBL           BDO            THF
     1     0.0000        0.0000       0.12386E-05   0.37925E-10   0.82833
     2    0.50477E-11   0.12922E-10   0.23512E-03   0.29148E-07   0.82623
     3    0.50728E-11   0.12987E-10   0.23630E-03   0.29295E-07   0.81383
     4    0.51166E-11   0.13099E-10   0.23834E-03   0.29551E-07   0.79285
     5    0.52097E-11   0.13337E-10   0.24277E-03   0.30097E-07   0.75102
     6    0.53873E-11   0.13785E-10   0.25746E-03   0.31706E-07   0.65136
     7    0.96936E-12   0.24803E-11   0.52016E-03   0.15395E-06   0.22453
     8    0.98469E-12   0.25195E-11   0.53002E-03   0.15644E-06   0.17773
    14    0.10021E-11   0.25641E-11   0.58119E-03   0.16191E-06   0.70902E-04
    15    0.14264E-11   0.36497E-11   0.76261E-03   0.22635E-06   0.38102E-05

                        ****   MOLE-X-PROFILE     ****
  STAGE     WATER         NBUTANOL      PROPANOL
     1    0.17150       0.26168E-04   0.14252E-03
     2    0.17277       0.22116E-03   0.53943E-03
     3    0.18451       0.31216E-03   0.11137E-02
     4    0.20405       0.67926E-03   0.21903E-02
     5    0.24245       0.21186E-02   0.41705E-02
     6    0.33399       0.70385E-02   0.73598E-02
     7    0.76140       0.78779E-02   0.56749E-02
```

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                         U-O-S BLOCK SECTION

BLOCK:  D-500    MODEL: RADFRAC (CONTINUED)

                     ****   MOLE-X-PROFILE     ****
  STAGE     WATER         NBUTANOL      PROPANOL
    8    0.79193       0.15869E-01   0.13945E-01
   14    0.94365       0.41618E-01   0.14078E-01
   15    0.98897       0.74543E-02   0.28135E-02

                     ****   MOLE-Y-PROFILE     ****
  STAGE     MALEIC        SUCCINIC      GBL           BDO           THF
    1     0.0000        0.0000       0.65313E-08   0.49414E-13   0.82883
    2     0.0000        0.0000       0.12386E-05   0.37925E-10   0.82833
    3     0.0000        0.0000       0.12519E-05   0.38665E-10   0.82417
    4     0.0000        0.0000       0.12592E-05   0.39634E-10   0.81804
    5     0.0000        0.0000       0.12627E-05   0.41275E-10   0.80774
    6     0.0000        0.0000       0.13203E-05   0.45738E-10   0.78749
    7     0.0000        0.0000       0.45286E-05   0.35778E-09   0.73379
    8     0.0000        0.0000       0.59405E-05   0.40779E-09   0.70076
   14     0.0000        0.0000       0.56163E-04   0.27573E-08   0.17359E-02
   15     0.0000        0.0000       0.15272E-03   0.97269E-08   0.22937E-03

                     ****   MOLE-Y-PROFILE     ****
  STAGE     WATER         NBUTANOL      PROPANOL
    1    0.17113       0.30950E-05   0.37666E-04
    2    0.17150       0.26168E-04   0.14252E-03
    3    0.17550       0.37154E-04   0.29375E-03
    4    0.18130       0.81645E-04   0.57679E-03
    5    0.19089       0.26118E-03   0.11039E-02
    6    0.20949       0.95878E-03   0.20591E-02
    7    0.25882       0.34608E-02   0.39213E-02
    8    0.27872       0.87764E-02   0.11744E-01
   14    0.67544       0.23602       0.86748E-01
   15    0.83663       0.12231       0.40682E-01

                     ****   K-VALUES           ****
  STAGE     MALEIC        SUCCINIC      GBL           BDO           THF
    1    0.32528E-05   0.11937E-05   0.52730E-02   0.13029E-02    1.0006
    2    0.32510E-05   0.11930E-05   0.52680E-02   0.13011E-02    1.0025
    3    0.32496E-05   0.11923E-05   0.52981E-02   0.13199E-02    1.0127
    4    0.32214E-05   0.11817E-05   0.52830E-02   0.13412E-02    1.0318
    5    0.31501E-05   0.11552E-05   0.52014E-02   0.13714E-02    1.0755
    6    0.30445E-05   0.11158E-05   0.51281E-02   0.14426E-02    1.2090
    7    0.33242E-05   0.12156E-05   0.87059E-02   0.23240E-02    3.2682
    8    0.40025E-05   0.14614E-05   0.11203E-01   0.26065E-02    3.9436
   14    0.38954E-04   0.13967E-04   0.96634E-01   0.17029E-01    24.483
   15    0.84492E-04   0.30164E-04   0.20025       0.42974E-01    60.198

                     ****   K-VALUES           ****
  STAGE     WATER         NBUTANOL      PROPANOL
    1    0.99786       0.11828       0.26428
    2    0.99262       0.11832       0.26421
    3    0.95115       0.11902       0.26376
    4    0.88853       0.12020       0.26334
    5    0.78735       0.12328       0.26469
    6    0.62724       0.13622       0.27978
    7    0.33993       0.43930       0.69099
```

```
                         U-O-S BLOCK SECTION

BLOCK:  D-500    MODEL: RADFRAC (CONTINUED)

                     ****   K-VALUES           ****
  STAGE     WATER         NBUTANOL      PROPANOL
    8    0.35195       0.55278       0.84182
   14    0.71577        5.6710        6.1621
   15    0.84596        16.408        14.460

                     ****   MASS-X-PROFILE     ****
  STAGE     MALEIC        SUCCINIC      GBL           BDO           THF
    1     0.0000        0.0000       0.16972E-05   0.54400E-10   0.95066
    2    0.93358E-11   0.24315E-10   0.32254E-03   0.41857E-07   0.94930
    3    0.94791E-11   0.24689E-10   0.32750E-03   0.42503E-07   0.94471
    4    0.97285E-11   0.25338E-10   0.33611E-03   0.43625E-07   0.93647
    5    0.10258E-10   0.26717E-10   0.35454E-03   0.46012E-07   0.91864
    6    0.11586E-10   0.30161E-10   0.41069E-03   0.52944E-07   0.87024
    7    0.36441E-11   0.94860E-11   0.14503E-02   0.44935E-06   0.52435
    8    0.39220E-11   0.10210E-10   0.15658E-02   0.48380E-06   0.43975
   14    0.55428E-11   0.14428E-10   0.23842E-02   0.69531E-06   0.24362E-03
   15    0.88994E-11   0.23167E-10   0.35290E-02   0.10965E-05   0.14768E-04

                     ****   MASS-X-PROFILE     ****
  STAGE     WATER         NBUTANOL      PROPANOL
    1    0.49176E-01   0.30872E-04   0.13632E-03
    2    0.49596E-01   0.26121E-03   0.51654E-03
    3    0.53512E-01   0.37249E-03   0.10775E-02
    4    0.60214E-01   0.82473E-03   0.21561E-02
    5    0.74093E-01   0.26639E-02   0.42516E-02
    6    0.11148       0.96667E-02   0.81952E-02
    7    0.44424       0.18912E-01   0.11045E-01
    8    0.48956       0.40364E-01   0.28757E-01
   14    0.81006       0.14699       0.40313E-01
   15    0.95767       0.29699E-01   0.90884E-02

                     ****   MASS-Y-PROFILE     ****
  STAGE     MALEIC        SUCCINIC      GBL           BDO           THF
    1     0.0000        0.0000       0.89464E-08   0.70857E-13   0.95091
    2     0.0000        0.0000       0.16972E-05   0.54400E-10   0.95066
    3     0.0000        0.0000       0.17214E-05   0.55655E-10   0.94918
    4     0.0000        0.0000       0.17402E-05   0.57341E-10   0.94691
    5     0.0000        0.0000       0.17599E-05   0.60222E-10   0.94294
    6     0.0000        0.0000       0.18709E-05   0.67850E-10   0.93467
    7     0.0000        0.0000       0.67142E-05   0.55529E-09   0.91122
    8     0.0000        0.0000       0.89869E-05   0.64581E-09   0.88792
   14     0.0000        0.0000       0.13812E-03   0.70986E-08   0.35758E-02
   15     0.0000        0.0000       0.49403E-03   0.32940E-07   0.62147E-03

                     ****   MASS-Y-PROFILE     ****
  STAGE     WATER         NBUTANOL      PROPANOL
    1    0.49054E-01   0.36502E-05   0.36015E-04
    2    0.49176E-01   0.30872E-04   0.13632E-03
    3    0.50497E-01   0.43985E-04   0.28195E-03
    4    0.52432E-01   0.97149E-04   0.55645E-03
    5    0.55675E-01   0.31342E-03   0.10740E-02
    6    0.62120E-01   0.11698E-02   0.20369E-02
    7    0.80300E-01   0.44177E-02   0.40584E-02
```

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                             U-O-S BLOCK SECTION

BLOCK:  D-500    MODEL: RADFRAC (CONTINUED)

                        ****   MASS-Y-PROFILE     ****
  STAGE     WATER         NBUTANOL      PROPANOL
     8    0.88233E-01   0.11431E-01   0.12402E-01
    14    0.34761       0.49976       0.14892
    15    0.56635       0.34066       0.91868E-01


  **** THERMOSYPHON REBOILER ****

TEMPERATURE   PRESSURE     FLOW RATE     MASS FLOW     VFRAC        HEAT DUTY
    F         PSIA         LBMOL/HR      LB/HR                        BTU/HR
  217.94       17.000       2067.8       38469.      0.30000      0.11195E+08

                        ****   LIQUID MOLE-FRAC   ****
        MALEIC      SUCCINIC    GBL         BDO         THF         WATER
     .20376E-11  .52138E-11  .97957E-03  .31501E-06  .15298E-06  .99764

                        ****   LIQUID MOLE-FRAC   ****
        NBUTANOL    PROPANOL
     .95167E-03  .42954E-03

                        ****   VAPOR MOLE-FRAC    ****
        MALEIC      SUCCINIC    GBL         BDO         THF         WATER
     0.0000      0.0000      .25637E-03  .19460E-07  .12344E-04  .96873

                        ****   VAPOR MOLE-FRAC    ****
        NBUTANOL    PROPANOL
     .22627E-01  .83761E-02
```

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                             U-O-S BLOCK SECTION

BLOCK:  D-500    MODEL: RADFRAC (CONTINUED)


                   ********************************
                   ***** HYDRAULIC PARAMETERS *****
                   ********************************


      *** DEFINITIONS ***

       MARANGONI INDEX = SIGMA - SIGMATO
       FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
       QR = QV*SQRT(RHOV/(RHOL-RHOV))
       F FACTOR = QV*SQRT(RHOV)
         WHERE:
         SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
         SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
         ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
         MV IS THE MASS FLOW OF VAPOR TO THE STAGE
         RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
         RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
         QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE


                    TEMPERATURE
                        F
STAGE       LIQUID FROM       VAPOR TO
   1         147.26            147.29
   2         147.29            147.86
   3         147.86            148.47
   4         148.47            149.25
   5         149.25            150.65
   6         150.65            154.81
   7         155.25            158.72
   8         158.72            169.13
  14         200.78            210.82
  15         210.82            217.94


             MASS FLOW                VOLUME FLOW         MOLECULAR WEIGHT
              LB/HR                     CUFT/HR
STAGE LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO
   1   50536.      50536.      946.27     0.34157E+06  62.829      62.829
   2   25004.      50381.      468.11     0.33852E+06  62.758      62.611
   3   24626.      50002.      460.53     0.33461E+06  62.117      62.293
   4   23995.      49371.      447.83     0.33032E+06  61.048      61.769
   5   22756.      48133.      422.97     0.32502E+06  58.950      60.753
   6   20184.      45233.      371.50     0.32077E+06  53.970      58.315
   7   64174.      37897.      1125.6     0.27190E+06  30.877      56.907
   8   59626.      33348.      1050.5     0.26101E+06  29.142      52.635
  14   42192.      15915.      763.37     0.25046E+06  20.986      26.613
  15   26277.      12193.      462.26     0.26311E+06  18.604      19.655
```

```
BLOCK:  D-500    MODEL: RADFRAC (CONTINUED)


              DENSITY                  VISCOSITY         SURFACE TENSION
              LB/CUFT                  CP                    DYNE/CM
STAGE LIQUID FROM  VAPOR TO     LIQUID FROM  VAPOR TO      LIQUID FROM
   1   53.406      0.14795      0.33754      0.98757E-02    29.153
   2   53.415      0.14883      0.33792      0.98964E-02    29.208
   3   53.473      0.14943      0.33848      0.99224E-02    29.675
   4   53.580      0.14947      0.34009      0.99609E-02    30.475
   5   53.801      0.14809      0.34421      0.10033E-01    32.079
   6   54.330      0.14101      0.35493      0.10219E-01    35.930
   7   57.016      0.13938      0.39354      0.10337E-01    54.005
   8   56.758      0.12777      0.39363      0.10643E-01    54.967
  14   55.271      0.63543E-01  0.31092      0.12167E-01    57.110
  15   56.845      0.46342E-01  0.28345      0.12669E-01    57.899


      MARANGONI INDEX   FLOW PARAM         QR         REDUCED F-FACTOR
STAGE    DYNE/CM                          CUFT/HR       (LB-CUFT)**.5/HR
   1                    0.52634E-01       18003.          0.13138E+06
   2   0.17289          0.26197E-01       17894.          0.13059E+06
   3   0.46698          0.26035E-01       17714.          0.12935E+06
   4   0.80037          0.25669E-01       17471.          0.12770E+06
   5    1.6033          0.24804E-01       17076.          0.12508E+06
   6    3.8271          0.22733E-01       16363.          0.12046E+06
   7   0.43387          0.83726E-01       13460.          0.10151E+06
   8   0.96204          0.84831E-01       12398.           93296.
  14    1.8388          0.89891E-01       8497.1           63135.
  15    1.6737          0.61534E-01       7515.4           56640.
```

```
BLOCK:  D-500    MODEL: RADFRAC (CONTINUED)


                ************************************
                ***** TRAY SIZING CALCULATIONS *****
                ************************************


   *******************
   *** SECTION   1 ***
   *******************

   STARTING STAGE NUMBER                                                2
   ENDING STAGE NUMBER                                                 14
   FLOODING CALCULATION METHOD                                       B960

   DESIGN PARAMETERS
   -----------------
   PEAK CAPACITY FACTOR                                              1.00000
   SYSTEM FOAMING FACTOR                                             1.00000
   FLOODING FACTOR                                                   0.80000
   MINIMUM COLUMN DIAMETER         FT                                1.00000
   MINIMUM DC AREA/COLUMN AREA                                       0.100000

   TRAY SPECIFICATIONS
   -------------------
   TRAY TYPE                                                         FLEXI
   NUMBER OF PASSES                                                     1
   TRAY SPACING                    FT                                2.00000


           ***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

   STAGE WITH MAXIMUM DIAMETER                                          2
   COLUMN DIAMETER                 FT                                4.56597
   DC AREA/COLUMN AREA                                               0.100000
   DOWNCOMER VELOCITY              FT/SEC                            0.079413
   WEIR LENGTH                     FT                                3.31768


                          **** SIZING PROFILES ****

      STAGE    DIAMETER      TOTAL AREA    ACTIVE AREA   SIDE DC AREA
                 FT            SQFT          SQFT           SQFT
        2       4.5660        16.374        13.099         1.6374
        3       4.5402        16.190        12.952         1.6190
        4       4.5032        15.927        12.741         1.5927
        5       4.4404        15.486        12.389         1.5486
        6       4.3221        14.672        11.737         1.4672
        7       4.2686        14.310        11.448         1.4310
        8       4.0754        13.045        10.436         1.3045
        9       3.7692        11.158        8.9263         1.1158
       10       3.6150        10.264        8.2109         1.0264
       11       3.5826        10.081        8.0644         1.0081
       12       3.5738        10.031        8.0250         1.0031
```

```
                             U-O-S BLOCK SECTION

BLOCK:  D-500    MODEL: RADFRAC (CONTINUED)

      STAGE    DIAMETER      TOTAL AREA   ACTIVE AREA   SIDE DC AREA
                  FT            SQFT         SQFT           SQFT
        13      3.5646        9.9795       7.9836       0.99795
        14      3.3013        8.5595       6.8476       0.85595

                    ***  ASSOCIATED  UTILITIES  ***

UTILITY USAGE:  CW1       (WATER)
------------------------------
CONDENSER                 3.6727+05                    3672.6850
                      -------------                -------------
TOTAL:                    3.6727+05  LB/HR             3672.6850  $/HR
                      =============
UTILITY USAGE:  50PSIG    (STEAM)
------------------------------
REBOILER                  1.2281+04                     122.8101
                      -------------                -------------
TOTAL:                    1.2281+04  LB/HR              122.8101  $/HR
                      =============

BLOCK:  D-501    MODEL: RADFRAC
-------------------------------
   INLETS   - 510      STAGE   5
   OUTLETS  - S-515A   STAGE   1
              S-518    STAGE  10
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG
  HENRY-COMPS ID:        HC-1

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           422.360         422.360        0.403756E-15
      MASS(LB/HR   )           26536.2         26536.2       -0.888209E-11
      ENTHALPY(BTU/HR  )      -0.404879E+08   -0.385751E+08   -0.472441E-01
```

```
                             U-O-S BLOCK SECTION

BLOCK:  D-501    MODEL: RADFRAC (CONTINUED)


                        **********************
                        ****  INPUT DATA  ****
                        **********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                                               10
   ALGORITHM OPTION                                             NONIDEAL
   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                         45
   MAXIMUM NO. OF INSIDE LOOP ITERATIONS                          10
   MAXIMUM NUMBER OF FLASH ITERATIONS                             50
   FLASH TOLERANCE                                                   0.000100000
   OUTSIDE LOOP CONVERGENCE TOLERANCE                                0.000100000

  ****   COL-SPECS   ****

   MOLAR VAPOR DIST / TOTAL DIST                                     0.0
   MASS REFLUX RATE              LB/HR                       12,000.0
   MASS BOTTOMS RATE             LB/HR                       12,500.0

  ****   THERMOSYPHON REBOILER   ****

   VAPOR FRACTION                                                    0.30000

  ****    PROFILES   ****

   P-SPEC          STAGE   1  PRES, PSIA                   115.000
                           2                               115.000
```

```
                             U-O-S BLOCK SECTION

BLOCK:  D-501    MODEL: RADFRAC (CONTINUED)

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


  ***   COMPONENT SPLIT FRACTIONS   ***

                           OUTLET STREAMS
                           --------------
                S-515A       S-518
   COMPONENT:
   GBL         .99328       .67211E-02
   BDO         .15860E-07   1.0000
   THF         .50465       .49535
   WATER       .99971       .29306E-03
   NBUTANOL    .27216E-01   .97278
   PROPANOL    .22974       .77026


  ***    SUMMARY OF KEY RESULTS    ***

   TOP STAGE TEMPERATURE          F                         274.480
   BOTTOM STAGE TEMPERATURE       F                         298.475
   TOP STAGE LIQUID FLOW          LBMOL/HR                  212.863
   BOTTOM STAGE LIQUID FLOW       LBMOL/HR                2,581.29
   TOP STAGE VAPOR FLOW           LBMOL/HR                    0.0
   BOTTOM STAGE VAPOR FLOW        LBMOL/HR                  721.337
   MOLAR REFLUX RATIO                                         0.85493
   MOLAR BOILUP RATIO                                         4.16051
   CONDENSER DUTY (W/O SUBCOOL)   BTU/HR           -5,727,470.
   REBOILER DUTY                  BTU/HR            7,640,280.

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

   DEW POINT                       0.33069E-05  STAGE=  1
   BUBBLE POINT                    0.48405E-05  STAGE=  2
   COMPONENT MASS BALANCE          0.55288E-06  STAGE=  4 COMP=NBUTANOL
   ENERGY BALANCE                  0.11064E-04  STAGE=  2
```

```
                             U-O-S BLOCK SECTION

BLOCK:  D-501    MODEL: RADFRAC (CONTINUED)

  ****    PROFILES   ****

  **NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS
           FROM THE STAGE EXCLUDING ANY SIDE PRODUCT.  FOR THE FIRST STAGE,
           THE REPORTED VAPOR FLOW IS THE VAPOR DISTILLATE FLOW.  FOR THE
           LAST STAGE, THE REPORTED LIQUID FLOW IS THE LIQUID BOTTOMS FLOW.

                                            ENTHALPY
STAGE TEMPERATURE   PRESSURE             BTU/LBMOL          HEAT DUTY
      F             PSIA           LIQUID       VAPOR        BTU/HR

  1   274.48        115.00       -95581.      -84191.      -.57275+07
  2   275.53        115.00       -92376.      -83180.
  4   280.59        115.50       -88720.      -80873.
  5   282.04        115.75       -88233.      -80361.
  6   290.02        116.00       -86361.      -77441.
  8   297.39        116.50       -85329.      -74923.
  9   298.13        116.75       -85255.      -74725.
 10   298.48        117.00       -85231.      -74669.       .76403+07

STAGE     FLOW RATE                  FEED RATE               PRODUCT RATE
           LBMOL/HR                  LBMOL/HR                  LBMOL/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID    VAPOR
  1  212.9      0.000                                      248.9827
  2  221.0      461.8
  4  231.8      476.8
  5  833.1      480.8      422.3597
  6  865.1      659.7
  8  892.3      711.4
  9  894.7      718.9
 10  173.4      721.3                                      173.3770

   ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE                  FEED RATE               PRODUCT RATE
           LB/HR                      LB/HR                     LB/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID    VAPOR
  1 0.1200E+05  0.000                                     .14036+05
  2 0.1361E+05 0.2604E+05
  4 0.1562E+05 0.2896E+05
  5 0.5674E+05 0.2966E+05  .26536+05
  6 0.6120E+05 0.4424E+05
  8 0.6425E+05 0.5096E+05
  9 0.6449E+05 0.5175E+05
 10 0.1250E+05 0.5199E+05                                 .12500+05
```

```
                         U-O-S BLOCK SECTION

BLOCK:  D-501    MODEL: RADFRAC (CONTINUED)

                        ****   MOLE-X-PROFILE     ****
  STAGE     GBL            BDO           THF           WATER         NBUTANOL
     1    0.20870E-05    0.0000       0.70910       0.29084       0.12081E-05
     2    0.73998E-05    0.0000       0.80560       0.19427       0.41367E-05
     4    0.66615E-05   0.36039E-12   0.91249       0.87313E-01   0.13516E-04
     5    0.45339E-05   0.19378E-10   0.92591       0.73874E-01   0.20325E-04
     6    0.25549E-05   0.18679E-10   0.97468       0.25079E-01   0.21624E-04
     8    0.27057E-06   0.18128E-10   0.99783       0.18971E-02   0.27813E-04
     9    0.76167E-07   0.18776E-10   0.99922       0.49214E-03   0.37919E-04
    10    0.20280E-07   0.92388E-10   0.99955       0.12244E-03   0.62011E-04

                        ****   MOLE-X-PROFILE     ****
  STAGE     PROPANOL
     1    0.55542E-04
     2    0.11740E-03
     4    0.18031E-03
     5    0.18916E-03
     6    0.21739E-03
     8    0.24287E-03
     9    0.25387E-03
    10    0.26743E-03

                        ****   MOLE-Y-PROFILE     ****
  STAGE     GBL            BDO           THF           WATER         NBUTANOL
     1    0.32433E-06    0.0000       0.67276       0.32722       0.35662E-06
     2    0.20870E-05    0.0000       0.70910       0.29084       0.12081E-05
     4    0.52474E-05   0.31684E-14   0.78961       0.21028       0.45679E-05
     5    0.42926E-05   0.17376E-12   0.80716       0.19271       0.71426E-05
     6    0.57201E-05   0.19078E-12   0.90656       0.93255E-01   0.93697E-05
     8    0.11194E-05   0.20936E-12   0.99094       0.88233E-02   0.14170E-04
     9    0.33093E-06   0.21919E-12   0.99742       0.23250E-02   0.19565E-04
    10    0.89599E-07   0.10829E-11   0.99914       0.58100E-03   0.32129E-04

                        ****   MOLE-Y-PROFILE     ****
  STAGE     PROPANOL
     1    0.25131E-04
     2    0.55542E-04
     4    0.10522E-03
     5    0.11570E-03
     6    0.16859E-03
     8    0.22378E-03
     9    0.23695E-03
    10    0.25061E-03

                        ****   K-VALUES           ****
  STAGE     GBL            BDO           THF           WATER         NBUTANOL
     1    0.15541       0.90919E-02   0.94874        1.1251       0.29519
     2    0.28222       0.85479E-02   0.88022        1.4970       0.29205
     4    0.78775       0.87917E-02   0.86533        2.4083       0.33795
     5    0.94673       0.89671E-02   0.87175        2.6086       0.35142
     6     2.2388       0.10213E-01   0.93011        3.7184       0.43330
     8     4.1370       0.11549E-01   0.99309        4.6510       0.50947
     9     4.3448       0.11674E-01   0.99820        4.7243       0.51597
    10     4.4181       0.11721E-01   0.99959        4.7452       0.51811
```

```
                         U-O-S BLOCK SECTION

BLOCK:  D-501    MODEL: RADFRAC (CONTINUED)

                        ****   K-VALUES           ****
  STAGE     PROPANOL
     1    0.45247
     2    0.47314
     4    0.58359
     5    0.61164
     6    0.77549
     8    0.92137
     9    0.93337
    10    0.93709

                        ****   MASS-X-PROFILE     ****
  STAGE     GBL            BDO           THF           WATER         NBUTANOL
     1    0.31871E-05    0.0000       0.90699       0.92942E-01   0.15885E-05
     2    0.10342E-04    0.0000       0.94305       0.56819E-01   0.49779E-05
     4    0.85111E-05   0.48201E-12   0.97647       0.23344E-01   0.14869E-04
     5    0.57309E-05   0.25641E-10   0.98027       0.19540E-01   0.22119E-04
     6    0.31089E-05   0.23795E-10   0.99340       0.63862E-02   0.22656E-04
     8    0.32352E-06   0.22691E-10   0.99929       0.47466E-03   0.28632E-04
     9    0.90975E-07   0.23477E-10   0.99963       0.12301E-03   0.38995E-04
    10    0.24216E-07   0.11549E-09   0.99968       0.30594E-04   0.63754E-04

                        ****   MASS-X-PROFILE     ****
  STAGE     PROPANOL
     1    0.59208E-04
     2    0.11454E-03
     4    0.16081E-03
     5    0.16690E-03
     6    0.18466E-03
     8    0.20271E-03
     9    0.21167E-03
    10    0.22291E-03

                        ****   MASS-Y-PROFILE     ****
  STAGE     GBL            BDO           THF           WATER         NBUTANOL
     1    0.51320E-06    0.0000       0.89162       0.10835       0.48586E-06
     2    0.31871E-05    0.0000       0.90699       0.92942E-01   0.15885E-05
     4    0.74385E-05   0.47017E-14   0.93751       0.62377E-01   0.55751E-05
     5    0.59913E-05   0.25388E-12   0.94359       0.56284E-01   0.85832E-05
     6    0.73433E-05   0.25638E-12   0.97478       0.25052E-01   0.10356E-04
     8    0.13454E-05   0.26342E-12   0.99758       0.22192E-02   0.14663E-04
     9    0.39582E-06   0.27444E-12   0.99920       0.58193E-03   0.20148E-04
    10    0.10703E-06   0.13541E-11   0.99961       0.14523E-03   0.33043E-04

                        ****   MASS-Y-PROFILE     ****
  STAGE     PROPANOL
     1    0.27759E-04
     2    0.59208E-04
     4    0.10412E-03
     5    0.11272E-03
     6    0.15108E-03
     8    0.18775E-03
     9    0.19783E-03
    10    0.20896E-03
```

```
                             U-O-S BLOCK SECTION

BLOCK:  D-501    MODEL: RADFRAC (CONTINUED)


  **** THERMOSYPHON REBOILER ****

TEMPERATURE   PRESSURE     FLOW RATE     MASS FLOW     VFRAC        HEAT DUTY
    F         PSIA         LBMOL/HR      LB/HR                        BTU/HR
  298.50       117.00       2407.9      0.17360E+06  0.30000      0.76403E+07

                        ****   LIQUID MOLE-FRAC   ****
         GBL         BDO          THF          WATER       NBUTANOL    PROPANOL
      .10004E-07  .13132E-09  .99960      .57632E-04  .72484E-04  .27253E-03

                        ****   VAPOR MOLE-FRAC    ****
         GBL         BDO          THF          WATER       NBUTANOL    PROPANOL
      .44258E-07  .15399E-11  .99943      .27366E-03  .37575E-04  .25553E-03




                   ********************************
                   ***** HYDRAULIC PARAMETERS *****
                   ********************************


      *** DEFINITIONS ***

       MARANGONI INDEX = SIGMA - SIGMATO
       FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
       QR = QV*SQRT(RHOV/(RHOL-RHOV))
       F FACTOR = QV*SQRT(RHOV)
         WHERE:
         SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
         SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
         ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
         MV IS THE MASS FLOW OF VAPOR TO THE STAGE
         RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
         RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
         QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE


                    TEMPERATURE
                        F
STAGE       LIQUID FROM       VAPOR TO
   1         274.48            275.53
   2         275.53            278.09
   4         280.59            282.04
   5         282.04            290.02
   6         290.02            295.32
   8         297.39            298.13
   9         298.13            298.48
  10         298.48            298.50
```

```
                             U-O-S BLOCK SECTION

BLOCK:  D-501    MODEL: RADFRAC (CONTINUED)


             MASS FLOW                VOLUME FLOW          MOLECULAR WEIGHT
               LB/HR                    CUFT/HR
STAGE LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO
   1   26036.      26036.      538.55      28616.      56.374      56.374
   2   13615.      27651.      285.53      29048.      61.597      58.830
   4   15620.      29657.      334.06      29615.      67.382      61.682
   5   56742.      44242.      1217.5      40683.      68.109      67.061
   6   61203.      48703.      1333.3      42665.      70.748      70.410
   8   64245.      51745.      1415.5      44205.      72.001      71.978
   9   64489.      51989.      1422.4      44265.      72.077      72.073
  10   12500.      52075.      275.82      44330.      72.097      72.089


               DENSITY                  VISCOSITY          SURFACE TENSION
               LB/CUFT                     CP                  DYNE/CM
STAGE LIQUID FROM  VAPOR TO     LIQUID FROM  VAPOR TO       LIQUID FROM
   1   48.345      0.90984      0.19899      0.12804E-01    24.379
   2   47.683      0.95191      0.19796      0.12713E-01    20.627
   4   46.760       1.0014      0.19446      0.12625E-01    16.216
   5   46.604       1.0875      0.19356      0.12463E-01    15.612
   6   45.902       1.1415      0.18886      0.12367E-01    13.256
   8   45.386       1.1706      0.18482      0.12329E-01    11.925
   9   45.339       1.1745      0.18443      0.12330E-01    11.826
  10   45.319       1.1747      0.18424      0.12330E-01    11.791


      MARANGONI INDEX   FLOW PARAM          QR          REDUCED F-FACTOR
STAGE    DYNE/CM                          CUFT/HR       (LB-CUFT)**.5/HR
   1                    0.13718           3963.2           27296.
   2   -3.7525          0.69569E-01       4145.8           28341.
   4   -1.4930          0.77079E-01       4381.1           29636.
   5   -8.4764          0.19592           6288.4           42425.
   6   -2.3555          0.19817           6813.4           45584.
   8   -.32417          0.19939           7192.7           47827.
   9   -.98387E-01      0.19965           7218.5           47972.
  10   -.15085E-02      0.38646E-01       7231.5           48047.
```

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ASPEN PLUS   PLAT: WIN32     VER: 21.0                  04/02/2009  PAGE 44

                             U-O-S BLOCK SECTION

BLOCK:  D-501    MODEL: RADFRAC (CONTINUED)


                ************************************
                ***** TRAY SIZING CALCULATIONS *****
                ************************************


   *******************
   *** SECTION   1 ***
   *******************

   STARTING STAGE NUMBER                                         2
   ENDING STAGE NUMBER                                           9
   FLOODING CALCULATION METHOD                               B960

   DESIGN PARAMETERS
   -----------------
   PEAK CAPACITY FACTOR                                      1.00000
   SYSTEM FOAMING FACTOR                                     1.00000
   FLOODING FACTOR                                           0.80000
   MINIMUM COLUMN DIAMETER         FT                        1.00000
   MINIMUM DC AREA/COLUMN AREA                               0.100000

   TRAY SPECIFICATIONS
   -------------------
   TRAY TYPE                                                 FLEXI
   NUMBER OF PASSES                                              1
   TRAY SPACING                    FT                        2.00000


           ***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

   STAGE WITH MAXIMUM DIAMETER                                   9
   COLUMN DIAMETER                 FT                        3.35559
   DC AREA/COLUMN AREA                                       0.11458
   DOWNCOMER VELOCITY              FT/SEC                    0.38990
   WEIR LENGTH                     FT                        2.53230


                         **** SIZING PROFILES ****

      STAGE    DIAMETER      TOTAL AREA   ACTIVE AREA   SIDE DC AREA
                  FT            SQFT         SQFT          SQFT
         2       2.1853        3.7506       3.0005       0.37506
         3       2.2357        3.9256       3.1405       0.39256
         4       2.2632        4.0227       3.2182       0.40227
         5       3.0831        7.4654       5.7306       0.86741
         6       3.2386        8.2377       6.3379       0.94990
         7       3.3195        8.6542       6.6681       0.99308
         8       3.3476        8.8013       6.7844        1.0085
         9       3.3556        8.8436       6.8169        1.0133

                      ***  ASSOCIATED  UTILITIES  ***

UTILITY USAGE:  CW1       (WATER)
------------------------------
CONDENSER                 1.9168+05                    1916.8389
                      -------------                    -------------
TOTAL:                    1.9168+05  LB/HR             1916.8389  $/HR
```

```
                       =============
UTILITY USAGE:  150PSIG   (STEAM)
------------------------------
REBOILER                 8916.6389                      178.3328
                       -------------                  -------------
TOTAL:                   8916.6389  LB/HR               178.3328  $/HR
                       =============
```

```
BLOCK:  DUMSEP1  MODEL: SEP2
----------------------------
  INLET STREAM:          S-301A
  OUTLET STREAMS:        D1          S-301
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1636.87         1636.87         0.00000
      MASS(LB/HR   )            41780.2         41780.2       -0.174148E-15
      ENTHALPY(BTU/HR  )      -0.198781E+09   -0.198781E+09    0.207372E-06


                       ***  INPUT DATA  ***

  FLASH SPECS FOR STREAM D1
  TWO    PHASE  TP  FLASH
  PRESSURE DROP         PSI                                 0.0
  MAXIMUM NO. ITERATIONS                                  30
  CONVERGENCE TOLERANCE                                     0.000100000

  FLASH SPECS FOR STREAM S-301
  TWO    PHASE  TP  FLASH
  PRESSURE DROP         PSI                                 0.0
  MAXIMUM NO. ITERATIONS                                  30
  CONVERGENCE TOLERANCE                                     0.000100000

  SPLIT FRACTION
    SUBSTREAM= MIXED
      STREAM= D1        CPT= MALEIC    FRACTION=          0.0
                             HYDROGEN                     1.00000
                             SUCCINIC                     0.0
                             GBL                          0.0
                             BDO                          0.0
                             THF                          0.0
                             METHANE                      1.00000
                             NBUTANE                      1.00000
                             WATER                        0.0
                             PROPANE                      1.00000
                             NBUTANOL                     0.0
                             PROPANOL                     0.0
```

```
BLOCK:  DUMSEP1  MODEL: SEP2 (CONTINUED)


                          ***  RESULTS  ***

  HEAT DUTY             BTU/HR                                    -41.222

 STREAM=   D1         SUBSTREAM= MIXED
    COMPONENT = HYDROGEN  SPLIT FRACTION =          1.00000
    COMPONENT = METHANE   SPLIT FRACTION =          1.00000
    COMPONENT = NBUTANE   SPLIT FRACTION =          1.00000
    COMPONENT = PROPANE   SPLIT FRACTION =          1.00000

 STREAM=   S-301      SUBSTREAM= MIXED
    COMPONENT = MALEIC    SPLIT FRACTION =          1.00000
    COMPONENT = SUCCINIC  SPLIT FRACTION =          1.00000
    COMPONENT = GBL       SPLIT FRACTION =          1.00000
    COMPONENT = BDO       SPLIT FRACTION =          1.00000
    COMPONENT = THF       SPLIT FRACTION =          1.00000
    COMPONENT = WATER     SPLIT FRACTION =          1.00000
    COMPONENT = NBUTANOL  SPLIT FRACTION =          1.00000
    COMPONENT = PROPANOL  SPLIT FRACTION =          1.00000

BLOCK:  DUMSEP2  MODEL: SEP2
----------------------------
  INLET STREAM:          S-400A
  OUTLET STREAMS:        D2          S-400
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            16.9291         16.9291         0.00000
      MASS(LB/HR   )            1196.78         1196.78       -0.189988E-15
      ENTHALPY(BTU/HR  )      -0.154685E+07   -0.154652E+07   -0.214462E-03


                       ***  INPUT DATA  ***

  FLASH SPECS FOR STREAM D2
  TWO    PHASE  TP  FLASH
  PRESSURE DROP         PSI                                 0.0
  MAXIMUM NO. ITERATIONS                                  30
  CONVERGENCE TOLERANCE                                     0.000100000
```

```
BLOCK:  DUMSEP2  MODEL: SEP2 (CONTINUED)

  FLASH SPECS FOR STREAM S-400
  TWO    PHASE  TP  FLASH
  PRESSURE DROP         PSI                                 0.0
  MAXIMUM NO. ITERATIONS                                   30
  CONVERGENCE TOLERANCE                                     0.000100000

  SPLIT FRACTION
    SUBSTREAM= MIXED
      STREAM= D2        CPT= MALEIC    FRACTION=          0.0
                             HYDROGEN                     1.00000
                             SUCCINIC                     0.0
                             GBL                          0.0
                             BDO                          0.0
                             THF                          0.0
                             METHANE                      1.00000
                             NBUTANE                      1.00000
                             WATER                        0.0
                             PROPANE                      1.00000
                             NBUTANOL                     0.0
                             PROPANOL                     0.0


                          ***  RESULTS  ***

  HEAT DUTY             BTU/HR                               331.74

 STREAM=   D2         SUBSTREAM= MIXED
    COMPONENT = HYDROGEN  SPLIT FRACTION =         1.00000
    COMPONENT = METHANE   SPLIT FRACTION =         1.00000
    COMPONENT = NBUTANE   SPLIT FRACTION =         1.00000
    COMPONENT = PROPANE   SPLIT FRACTION =         1.00000

 STREAM=   S-400      SUBSTREAM= MIXED
    COMPONENT = MALEIC    SPLIT FRACTION =         1.00000
    COMPONENT = SUCCINIC  SPLIT FRACTION =         1.00000
    COMPONENT = GBL       SPLIT FRACTION =         1.00000
    COMPONENT = BDO       SPLIT FRACTION =         1.00000
    COMPONENT = THF       SPLIT FRACTION =         1.00000
    COMPONENT = WATER     SPLIT FRACTION =         1.00000
    COMPONENT = NBUTANOL  SPLIT FRACTION =         1.00000
    COMPONENT = PROPANOL  SPLIT FRACTION =         1.00000

BLOCK:  DUMSEP3  MODEL: SEP2
----------------------------
  INLET STREAM:          S-404A
  OUTLET STREAMS:        D3          S-404
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE
```

```
BLOCK:  DUMSEP3  MODEL: SEP2 (CONTINUED)

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            5.12618         5.12618       -0.173263E-15
      MASS(LB/HR   )            356.944         356.944        0.159250E-15
      ENTHALPY(BTU/HR  )       -470131.        -470353.        0.472922E-03


                         ***  INPUT DATA  ***

  FLASH SPECS FOR STREAM D3
  TWO    PHASE  TP  FLASH
  PRESSURE DROP         PSI                                 0.0
  MAXIMUM NO. ITERATIONS                                   30
  CONVERGENCE TOLERANCE                                     0.000100000

  FLASH SPECS FOR STREAM S-404
  TWO    PHASE  TP  FLASH
  PRESSURE DROP         PSI                                 0.0
  MAXIMUM NO. ITERATIONS                                   30
  CONVERGENCE TOLERANCE                                     0.000100000

  SPLIT FRACTION
    SUBSTREAM= MIXED
      STREAM= D3        CPT= MALEIC    FRACTION=          0.0
                             HYDROGEN                     1.00000
                             SUCCINIC                     0.0
                             GBL                          0.0
                             BDO                          0.0
                             THF                          0.0
                             METHANE                      1.00000
                             NBUTANE                      1.00000
                             WATER                        0.0
                             PROPANE                      1.00000
                             NBUTANOL                     0.0
                             PROPANOL                     0.0
```

```
BLOCK:  DUMSEP3  MODEL: SEP2 (CONTINUED)


                        ***  RESULTS  ***

  HEAT DUTY             BTU/HR                              -222.44

 STREAM=   D3         SUBSTREAM= MIXED
    COMPONENT = HYDROGEN  SPLIT FRACTION =          1.00000
    COMPONENT = METHANE   SPLIT FRACTION =          1.00000
    COMPONENT = NBUTANE   SPLIT FRACTION =          1.00000
    COMPONENT = PROPANE   SPLIT FRACTION =          1.00000

 STREAM=   S-404      SUBSTREAM= MIXED
    COMPONENT = GBL       SPLIT FRACTION =          1.00000
    COMPONENT = BDO       SPLIT FRACTION =          1.00000
    COMPONENT = THF       SPLIT FRACTION =          1.00000
    COMPONENT = WATER     SPLIT FRACTION =          1.00000
    COMPONENT = NBUTANOL  SPLIT FRACTION =          1.00000
    COMPONENT = PROPANOL  SPLIT FRACTION =          1.00000

BLOCK:  F-200    MODEL: FLASH2
------------------------------
  INLET STREAM:           S-200
  OUTLET VAPOR STREAM:    S-201
  OUTLET LIQUID STREAM:   S-202
  PROPERTY OPTION SET:    PSRK      RKS-MHV1 EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            7439.21         7439.21        0.366770E-15
      MASS(LB/HR   )            55405.4         55405.4         0.00000
      ENTHALPY(BTU/HR  )      -0.200162E+09   -0.200162E+09    0.916614E-06

                        ***  INPUT DATA  ***
  TWO    PHASE  PQ  FLASH
  SPECIFIED PRESSURE    PSIA                              2,009.70
  SPECIFIED HEAT DUTY   BTU/HR                                0.0
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                       0.000100000
```

```
BLOCK:  F-200    MODEL: FLASH2 (CONTINUED)

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                           104.01
  OUTLET PRESSURE       PSIA                                        2009.7
  VAPOR FRACTION                                                   0.77605



  V-L PHASE EQUILIBRIUM :

     COMP             F(I)           X(I)           Y(I)           K(I)
     MALEIC          0.58913E-05    0.26306E-04    0.34835E-12    0.13243E-07
     HYDROGEN        0.77504        0.15710E-01    0.99416         63.289
     SUCCINIC        0.44661E-04    0.19942E-03    0.89179E-12    0.44724E-08
     GBL             0.60056E-02    0.26760E-01    0.16151E-04    0.60365E-03
     BDO             0.34753E-03    0.15518E-02    0.20092E-08    0.12949E-05
     THF             0.23679E-01    0.93620E-01    0.34956E-02    0.37344E-01
     METHANE         0.72415E-03    0.18046E-04    0.92792E-03     51.430
     NBUTANE         0.26969E-03    0.93738E-04    0.32047E-03     3.4196
     WATER           0.19188        0.85334        0.10008E-02    0.11728E-02
     PROPANE         0.45385E-04    0.99874E-05    0.55601E-04     5.5682
     NBUTANOL        0.14168E-02    0.62841E-02    0.12149E-04    0.19336E-02
     PROPANOL        0.54014E-03    0.23877E-02    0.69732E-05    0.29208E-02

BLOCK:  F-300    MODEL: FLASH2
------------------------------
  INLET STREAM:           S-202
  OUTLET VAPOR STREAM:    S-300
  OUTLET LIQUID STREAM:   S-301A
  PROPERTY OPTION SET:    RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1666.04         1666.04       -0.136476E-15
      MASS(LB/HR   )            42052.7         42052.7       -0.173020E-15
      ENTHALPY(BTU/HR  )      -0.199026E+09   -0.199026E+09    0.200198E-07

                        ***  INPUT DATA  ***
  TWO    PHASE  PQ  FLASH
  SPECIFIED PRESSURE    PSIA                                600.000
  SPECIFIED HEAT DUTY   BTU/HR                                0.0
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                       0.000100000
```

```
                             U-O-S BLOCK SECTION

BLOCK:  F-300    MODEL: FLASH2 (CONTINUED)

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                        78.155
  OUTLET PRESSURE       PSIA                                     600.00
  VAPOR FRACTION                                                 0.17506E-01


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)           X(I)           Y(I)           K(I)
     MALEIC          0.26306E-04    0.26775E-04    0.12527E-12    0.46793E-08
     HYDROGEN        0.15710E-01    0.81401E-04    0.89284         10968.
     SUCCINIC        0.19942E-03    0.20297E-03    0.22635E-12    0.11153E-08
     GBL             0.26760E-01    0.27237E-01    0.54857E-05    0.20142E-03
     BDO             0.15518E-02    0.15794E-02    0.39267E-09    0.24864E-06
     THF             0.93620E-01    0.93518E-01    0.99321E-01     1.0621
     METHANE         0.18046E-04    0.11369E-05    0.96700E-03     850.54
     NBUTANE         0.93738E-04    0.97966E-05    0.48047E-02     490.44
     WATER           0.85334        0.86853        0.93335E-03    0.10747E-02
     PROPANE         0.99874E-05    0.14988E-05    0.48638E-03     324.51
     NBUTANOL        0.62841E-02    0.63862E-02    0.55188E-03    0.86421E-01
     PROPANOL        0.23877E-02    0.24286E-02    0.91650E-04    0.37740E-01

BLOCK:  F-400    MODEL: FLASH2
------------------------------
  INLET STREAM:          S-203
  OUTLET VAPOR STREAM:   S-401
  OUTLET LIQUID STREAM:  S-400A
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           81.5000         81.5000         0.00000
      MASS(LB/HR   )           1580.91         1580.91        0.143825E-15
      ENTHALPY(BTU/HR  )      -0.188688E+07   -0.188688E+07   -0.230276E-07

                        ***  INPUT DATA  ***
  TWO    PHASE  PQ  FLASH
  SPECIFIED PRESSURE    PSIA                                  164.696
  SPECIFIED HEAT DUTY   BTU/HR                                  0.0
  MAXIMUM NO. ITERATIONS                                       30
  CONVERGENCE TOLERANCE                                         0.000100000
```

```
                             U-O-S BLOCK SECTION

BLOCK:  F-400    MODEL: FLASH2 (CONTINUED)

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                        89.988
  OUTLET PRESSURE       PSIA                                     164.70
  VAPOR FRACTION                                                 0.79228


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)           X(I)           Y(I)           K(I)
     MALEIC          0.24676E-10    0.11879E-09    0.87942E-17    0.74028E-07
     HYDROGEN        0.70423        0.87229E-02    0.88658         101.64
     SUCCINIC        0.63171E-10    0.30412E-09    0.52345E-17    0.17212E-07
     GBL             0.11441E-02    0.55049E-02    0.77182E-06    0.14020E-03
     BDO             0.14232E-06    0.68509E-06    0.20709E-10    0.30228E-04
     THF             0.21667        0.93654        0.27930E-01    0.29822E-01
     METHANE         0.52585E-01    0.22939E-02    0.65770E-01     28.672
     NBUTANE         0.19863E-01    0.34894E-01    0.15923E-01    0.45632
     WATER           0.70895E-03    0.32539E-02    0.41724E-04    0.12823E-01
     PROPANE         0.34462E-02    0.24087E-02    0.37182E-02     1.5436
     NBUTANOL        0.86056E-03    0.40918E-02    0.13409E-04    0.32771E-02
     PROPANOL        0.49395E-03    0.22883E-02    0.23503E-04    0.10271E-01

BLOCK:  F-401    MODEL: FLASH2
------------------------------
  INLET STREAM:          S-402
  OUTLET VAPOR STREAM:   S-403
  OUTLET LIQUID STREAM:  S-404A
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           93.7372         93.7372       -0.151603E-15
      MASS(LB/HR   )           656.587         656.587       -0.173148E-15
      ENTHALPY(BTU/HR  )      -717344.        -717344.         0.633966E-08

                        ***  INPUT DATA  ***
  TWO    PHASE  PQ  FLASH
  SPECIFIED PRESSURE    PSIA                                  164.696
  SPECIFIED HEAT DUTY   BTU/HR                                  0.0
  MAXIMUM NO. ITERATIONS                                       30
  CONVERGENCE TOLERANCE                                         0.000100000
```

```
BLOCK:  F-401    MODEL: FLASH2 (CONTINUED)

                         ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                  -0.20103E-03
  OUTLET PRESSURE       PSIA                                  164.70
  VAPOR FRACTION                                             0.94531



  V-L PHASE EQUILIBRIUM :

     COMP             F(I)           X(I)           Y(I)           K(I)
     MALEIC         0.38985E-13    0.71288E-12    0.10809E-22    0.15162E-10
     HYDROGEN       0.88853        0.77140E-02    0.93948         121.79
     SUCCINIC       0.70432E-13    0.12879E-11    0.25425E-23    0.19742E-11
     GBL            0.22385E-05    0.40932E-04    0.10201E-09    0.24922E-05
     BDO            0.13645E-09    0.24950E-08    0.40268E-15    0.16139E-06
     THF            0.50143E-01    0.88030        0.21184E-02    0.24065E-02
     METHANE        0.45606E-01    0.25113E-02    0.48100E-01     19.154
     NBUTANE        0.12463E-01    0.93383E-01    0.77821E-02    0.83336E-01
     WATER          0.31915E-03    0.57964E-02    0.22924E-05    0.39549E-03
     PROPANE        0.27126E-02    0.61408E-02    0.25143E-02    0.40945
     NBUTANOL       0.18096E-03    0.33053E-02    0.21194E-06    0.64122E-04
     PROPANOL       0.44707E-04    0.81331E-03    0.24321E-06    0.29903E-03

BLOCK:  M-200    MODEL: SEP2
----------------------------
  INLET STREAM:          S-201
  OUTLET STREAMS:        S-204       S-203
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            5773.18         5773.18       -0.472614E-15
      MASS(LB/HR   )            13352.7         13352.7       -0.544907E-15
      ENTHALPY(BTU/HR  )      -0.113564E+07   -0.134224E+07    0.153925


                        ***  INPUT DATA  ***

  INLET PRESSURE DROP   PSI                               300.000
```

```
BLOCK:  M-200    MODEL: SEP2 (CONTINUED)

  FLASH SPECS FOR STREAM S-204
  TWO    PHASE  TP  FLASH
  PRESSURE DROP         PSI                                 0.0
  MAXIMUM NO. ITERATIONS                                   30
  CONVERGENCE TOLERANCE                                     0.000100000

  FLASH SPECS FOR STREAM S-203
  TWO    PHASE  TP  FLASH
  PRESSURE DROP         PSI                                 0.0
  MAXIMUM NO. ITERATIONS                                   30
  CONVERGENCE TOLERANCE                                     0.000100000

  SPLIT FRACTION
    SUBSTREAM= MIXED
      STREAM= S-204     CPT= MALEIC    FRACTION=          0.0
                             HYDROGEN                     0.99000
                             SUCCINIC                     0.0
                             GBL                          0.0
                             BDO                          0.0
                             THF                          0.12500
                             METHANE                      0.20000
                             NBUTANE                      0.12500
                             WATER                        0.99000
                             PROPANE                      0.12500
                             NBUTANOL                     0.0
                             PROPANOL                     0.0


                        ***  RESULTS  ***

  HEAT DUTY             BTU/HR                            -0.20660E+06

 STREAM=   S-204      SUBSTREAM= MIXED
    COMPONENT = HYDROGEN  SPLIT FRACTION =          0.99000
    COMPONENT = THF       SPLIT FRACTION =          0.12500
    COMPONENT = METHANE   SPLIT FRACTION =          0.20000
    COMPONENT = NBUTANE   SPLIT FRACTION =          0.12500
    COMPONENT = WATER     SPLIT FRACTION =          0.99000
    COMPONENT = PROPANE   SPLIT FRACTION =          0.12500
```

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ASPEN PLUS   PLAT: WIN32     VER: 21.0                  04/02/2009  PAGE 55

                             U-O-S BLOCK SECTION

BLOCK:  M-200    MODEL: SEP2 (CONTINUED)

 STREAM=   S-203      SUBSTREAM= MIXED
    COMPONENT = MALEIC    SPLIT FRACTION =          1.00000
    COMPONENT = HYDROGEN  SPLIT FRACTION =          0.0100000
    COMPONENT = SUCCINIC  SPLIT FRACTION =          1.00000
    COMPONENT = GBL       SPLIT FRACTION =          1.00000
    COMPONENT = BDO       SPLIT FRACTION =          1.00000
    COMPONENT = THF       SPLIT FRACTION =          0.87500
    COMPONENT = METHANE   SPLIT FRACTION =          0.80000
    COMPONENT = NBUTANE   SPLIT FRACTION =          0.87500
    COMPONENT = WATER     SPLIT FRACTION =          0.0100000
    COMPONENT = PROPANE   SPLIT FRACTION =          0.87500
    COMPONENT = NBUTANOL  SPLIT FRACTION =          1.00000
    COMPONENT = PROPANOL  SPLIT FRACTION =          1.00000

BLOCK:  P-100    MODEL: PUMP
----------------------------
  INLET STREAM:          S-101
  OUTLET STREAM:         S-102
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1013.21         1013.21         0.00000
      MASS(LB/HR   )            37015.8         37015.8         0.00000
      ENTHALPY(BTU/HR  )      -0.162000E+09   -0.161476E+09   -0.323570E-02

                         ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIA                                  2,054.70
   DRIVER EFFICIENCY                                          1.00000

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

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ASPEN PLUS   PLAT: WIN32     VER: 21.0                  04/02/2009  PAGE 56

                             U-O-S BLOCK SECTION

BLOCK:  P-100    MODEL: PUMP (CONTINUED)

                          ***  RESULTS  ***
   VOLUMETRIC FLOW RATE  CUFT/HR                             725.200
   PRESSURE CHANGE  PSI                                    2,040.00
   NPSH AVAILABLE   FT-LBF/LB                                 12.8691
   FLUID POWER  HP                                           107.593
   BRAKE POWER  HP                                           206.012
   ELECTRICITY  KW                                           153.623
   PUMP EFFICIENCY USED                                        0.52227
   NET WORK REQUIRED  HP                                     206.012
   HEAD DEVELOPED FT-LBF/LB                                5,755.24

                      ***  ASSOCIATED  UTILITIES  ***

 UTILITY ID FOR ELECTRICITY              ELECTRIC
 RATE OF CONSUMPTION                     153.6230  KW
 COST                                      7.6811  $/HR

BLOCK:  P-300    MODEL: PUMP
----------------------------
  INLET STREAM:          S-311
  OUTLET STREAM:         S-312
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            71.4208         71.4208         0.00000
      MASS(LB/HR   )            4478.65         4478.65         0.00000
      ENTHALPY(BTU/HR  )      -0.114800E+08   -0.113900E+08   -0.783298E-02

                         ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIA                                  2,054.70
   DRIVER EFFICIENCY                                          1.00000

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

```
                             U-O-S BLOCK SECTION

BLOCK:  P-300    MODEL: PUMP (CONTINUED)

                          ***  RESULTS  ***
   VOLUMETRIC FLOW RATE  CUFT/HR                          70.6798
   PRESSURE CHANGE  PSI                                2,032.70
   NPSH AVAILABLE   FT-LBF/LB                              0.0
   FLUID POWER  HP                                        10.4488
   BRAKE POWER  HP                                        35.3408
   ELECTRICITY  KW                                        26.3536
   PUMP EFFICIENCY USED                                    0.29566
   NET WORK REQUIRED  HP                                  35.3408
   HEAD DEVELOPED FT-LBF/LB                            4,619.38

                      ***  ASSOCIATED  UTILITIES  ***

 UTILITY ID FOR ELECTRICITY              ELECTRIC
 RATE OF CONSUMPTION                      26.3536  KW
 COST                                      1.3177  $/HR

BLOCK:  P-502    MODEL: PUMP
----------------------------
  INLET STREAM:          S-504
  OUTLET STREAM:         510
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           422.360         422.360         0.00000
      MASS(LB/HR   )           26536.2         26536.2       -0.137095E-15
      ENTHALPY(BTU/HR  )      -0.405085E+08   -0.404879E+08   -0.506444E-03

                         ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIA                                 120.000
   DRIVER EFFICIENCY                                       1.00000

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

```
                             U-O-S BLOCK SECTION

BLOCK:  P-502    MODEL: PUMP (CONTINUED)

                          ***  RESULTS  ***
   VOLUMETRIC FLOW RATE  CUFT/HR                          496.880
   PRESSURE CHANGE  PSI                                   105.000
   NPSH AVAILABLE   FT-LBF/LB                               0.0
   FLUID POWER  HP                                          3.79435
   BRAKE POWER  HP                                          8.06280
   ELECTRICITY  KW                                          6.01243
   PUMP EFFICIENCY USED                                     0.47060
   NET WORK REQUIRED  HP                                    8.06280
   HEAD DEVELOPED FT-LBF/LB                               283.115

                      ***  ASSOCIATED  UTILITIES  ***

 UTILITY ID FOR ELECTRICITY              ELECTRIC
 RATE OF CONSUMPTION                        6.0124  KW
 COST                                       0.3006  $/HR

BLOCK:  R-100    MODEL: RSTOIC
------------------------------
  INLET STREAMS:         S-102       S-104       S-312       S-206
  OUTLET STREAM:         DUMMY
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                IN          OUT       GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)         7839.31       7803.87      -33.5822      0.237842E-03
  MASS(LB/HR   )         55409.0       55405.4                    0.663702E-04
  ENTHALPY(BTU/HR  )   -0.151047E+09 -0.151144E+09                0.639597E-03

                         ***  INPUT DATA  ***
```

```
BLOCK:  R-100    MODEL: RSTOIC (CONTINUED)
  STOICHIOMETRY MATRIX:

   REACTION #   1:
    SUBSTREAM MIXED   :
    HYDROGEN  -2.00    SUCCINIC  -1.00    GBL        1.00    WATER      2.00

   REACTION #   2:
    SUBSTREAM MIXED   :
    HYDROGEN  -4.00    SUCCINIC  -1.00    BDO        1.00    WATER      2.00

   REACTION #   3:
    SUBSTREAM MIXED   :
    HYDROGEN  -4.00    SUCCINIC  -1.00    THF        1.00    WATER      3.00

   REACTION #   4:
    SUBSTREAM MIXED   :
    HYDROGEN  -7.00    SUCCINIC  -1.00    METHANE    1.00    WATER      4.00
    PROPANE    1.00

   REACTION #   5:
    SUBSTREAM MIXED   :
    HYDROGEN  -6.00    SUCCINIC  -1.00    NBUTANE    1.00    WATER      4.00

   REACTION #   6:
    SUBSTREAM MIXED   :
    HYDROGEN  -6.00    SUCCINIC  -1.00    METHANE    1.00    WATER      3.00
    PROPANOL   1.00

   REACTION #   7:
    SUBSTREAM MIXED   :
    HYDROGEN  -5.00    SUCCINIC  -1.00    WATER      3.00    NBUTANOL   1.00

   REACTION #   8:
    SUBSTREAM MIXED   :
    HYDROGEN  -2.00    GBL       -1.00    BDO        1.00

   REACTION #   9:
    SUBSTREAM MIXED   :
    HYDROGEN  -2.00    GBL       -1.00    THF        1.00    WATER      1.00

   REACTION #  10:
    SUBSTREAM MIXED   :
    HYDROGEN  -5.00    GBL       -1.00    METHANE    1.00    WATER      2.00
    PROPANE    1.00

   REACTION #  11:
    SUBSTREAM MIXED   :
    HYDROGEN  -4.00    GBL       -1.00    NBUTANE    1.00    WATER      2.00

   REACTION #  12:
    SUBSTREAM MIXED   :
    HYDROGEN  -4.00    GBL       -1.00    METHANE    1.00    WATER      1.00
    PROPANOL   1.00

   REACTION #  13:
    SUBSTREAM MIXED   :
    HYDROGEN  -3.00    GBL       -1.00    WATER      1.00    NBUTANOL   1.00

   REACTION #  14:
    SUBSTREAM MIXED   :
    BDO       -1.00    THF        1.00    WATER      1.00

   REACTION #  15:
    SUBSTREAM MIXED   :
    HYDROGEN  -2.00    BDO       -1.00    NBUTANE    1.00    WATER      2.00

   REACTION #  16:
    SUBSTREAM MIXED   :
    HYDROGEN  -1.00    BDO       -1.00    WATER      1.00    NBUTANOL   1.00
```

```
                        U-O-S BLOCK SECTION

BLOCK:  R-100    MODEL: RSTOIC (CONTINUED)
  REACTION CONVERSION SPECS: NUMBER=   16
    REACTION #   1:
    SUBSTREAM:MIXED    KEY COMP:SUCCINIC CONV FRAC: 0.1765
    REACTION #   2:
    SUBSTREAM:MIXED    KEY COMP:SUCCINIC CONV FRAC: 0.1015E-01
    REACTION #   3:
    SUBSTREAM:MIXED    KEY COMP:SUCCINIC CONV FRAC: 0.7454
    REACTION #   4:
    SUBSTREAM:MIXED    KEY COMP:SUCCINIC CONV FRAC: 0.1230E-02
    REACTION #   5:
    SUBSTREAM:MIXED    KEY COMP:SUCCINIC CONV FRAC: 0.7948E-02
    REACTION #   6:
    SUBSTREAM:MIXED    KEY COMP:SUCCINIC CONV FRAC: 0.1270E-01
    REACTION #   7:
    SUBSTREAM:MIXED    KEY COMP:SUCCINIC CONV FRAC: 0.4434E-01
    REACTION #   8:
    SUBSTREAM:MIXED    KEY COMP:GBL      CONV FRAC: 0.1406E-01
    REACTION #   9:
    SUBSTREAM:MIXED    KEY COMP:GBL      CONV FRAC: 0.6858
    REACTION #  10:
    SUBSTREAM:MIXED    KEY COMP:GBL      CONV FRAC: 0.5810E-03
    REACTION #  11:
    SUBSTREAM:MIXED    KEY COMP:GBL      CONV FRAC: 0.5172E-02
    REACTION #  12:
    SUBSTREAM:MIXED    KEY COMP:GBL      CONV FRAC: 0.3632E-02
    REACTION #  13:
    SUBSTREAM:MIXED    KEY COMP:GBL      CONV FRAC: 0.4202E-01
    REACTION #  14:
    SUBSTREAM:MIXED    KEY COMP:BDO      CONV FRAC: 0.9000
    REACTION #  15:
    SUBSTREAM:MIXED    KEY COMP:BDO      CONV FRAC: 0.1000E-01
    REACTION #  16:
    SUBSTREAM:MIXED    KEY COMP:BDO      CONV FRAC: 0.8000E-01




  THREE  PHASE  PQ  FLASH
  SPECIFIED PRESSURE    PSIA                          2,034.70
  SPECIFIED HEAT DUTY   BTU/HR                             0.0
  MAXIMUM NO. ITERATIONS                                 30
  CONVERGENCE TOLERANCE                                    0.000100000
  SIMULTANEOUS REACTIONS
  GENERATE COMBUSTION REACTIONS FOR FEED SPECIES          NO
```

```
                        U-O-S BLOCK SECTION

BLOCK:  R-100    MODEL: RSTOIC (CONTINUED)

                             ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                          345.31
  OUTLET PRESSURE       PSIA                                       2034.7
  VAPOR FRACTION                                                  0.91539
  1ST LIQUID/TOTAL LIQUID                                          1.0000

  REACTION EXTENTS:

     REACTION          REACTION
     NUMBER            EXTENT
                       LBMOL/HR
     1                 0.58633E-01
     2                 0.33736E-02
     3                 0.24766
     4                 0.40865E-03
     5                 0.26406E-02
     6                 0.42201E-02
     7                 0.14732E-01
     8                 0.61296
     9                  29.902
     10                0.25331E-01
     11                0.22550
     12                0.15835
     13                 1.8319
     14                 2.3265
     15                0.25850E-01
     16                0.20680

  V-L1-L2 PHASE EQUILIBRIUM :

     COMP           F(I)       X1(I)      X2(I)      Y(I)       K1(I)      K2(I)
     MALEIC       0.245E-01 0.288      0.288      0.130E-03 0.450E-03 0.258
     HYDROGEN     0.855      0.467E-01 0.467E-01 0.930      19.9       3.62
     SUCCINIC     0.732E-07 0.863E-06 0.863E-06 0.199E-09 0.231E-03 0.254
     GBL          0.140E-02 0.129E-01 0.129E-01 0.333E-03 0.258E-01 0.950
     BDO          0.823E-04 0.937E-03 0.937E-03 0.330E-05 0.352E-02 0.693
     THF          0.448E-02 0.995E-02 0.995E-02 0.398E-02 0.400      1.32
     METHANE      0.161E-03 0.112E-04 0.112E-04 0.175E-03  15.6      3.93
     NBUTANE      0.622E-04 0.829E-05 0.829E-05 0.671E-04  8.10      3.20
```

```
BLOCK:  R-100    MODEL: RSTOIC (CONTINUED)

  V-L1-L2 PHASE EQUILIBRIUM :

     COMP           F(I)      X1(I)     X2(I)     Y(I)      K1(I)     K2(I)
     WATER         0.114     0.640     0.640     0.652E-01 0.102      1.23
     PROPANE       0.844E-05 0.853E-06 0.853E-06 0.914E-05  10.7      3.25
     NBUTANOL      0.263E-03 0.101E-02 0.101E-02 0.194E-03 0.193      1.57
     PROPANOL      0.208E-04 0.668E-04 0.668E-04 0.166E-04 0.248      1.61

BLOCK:  R-100A   MODEL: RSTOIC
------------------------------
  INLET STREAM:          DUMMY
  OUTLET STREAM:         S-105
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                      ***  MASS AND ENERGY BALANCE  ***
                              IN          OUT       GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)         7803.87       7439.21      -364.651       0.00000
  MASS(LB/HR   )         55405.4       55405.4                     0.00000
  ENTHALPY(BTU/HR  )   -0.151144E+09 -0.151144E+09               0.197179E-15

                          ***  INPUT DATA  ***
```

```
BLOCK:  R-100A   MODEL: RSTOIC (CONTINUED)
  STOICHIOMETRY MATRIX:

   REACTION #   1:
    SUBSTREAM MIXED   :
    MALEIC    -1.00    HYDROGEN  -1.00    SUCCINIC   1.00

   REACTION #   2:
    SUBSTREAM MIXED   :
    MALEIC    -1.00    HYDROGEN  -5.00    THF        1.00    WATER      3.00

   REACTION #   3:
    SUBSTREAM MIXED   :
    MALEIC    -1.00    HYDROGEN  -3.00    GBL        1.00    WATER      2.00

   REACTION #   4:
    SUBSTREAM MIXED   :
    MALEIC    -1.00    HYDROGEN  -5.00    BDO        1.00    WATER      2.00

   REACTION #   5:
    SUBSTREAM MIXED   :
    MALEIC    -1.00    HYDROGEN  -6.00    WATER      3.00    NBUTANOL   1.00

   REACTION #   6:
    SUBSTREAM MIXED   :
    MALEIC    -1.00    HYDROGEN  -7.00    METHANE    1.00    WATER      3.00
    PROPANOL   1.00

   REACTION #   7:
    SUBSTREAM MIXED   :
    MALEIC    -1.00    HYDROGEN  -7.00    NBUTANE    1.00    WATER      4.00

   REACTION #   8:
    SUBSTREAM MIXED   :
    MALEIC    -1.00    HYDROGEN  -8.00    METHANE    1.00    WATER      4.00
    PROPANE    1.00


  REACTION CONVERSION SPECS: NUMBER=    8
    REACTION #   1:
    SUBSTREAM:MIXED    KEY COMP:MALEIC   CONV FRAC: 0.1733E-02
    REACTION #   2:
    SUBSTREAM:MIXED    KEY COMP:MALEIC   CONV FRAC: 0.7376
    REACTION #   3:
    SUBSTREAM:MIXED    KEY COMP:MALEIC   CONV FRAC: 0.1765
    REACTION #   4:
    SUBSTREAM:MIXED    KEY COMP:MALEIC   CONV FRAC: 0.1015E-01
    REACTION #   5:
    SUBSTREAM:MIXED    KEY COMP:MALEIC   CONV FRAC: 0.4434E-01
    REACTION #   6:
    SUBSTREAM:MIXED    KEY COMP:MALEIC   CONV FRAC: 0.2015E-01
    REACTION #   7:
    SUBSTREAM:MIXED    KEY COMP:MALEIC   CONV FRAC: 0.7948E-02
    REACTION #   8:
    SUBSTREAM:MIXED    KEY COMP:MALEIC   CONV FRAC: 0.1420E-02
```

```
                              U-O-S BLOCK SECTION

BLOCK:  R-100A   MODEL: RSTOIC (CONTINUED)
  THREE  PHASE  PQ  FLASH
  SPECIFIED PRESSURE    PSIA                           2,014.70
  SPECIFIED HEAT DUTY   BTU/HR                             0.0
  MAXIMUM NO. ITERATIONS                                  30
  CONVERGENCE TOLERANCE                                    0.000100000
  SIMULTANEOUS REACTIONS
  GENERATE COMBUSTION REACTIONS FOR FEED SPECIES          NO

                           ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                   480.40
  OUTLET PRESSURE       PSIA                                2014.7
  VAPOR FRACTION                                            1.0000
  1ST LIQUID/TOTAL LIQUID                                   1.0000

  REACTION EXTENTS:

     REACTION          REACTION
     NUMBER            EXTENT
                       LBMOL/HR
     1                 0.33167
     2                  141.16
     3                  33.775
     4                  1.9431
     5                  8.4861
     6                  3.8556
     7                  1.5211
     8                 0.27176

  V-L1-L2 PHASE EQUILIBRIUM :

     COMP           F(I)      X1(I)     X2(I)     Y(I)      K1(I)     K2(I)
     MALEIC       0.589E-05 0.269E-02 0.269E-02 0.589E-05 0.219E-02 0.219E-02
     HYDROGEN     0.775     0.231E-01 0.231E-01 0.775      33.6      33.6
     SUCCINIC     0.447E-04 0.275E-01 0.275E-01 0.447E-04 0.162E-02 0.162E-02
     GBL          0.601E-02 0.390E-01 0.390E-01 0.601E-02 0.154     0.154
     BDO          0.348E-03 0.148E-01 0.148E-01 0.348E-03 0.235E-01 0.235E-01
     THF          0.237E-01 0.200E-01 0.200E-01 0.237E-01  1.18      1.18
     METHANE      0.724E-03 0.154E-04 0.154E-04 0.724E-03  47.1      47.1
     NBUTANE      0.270E-03 0.170E-04 0.170E-04 0.270E-03  15.8      15.8
     WATER        0.192     0.870     0.870     0.192     0.221     0.221
```

```
                              U-O-S BLOCK SECTION

BLOCK:  R-100A   MODEL: RSTOIC (CONTINUED)

  V-L1-L2 PHASE EQUILIBRIUM :

     COMP           F(I)      X1(I)     X2(I)     Y(I)      K1(I)     K2(I)
     PROPANE      0.454E-04 0.262E-05 0.262E-05 0.454E-04  17.3      17.3
     NBUTANOL     0.142E-02 0.216E-02 0.216E-02 0.142E-02 0.657     0.657
     PROPANOL     0.540E-03 0.757E-03 0.757E-03 0.540E-03 0.714     0.714

BLOCK:  V-600    MODEL: VALVE
-----------------------------
  INLET STREAM:          S-518
  OUTLET STREAM:         S-600
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                   ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           173.377         173.377         0.00000
      MASS(LB/HR   )           12500.0         12500.0         0.00000
      ENTHALPY(BTU/HR  )      -0.147771E+08   -0.147771E+08     0.00000

                       ***  INPUT DATA  ***

   VALVE OUTLET PRESSURE     PSIA                        21.0000
   VALVE FLOW COEF CALC.                                 NO

                       FLASH SPECIFICATIONS:
   NPHASE                                                 2
   MAX NUMBER OF ITERATIONS                              30
   CONVERGENCE TOLERANCE                                  0.000100000

                       ***  RESULTS  ***

   VALVE PRESSURE DROP       PSI                         96.0000
```

```
                             U-O-S BLOCK SECTION

BLOCK:  X-100    MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:          U-100
  OUTLET STREAM:         U-101
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE
  COLD SIDE:
  ----------
  INLET STREAM:          S-100
  OUTLET STREAM:         S-101
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1174.24         1174.24         0.00000
      MASS(LB/HR   )            39916.8         39916.8         0.00000
      ENTHALPY(BTU/HR  )      -0.181255E+09   -0.181255E+09     0.00000

                       ***  INPUT DATA  ***

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

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

  FLOW DIRECTION AND SPECIFICATION:
    COUNTERCURRENT   HEAT EXCHANGER
    SPECIFIED HOT VAPOR FRACTION
    SPECIFIED VALUE                                      0.0000
    LMTD CORRECTION FACTOR                               1.00000

  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                   0.0000
    COLD SIDE PRESSURE DROP        PSI                   5.0000

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT           BTU/HR-SQFT-R          150.0000
```

```
                             U-O-S BLOCK SECTION

BLOCK:  X-100    MODEL: HEATX (CONTINUED)

                       ***  OVERALL RESULTS  ***

  STREAMS:
                 --------------------------------------
                |                                      |
  U-100     ----->|                HOT                 |-----> U-101
  T=  3.0015D+02  |                                    |       T=  3.0016D+02
  P=  6.4696D+01  |                                    |       P=  6.4696D+01
  V=  1.0000D+00  |                                    |       V=  0.0000D+00
                |                                      |
  S-101     <-----|                COLD                |<----- S-100
  T=  2.0120D+02  |                                    |       T=  1.0400D+02
  P=  1.4696D+01  |                                    |       P=  1.9696D+01
  V=  0.0000D+00  |                                    |       V=  0.0000D+00
                 --------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR            2786743.4316
    CALCULATED (REQUIRED) AREA     SQFT                  130.7831
    ACTUAL EXCHANGER AREA          SQFT                  130.7831
    PER CENT OVER-DESIGN                                   0.0000

  HEAT TRANSFER COEFFICIENT:
    AVERAGE COEFFICIENT (DIRTY)    BTU/HR-SQFT-R         150.0000
    UA (DIRTY)                     BTU/HR-R            19617.4660

  LOG-MEAN TEMPERATURE DIFFERENCE:
    LMTD CORRECTION FACTOR                                 1.0000
    LMTD (CORRECTED)               F                     142.0542
    NUMBER OF SHELLS IN SERIES                             1

  PRESSURE DROP:
    HOTSIDE, TOTAL                 PSI                     0.0000
    COLDSIDE, TOTAL                PSI                     5.0000

  PRESSURE DROP PARAMETER:
    HOT SIDE:                                            0.0000
    COLD SIDE:                                           0.18336E+07

BLOCK:  X-200    MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:          S-105
  OUTLET STREAM:         S-200
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE
  COLD SIDE:
  ----------
  INLET STREAM:          U-200
  OUTLET STREAM:         U-201
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE
```

```
                             U-O-S BLOCK SECTION

BLOCK:  X-200    MODEL: HEATX (CONTINUED)

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            9841.31         9841.31         0.00000
      MASS(LB/HR   )            98679.8         98679.8         0.00000
      ENTHALPY(BTU/HR  )      -0.445850E+09   -0.445850E+09   -0.267376E-15

                         ***  INPUT DATA  ***

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

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

  FLOW DIRECTION AND SPECIFICATION:
    COUNTERCURRENT   HEAT EXCHANGER
    SPECIFIED HOT APPROACH TEMP
    SPECIFIED VALUE               F                       14.0000
    TEMPERATURE TOLERANCE         F                        0.01800
    LMTD CORRECTION FACTOR                                 1.00000

  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP       PSI                      2.0000
    COLD SIDE PRESSURE DROP       PSI                      2.0000

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT           BTU/HR-SQFT-R           60.0000

                       ***  OVERALL RESULTS  ***

  STREAMS:
                --------------------------------------
                |                                    |
  S-105     ----->|             HOT                   |-----> S-200
  T=  4.8040D+02  |                                    |       T=  1.0400D+02
  P=  2.0147D+03  |                                    |       P=  2.0127D+03
  V=  1.0000D+00  |                                    |       V=  7.7604D-01
                |                                    |
  U-201     <-----|             COLD                  |<----- U-200
  T=  2.9772D+02  |                                    |       T=  9.0000D+01
  P=  6.2696D+01  |                                    |       P=  6.4696D+01
  V=  1.0000D+00  |                                    |       V=  0.0000D+00
                --------------------------------------
```

```
                             U-O-S BLOCK SECTION

BLOCK:  X-200    MODEL: HEATX (CONTINUED)

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR           49017997.3173
    CALCULATED (REQUIRED) AREA     SQFT                12440.8998
    ACTUAL EXCHANGER AREA          SQFT                12440.8998
    PER CENT OVER-DESIGN                                   0.0000

  HEAT TRANSFER COEFFICIENT:
    AVERAGE COEFFICIENT (DIRTY)    BTU/HR-SQFT-R          60.0000
    UA (DIRTY)                     BTU/HR-R           746453.9813

  LOG-MEAN TEMPERATURE DIFFERENCE:
    LMTD CORRECTION FACTOR                                 1.0000
    LMTD (CORRECTED)               F                      65.6678
    NUMBER OF SHELLS IN SERIES                               1

  PRESSURE DROP:
    HOTSIDE, TOTAL                 PSI                     2.0000
    COLDSIDE, TOTAL                PSI                     2.0000

  PRESSURE DROP PARAMETER:
    HOT SIDE:                                            8787.9
    COLD SIDE:                                           2113.9

BLOCK:  X-201    MODEL: HEATER
------------------------------
  INLET STREAM:          S-205
  OUTLET STREAM:         S-206
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            5691.68         5691.68         0.00000
      MASS(LB/HR   )            11771.8         11771.8         0.00000
      ENTHALPY(BTU/HR  )      0.236869E+07    0.194076E+08   -0.877951

                         ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE               F                     572.000
  SPECIFIED PRESSURE                  PSIA                2,054.70
  MAXIMUM NO. ITERATIONS                                     30
  CONVERGENCE TOLERANCE                                       0.000100000
```

```
ASPEN PLUS   PLAT: WIN32     VER: 21.0                  04/02/2009  PAGE 70

                             U-O-S BLOCK SECTION

BLOCK:  X-201    MODEL: HEATER (CONTINUED)

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                      572.00
  OUTLET PRESSURE       PSIA                                   2054.7
  HEAT DUTY             BTU/HR                               0.17039E+08
  OUTLET VAPOR FRACTION                                        1.0000
  PRESSURE-DROP CORRELATION PARAMETER                          0.0000


  V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     HYDROGEN         0.99832        0.99857        0.99832         5.8247
     THF              0.44321E-03    0.58678E-03    0.44321E-03     4.4007
     METHANE          0.18824E-03    0.16135E-03    0.18824E-03     6.7972
     NBUTANE          0.40632E-04    0.34067E-04    0.40632E-04     6.9490
     WATER            0.10050E-02    0.63846E-03    0.10050E-02     9.1709
     PROPANE          0.70496E-05    0.64050E-05    0.70496E-05     6.4126

BLOCK:  X-400    MODEL: HEATER
------------------------------
  INLET STREAMS:         S-300       S-401
  OUTLET STREAM:         S-402
  PROPERTY OPTION SET:   PSRK      RKS-MHV1 EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           93.7372         93.7372         0.00000
      MASS(LB/HR   )           656.587         656.587        0.173148E-15
      ENTHALPY(BTU/HR  )      -584812.        -717344.        0.184753

                         ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE               F                           0.0
  SPECIFIED PRESSURE                  PSIA                      164.696
  MAXIMUM NO. ITERATIONS                                        30
  CONVERGENCE TOLERANCE                                           0.000100000
```

```
ASPEN PLUS   PLAT: WIN32     VER: 21.0                  04/02/2009  PAGE 71

                             U-O-S BLOCK SECTION

BLOCK:  X-400    MODEL: HEATER (CONTINUED)

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                      0.0000
  OUTLET PRESSURE       PSIA                                   164.70
  HEAT DUTY             BTU/HR                              -0.13253E+06
  OUTLET VAPOR FRACTION                                       0.94531
  PRESSURE-DROP CORRELATION PARAMETER                          0.0000


  V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     MALEIC           0.38985E-13    0.71288E-12    0.10811E-22    0.15163E-10
     HYDROGEN         0.88853        0.77141E-02    0.93948         121.79
     SUCCINIC         0.70432E-13    0.12879E-11    0.25431E-23    0.19742E-11
     GBL              0.22385E-05    0.40932E-04    0.10202E-09    0.24923E-05
     BDO              0.13645E-09    0.24950E-08    0.40274E-15    0.16140E-06
     THF              0.50143E-01    0.88029        0.21184E-02    0.24065E-02
     METHANE          0.45606E-01    0.25114E-02    0.48100E-01     19.154
     NBUTANE          0.12463E-01    0.93386E-01    0.77819E-02    0.83336E-01
     WATER            0.31915E-03    0.57964E-02    0.22926E-05    0.39550E-03
     PROPANE          0.27126E-02    0.61411E-02    0.25143E-02    0.40945
     NBUTANOL         0.18096E-03    0.33053E-02    0.21195E-06    0.64123E-04
     PROPANOL         0.44707E-04    0.81330E-03    0.24322E-06    0.29904E-03

                      ***  ASSOCIATED  UTILITIES  ***

 UTILITY ID FOR ELECTRICITY             ELECTRIC
 RATE OF CONSUMPTION                     38.8412  KW
 COST                                     1.9421  $/HR

BLOCK:  X-600    MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:          S-600
  OUTLET STREAM:         S-601
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG
  COLD SIDE:
  ----------
  INLET STREAM:          U-600
  OUTLET STREAM:         U-601
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
```

```
                             U-O-S BLOCK SECTION

BLOCK:  X-600    MODEL: HEATX (CONTINUED)
   TOTAL BALANCE
      MOLE(LBMOL/HR)            2099.80         2099.80         0.00000
      MASS(LB/HR   )            47205.0         47205.0         0.00000
      ENTHALPY(BTU/HR  )      -0.253638E+09   -0.253638E+09   -0.234999E-15

                         ***  INPUT DATA  ***

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

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

  FLOW DIRECTION AND SPECIFICATION:
    COUNTERCURRENT   HEAT EXCHANGER
    SPECIFIED HOT APPROACH TEMP
    SPECIFIED VALUE                F                         14.0000
    TEMPERATURE TOLERANCE          F                          0.01800
    LMTD CORRECTION FACTOR                                    1.00000

  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                        1.0000
    COLD SIDE PRESSURE DROP        PSI                       10.0000

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT            BTU/HR-SQFT-R            100.0000

                       ***  OVERALL RESULTS  ***

  STREAMS:
                  --------------------------------------
                  |                                    |
  S-600     ----->|               HOT                  |-----> S-601
  T=  1.7133D+02  |                                    |       T=  1.0400D+02
  P=  2.1000D+01  |                                    |       P=  2.0000D+01
  V=  3.7695D-01  |                                    |       V=  0.0000D+00
                  |                                    |
  U-601     <-----|               COLD                 |<----- U-600
  T=  1.2000D+02  |                                    |       T=  9.0000D+01
  P=  6.9696D+01  |                                    |       P=  7.9696D+01
  V=  0.0000D+00  |                                    |       V=  0.0000D+00
                  --------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR               1199440.0765
    CALCULATED (REQUIRED) AREA     SQFT                     417.4421
    ACTUAL EXCHANGER AREA          SQFT                     417.4421
    PER CENT OVER-DESIGN                                      0.0000
```

```
                             U-O-S BLOCK SECTION

BLOCK:  X-600    MODEL: HEATX (CONTINUED)

  HEAT TRANSFER COEFFICIENT:
    AVERAGE COEFFICIENT (DIRTY)    BTU/HR-SQFT-R            100.0000
    UA (DIRTY)                     BTU/HR-R               41744.2103

  LOG-MEAN TEMPERATURE DIFFERENCE:
    LMTD CORRECTION FACTOR                                    1.0000
    LMTD (CORRECTED)               F                         28.7331
    NUMBER OF SHELLS IN SERIES                                 1

  PRESSURE DROP:
    HOTSIDE, TOTAL                 PSI                        1.0000
    COLDSIDE, TOTAL                PSI                       10.0000

  PRESSURE DROP PARAMETER:
    HOT SIDE:                                               53574.
    COLD SIDE:                                             0.35291E+07
```

```
                                STREAM SECTION

510 D1 D2 D3 DUMMY
------------------

STREAM ID               510        D1         D2         D3         DUMMY
FROM :                  P-502      DUMSEP1    DUMSEP2    DUMSEP3    R-100
TO   :                  D-501      ----       ----       ----       R-100A


MAX CONV. ERROR:         0.0        0.0        0.0        0.0     7.0593-04
SUBSTREAM: MIXED
PHASE:                  LIQUID     VAPOR      MIXED      MIXED      MIXED
COMPONENTS: LBMOL/HR
  MALEIC              6.9308-15      0.0        0.0        0.0     191.3836
  HYDROGEN               0.0       0.1332     0.1477  3.9543-02  6673.5377
  SUCCINIC            6.5115-15      0.0        0.0        0.0    5.7145-04
  GBL                 5.2315-04      0.0        0.0        0.0      10.9018
  BDO                 1.6018-08      0.0        0.0        0.0       0.6422
  THF                  349.8530      0.0        0.0        0.0      34.9996
  METHANE                0.0    1.8610-03  3.8834-02  1.2873-02     1.2597
  NBUTANE                0.0    1.6036-02     0.5907     0.4787     0.4852
  WATER                 72.4349      0.0        0.0        0.0     888.3729
  PROPANE                0.0    2.4533-03  4.0778-02  3.1479-02  6.5866-02
  NBUTANOL            1.1052-02      0.0        0.0        0.0       2.0535
  PROPANOL            6.0195-02      0.0        0.0        0.0       0.1626
COMPONENTS: MOLE FRAC
  MALEIC              1.6410-17      0.0        0.0        0.0    2.4524-02
  HYDROGEN               0.0       0.8675     0.1805  7.0288-02     0.8552
  SUCCINIC            1.5417-17      0.0        0.0        0.0    7.3227-08
  GBL                 1.2386-06      0.0        0.0        0.0    1.3970-03
  BDO                 3.7925-11      0.0        0.0        0.0    8.2292-05
  THF                    0.8283      0.0        0.0        0.0    4.4849-03
  METHANE                0.0    1.2116-02  4.7474-02  2.2882-02  1.6143-04
  NBUTANE                0.0       0.1044     0.7221     0.8509  6.2172-05
  WATER                  0.1715      0.0        0.0        0.0       0.1138
  PROPANE                0.0    1.5973-02  4.9851-02  5.5953-02  8.4402-06
  NBUTANOL            2.6168-05      0.0        0.0        0.0    2.6314-04
  PROPANOL            1.4252-04      0.0        0.0        0.0    2.0833-05
COMPONENTS: LB/HR
  MALEIC              8.0449-13      0.0        0.0        0.0    2.2215+04
  HYDROGEN               0.0       0.2686     0.2977  7.9715-02  1.3453+04
  SUCCINIC            7.6894-13      0.0        0.0        0.0    6.7482-02
  GBL                 4.5038-02      0.0        0.0        0.0     938.5410
  BDO                 1.4436-06      0.0        0.0        0.0      57.8761
  THF                 2.5227+04      0.0        0.0        0.0    2523.7101
  METHANE                0.0    2.9855-02     0.6230     0.2065    20.2098
  NBUTANE                0.0       0.9321    34.3348    27.8235    28.2005
  WATER               1304.9358      0.0        0.0        0.0    1.6004+04
  PROPANE                0.0       0.1082     1.7982     1.3881     2.9045
  NBUTANOL               0.8192      0.0        0.0        0.0     152.2091
  PROPANOL               3.6175      0.0        0.0        0.0       9.7701
COMPONENTS: MASS FRAC
  MALEIC              3.0316-17      0.0        0.0        0.0       0.4009
  HYDROGEN               0.0       0.2006  8.0340-03  2.7024-03     0.2428
  SUCCINIC            2.8977-17      0.0        0.0        0.0    1.2180-06
  GBL                 1.6972-06      0.0        0.0        0.0    1.6940-02
  BDO                 5.4400-11      0.0        0.0        0.0    1.0446-03
```

```
                                STREAM SECTION

510 D1 D2 D3 DUMMY (CONTINUED)

STREAM ID               510        D1         D2         D3         DUMMY

  THF                    0.9507      0.0        0.0        0.0    4.5550-02
  METHANE                0.0    2.2302-02  1.6813-02  7.0012-03  3.6476-04
  NBUTANE                0.0       0.6962     0.9266     0.9432  5.0899-04
  WATER               4.9176-02      0.0        0.0        0.0       0.2889
  PROPANE                0.0    8.0813-02  4.8529-02  4.7058-02  5.2422-05
  NBUTANOL            3.0872-05      0.0        0.0        0.0    2.7472-03
  PROPANOL            1.3632-04      0.0        0.0        0.0    1.7634-04
COMPONENTS: STD CUFT/HR
  MALEIC              1.0085-14      0.0        0.0        0.0     278.4703
  HYDROGEN               0.0       0.1143     0.1267  3.3925-02  5725.3192
  SUCCINIC            1.0165-14      0.0        0.0        0.0    8.9206-04
  GBL                 6.4139-04      0.0        0.0        0.0      13.3658
  BDO                 2.2798-08      0.0        0.0        0.0       0.9140
  THF                  459.2101      0.0        0.0        0.0      45.9397
  METHANE                0.0    1.5965-03  3.3316-02  1.1044-02     1.0808
  NBUTANE                0.0    2.5613-02     0.9435     0.7646     0.7750
  WATER                 20.9434      0.0        0.0        0.0     256.8582
  PROPANE                0.0    3.4247-03  5.6923-02  4.3942-02  9.1944-02
  NBUTANOL            1.6164-02      0.0        0.0        0.0       3.0032
  PROPANOL            7.1909-02      0.0        0.0        0.0       0.1942
  TOTAL CUFT/HR        480.2422    0.1449     1.1605     0.8535  6326.0131
TOTAL FLOW:
  LBMOL/HR             422.3598    0.1536     0.8180     0.5626  7803.8653
  LB/HR               2.6536+04    1.3387    37.0536    29.4978  5.5405+04
  CUFT/HR              497.3366    1.5725    10.2558     2.2048  3.2450+04
STATE VARIABLES:
  TEMP   F             148.4294  108.7651    89.9881 -2.0103-04   345.3050
  PRES   PSIA          120.0000  600.0000   164.6959   164.6959  2034.6959
  VFRAC                  0.0       1.0000     0.3273  8.2463-02     0.9154
  LFRAC                  1.0000      0.0      0.6727     0.9175  8.4614-02
  SFRAC                  0.0         0.0        0.0        0.0        0.0
ENTHALPY:
  BTU/LBMOL          -9.5861+04 -6527.3507 -4.8596+04 -5.9807+04 -1.9368+04
  BTU/LB             -1525.7604  -748.9067 -1072.8116 -1140.6528 -2727.9611
  BTU/HR             -4.0488+07 -1002.5561 -3.9752+04 -3.3647+04 -1.5114+08
ENTROPY:
  BTU/LBMOL-R          -90.6326  -16.3994   -79.7750   -99.9110   -10.9885
  BTU/LB-R              -1.4425   -1.8816    -1.7611    -1.9055    -1.5477
DENSITY:
  LBMOL/CUFT             0.8492 9.7673-02  7.9760-02     0.2552     0.2405
  LB/CUFT               53.3567    0.8513     3.6130    13.3788     1.7074
AVG MW                  62.8285    8.7158    45.2976    52.4320     7.0997
```

```
                                STREAM SECTION

S-100 S-101 S-102 S-103 S-104
-----------------------------

STREAM ID               S-100      S-101      S-102      S-103      S-104
FROM :                  ----       X-100      P-100      ----       C-100
TO   :                  X-100      P-100      R-100      C-100      R-100

SUBSTREAM: MIXED
PHASE:                  LIQUID     LIQUID     LIQUID     VAPOR      VAPOR
COMPONENTS: LBMOL/HR
  MALEIC               191.3398   191.3398   191.3398     0.0        0.0
  HYDROGEN               0.0        0.0        0.0     1063.0000  1063.0000
  SUCCINIC               0.0        0.0        0.0        0.0        0.0
  GBL                    0.0        0.0        0.0        0.0        0.0
  BDO                    0.0        0.0        0.0        0.0        0.0
  THF                    0.0        0.0        0.0        0.0        0.0
  METHANE                0.0        0.0        0.0        0.0        0.0
  NBUTANE                0.0        0.0        0.0        0.0        0.0
  WATER                821.8747   821.8747   821.8747     0.0        0.0
  PROPANE                0.0        0.0        0.0        0.0        0.0
  NBUTANOL               0.0        0.0        0.0        0.0        0.0
  PROPANOL               0.0        0.0        0.0        0.0        0.0
COMPONENTS: MOLE FRAC
  MALEIC                 0.1888     0.1888     0.1888     0.0        0.0
  HYDROGEN               0.0        0.0        0.0        1.0000     1.0000
  SUCCINIC               0.0        0.0        0.0        0.0        0.0
  GBL                    0.0        0.0        0.0        0.0        0.0
  BDO                    0.0        0.0        0.0        0.0        0.0
  THF                    0.0        0.0        0.0        0.0        0.0
  METHANE                0.0        0.0        0.0        0.0        0.0
  NBUTANE                0.0        0.0        0.0        0.0        0.0
  WATER                  0.8112     0.8112     0.8112     0.0        0.0
  PROPANE                0.0        0.0        0.0        0.0        0.0
  NBUTANOL               0.0        0.0        0.0        0.0        0.0
  PROPANOL               0.0        0.0        0.0        0.0        0.0
COMPONENTS: LB/HR
  MALEIC               2.2209+04  2.2209+04  2.2209+04    0.0        0.0
  HYDROGEN               0.0        0.0        0.0     2142.8804  2142.8804
  SUCCINIC               0.0        0.0        0.0        0.0        0.0
  GBL                    0.0        0.0        0.0        0.0        0.0
  BDO                    0.0        0.0        0.0        0.0        0.0
  THF                    0.0        0.0        0.0        0.0        0.0
  METHANE                0.0        0.0        0.0        0.0        0.0
  NBUTANE                0.0        0.0        0.0        0.0        0.0
  WATER                1.4806+04  1.4806+04  1.4806+04    0.0        0.0
  PROPANE                0.0        0.0        0.0        0.0        0.0
  NBUTANOL               0.0        0.0        0.0        0.0        0.0
  PROPANOL               0.0        0.0        0.0        0.0        0.0
COMPONENTS: MASS FRAC
  MALEIC                 0.6000     0.6000     0.6000     0.0        0.0
  HYDROGEN               0.0        0.0        0.0        1.0000     1.0000
  SUCCINIC               0.0        0.0        0.0        0.0        0.0
  GBL                    0.0        0.0        0.0        0.0        0.0
  BDO                    0.0        0.0        0.0        0.0        0.0
  THF                    0.0        0.0        0.0        0.0        0.0
  METHANE                0.0        0.0        0.0        0.0        0.0
```

```
                                STREAM SECTION

S-100 S-101 S-102 S-103 S-104 (CONTINUED)

STREAM ID               S-100      S-101      S-102      S-103      S-104

  NBUTANE                0.0        0.0        0.0        0.0        0.0
  WATER                  0.4000     0.4000     0.4000     0.0        0.0
  PROPANE                0.0        0.0        0.0        0.0        0.0
  NBUTANOL               0.0        0.0        0.0        0.0        0.0
  PROPANOL               0.0        0.0        0.0        0.0        0.0
COMPONENTS: STD CUFT/HR
  MALEIC               278.4065   278.4065   278.4065     0.0        0.0
  HYDROGEN               0.0        0.0        0.0      911.9622   911.9622
  SUCCINIC               0.0        0.0        0.0        0.0        0.0
  GBL                    0.0        0.0        0.0        0.0        0.0
  BDO                    0.0        0.0        0.0        0.0        0.0
  THF                    0.0        0.0        0.0        0.0        0.0
  METHANE                0.0        0.0        0.0        0.0        0.0
  NBUTANE                0.0        0.0        0.0        0.0        0.0
  WATER                237.6313   237.6313   237.6313     0.0        0.0
  PROPANE                0.0        0.0        0.0        0.0        0.0
  NBUTANOL               0.0        0.0        0.0        0.0        0.0
  PROPANOL               0.0        0.0        0.0        0.0        0.0
  TOTAL CUFT/HR        516.0378   516.0378   516.0378   911.9622   911.9622
TOTAL FLOW:
  LBMOL/HR            1013.2145  1013.2145  1013.2145  1063.0000  1063.0000
  LB/HR               3.7016+04  3.7016+04  3.7016+04  2142.8804  2142.8804
  CUFT/HR              498.5682   526.4480   725.2913  2.3003+04  5015.1221
STATE VARIABLES:
  TEMP   F             104.0000   201.2000   218.8406    68.0000   389.6654
  PRES   PSIA           19.6959    14.6959  2054.6959   264.6959  2054.6959
  VFRAC                  0.0        0.0        0.0        1.0000     1.0000
  LFRAC                  1.0000     1.0000     1.0000     0.0        0.0
  SFRAC                  0.0        0.0        0.0        0.0        0.0
ENTHALPY:
  BTU/LBMOL           -1.6264+05 -1.5989+05 -1.5937+05   -55.3587  2268.0826
  BTU/LB              -4451.7941 -4376.5088 -4362.3477   -27.4613  1125.1079
  BTU/HR              -1.6479+08 -1.6200+08 -1.6148+08 -5.8846+04  2.4110+06
ENTROPY:
  BTU/LBMOL-R          -51.8097   -47.3082   -46.6563    -5.8678    -6.6356
  BTU/LB-R              -1.4182    -1.2949    -1.2771    -2.9108    -3.2917
DENSITY:
  LBMOL/CUFT             2.0322     1.9246     1.3970  4.6212-02     0.2120
  LB/CUFT               74.2441    70.3123    51.0357  9.3158-02     0.4273
AVG MW                  36.5330    36.5330    36.5330     2.0159     2.0159
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                                STREAM SECTION

S-105 S-200 S-201 S-202 S-203
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STREAM ID               S-105      S-200      S-201      S-202      S-203
FROM :                  R-100A     X-200      F-200      F-200      M-200
TO   :                  X-200      F-200      M-200      F-300      F-400

SUBSTREAM: MIXED
PHASE:                  VAPOR      MIXED      VAPOR      LIQUID     MIXED
COMPONENTS: LBMOL/HR
  MALEIC              4.3827-02  4.3827-02  2.0111-09  4.3827-02  2.0111-09
  HYDROGEN            5765.6601  5765.6601  5739.4860    26.1741    57.3949
  SUCCINIC               0.3322     0.3322  5.1485-09     0.3322  5.1485-09
  GBL                   44.6766    44.6766  9.3243-02    44.5834  9.3243-02
  BDO                    2.5853     2.5853  1.1599-05     2.5853  1.1599-05
  THF                  176.1551   176.1551    20.1809   155.9742    17.6583
  METHANE                5.3871     5.3871     5.3571  3.0065-02     4.2856
  NBUTANE                2.0063     2.0063     1.8501     0.1562     1.6189
  WATER               1427.4723  1427.4723     5.7780  1421.6943  5.7780-02
  PROPANE                0.3376     0.3376     0.3210  1.6639-02     0.2809
  NBUTANOL              10.5396    10.5396  7.0136-02    10.4695  7.0136-02
  PROPANOL               4.0182     4.0182  4.0257-02     3.9779  4.0257-02
COMPONENTS: MOLE FRAC
  MALEIC              5.8913-06  5.8913-06  3.4835-13  2.6306-05  2.4676-11
  HYDROGEN               0.7750     0.7750     0.9942  1.5710-02     0.7042
  SUCCINIC            4.4661-05  4.4661-05  8.9179-13  1.9942-04  6.3171-11
  GBL                 6.0056-03  6.0056-03  1.6151-05  2.6760-02  1.1441-03
  BDO                 3.4753-04  3.4753-04  2.0092-09  1.5518-03  1.4232-07
  THF                 2.3679-02  2.3679-02  3.4956-03  9.3620-02     0.2167
  METHANE             7.2415-04  7.2415-04  9.2792-04  1.8046-05  5.2585-02
  NBUTANE             2.6969-04  2.6969-04  3.2047-04  9.3738-05  1.9863-02
  WATER                  0.1919     0.1919  1.0008-03     0.8533  7.0895-04
  PROPANE             4.5385-05  4.5385-05  5.5601-05  9.9874-06  3.4462-03
  NBUTANOL            1.4168-03  1.4168-03  1.2149-05  6.2841-03  8.6056-04
  PROPANOL            5.4014-04  5.4014-04  6.9732-06  2.3877-03  4.9395-04
COMPONENTS: LB/HR
  MALEIC                 5.0871     5.0871  2.3343-07     5.0871  2.3343-07
  HYDROGEN            1.1623+04  1.1623+04  1.1570+04    52.7638   115.7012
  SUCCINIC              39.2339    39.2339  6.0798-07    39.2339  6.0798-07
  GBL                 3846.2291  3846.2291     8.0273  3838.2018     8.0273
  BDO                  232.9941   232.9941  1.0454-03   232.9931  1.0454-03
  THF                 1.2702+04  1.2702+04  1455.1831  1.1247+04  1273.2852
  METHANE               86.4244    86.4244    85.9420     0.4823    68.7536
  NBUTANE              116.6130   116.6130   107.5358     9.0772    94.0938
  WATER               2.5716+04  2.5716+04   104.0914  2.5612+04     1.0409
  PROPANE               14.8884    14.8884    14.1546     0.7337    12.3853
  NBUTANOL             781.2257   781.2257     5.1987   776.0270     5.1987
  PROPANOL             241.4768   241.4768     2.4193   239.0575     2.4193
COMPONENTS: MASS FRAC
  MALEIC              9.1817-05  9.1817-05  1.7482-11  1.2097-04  1.4766-10
  HYDROGEN               0.2098     0.2098     0.8665  1.2547-03  7.3187-02
  SUCCINIC            7.0812-04  7.0812-04  4.5532-11  9.3297-04  3.8458-10
  GBL                 6.9420-02  6.9420-02  6.0118-04  9.1271-02  5.0777-03
  BDO                 4.2053-03  4.2053-03  7.8288-08  5.5405-03  6.6124-07
  THF                    0.2293     0.2293     0.1090     0.2674     0.8054
  METHANE             1.5599-03  1.5599-03  6.4363-03  1.1470-05  4.3490-02
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                                STREAM SECTION

S-105 S-200 S-201 S-202 S-203 (CONTINUED)

STREAM ID               S-105      S-200      S-201      S-202      S-203

  NBUTANE             2.1047-03  2.1047-03  8.0535-03  2.1585-04  5.9519-02
  WATER                  0.4641     0.4641  7.7956-03     0.6091  6.5843-04
  PROPANE             2.6872-04  2.6872-04  1.0601-03  1.7448-05  7.8343-03
  NBUTANOL            1.4100-02  1.4100-02  3.8934-04  1.8454-02  3.2884-03
  PROPANOL            4.3584-03  4.3584-03  1.8118-04  5.6847-03  1.5303-03
COMPONENTS: STD CUFT/HR
  MALEIC              6.3770-02  6.3770-02  2.9262-09  6.3770-02  2.9262-09
  HYDROGEN            4946.4386  4946.4386  4923.9834    22.4551    49.2398
  SUCCINIC               0.5186     0.5186  8.0370-09     0.5186  8.0370-09
  GBL                   54.7743    54.7743     0.1143    54.6600     0.1143
  BDO                    3.6796     3.6796  1.6509-05     3.6796  1.6509-05
  THF                  231.2177   231.2177    26.4891   204.7287    23.1779
  METHANE                4.6217     4.6217     4.5959  2.5793-02     3.6767
  NBUTANE                3.2046     3.2046     2.9551     0.2494     2.5857
  WATER                412.7297   412.7297     1.6706   411.0591  1.6706-02
  PROPANE                0.4713     0.4713     0.4481  2.3227-02     0.3921
  NBUTANOL              15.4143    15.4143     0.1026    15.3117     0.1026
  PROPANOL               4.8001     4.8001  4.8091-02     4.7520  4.8091-02
  TOTAL CUFT/HR       5677.9343  5677.9343  4960.4072   717.5271    79.3540
TOTAL FLOW:
  LBMOL/HR            7439.2144  7439.2144  5773.1767  1666.0377    81.5000
  LB/HR               5.5405+04  5.5405+04  1.3353+04  4.2053+04  1580.9064
  CUFT/HR             3.7463+04  1.9690+04  1.8832+04   884.2073   256.8326
STATE VARIABLES:
  TEMP   F             480.3974   104.0000   104.0086   104.0086   105.2487
  PRES   PSIA         2014.6959  2012.6959  2009.6959  2009.6959  1709.6959
  VFRAC                  1.0000     0.7760     1.0000     0.0        0.7395
  LFRAC                  0.0        0.2240     0.0        1.0000     0.2605
  SFRAC                  0.0        0.0        0.0        0.0        0.0
ENTHALPY:
  BTU/LBMOL          -2.0317+04 -2.6906+04  -196.7090 -1.1946+05 -2.3152+04
  BTU/LB             -2727.9611 -3612.6767   -85.0494 -4732.7813 -1193.5427
  BTU/HR             -1.5114+08 -2.0016+08 -1.1356+06 -1.9903+08 -1.8869+06
ENTROPY:
  BTU/LBMOL-R           -9.1735   -17.9211    -9.7687   -46.1593   -32.4836
  BTU/LB-R              -1.2317    -2.4062    -4.2236    -1.8287    -1.6746
DENSITY:
  LBMOL/CUFT             0.1986     0.3778     0.3066     1.8842     0.3173
  LB/CUFT                1.4789     2.8139     0.7091    47.5598     6.1554
AVG MW                   7.4477     7.4477     2.3129    25.2411    19.3976
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                                STREAM SECTION

S-204 S-205 S-206 S-300 S-301
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STREAM ID               S-204      S-205      S-206      S-300      S-301
FROM :                  M-200      C-200      X-201      F-300      DUMSEP1
TO   :                  C-200      X-201      R-100      X-400      D-300

SUBSTREAM: MIXED
PHASE:                  MIXED      VAPOR      VAPOR      VAPOR      LIQUID
COMPONENTS: LBMOL/HR
  MALEIC                  0.0        0.0        0.0     3.6538-12  4.3827-02
  HYDROGEN             5682.0912  5682.0912  5682.0912    26.0408      0.0
  SUCCINIC                0.0        0.0        0.0     6.6018-12     0.3322
  GBL                     0.0        0.0        0.0     1.6000-04    44.5832
  BDO                     0.0        0.0        0.0     1.1453-08     2.5853
  THF                     2.5226     2.5226     2.5226     2.8968   153.0774
  METHANE                 1.0714     1.0714     1.0714  2.8204-02      0.0
  NBUTANE                 0.2313     0.2313     0.2313     0.1401      0.0
  WATER                   5.7202     5.7202     5.7202  2.7223-02  1421.6671
  PROPANE              4.0124-02  4.0124-02  4.0124-02  1.4186-02      0.0
  NBUTANOL                0.0        0.0        0.0     1.6096-02    10.4534
  PROPANOL                0.0        0.0        0.0     2.6731-03     3.9753
COMPONENTS: MOLE FRAC
  MALEIC                  0.0        0.0        0.0     1.2527-13  2.6777-05
  HYDROGEN                0.9983     0.9983     0.9983     0.8928      0.0
  SUCCINIC                0.0        0.0        0.0     2.2635-13  2.0299-04
  GBL                     0.0        0.0        0.0     5.4857-06  2.7239-02
  BDO                     0.0        0.0        0.0     3.9267-10  1.5796-03
  THF                  4.4321-04  4.4321-04  4.4321-04  9.9321-02  9.3527-02
  METHANE              1.8824-04  1.8824-04  1.8824-04  9.6700-04      0.0
  NBUTANE              4.0632-05  4.0632-05  4.0632-05  4.8047-03      0.0
  WATER                1.0050-03  1.0050-03  1.0050-03  9.3335-04     0.8686
  PROPANE              7.0496-06  7.0496-06  7.0496-06  4.8638-04      0.0
  NBUTANOL                0.0        0.0        0.0     5.5188-04  6.3868-03
  PROPANOL                0.0        0.0        0.0     9.1650-05  2.4288-03
COMPONENTS: LB/HR
  MALEIC                  0.0        0.0        0.0     4.2411-10     5.0871
  HYDROGEN             1.1454+04  1.1454+04  1.1454+04    52.4952      0.0
  SUCCINIC                0.0        0.0        0.0     7.7960-10    39.2339
  GBL                     0.0        0.0        0.0     1.3774-02  3838.1880
  BDO                     0.0        0.0        0.0     1.0321-06   232.9931
  THF                   181.8979   181.8979   181.8979   208.8805  1.1038+04
  METHANE                17.1884    17.1884    17.1884     0.4525      0.0
  NBUTANE                13.4420    13.4420    13.4420     8.1452      0.0
  WATER                 103.0505   103.0505   103.0505     0.4904  2.5612+04
  PROPANE                 1.7693     1.7693     1.7693     0.6256      0.0
  NBUTANOL                0.0        0.0        0.0        1.1931   774.8339
  PROPANOL                0.0        0.0        0.0        0.1606   238.8969
COMPONENTS: MASS FRAC
  MALEIC                  0.0        0.0        0.0     1.5566-12  1.2176-04
  HYDROGEN                0.9730     0.9730     0.9730     0.1927      0.0
  SUCCINIC                0.0        0.0        0.0     2.8614-12  9.3908-04
  GBL                     0.0        0.0        0.0     5.0556-05  9.1869-02
  BDO                     0.0        0.0        0.0     3.7883-09  5.5768-03
  THF                  1.5452-02  1.5452-02  1.5452-02     0.7667     0.2642
  METHANE              1.4601-03  1.4601-03  1.4601-03  1.6607-03      0.0
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                                STREAM SECTION

S-204 S-205 S-206 S-300 S-301 (CONTINUED)

STREAM ID               S-204      S-205      S-206      S-300      S-301

  NBUTANE              1.1419-03  1.1419-03  1.1419-03  2.9895-02      0.0
  WATER                8.7540-03  8.7540-03  8.7540-03  1.8000-03     0.6130
  PROPANE              1.5030-04  1.5030-04  1.5030-04  2.2960-03      0.0
  NBUTANOL                0.0        0.0        0.0     4.3791-03  1.8546-02
  PROPANOL                0.0        0.0        0.0     5.8961-04  5.7181-03
COMPONENTS: STD CUFT/HR
  MALEIC                  0.0        0.0        0.0     5.3164-12  6.3770-02
  HYDROGEN             4874.7436  4874.7436  4874.7436    22.3408      0.0
  SUCCINIC                0.0        0.0        0.0     1.0306-11     0.5186
  GBL                     0.0        0.0        0.0     1.9616-04    54.6598
  BDO                     0.0        0.0        0.0     1.6300-08     3.6796
  THF                     3.3111     3.3111     3.3111     3.8023   200.9264
  METHANE                 0.9192     0.9192     0.9192  2.4197-02      0.0
  NBUTANE                 0.3694     0.3694     0.3694     0.2238      0.0
  WATER                   1.6539     1.6539     1.6539  7.8709-03   411.0513
  PROPANE              5.6010-02  5.6010-02  5.6010-02  1.9802-02      0.0
  NBUTANOL                0.0        0.0        0.0     2.3541-02    15.2882
  PROPANOL                0.0        0.0        0.0     3.1933-03     4.7488
  TOTAL CUFT/HR        4881.0532  4881.0532  4881.0532    26.4457   690.9364
TOTAL FLOW:
  LBMOL/HR             5691.6768  5691.6768  5691.6768    29.1663  1636.7177
  LB/HR                1.1772+04  1.1772+04  1.1772+04   272.4569  4.1779+04
  CUFT/HR              2.1650+04  1.9596+04  3.2304+04   283.9673   872.7619
STATE VARIABLES:
  TEMP   F              105.2487   148.7928   572.0000    78.1551   108.7651
  PRES   PSIA          1709.6959  2054.6959  2054.6959   600.0000   600.0000
  VFRAC                   0.9999     1.0000     1.0000     1.0000      0.0
  LFRAC                5.1260-05     0.0        0.0        0.0        1.0000
  SFRAC                   0.0        0.0        0.0        0.0        0.0
ENTHALPY:
  BTU/LBMOL              95.6905   416.1673  3409.8292 -8392.6996 -1.2145+05
  BTU/LB                 46.2666   201.2180  1648.6611  -898.4332 -4757.9154
  BTU/HR               5.4464+05  2.3687+06  1.9408+07 -2.4478+05 -1.9878+08
ENTROPY:
  BTU/LBMOL-R            -9.1747    -9.0217    -5.2860   -15.5717   -46.4594
  BTU/LB-R               -4.4360    -4.3620    -2.5558    -1.6669    -1.8201
DENSITY:
  LBMOL/CUFT              0.2629     0.2905     0.1762     0.1027     1.8753
  LB/CUFT                 0.5437     0.6007     0.3644     0.9595    47.8698
AVG MW                    2.0682     2.0682     2.0682     9.3415    25.5260
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                          STREAM SECTION

S-301A S-306 S-311 S-312 S-400
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STREAM ID               S-301A     S-306      S-311      S-312      S-400
FROM :                  F-300      D-300      D-300      P-300      DUMSEP2
TO   :                  DUMSEP1    D-500      P-300      R-100      D-500

SUBSTREAM: MIXED
PHASE:                  LIQUID     LIQUID     LIQUID     LIQUID     LIQUID
COMPONENTS: LBMOL/HR
  MALEIC              4.3827-02  1.5195-16  4.3827-02  4.3827-02  2.0111-09
  HYDROGEN               0.1332     0.0        0.0        0.0        0.0
  SUCCINIC               0.3322  1.8365-17     0.3322     0.3322  5.1485-09
  GBL                   44.5832     0.9838    43.5995    43.5995  9.3193-02
  BDO                    2.5853  3.0811-04     2.5850     2.5850  1.1598-05
  THF                  153.0774   153.0774  2.4737-09  2.4737-09    15.8548
  METHANE             1.8610-03     0.0        0.0        0.0        0.0
  NBUTANE             1.6036-02     0.0        0.0        0.0        0.0
  WATER               1421.6671  1396.8069    24.8602    24.8602  5.5085-02
  PROPANE             2.4533-03     0.0        0.0        0.0        0.0
  NBUTANOL              10.4534    10.4534  2.0007-07  2.0007-07  6.9270-02
  PROPANOL               3.9753     3.9753  8.9243-08  8.9243-08  3.8740-02
COMPONENTS: MOLE FRAC
  MALEIC              2.6775-05  9.7071-20  6.1364-04  6.1364-04  1.2482-10
  HYDROGEN            8.1401-05     0.0        0.0        0.0        0.0
  SUCCINIC            2.0297-04  1.1732-20  4.6519-03  4.6519-03  3.1956-10
  GBL                 2.7237-02  6.2848-04     0.6105     0.6105  5.7844-03
  BDO                 1.5794-03  1.9684-07  3.6194-02  3.6194-02  7.1987-07
  THF                 9.3518-02  9.7794-02  3.4635-11  3.4635-11     0.9841
  METHANE             1.1369-06     0.0        0.0        0.0        0.0
  NBUTANE             9.7966-06     0.0        0.0        0.0        0.0
  WATER                  0.8685     0.8924     0.3481     0.3481  3.4191-03
  PROPANE             1.4988-06     0.0        0.0        0.0        0.0
  NBUTANOL            6.3862-03  6.6782-03  2.8013-09  2.8013-09  4.2995-03
  PROPANOL            2.4286-03  2.5396-03  1.2495-09  1.2495-09  2.4045-03
COMPONENTS: LB/HR
  MALEIC                 5.0871  1.7637-14     5.0871     5.0871  2.3343-07
  HYDROGEN               0.2686     0.0        0.0        0.0        0.0
  SUCCINIC              39.2339  2.1687-15    39.2339    39.2339  6.0798-07
  GBL                 3838.1880    84.6917  3753.4963  3753.4963     8.0230
  BDO                  232.9931  2.7768-02   232.9653   232.9653  1.0452-03
  THF                 1.1038+04  1.1038+04  1.7837-07  1.7837-07  1143.2438
  METHANE             2.9855-02     0.0        0.0        0.0        0.0
  NBUTANE                0.9321     0.0        0.0        0.0        0.0
  WATER               2.5612+04  2.5164+04   447.8643   447.8643     0.9924
  PROPANE                0.1082     0.0        0.0        0.0        0.0
  NBUTANOL             774.8339   774.8339  1.4830-05  1.4830-05     5.1345
  PROPANOL             238.8969   238.8969  5.3631-06  5.3631-06     2.3281
COMPONENTS: MASS FRAC
  MALEIC              1.2176-04  4.7283-19  1.1359-03  1.1359-03  2.0128-10
  HYDROGEN            6.4289-06     0.0        0.0        0.0        0.0
  SUCCINIC            9.3905-04  5.8141-20  8.7602-03  8.7602-03  5.2425-10
  GBL                 9.1866-02  2.2705-03     0.8381     0.8381  6.9181-03
  BDO                 5.5766-03  7.4443-07  5.2017-02  5.2017-02  9.0128-07
  THF                    0.2642     0.2959  3.9827-11  3.9827-11     0.9858
  METHANE             7.1457-07     0.0        0.0        0.0        0.0
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                          STREAM SECTION

S-301A S-306 S-311 S-312 S-400 (CONTINUED)

STREAM ID                S-301A     S-306      S-311      S-312      S-400

  NBUTANE             2.2308-05     0.0        0.0        0.0        0.0
  WATER                  0.6130     0.6746     0.1000     0.1000  8.5570-04
  PROPANE             2.5894-06     0.0        0.0        0.0        0.0
  NBUTANOL            1.8545-02  2.0773-02  3.3113-09  3.3113-09  4.4273-03
  PROPANOL            5.7179-03  6.4047-03  1.1975-09  1.1975-09  2.0075-03
COMPONENTS: STD CUFT/HR
  MALEIC              6.3770-02  2.2109-16  6.3770-02  6.3770-02  2.9262-09
  HYDROGEN               0.1143     0.0        0.0        0.0        0.0
  SUCCINIC               0.5186  2.8668-17     0.5186     0.5186  8.0370-09
  GBL                   54.6598     1.2061    53.4537    53.4537     0.1143
  BDO                    3.6796  4.3852-04     3.6791     3.6791  1.6507-05
  THF                  200.9264   200.9264  3.2469-09  3.2469-09    20.8108
  METHANE             1.5965-03     0.0        0.0        0.0        0.0
  NBUTANE             2.5613-02     0.0        0.0        0.0        0.0
  WATER                411.0513   403.8633     7.1879     7.1879  1.5927-02
  PROPANE             3.4247-03     0.0        0.0        0.0        0.0
  NBUTANOL              15.2882    15.2882  2.9261-07  2.9261-07     0.1013
  PROPANOL               4.7488     4.7488  1.0661-07  1.0661-07  4.6278-02
  TOTAL CUFT/HR        691.0813   626.0332    64.9032    64.9032    21.0885
TOTAL FLOW:
  LBMOL/HR            1636.8713  1565.2970    71.4208    71.4208    16.1111
  LB/HR               4.1780+04  3.7300+04  4478.6470  4478.6470  1159.7229
  CUFT/HR              676.2051   648.5590    70.6798    71.9610    23.3677
STATE VARIABLES:
  TEMP   F              78.1551   168.5268   255.1916   286.7685    89.9881
  PRES   PSIA          600.0000    20.0000    22.0000  2054.6959   164.6959
  VFRAC                   0.0        0.0        0.0        0.0        0.0
  LFRAC                  1.0000     1.0000     1.0000     1.0000     1.0000
  SFRAC                   0.0        0.0        0.0        0.0        0.0
ENTHALPY:
  BTU/LBMOL          -1.2144+05 -1.1844+05 -1.6074+05 -1.5948+05 -9.3523+04
  BTU/LB             -4757.7859 -4970.4185 -2563.2644 -2543.1864 -1299.2484
  BTU/HR             -1.9878+08 -1.8540+08 -1.1480+07 -1.1390+07 -1.5068+06
ENTROPY:
  BTU/LBMOL-R          -47.0338   -43.2715   -73.0364   -71.8181  -105.3761
  BTU/LB-R              -1.8427    -1.8159    -1.1647    -1.1453    -1.4639
DENSITY:
  LBMOL/CUFT             2.4207     2.4135     1.0105     0.9925     0.6895
  LB/CUFT               61.7864    57.5125    63.3653    62.2371    49.6293
AVG MW                  25.5245    23.8295    62.7079    62.7079    71.9827
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                          STREAM SECTION

S-400A S-401 S-402 S-403 S-404
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STREAM ID               S-400A     S-401      S-402      S-403      S-404
FROM :                  F-400      F-400      X-400      F-401      DUMSEP3
TO   :                  DUMSEP2    X-400      F-401      ----       D-500

SUBSTREAM: MIXED
PHASE:                  LIQUID     VAPOR      MIXED      VAPOR      LIQUID
COMPONENTS: LBMOL/HR
  MALEIC              2.0111-09  5.6785-16  3.6544-12  9.5777-22  3.6544-12
  HYDROGEN               0.1477    57.2472    83.2880    83.2485     0.0
  SUCCINIC            5.1485-09  3.3799-16  6.6021-12  2.2530-22  6.6021-12
  GBL                 9.3193-02  4.9837-05  2.0983-04  9.0394-09  2.0982-04
  BDO                 1.1598-05  1.3372-09  1.2790-08  3.5682-14  1.2790-08
  THF                   15.8548     1.8035     4.7003     0.1877     4.5126
  METHANE             3.8834-02     4.2468     4.2750     4.2621     0.0
  NBUTANE                0.5907     1.0281     1.1683     0.6896     0.0
  WATER               5.5085-02  2.6941-03  2.9917-02  2.0314-04  2.9714-02
  PROPANE             4.0778-02     0.2401     0.2543     0.2228     0.0
  NBUTANOL            6.9270-02  8.6584-04  1.6962-02  1.8780-05  1.6943-02
  PROPANOL            3.8740-02  1.5176-03  4.1907-03  2.1551-05  4.1692-03
COMPONENTS: MOLE FRAC
  MALEIC              1.1879-10  8.7942-18  3.8985-14  1.0809-23  8.0076-13
  HYDROGEN            8.7229-03     0.8866     0.8885     0.9395     0.0
  SUCCINIC            3.0412-10  5.2345-18  7.0432-14  2.5425-24  1.4467-12
  GBL                 5.5049-03  7.7182-07  2.2385-06  1.0201-10  4.5978-05
  BDO                 6.8509-07  2.0709-11  1.3645-10  4.0268-16  2.8026-09
  THF                    0.9365  2.7930-02  5.0143-02  2.1184-03     0.9888
  METHANE             2.2939-03  6.5770-02  4.5606-02  4.8100-02     0.0
  NBUTANE             3.4894-02  1.5923-02  1.2463-02  7.7821-03     0.0
  WATER               3.2539-03  4.1724-05  3.1915-04  2.2924-06  6.5110-03
  PROPANE             2.4087-03  3.7182-03  2.7126-03  2.5143-03     0.0
  NBUTANOL            4.0918-03  1.3409-05  1.8096-04  2.1194-07  3.7128-03
  PROPANOL            2.2883-03  2.3503-05  4.4707-05  2.4321-07  9.1357-04
COMPONENTS: LB/HR
  MALEIC              2.3343-07  6.5912-14  4.2417-10  1.1117-19  4.2417-10
  HYDROGEN               0.2977   115.4035   167.8987   167.8190     0.0
  SUCCINIC            6.0798-07  3.9913-14  7.7964-10  2.6605-20  7.7964-10
  GBL                    8.0230  4.2905-03  1.8065-02  7.7821-07  1.8064-02
  BDO                 1.0452-03  1.2051-07  1.1527-06  3.2157-12  1.1527-06
  THF                 1143.2438   130.0414   338.9219    13.5354   325.3866
  METHANE                0.6230    68.1306    68.5831    68.3766     0.0
  NBUTANE               34.3348    59.7590    67.9042    40.0807     0.0
  WATER                  0.9924  4.8535-02     0.5390  3.6595-03     0.5353
  PROPANE                1.7982    10.5871    11.2127     9.8246     0.0
  NBUTANOL               5.1345  6.4178-02     1.2573  1.3921-03     1.2559
  PROPANOL               2.3281  9.1201-02     0.2518  1.2951-03     0.2505
COMPONENTS: MASS FRAC
  MALEIC              1.9505-10  1.7159-16  6.4603-13  3.7102-22  1.2954-12
  HYDROGEN            2.4874-04     0.3004     0.2557     0.5601     0.0
  SUCCINIC            5.0801-10  1.0391-16  1.1874-12  8.8790-23  2.3810-12
  GBL                 6.7039-03  1.1169-05  2.7513-05  2.5971-09  5.5166-05
  BDO                 8.7338-07  3.1373-10  1.7555-09  1.0732-14  3.5201-09
  THF                    0.9553     0.3385     0.5162  4.5172-02     0.9937
  METHANE             5.2057-04     0.1774     0.1045     0.2282     0.0
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                          STREAM SECTION

S-400A S-401 S-402 S-403 S-404 (CONTINUED)

STREAM ID               S-400A     S-401      S-402      S-403      S-404

  NBUTANE             2.8689-02     0.1556     0.1034     0.1338     0.0
  WATER               8.2921-04  1.2635-04  8.2085-04  1.2213-05  1.6348-03
  PROPANE             1.5025-03  2.7561-02  1.7077-02  3.2788-02     0.0
  NBUTANOL            4.2903-03  1.6707-04  1.9149-03  4.6457-06  3.8354-03
  PROPANOL            1.9453-03  2.3742-04  3.8357-04  4.3222-06  7.6516-04
COMPONENTS: STD CUFT/HR
  MALEIC              2.9262-09  8.2624-16  5.3172-12  1.3936-21  5.3172-12
  HYDROGEN               0.1267    49.1131    71.4539    71.4200     0.0
  SUCCINIC            8.0370-09  5.2762-16  1.0306-11  3.5170-22  1.0306-11
  GBL                    0.1143  6.1101-05  2.5726-04  1.1082-08  2.5725-04
  BDO                 1.6507-05  1.9032-09  1.8203-08  5.0784-14  1.8203-08
  THF                   20.8108     2.3672     6.1695     0.2464     5.9231
  METHANE             3.3316-02     3.6434     3.6676     3.6566     0.0
  NBUTANE                0.9435     1.6422     1.8660     1.1014     0.0
  WATER               1.5927-02  7.7896-04  8.6499-03  5.8733-05  8.5912-03
  PROPANE             5.6923-02     0.3351     0.3549     0.3110     0.0
  NBUTANOL               0.1013  1.2663-03  2.4807-02  2.7467-05  2.4780-02
  PROPANOL            4.6278-02  1.8129-03  5.0062-03  2.5744-05  4.9804-03
  TOTAL CUFT/HR         22.2490    57.1050    83.5507    76.7355     5.9617
TOTAL FLOW:
  LBMOL/HR              16.9291    64.5708    93.7372    88.6110     4.5636
  LB/HR               1196.7765   384.1299   656.5868   299.6426   327.4464
  CUFT/HR               24.5622  2319.8343  2677.8932  2670.8030     6.2668
STATE VARIABLES:
  TEMP   F              89.9881    89.9881     0.0    -2.0103-04 -2.0103-04
  PRES   PSIA          164.6959   164.6959   164.6959   164.6959   164.6959
  VFRAC                  0.0        1.0000     0.9453     1.0000     0.0
  LFRAC                  1.0000     0.0     5.4687-02     0.0        1.0000
  SFRAC                  0.0        0.0        0.0        0.0        0.0
ENTHALPY:
  BTU/LBMOL          -9.1372+04 -5265.9681 -7652.7147 -2789.8687 -9.5694+04
  BTU/LB             -1292.5149  -885.1898 -1092.5345  -825.0262 -1333.6730
  BTU/HR             -1.5469+06 -3.4003+05 -7.1734+05 -2.4721+05 -4.3671+05
ENTROPY:
  BTU/LBMOL-R         -103.8847    -8.9379   -12.8672    -7.3191  -110.5782
  BTU/LB-R              -1.4695    -1.5024    -1.8370    -2.1644    -1.5411
DENSITY:
  LBMOL/CUFT             0.6892  2.7834-02  3.5004-02  3.3178-02     0.7282
  LB/CUFT               48.7242     0.1656     0.2452     0.1122    52.2507
AVG MW                  70.6933     5.9490     7.0046     3.3816    71.7519
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S-404A S-504 S-508 S-515 S-515A
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STREAM ID               S-404A     S-504      S-508      S-515      S-515A
FROM :                  F-401      D-500      D-500      ----       D-501
TO   :                  DUMSEP3    P-502      ----       D-500      ----

SUBSTREAM: MIXED
PHASE:                  LIQUID     LIQUID     LIQUID     LIQUID     LIQUID
COMPONENTS: LBMOL/HR
  MALEIC              3.6544-12  6.9308-15  2.0147-09     0.0        0.0
  HYDROGEN            3.9543-02     0.0        0.0        0.0        0.0
  SUCCINIC            6.6021-12  6.5115-15  5.1551-09     0.0        0.0
  GBL                 2.0982-04  5.2315-04     1.0772  5.1898-04  5.1963-04
  BDO                 1.2790-08  1.6018-08  3.1970-04  2.5276-16  2.5404-16
  THF                    4.5126   349.8530  5.3817-03   176.4136   176.5544
  METHANE             1.2873-02     0.0        0.0        0.0        0.0
  NBUTANE                0.4787     0.0        0.0        0.0        0.0
  WATER               2.9714-02    72.4349  1396.8746    72.4179    72.4137
  PROPANE             3.1479-02     0.0        0.0        0.0        0.0
  NBUTANOL            1.6943-02  1.1052-02    10.5288  3.0344-04  3.0080-04
  PROPANOL            4.1692-03  6.0195-02     3.9740  1.5996-02  1.3829-02
COMPONENTS: MOLE FRAC
  MALEIC              7.1288-13  1.6410-17  1.4264-12     0.0        0.0
  HYDROGEN            7.7140-03     0.0        0.0        0.0        0.0
  SUCCINIC            1.2879-12  1.5417-17  3.6497-12     0.0        0.0
  GBL                 4.0932-05  1.2386-06  7.6261-04  2.0855-06  2.0870-06
  BDO                 2.4950-09  3.7925-11  2.2635-07  1.0157-18  1.0203-18
  THF                    0.8803     0.8283  3.8102-06     0.7089     0.7091
  METHANE             2.5113-03     0.0        0.0        0.0        0.0
  NBUTANE             9.3383-02     0.0        0.0        0.0        0.0
  WATER               5.7964-03     0.1715     0.9890     0.2910     0.2908
  PROPANE             6.1408-03     0.0        0.0        0.0        0.0
  NBUTANOL            3.3053-03  2.6168-05  7.4543-03  1.2194-06  1.2081-06
  PROPANOL            8.1331-04  1.4252-04  2.8135-03  6.4279-05  5.5542-05
COMPONENTS: LB/HR
  MALEIC              4.2417-10  8.0449-13  2.3385-07     0.0        0.0
  HYDROGEN            7.9715-02     0.0        0.0        0.0        0.0
  SUCCINIC            7.7964-10  7.6894-13  6.0876-07     0.0        0.0
  GBL                 1.8064-02  4.5038-02    92.7324  4.4679-02  4.4735-02
  BDO                 1.1527-06  1.4436-06  2.8813-02  2.2779-14  2.2894-14
  THF                  325.3866  2.5227+04     0.3881  1.2721+04  1.2731+04
  METHANE                0.2065     0.0        0.0        0.0        0.0
  NBUTANE               27.8235     0.0        0.0        0.0        0.0
  WATER                  0.5353  1304.9358  2.5165+04  1304.6286  1304.5533
  PROPANE                1.3881     0.0        0.0        0.0        0.0
  NBUTANOL               1.2559     0.8192   780.4275  2.2492-02  2.2296-02
  PROPANOL               0.2505     3.6175   238.8193     0.9613     0.8311
COMPONENTS: MASS FRAC
  MALEIC              1.1883-12  3.0316-17  8.8994-12     0.0        0.0
  HYDROGEN            2.2333-04     0.0        0.0        0.0        0.0
  SUCCINIC            2.1842-12  2.8977-17  2.3167-11     0.0        0.0
  GBL                 5.0607-05  1.6972-06  3.5290-03  3.1854-06  3.1871-06
  BDO                 3.2292-09  5.4400-11  1.0965-06  1.6240-18  1.6311-18
  THF                    0.9116     0.9507  1.4768-05     0.9069     0.9070
  METHANE             5.7858-04     0.0        0.0        0.0        0.0
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S-404A S-504 S-508 S-515 S-515A (CONTINUED)

STREAM ID               S-404A     S-504      S-508      S-515      S-515A

  NBUTANE             7.7949-02     0.0        0.0        0.0        0.0
  WATER               1.4997-03  4.9176-02     0.9577  9.3013-02  9.2942-02
  PROPANE             3.8888-03     0.0        0.0        0.0        0.0
  NBUTANOL            3.5185-03  3.0872-05  2.9699-02  1.6035-06  1.5885-06
  PROPANOL            7.0193-04  1.3632-04  9.0884-03  6.8534-05  5.9208-05
COMPONENTS: STD CUFT/HR
  MALEIC              5.3172-12  1.0085-14  2.9315-09     0.0        0.0
  HYDROGEN            3.3925-02     0.0        0.0        0.0        0.0
  SUCCINIC            1.0306-11  1.0165-14  8.0473-09     0.0        0.0
  GBL                 2.5725-04  6.4139-04     1.3206  6.3628-04  6.3708-04
  BDO                 1.8203-08  2.2798-08  4.5502-04  3.5974-16  3.6156-16
  THF                    5.9231   459.2101  7.0640-03   231.5570   231.7417
  METHANE             1.1044-02     0.0        0.0        0.0        0.0
  NBUTANE                0.7646     0.0        0.0        0.0        0.0
  WATER               8.5912-03    20.9434   403.8829    20.9384    20.9372
  PROPANE             4.3942-02     0.0        0.0        0.0        0.0
  NBUTANOL            2.4780-02  1.6164-02    15.3985  4.4378-04  4.3992-04
  PROPANOL            4.9804-03  7.1909-02     4.7473  1.9108-02  1.6520-02
  TOTAL CUFT/HR          6.8152   480.2422   425.3569   252.5156   252.6966
TOTAL FLOW:
  LBMOL/HR               5.1262   422.3598  1412.4603   248.8483   248.9827
  LB/HR                356.9442  2.6536+04  2.6277+04  1.4026+04  1.4036+04
  CUFT/HR                7.0896   496.8797   462.2625   290.1198   290.3325
STATE VARIABLES:
  TEMP   F           -2.0103-04   147.2576   210.8186   274.4779   274.4802
  PRES   PSIA          164.6959    15.0000    17.0000   115.0000   115.0000
  VFRAC                  0.0        0.0        0.0        0.0        0.0
  LFRAC                  1.0000     1.0000     1.0000     1.0000     1.0000
  SFRAC                  0.0        0.0        0.0        0.0        0.0
ENTHALPY:
  BTU/LBMOL          -9.1712+04 -9.5910+04 -1.2064+05 -9.5587+04 -9.5581+04
  BTU/LB             -1317.0986 -1526.5335 -6484.5709 -1695.8669 -1695.4723
  BTU/HR             -4.7013+05 -4.0508+07 -1.7040+08 -2.3787+07 -2.3798+07
ENTROPY:
  BTU/LBMOL-R         -108.7711   -90.6739   -35.7881   -76.8872   -76.8981
  BTU/LB-R              -1.5621    -1.4432    -1.9237    -1.3641    -1.3641
DENSITY:
  LBMOL/CUFT             0.7231     0.8500     3.0555     0.8577     0.8576
  LB/CUFT               50.3477    53.4058    56.8454    48.3466    48.3454
AVG MW                  69.6316    62.8285    18.6041    56.3649    56.3744
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S-518 S-600 S-601 U-100 U-101
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STREAM ID               S-518      S-600      S-601      U-100      U-101
FROM :                  D-501      V-600      X-600      ----       X-100
TO   :                  V-600      X-600      ----       X-100      ----

SUBSTREAM: MIXED
PHASE:                  LIQUID     MIXED      LIQUID     VAPOR      LIQUID
COMPONENTS: LBMOL/HR
  MALEIC                  0.0        0.0        0.0        0.0        0.0
  HYDROGEN                0.0        0.0        0.0        0.0        0.0
  SUCCINIC                0.0        0.0        0.0        0.0        0.0
  GBL                  3.5161-06  3.5161-06  3.5161-06     0.0        0.0
  BDO                  1.6018-08  1.6018-08  1.6018-08     0.0        0.0
  THF                   173.2987   173.2987   173.2987     0.0        0.0
  METHANE                 0.0        0.0        0.0        0.0        0.0
  NBUTANE                 0.0        0.0        0.0        0.0        0.0
  WATER                2.1228-02  2.1228-02  2.1228-02   161.0299   161.0299
  PROPANE                 0.0        0.0        0.0        0.0        0.0
  NBUTANOL             1.0751-02  1.0751-02  1.0751-02     0.0        0.0
  PROPANOL             4.6366-02  4.6366-02  4.6366-02     0.0        0.0
COMPONENTS: MOLE FRAC
  MALEIC                  0.0        0.0        0.0        0.0        0.0
  HYDROGEN                0.0        0.0        0.0        0.0        0.0
  SUCCINIC                0.0        0.0        0.0        0.0        0.0
  GBL                  2.0280-08  2.0280-08  2.0280-08     0.0        0.0
  BDO                  9.2388-11  9.2388-11  9.2388-11     0.0        0.0
  THF                     0.9995     0.9995     0.9995     0.0        0.0
  METHANE                 0.0        0.0        0.0        0.0        0.0
  NBUTANE                 0.0        0.0        0.0        0.0        0.0
  WATER                1.2244-04  1.2244-04  1.2244-04     1.0000     1.0000
  PROPANE                 0.0        0.0        0.0        0.0        0.0
  NBUTANOL             6.2011-05  6.2011-05  6.2011-05     0.0        0.0
  PROPANOL             2.6743-04  2.6743-04  2.6743-04     0.0        0.0
COMPONENTS: LB/HR
  MALEIC                  0.0        0.0        0.0        0.0        0.0
  HYDROGEN                0.0        0.0        0.0        0.0        0.0
  SUCCINIC                0.0        0.0        0.0        0.0        0.0
  GBL                  3.0270-04  3.0270-04  3.0270-04     0.0        0.0
  BDO                  1.4436-06  1.4436-06  1.4436-06     0.0        0.0
  THF                  1.2496+04  1.2496+04  1.2496+04     0.0        0.0
  METHANE                 0.0        0.0        0.0        0.0        0.0
  NBUTANE                 0.0        0.0        0.0        0.0        0.0
  WATER                   0.3824     0.3824     0.3824  2900.9992  2900.9992
  PROPANE                 0.0        0.0        0.0        0.0        0.0
  NBUTANOL                0.7969     0.7969     0.7969     0.0        0.0
  PROPANOL                2.7864     2.7864     2.7864     0.0        0.0
COMPONENTS: MASS FRAC
  MALEIC                  0.0        0.0        0.0        0.0        0.0
  HYDROGEN                0.0        0.0        0.0        0.0        0.0
  SUCCINIC                0.0        0.0        0.0        0.0        0.0
  GBL                  2.4216-08  2.4216-08  2.4216-08     0.0        0.0
  BDO                  1.1549-10  1.1549-10  1.1549-10     0.0        0.0
  THF                     0.9997     0.9997     0.9997     0.0        0.0
  METHANE                 0.0        0.0        0.0        0.0        0.0
```

```
S-518 S-600 S-601 U-100 U-101 (CONTINUED)

STREAM ID               S-518      S-600      S-601      U-100      U-101

  NBUTANE                 0.0        0.0        0.0        0.0        0.0
  WATER                3.0594-05  3.0594-05  3.0594-05     1.0000     1.0000
  PROPANE                 0.0        0.0        0.0        0.0        0.0
  NBUTANOL             6.3754-05  6.3754-05  6.3754-05     0.0        0.0
  PROPANOL             2.2291-04  2.2291-04  2.2291-04     0.0        0.0
COMPONENTS: STD CUFT/HR
  MALEIC                  0.0        0.0        0.0        0.0        0.0
  HYDROGEN                0.0        0.0        0.0        0.0        0.0
  SUCCINIC                0.0        0.0        0.0        0.0        0.0
  GBL                  4.3108-06  4.3108-06  4.3108-06     0.0        0.0
  BDO                  2.2798-08  2.2798-08  2.2798-08     0.0        0.0
  THF                   227.4684   227.4684   227.4684     0.0        0.0
  METHANE                 0.0        0.0        0.0        0.0        0.0
  NBUTANE                 0.0        0.0        0.0        0.0        0.0
  WATER                6.1378-03  6.1378-03  6.1378-03    46.5591    46.5591
  PROPANE                 0.0        0.0        0.0        0.0        0.0
  NBUTANOL             1.5724-02  1.5724-02  1.5724-02     0.0        0.0
  PROPANOL             5.5389-02  5.5389-02  5.5389-02     0.0        0.0
  TOTAL CUFT/HR         227.5457   227.5457   227.5457    46.5591    46.5591
TOTAL FLOW:
  LBMOL/HR              173.3770   173.3770   173.3770   161.0299   161.0299
  LB/HR                1.2500+04  1.2500+04  1.2500+04  2900.9992  2900.9992
  CUFT/HR               275.8220  2.0545+04   232.0623  1.9751+04    53.7618
STATE VARIABLES:
  TEMP   F              298.4753   171.3312   104.0000   300.1523   300.1563
  PRES   PSIA           117.0000    21.0000    20.0000    64.6959    64.6959
  VFRAC                   0.0        0.3769     0.0        1.0000     0.0
  LFRAC                   1.0000     0.6231     1.0000     0.0        1.0000
  SFRAC                   0.0        0.0        0.0        0.0        0.0
ENTHALPY:
  BTU/LBMOL           -8.5231+04 -8.5231+04 -9.2149+04 -1.0227+05 -1.1957+05
  BTU/LB              -1182.1657 -1182.1657 -1278.1209 -5676.6816 -6637.2966
  BTU/HR              -1.4777+07 -1.4777+07 -1.5977+07 -1.6468+07 -1.9255+07
ENTROPY:
  BTU/LBMOL-R           -94.4205   -93.6536  -104.7862   -10.8184   -33.5945
  BTU/LB-R               -1.3096    -1.2990    -1.4534    -0.6005    -1.8648
DENSITY:
  LBMOL/CUFT              0.6286  8.4390-03     0.7471  8.1531-03     2.9952
  LB/CUFT                45.3191     0.6084    53.8649     0.1469    53.9602
AVG MW                   72.0972    72.0972    72.0972    18.0153    18.0153
```

```
                                STREAM SECTION

U-200 U-201 U-600 U-601
-----------------------

STREAM ID               U-200      U-201      U-600      U-601
FROM :                  ----       X-200      ----       X-600
TO   :                  X-200      ----       X-600      ----

SUBSTREAM: MIXED
PHASE:                  LIQUID     VAPOR      LIQUID     LIQUID
COMPONENTS: LBMOL/HR
  MALEIC                 0.0        0.0        0.0        0.0
  HYDROGEN               0.0        0.0        0.0        0.0
  SUCCINIC               0.0        0.0        0.0        0.0
  GBL                    0.0        0.0        0.0        0.0
  BDO                    0.0        0.0        0.0        0.0
  THF                    0.0        0.0        0.0        0.0
  METHANE                0.0        0.0        0.0        0.0
  NBUTANE                0.0        0.0        0.0        0.0
  WATER              2402.0935  2402.0935  1926.4221  1926.4221
  PROPANE                0.0        0.0        0.0        0.0
  NBUTANOL               0.0        0.0        0.0        0.0
  PROPANOL               0.0        0.0        0.0        0.0
COMPONENTS: MOLE FRAC
  MALEIC                 0.0        0.0        0.0        0.0
  HYDROGEN               0.0        0.0        0.0        0.0
  SUCCINIC               0.0        0.0        0.0        0.0
  GBL                    0.0        0.0        0.0        0.0
  BDO                    0.0        0.0        0.0        0.0
  THF                    0.0        0.0        0.0        0.0
  METHANE                0.0        0.0        0.0        0.0
  NBUTANE                0.0        0.0        0.0        0.0
  WATER                  1.0000     1.0000     1.0000     1.0000
  PROPANE                0.0        0.0        0.0        0.0
  NBUTANOL               0.0        0.0        0.0        0.0
  PROPANOL               0.0        0.0        0.0        0.0
COMPONENTS: LB/HR
  MALEIC                 0.0        0.0        0.0        0.0
  HYDROGEN               0.0        0.0        0.0        0.0
  SUCCINIC               0.0        0.0        0.0        0.0
  GBL                    0.0        0.0        0.0        0.0
  BDO                    0.0        0.0        0.0        0.0
  THF                    0.0        0.0        0.0        0.0
  METHANE                0.0        0.0        0.0        0.0
  NBUTANE                0.0        0.0        0.0        0.0
  WATER              4.3274+04  4.3274+04  3.4705+04  3.4705+04
  PROPANE                0.0        0.0        0.0        0.0
  NBUTANOL               0.0        0.0        0.0        0.0
  PROPANOL               0.0        0.0        0.0        0.0
COMPONENTS: MASS FRAC
  MALEIC                 0.0        0.0        0.0        0.0
  HYDROGEN               0.0        0.0        0.0        0.0
  SUCCINIC               0.0        0.0        0.0        0.0
  GBL                    0.0        0.0        0.0        0.0
  BDO                    0.0        0.0        0.0        0.0
  THF                    0.0        0.0        0.0        0.0
  METHANE                0.0        0.0        0.0        0.0
```

```
                                STREAM SECTION

U-200 U-201 U-600 U-601 (CONTINUED)

STREAM ID               U-200      U-201      U-600      U-601

  NBUTANE                0.0        0.0        0.0        0.0
  WATER                  1.0000     1.0000     1.0000     1.0000
  PROPANE                0.0        0.0        0.0        0.0
  NBUTANOL               0.0        0.0        0.0        0.0
  PROPANOL               0.0        0.0        0.0        0.0
COMPONENTS: STD CUFT/HR
  MALEIC                 0.0        0.0        0.0        0.0
  HYDROGEN               0.0        0.0        0.0        0.0
  SUCCINIC               0.0        0.0        0.0        0.0
  GBL                    0.0        0.0        0.0        0.0
  BDO                    0.0        0.0        0.0        0.0
  THF                    0.0        0.0        0.0        0.0
  METHANE                0.0        0.0        0.0        0.0
  NBUTANE                0.0        0.0        0.0        0.0
  WATER                 694.5251   694.5251   556.9927   556.9927
  PROPANE                0.0        0.0        0.0        0.0
  NBUTANOL               0.0        0.0        0.0        0.0
  PROPANOL               0.0        0.0        0.0        0.0
  TOTAL CUFT/HR         694.5251   694.5251   556.9927   556.9927
TOTAL FLOW:
  LBMOL/HR           2402.0935  2402.0935  1926.4221  1926.4221
  LB/HR              4.3274+04  4.3274+04  3.4705+04  3.4705+04
  CUFT/HR               925.1872  3.0327+05   563.2646   572.7572
STATE VARIABLES:
  TEMP   F              90.0000   297.7181    90.0000   119.9999
  PRES   PSIA           64.6959    62.6959    79.6959    69.6959
  VFRAC                  0.0        1.0000     0.0        0.0
  LFRAC                  1.0000     0.0        1.0000     1.0000
  SFRAC                  0.0        0.0        0.0        0.0
ENTHALPY:
  BTU/LBMOL          -1.2269+05 -1.0228+05 -1.2399+05 -1.2337+05
  BTU/LB             -6810.1692 -5677.4438 -6882.6002 -6848.0392
  BTU/HR             -2.9471+08 -2.4569+08 -2.3886+08 -2.3766+08
ENTROPY:
  BTU/LBMOL-R          -38.6189   -10.7760   -40.3969   -39.2928
  BTU/LB-R              -2.1437    -0.5982    -2.2424    -2.1811
DENSITY:
  LBMOL/CUFT             2.5963  7.9205-03     3.4201     3.3634
  LB/CUFT               46.7737     0.1427    61.6141    60.5929
AVG MW                  18.0153    18.0153    18.0153    18.0153
```

```
ASPEN PLUS   PLAT: WIN32     VER: 21.0                  04/02/2009  PAGE 92

                              UTILITY SECTION

UTILITY USAGE:  150PSIG   (STEAM)
---------------------------------

 INPUT DATA:

   INLET PRESSURE                    164.6959  PSIA
   OUTLET PRESSURE                   164.6959  PSIA
   INLET VAPOR FRACTION                1.0000
   OUTLET VAPOR FRACTION              0.0
   PRICE                            2.0000-02  $/LB
   INDEX TYPE                            FUEL

 RESULT:

   HEATING VALUE                     856.8563  BTU/LB
   INDEXED PRICE                    2.0000-02  $/LB

 THIS UTILITY IS PURCHASED

 USAGE:

 UOS BLOCK ID     MODEL            USAGE RATE (LB/HR )    COST ($/HR)
 -------------    ------------    -------------------    -------------
 D-501            RADFRAC                    8916.6389         178.3328
                                         -------------    -------------
                              TOTAL:         8916.6389         178.3328
                                         =============    =============
```

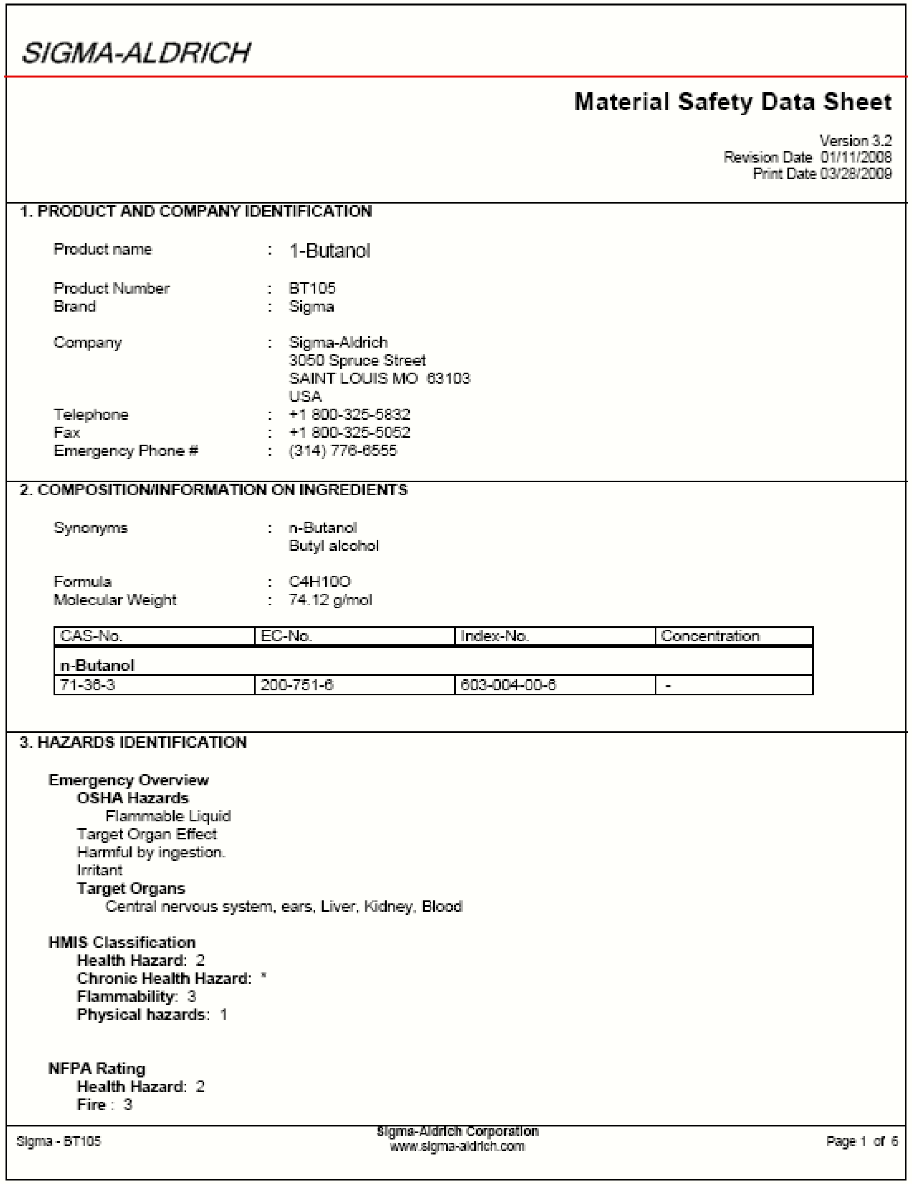
```
ASPEN PLUS   PLAT: WIN32     VER: 21.0                  04/02/2009  PAGE 93

                              UTILITY SECTION

UTILITY USAGE:  50PSIG    (STEAM)
---------------------------------

 INPUT DATA:

   INLET PRESSURE                     64.6959  PSIA
   OUTLET PRESSURE                    64.6959  PSIA
   INLET VAPOR FRACTION                1.0000
   OUTLET VAPOR FRACTION              0.0
   PRICE                            1.0000-02  $/LB
   INDEX TYPE                            FUEL

 RESULT:

   HEATING VALUE                     911.5911  BTU/LB
   INDEXED PRICE                    1.0000-02  $/LB

 THIS UTILITY IS PURCHASED

 USAGE:

 UOS BLOCK ID     MODEL            USAGE RATE (LB/HR )    COST ($/HR)
 -------------    ------------    -------------------    -------------
 D-300            RADFRAC                   5.1829+04          518.2934
 D-500            RADFRAC                   1.2281+04          122.8101
                                         -------------    -------------
                              TOTAL:        6.4110+04          641.1035
                                         =============    =============
```

```
                                UTILITY SECTION

UTILITY USAGE:  CW1       (WATER)
---------------------------------

 INPUT DATA:

   INLET TEMPERATURE                   90.0000  F
   OUTLET TEMPERATURE                 120.0000  F
   INLET PRESSURE                      65.0000  PSIA
   OUTLET PRESSURE                     60.0000  PSIA
   PRICE                             1.0000-02  $/LB
   INDEX TYPE                             FUEL

 RESULT:

   COOLING VALUE                       29.8798  BTU/LB
   INDEXED PRICE                     1.0000-02  $/LB

 THIS UTILITY IS PURCHASED

 USAGE:

 UOS BLOCK ID     MODEL            USAGE RATE (LB/HR )    COST ($/HR)
 -------------    ------------     -------------------    -------------
 D-300            RADFRAC                   1.5176+06       1.5176+04
 D-500            RADFRAC                   3.6727+05       3672.6850
 D-501            RADFRAC                   1.9168+05       1916.8389
 C-100            MCOMPR                    5.7348+04        573.4828
                                        -------------     -------------
                              TOTAL:        2.1339+06       2.1339+04
                                        =============     =============
```

```
                                UTILITY SECTION

UTILITY USAGE:  ELECTRIC  (ELECTRICITY)
---------------------------------------

 INPUT DATA:

   PRICE                             5.0000-02  $/KWHR
   INDEX TYPE                             FUEL

 RESULT:

   INDEXED PRICE                     5.0000-02  $/KWHR

 THIS UTILITY IS PURCHASED

 USAGE:

 UOS BLOCK ID     MODEL            USAGE RATE (KW    )    COST ($/HR)
 -------------    ------------     -------------------    -------------
 X-400            HEATER                      38.8412          1.9421
 P-100            PUMP                       153.6230          7.6811
 P-300            PUMP                        26.3536          1.3177
 P-502            PUMP                         6.0124          0.3006
 C-200            COMPR                      534.5764         26.7288
 C-100            MCOMPR                    1226.0253         61.3013
                                        -------------     -------------
                              TOTAL:        1985.4318         99.2716
                                        =============     =============
```

```
                            PROBLEM STATUS SECTION

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

****************************************************************************
*                                                                          *
* Calculations were completed with errors                                  *
*                                                                          *
* All Unit Operation blocks were completed normally                        *
*                                                                          *
* All streams were flashed normally                                        *
*                                                                          *
* All Utility blocks were completed normally                               *
*                                                                          *
* The following Convergence blocks were                                    *
* completed with errors:                                                   *
*   $OLVER01  $OLVER05                                                     *
*                                                                          *
****************************************************************************
```

A.4 MSDS and Compound Data



SIGMA-ALDRICH

Material Safety Data Sheet

Version 3.2
Revision Date 01/11/2008
Print Date 03/28/2009

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : 1-Butanol

Product Number : BT105
Brand : Sigma

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA
Telephone : +1 800-325-5832
Fax : +1 800-325-5052
Emergency Phone # : (314) 776-6555

2. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : n-Butanol
Butyl alcohol

Formula : $C_4H_{10}O$
Molecular Weight : 74.12 g/mol

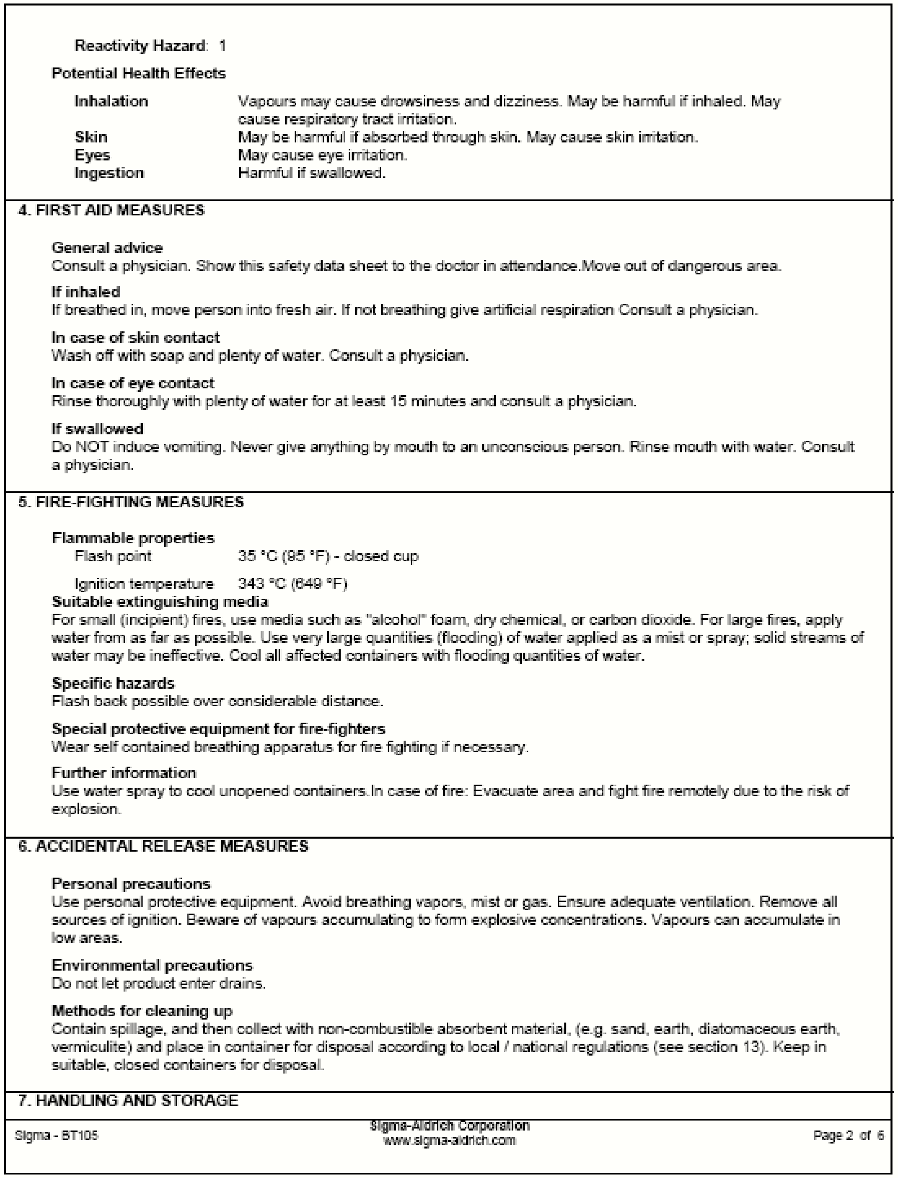
CAS-No.	EC-No.	Index-No.	Concentration
n-Butanol			
71-36-3	200-751-6	603-004-00-6	-

3. HAZARDS IDENTIFICATION

Emergency Overview
OSHA Hazards
Flammable Liquid
Target Organ Effect
Harmful by ingestion.
Irritant
Target Organs
Central nervous system, ears, Liver, Kidney, Blood

HMIS Classification
Health Hazard: 2
Chronic Health Hazard: *
Flammability: 3
Physical hazards: 1

NFPA Rating
Health Hazard: 2
Fire : 3



Reactivity Hazard: 1

Potential Health Effects

Inhalation	Vapours may cause drowsiness and dizziness. 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	Harmful if swallowed.

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. FIRE-FIGHTING MEASURES

Flammable properties
Flash point 35 °C (95 °F) - closed cup

Ignition temperature 343 °C (649 °F)

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.

Specific hazards
Flash back possible over considerable distance.

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

Further information
Use water spray to cool unopened containers.In case of fire: Evacuate area and fight fire remotely due to the risk of explosion.

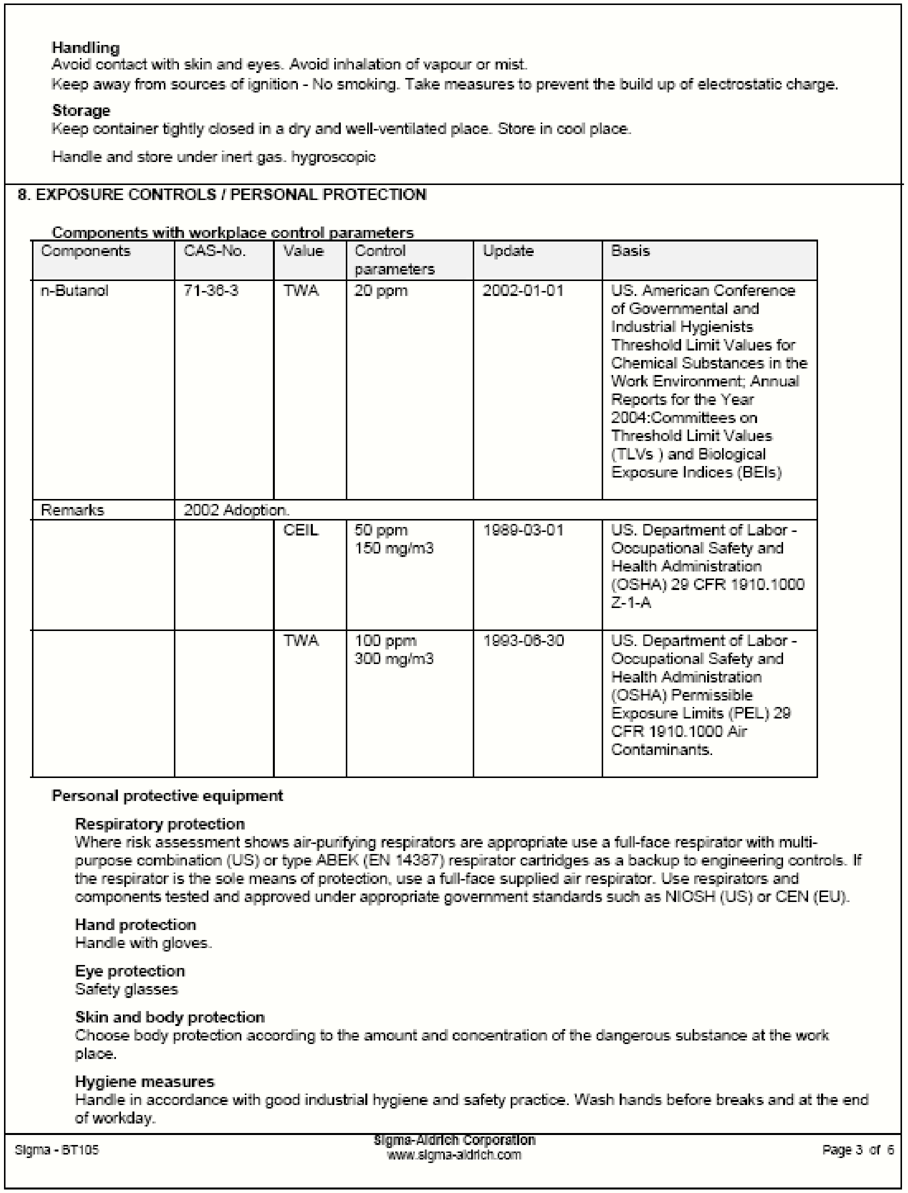
6. ACCIDENTAL RELEASE MEASURES

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

Environmental precautions
Do not let product enter drains.

Methods for cleaning up
Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

7. HANDLING AND STORAGE



Handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Storage
Keep container tightly closed in a dry and well-ventilated place. Store in cool place.

Handle and store under inert gas. hygroscopic

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Update	Basis
n-Butanol	71-36-3	TWA	20 ppm	2002-01-01	US. American Conference of Governmental and Industrial Hygienists Threshold Limit Values for Chemical Substances in the Work Environment; Annual Reports for the Year 2004:Committees on Threshold Limit Values (TLVs) and Biological Exposure Indices (BEIs)
Remarks	2002 Adoption.				
		CEIL	50 ppm 150 mg/m3	1989-03-01	US. Department of Labor - Occupational Safety and Health Administration (OSHA) 29 CFR 1910.1000 Z-1-A
		TWA	100 ppm 300 mg/m3	1993-06-30	US. Department of Labor - Occupational Safety and Health Administration (OSHA) Permissible Exposure Limits (PEL) 29 CFR 1910.1000 Air Contaminants.

Personal protective equipment

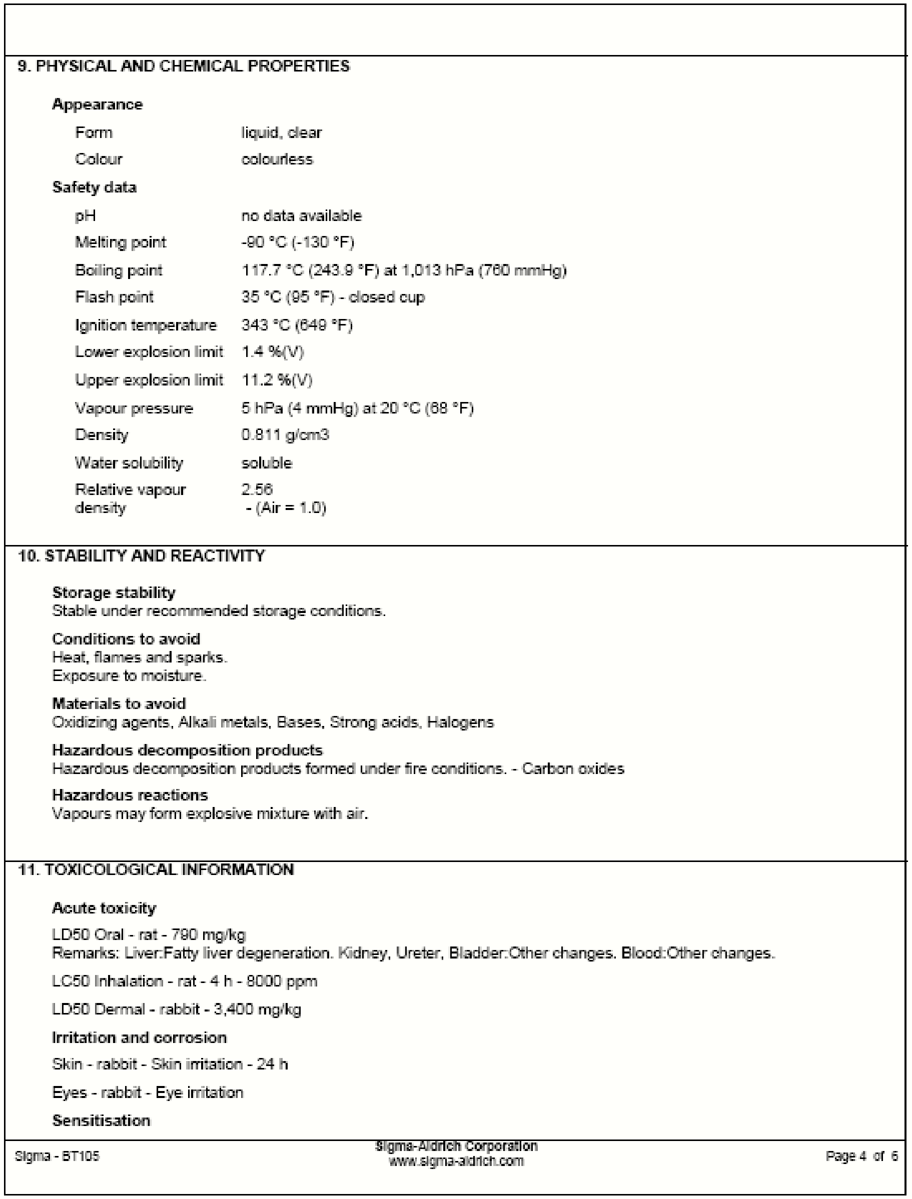
Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face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

Eye protection
Safety glasses

Skin and body protection
Choose body protection according to the amount and concentration of the dangerous substance at the work place.

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	liquid, clear
Colour	colourless

Safety data

pH	no data available
Melting point	-90 °C (-130 °F)
Boiling point	117.7 °C (243.9 °F) at 1,013 hPa (760 mmHg)
Flash point	35 °C (95 °F) - closed cup
Ignition temperature	343 °C (649 °F)
Lower explosion limit	1.4 %(V)
Upper explosion limit	11.2 %(V)
Vapour pressure	5 hPa (4 mmHg) at 20 °C (68 °F)
Density	0.811 g/cm3
Water solubility	soluble
Relative vapour density	2.56 - (Air = 1.0)

10. STABILITY AND REACTIVITY

Storage stability
Stable under recommended storage conditions.

Conditions to avoid
Heat, flames and sparks.
Exposure to moisture.

Materials to avoid
Oxidizing agents, Alkali metals, Bases, Strong acids, Halogens

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

Hazardous reactions
Vapours may form explosive mixture with air.

11. TOXICOLOGICAL INFORMATION

Acute toxicity

LD50 Oral - rat - 790 mg/kg
Remarks: Liver:Fatty liver degeneration. Kidney, Ureter, Bladder:Other changes. Blood:Other changes.

LC50 Inhalation - rat - 4 h - 8000 ppm

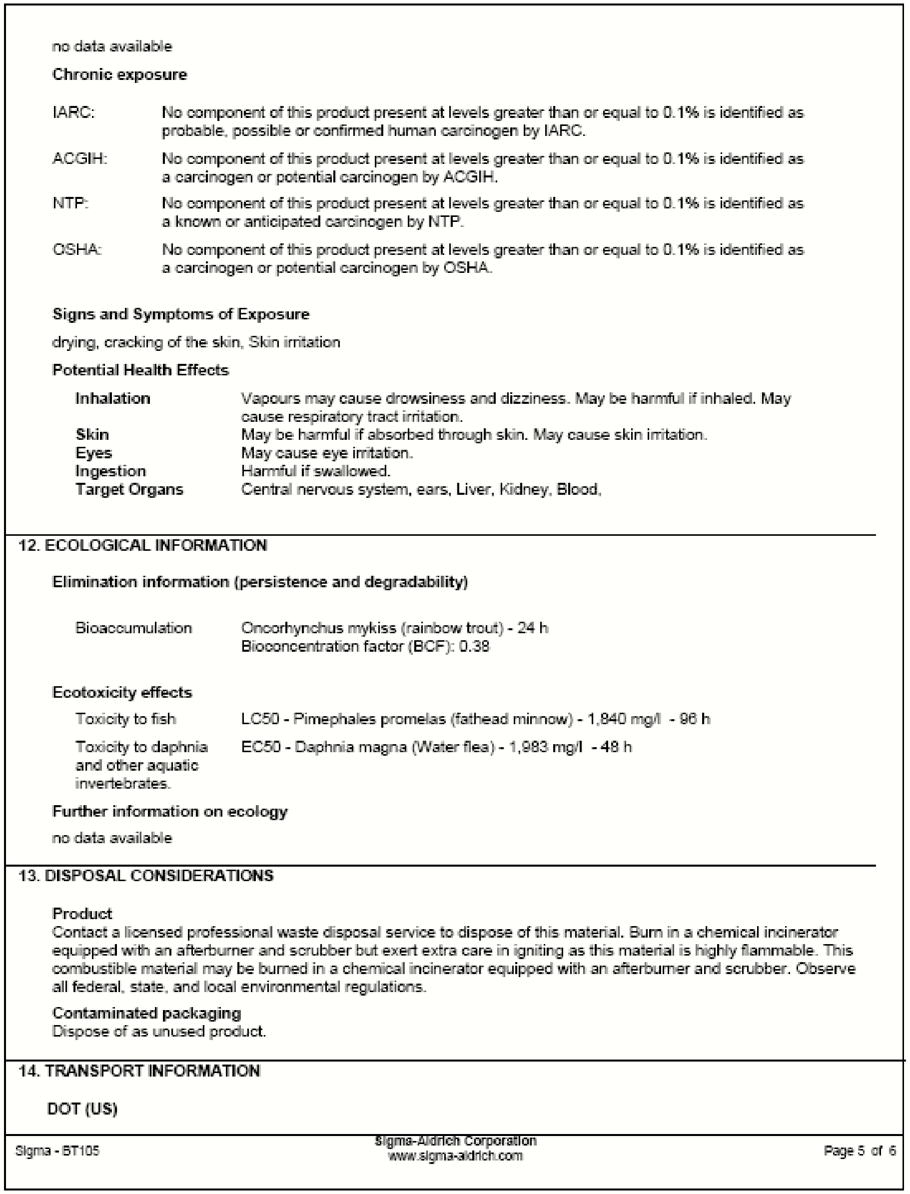
LD50 Dermal - rabbit - 3,400 mg/kg

Irritation and corrosion

Skin - rabbit - Skin irritation - 24 h

Eyes - rabbit - Eye irritation

Sensitisation



no data available

Chronic exposure

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.

Signs and Symptoms of Exposure

drying, cracking of the skin, Skin irritation

Potential Health Effects

Inhalation	Vapours may cause drowsiness and dizziness. 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	Harmful if swallowed.
Target Organs	Central nervous system, ears, Liver, Kidney, Blood,

12. ECOLOGICAL INFORMATION

Elimination information (persistence and degradability)

Bioaccumulation	Oncorhynchus mykiss (rainbow trout) - 24 h Bioconcentration factor (BCF): 0.38

Ecotoxicity effects

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 1,840 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates.	EC50 - Daphnia magna (Water flea) - 1,983 mg/l - 48 h

Further information on ecology

no data available

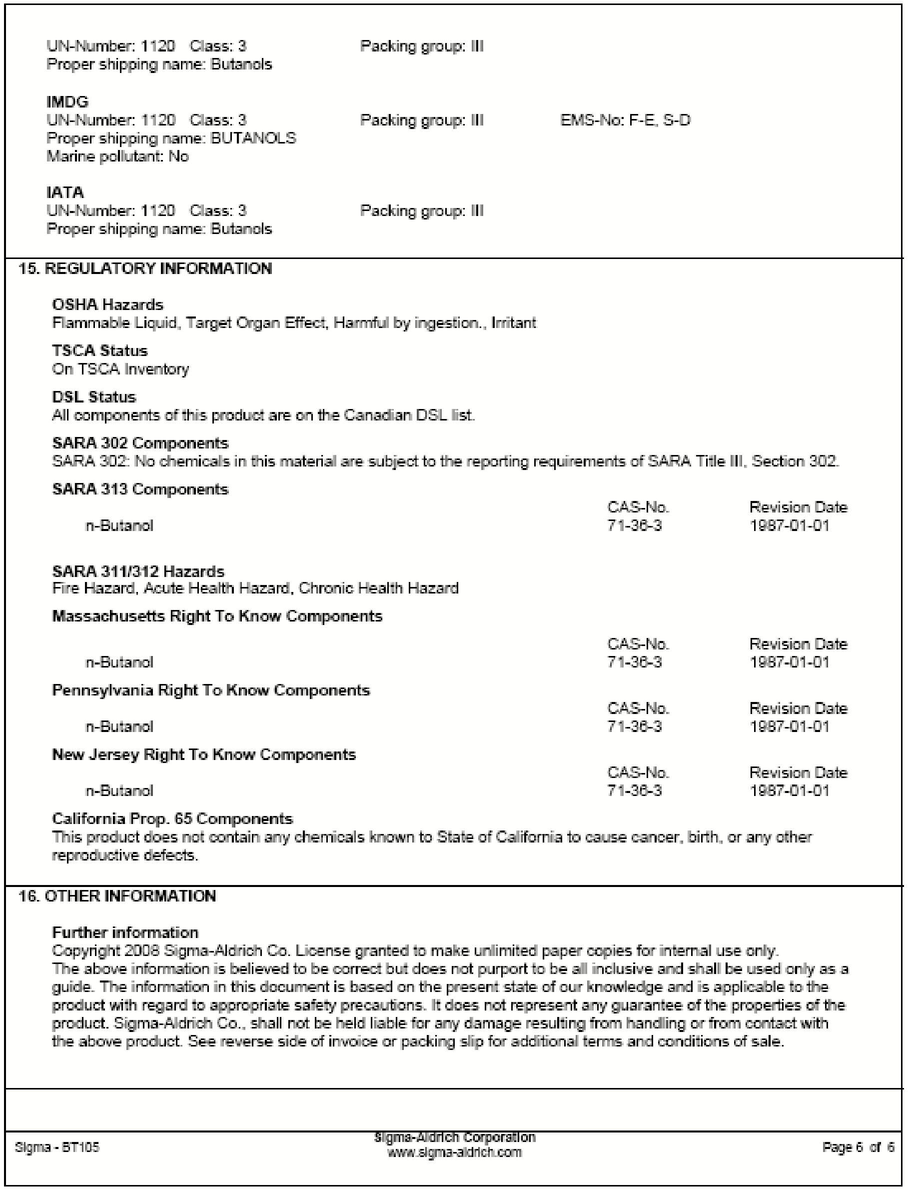
13. DISPOSAL CONSIDERATIONS

Product
Contact a licensed professional waste disposal service to dispose of this material. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)



UN-Number: 1120 Class: 3 Packing group: III
Proper shipping name: Butanols

IMDG
UN-Number: 1120 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: BUTANOLS
Marine pollutant: No

IATA
UN-Number: 1120 Class: 3 Packing group: III
Proper shipping name: Butanols

15. REGULATORY INFORMATION

OSHA Hazards
Flammable Liquid, Target Organ Effect, Harmful by ingestion., Irritant

TSCA Status
On TSCA Inventory

DSL Status
All components of this product are on the Canadian DSL list.

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

	CAS-No.	Revision Date
n-Butanol	71-36-3	1987-01-01

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

Massachusetts Right To Know Components

	CAS-No.	Revision Date
n-Butanol	71-36-3	1987-01-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
n-Butanol	71-36-3	1987-01-01

New Jersey Right To Know Components

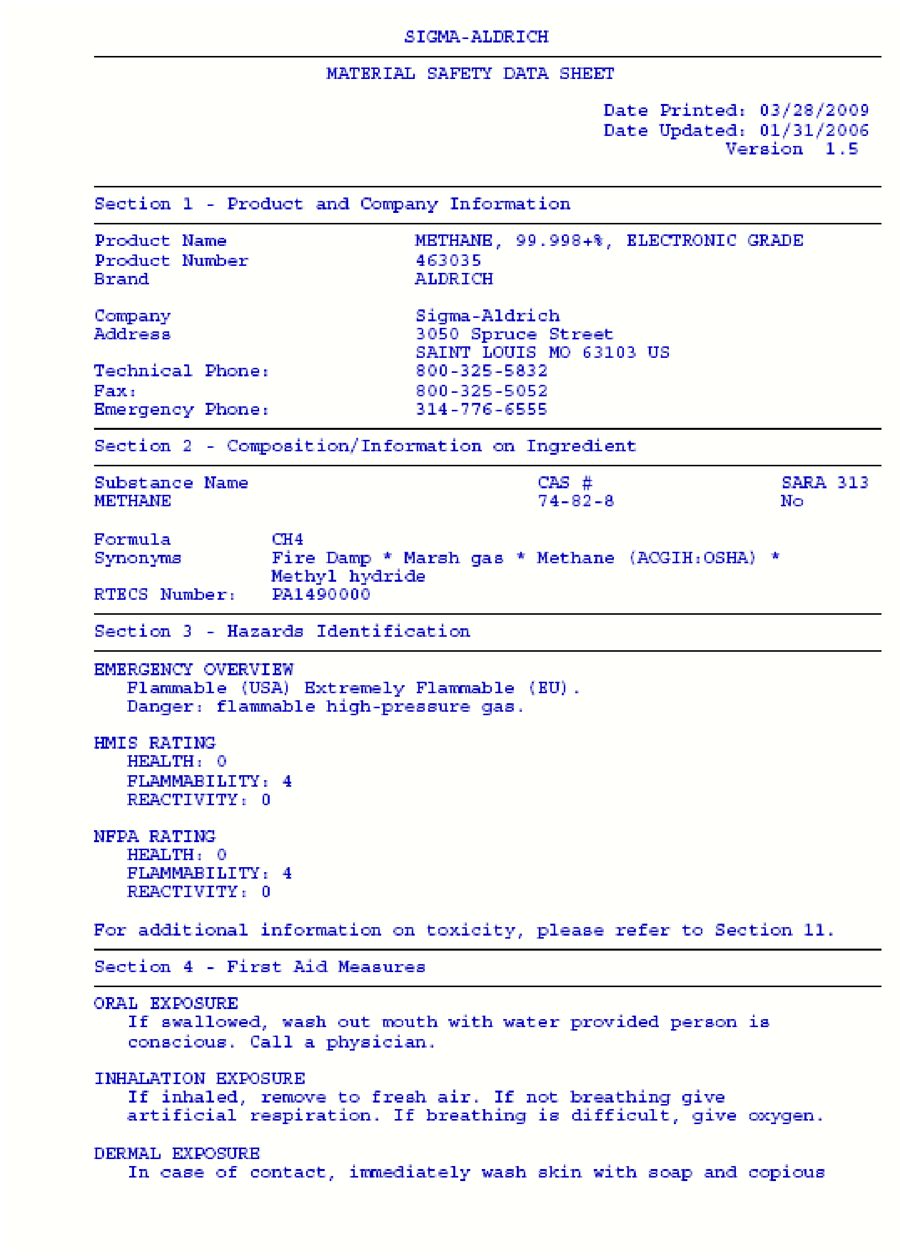
	CAS-No.	Revision Date
n-Butanol	71-36-3	1987-01-01

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

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 Co., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.



SIGMA-ALDRICH

MATERIAL SAFETY DATA SHEET

Date Printed: 03/28/2009
Date Updated: 01/31/2006
Version 1.5

Section 1 - Product and Company Information

Product Name	METHANE, 99.998+%, ELECTRONIC GRADE
Product Number	463035
Brand	ALDRICH
Company	Sigma-Aldrich
Address	3050 Spruce Street SAINT LOUIS MO 63103 US
Technical Phone:	800-325-5832
Fax:	800-325-5052
Emergency Phone:	314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
METHANE	74-82-8	No

Formula	CH4
Synonyms	Fire Damp * Marsh gas * Methane (ACGIH:OSHA) * Methyl hydride
RTECS Number:	PA1490000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW
Flammable (USA) Extremely Flammable (EU).
Danger: flammable high-pressure gas.

HMIS RATING
HEALTH: 0
FLAMMABILITY: 4
REACTIVITY: 0

NFPA RATING
HEALTH: 0
FLAMMABILITY: 4
REACTIVITY: 0

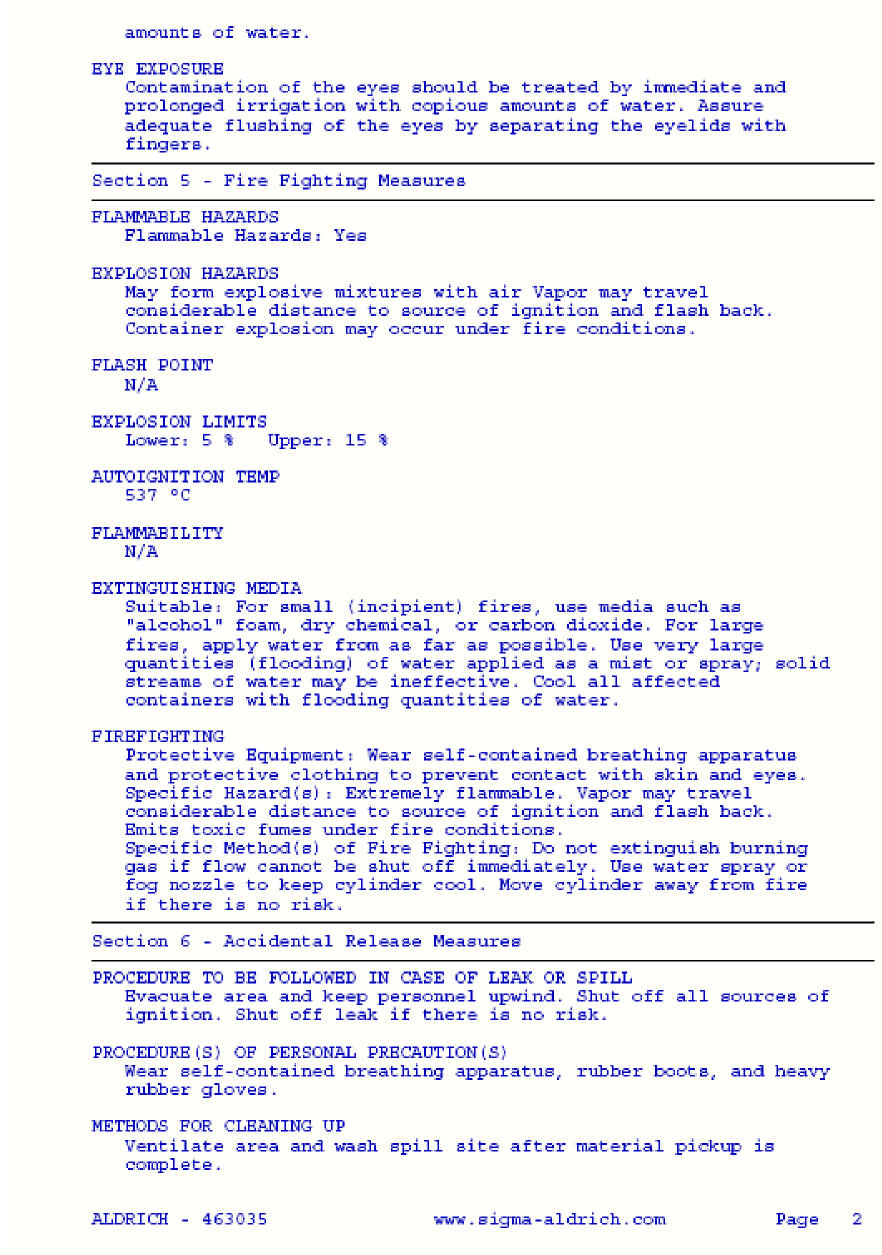
For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE
If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE
If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE
In case of contact, immediately wash skin with soap and copious



amounts of water.

EYE EXPOSURE
Contamination of the eyes should be treated by immediate and prolonged irrigation with copious amounts of water. Assure adequate flushing of the eyes by separating the eyelids with fingers.

Section 5 - Fire Fighting Measures

FLAMMABLE HAZARDS
Flammable Hazards: Yes

EXPLOSION HAZARDS
May form explosive mixtures with air Vapor may travel considerable distance to source of ignition and flash back. Container explosion may occur under fire conditions.

FLASH POINT
N/A

EXPLOSION LIMITS
Lower: 5 %   Upper: 15 %

AUTOIGNITION TEMP
537 °C

FLAMMABILITY
N/A

EXTINGUISHING MEDIA
Suitable: 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.

FIREFIGHTING
Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Extremely flammable. Vapor may travel considerable distance to source of ignition and flash back. Emits toxic fumes under fire conditions.
Specific Method(s) of Fire Fighting: Do not extinguish burning gas if flow cannot be shut off immediately. Use water spray or fog nozzle to keep cylinder cool. Move cylinder away from fire if there is no risk.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL
Evacuate area and keep personnel upwind. Shut off all sources of ignition. Shut off leak if there is no risk.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)
Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP
Ventilate area and wash spill site after material pickup is complete.

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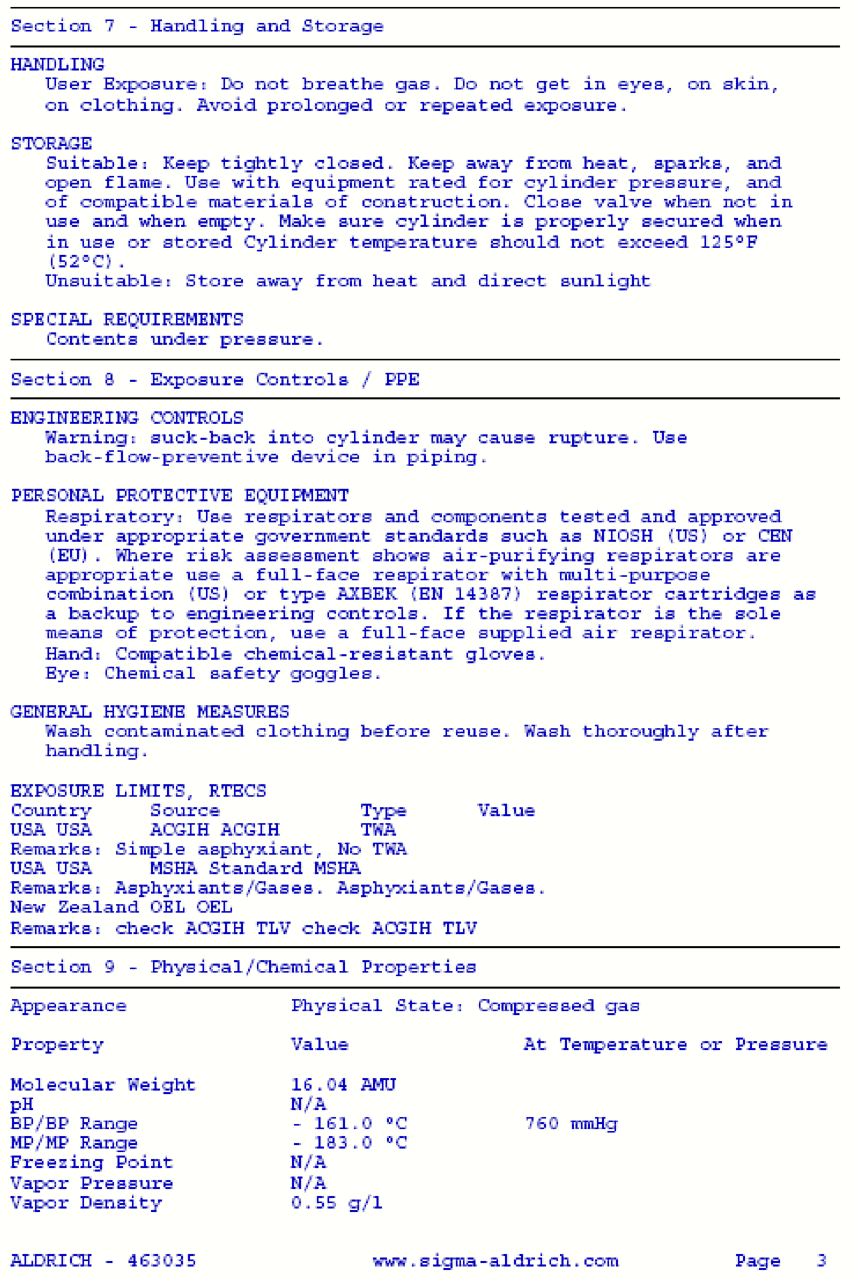


Section 7 - Handling and Storage

HANDLING
User Exposure: Do not breathe gas. Do not get in eyes, on skin, on clothing. Avoid prolonged or repeated exposure.

STORAGE
Suitable: Keep tightly closed. Keep away from heat, sparks, and open flame. Use with equipment rated for cylinder pressure, and of compatible materials of construction. Close valve when not in use and when empty. Make sure cylinder is properly secured when in use or stored Cylinder temperature should not exceed 125°F (52°C).
Unsuitable: Store away from heat and direct sunlight

SPECIAL REQUIREMENTS
Contents under pressure.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS
Warning: suck-back into cylinder may cause rupture. Use back-flow-preventive device in piping.

PERSONAL PROTECTIVE EQUIPMENT
Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (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.
Hand: Compatible chemical-resistant gloves.
Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES
Wash contaminated clothing before reuse. Wash thoroughly after handling.

EXPOSURE LIMITS, RTECS

Country	Source	Type	Value
USA USA	ACGIH ACGIH	TWA	
Remarks: Simple asphyxiant, No TWA			
USA USA	MSHA Standard MSHA		
Remarks: Asphyxiants/Gases. Asphyxiants/Gases.			
New Zealand OEL OEL			
Remarks: check ACGIH TLV check ACGIH TLV			

Section 9 - Physical/Chemical Properties

Appearance   Physical State: Compressed gas

Property	Value	At Temperature or Pressure
Molecular Weight	16.04 AMU	
pH	N/A	
BP/BP Range	- 161.0 °C	760 mmHg
MP/MP Range	- 183.0 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	0.55 g/l	

ALDRICH - 463035   www.sigma-aldrich.com   Page 3

Saturated Vapor Conc.	N/A
SG/Density	N/A
Bulk Density	N/A
Odor Threshold	N/A
Volatile%	N/A
VOC Content	N/A
Water Content	N/A
Solvent Content	N/A
Evaporation Rate	N/A
Viscosity	N/A
Surface Tension	N/A
Partition Coefficient	N/A
Decomposition Temp.	N/A
Flash Point	N/A
Explosion Limits	Lower: 5 % Upper: 15 %
Flammability	N/A
Autoignition Temp	537 °C
Refractive Index	N/A
Optical Rotation	N/A
Miscellaneous Data	N/A
Solubility	N/A

N/A = not available

Section 10 - Stability and Reactivity

STABILITY

Materials to Avoid: Strong oxidizing agents.

HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE

Skin Contact: May cause skin irritation.
Skin Absorption: May be harmful if absorbed through the skin.
Eye Contact: May cause eye irritation.
Inhalation: Can cause rapid suffocation. Material may be irritating to mucous membranes and upper respiratory tract. May be harmful if inhaled.
Ingestion: May be harmful if swallowed.

SIGNS AND SYMPTOMS OF EXPOSURE

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

CONDITIONS AGGRAVATED BY EXPOSURE

At high concentrations methane functions as a simple asphyxiant by displacing air.

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Observe all federal, state, and local environmental regulations.

APPROPRIATE METHOD OF DISPOSAL OF CONTAMINATED PACKAGING

Caution: no-return cylinder. Do not reuse. Empty cylinder will contain hazardous residue. Follow proper disposal techniques.

Section 14 - Transport Information

DOT

Proper Shipping Name: Methane, compressed [or] Natural gas, compressed [(with high methane content)]
UN#: 1971
Class: 2.1
Packing Group: None
Hazard Label: Flammable gas
PIH: Not PIH

IATA

Proper Shipping Name: Methane, compressed
IATA UN Number: 1971
Hazard Class: 2.1
Not Allowed - Aircraft: Cargo aircraft only. Not permitted on passenger aircraft.

Section 15 - Regulatory Information

EU DIRECTIVES CLASSIFICATION

Symbol of Danger: F+
Indication of Danger: Extremely Flammable.
R: 12
Risk Statements: Extremely flammable.
S: 9-16-33
Safety Statements: Keep container in a well-ventilated place. Keep away from sources of ignition - no smoking. Take precautionary measures against static discharges.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Flammable (USA) Extremely Flammable (EU).
Safety Statements: Keep in a cool place. Keep away from sources of ignition - no smoking. Take precautionary measures against static discharges.
US Statements: Danger: flammable high-pressure gas.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: No
TSCA INVENTORY ITEM: Yes Yes

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: No

Section 16 - Other Information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

The above information is believed to be correct but does not

SIGMA-ALDRICH

MATERIAL SAFETY DATA SHEET

Date Printed: 03/28/2009
Date Updated: 10/21/2008
Version 1.15

Section 1 - Product and Company Information

Product Name	TETRAHYDROFURAN, INHIBITOR-FREE, PURIFICATION GRADE
Product Number	644544
Brand	ALDRICH
Company	Sigma-Aldrich
Address	3050 Spruce Street SAINT LOUIS MO 63103 US
Technical Phone:	800-325-5832
Fax:	800-325-5052
Emergency Phone:	314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
TETRAHYDROFURAN (Inhibitor free)	109-99-9	No

Formula	C4H8O
Synonyms	Agrisynth THF * Butane, 1,4-epoxy- * Butane, alpha,delta-oxide * Cyclotetramethylene oxide * Diethylene oxide * 1,4-Epoxybutane * Furanidine * NCI-C60560 * Oxacyclopentane * Oxolane * RCRA waste number U213 * Tetrahydrofuraan (Dutch) * Tetrahydrofuran (ACGIH:OSHA) * Tetrahydrofuranne (French) * Tetraidrofurano (Italian) * Tetramethylene oxide
RTECS Number:	LU5950000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW
Flammable (USA) Highly Flammable (EU). Irritant.
May form explosive peroxides. Irritating to eyes and respiratory system.
Possible Carcinogen (US). Target organ(s): Liver. Nerves.

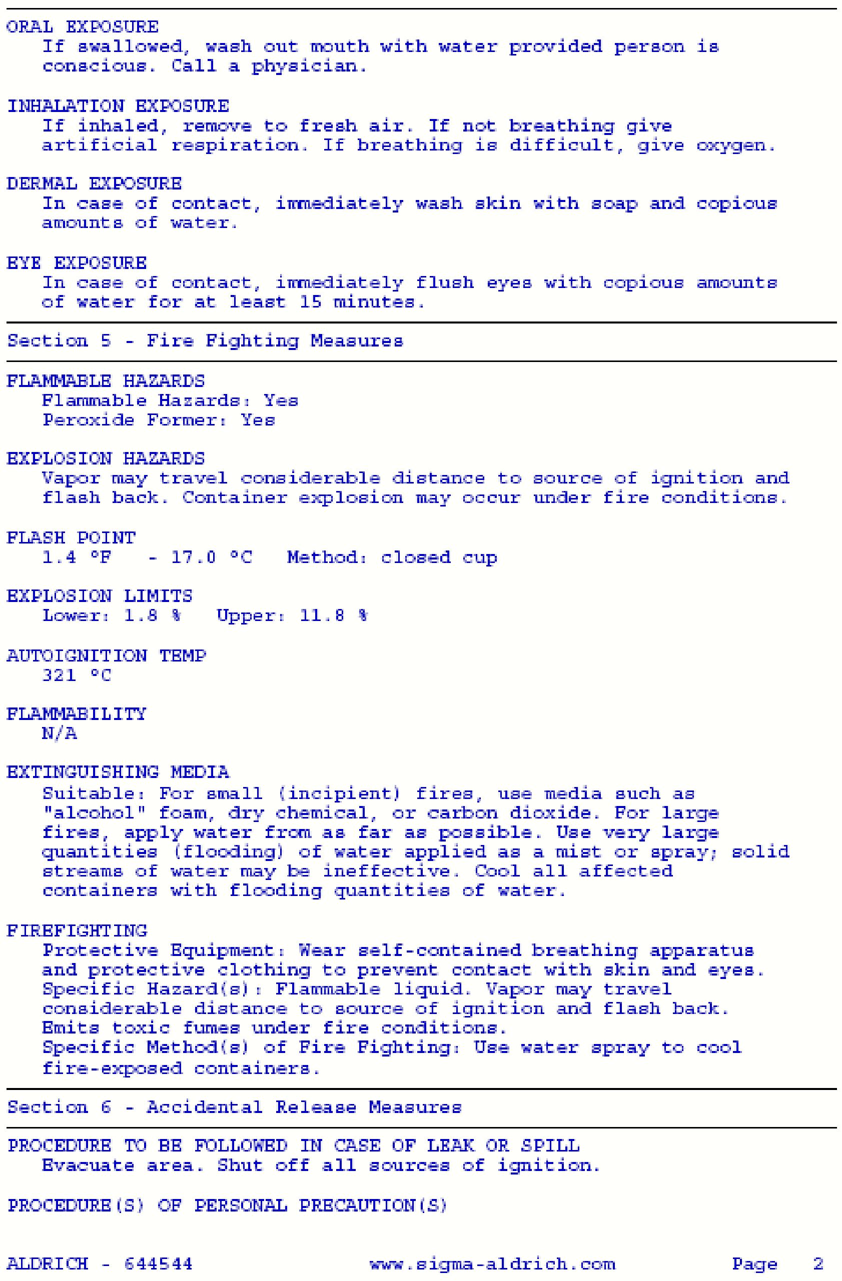
HMIS RATING
HEALTH: 2*
FLAMMABILITY: 3
REACTIVITY: 3

NFPA RATING
HEALTH: 2
FLAMMABILITY: 3
REACTIVITY: 3

*additional chronic hazards present.

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures



ORAL EXPOSURE
If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE
If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE
In case of contact, immediately wash skin with soap and copious amounts of water.

EYE EXPOSURE
In case of contact, immediately flush eyes with copious amounts of water for at least 15 minutes.

Section 5 - Fire Fighting Measures

FLAMMABLE HAZARDS
Flammable Hazards: Yes
Peroxide Former: Yes

EXPLOSION HAZARDS
Vapor may travel considerable distance to source of ignition and flash back. Container explosion may occur under fire conditions.

FLASH POINT
1.4 °F - 17.0 °C Method: closed cup

EXPLOSION LIMITS
Lower: 1.8 % Upper: 11.8 %

AUTOIGNITION TEMP
321 °C

FLAMMABILITY
N/A

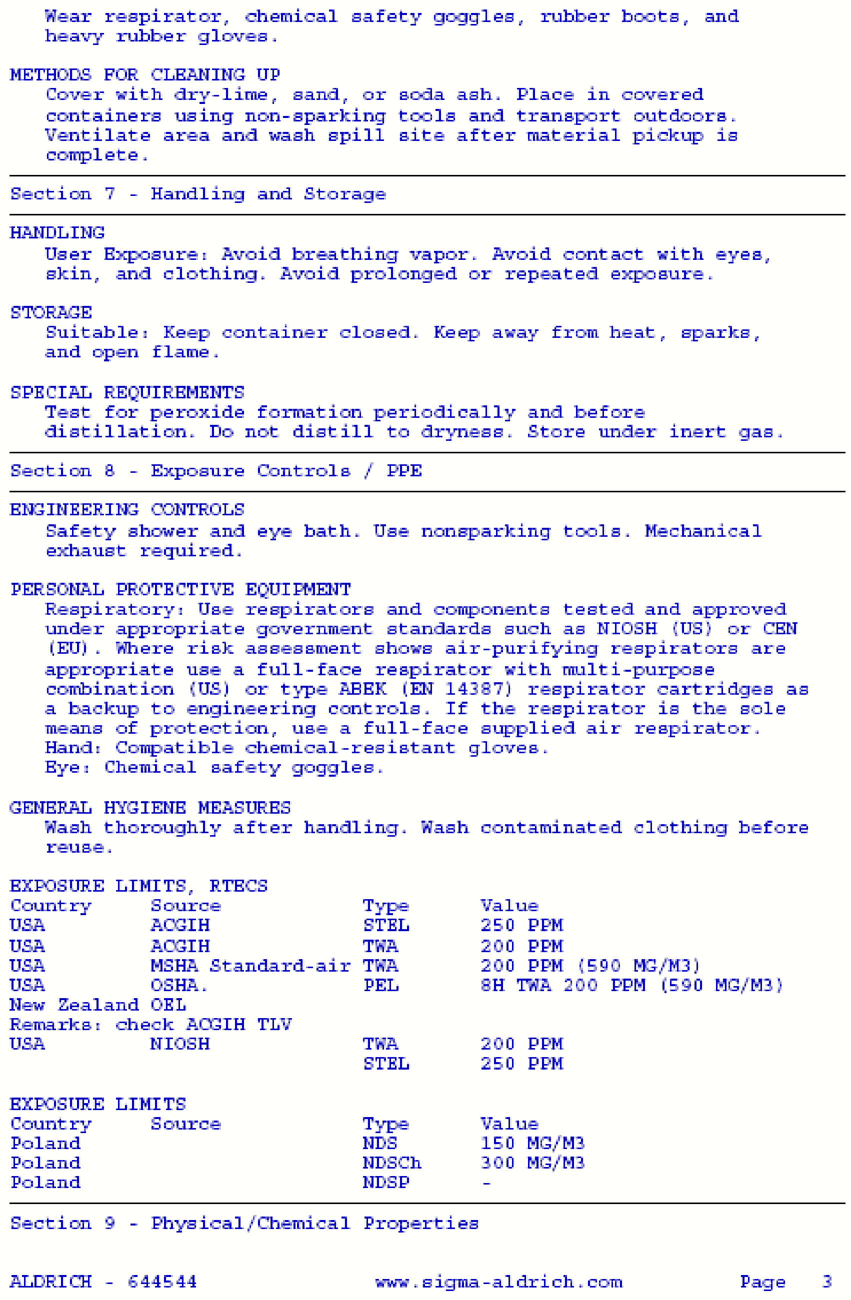
EXTINGUISHING MEDIA
Suitable: For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool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

FIREFIGHTING
Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Flammable liquid. Vapor may travel considerable distance to source of ignition and flash back. Emits toxic fumes under fire conditions.
Specific Method(s) of Fire Fighting: Use water spray to cool fire-exposed containers.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL
Evacuate area. Shut off all sources of ignition.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)



Wear respirator, chemical safety goggles, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP
Cover with dry-lime, sand, or soda ash. Place in covered containers using non-sparking tools and transport outdoors. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING
User Exposure: Avoid breathing vapor. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

STORAGE
Suitable: Keep container closed. Keep away from heat, sparks, and open flame.

SPECIAL REQUIREMENTS
Test for peroxide formation periodically and before distillation. Do not distill to dryness. Store under inert gas.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS
Safety shower and eye bath. Use nonsparking tools. Mechanical exhaust required.

PERSONAL PROTECTIVE EQUIPMENT
Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). 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.
Hand: Compatible chemical-resistant gloves.
Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES
Wash thoroughly after handling. Wash contaminated clothing before reuse.

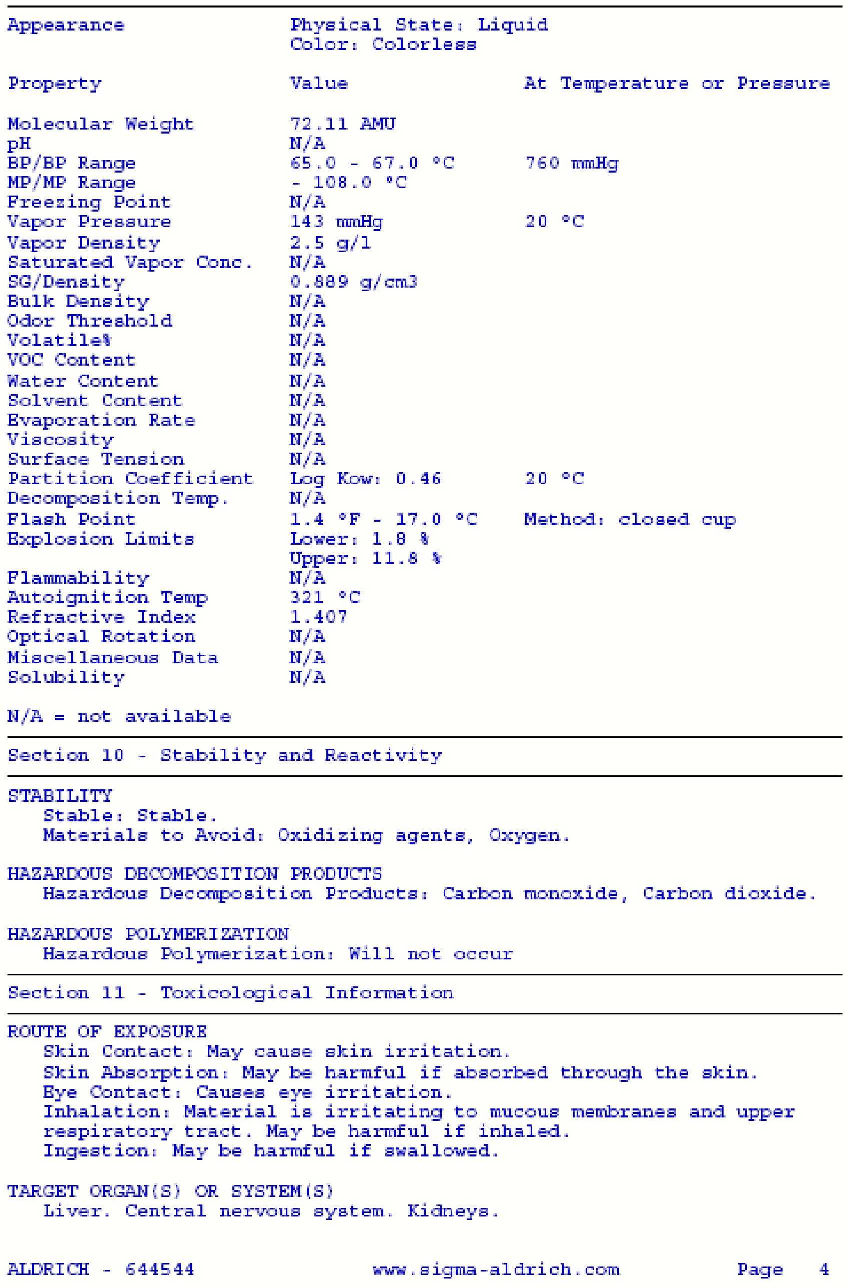
EXPOSURE LIMITS, RTECS

Country	Source	Type	Value
USA	ACGIH	STEL	250 PPM
USA	ACGIH	TWA	200 PPM
USA	MSHA Standard-air	TWA	200 PPM (590 MG/M3)
USA	OSHA.	PEL	8H TWA 200 PPM (590 MG/M3)
New Zealand	OEL		
Remarks: check ACGIH TLV			
USA	NIOSH	TWA	200 PPM
		STEL	250 PPM

EXPOSURE LIMITS

Country	Source	Type	Value
Poland		NDS	150 MG/M3
Poland		NDSCh	300 MG/M3
Poland		NDSP	-

Section 9 - Physical/Chemical Properties



Appearance	Physical State: Liquid Color: Colorless	
Property	Value	At Temperature or Pressure
Molecular Weight	72.11 AMU	
pH	N/A	
BP/BP Range	65.0 - 67.0 °C	760 mmHg
MP/MP Range	- 108.0 °C	
Freezing Point	N/A	
Vapor Pressure	143 mmHg	20 °C
Vapor Density	2.5 g/l	
Saturated Vapor Conc.	N/A	
SG/Density	0.889 g/cm3	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	Log Kow: 0.46	20 °C
Decomposition Temp.	N/A	
Flash Point	1.4 °F - 17.0 °C	Method: closed cup
Explosion Limits	Lower: 1.8 % Upper: 11.8 %	
Flammability	N/A	
Autoignition Temp	321 °C	
Refractive Index	1.407	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

N/A = not available

Section 10 - Stability and Reactivity

STABILITY
Stable: Stable.
Materials to Avoid: Oxidizing agents, Oxygen.

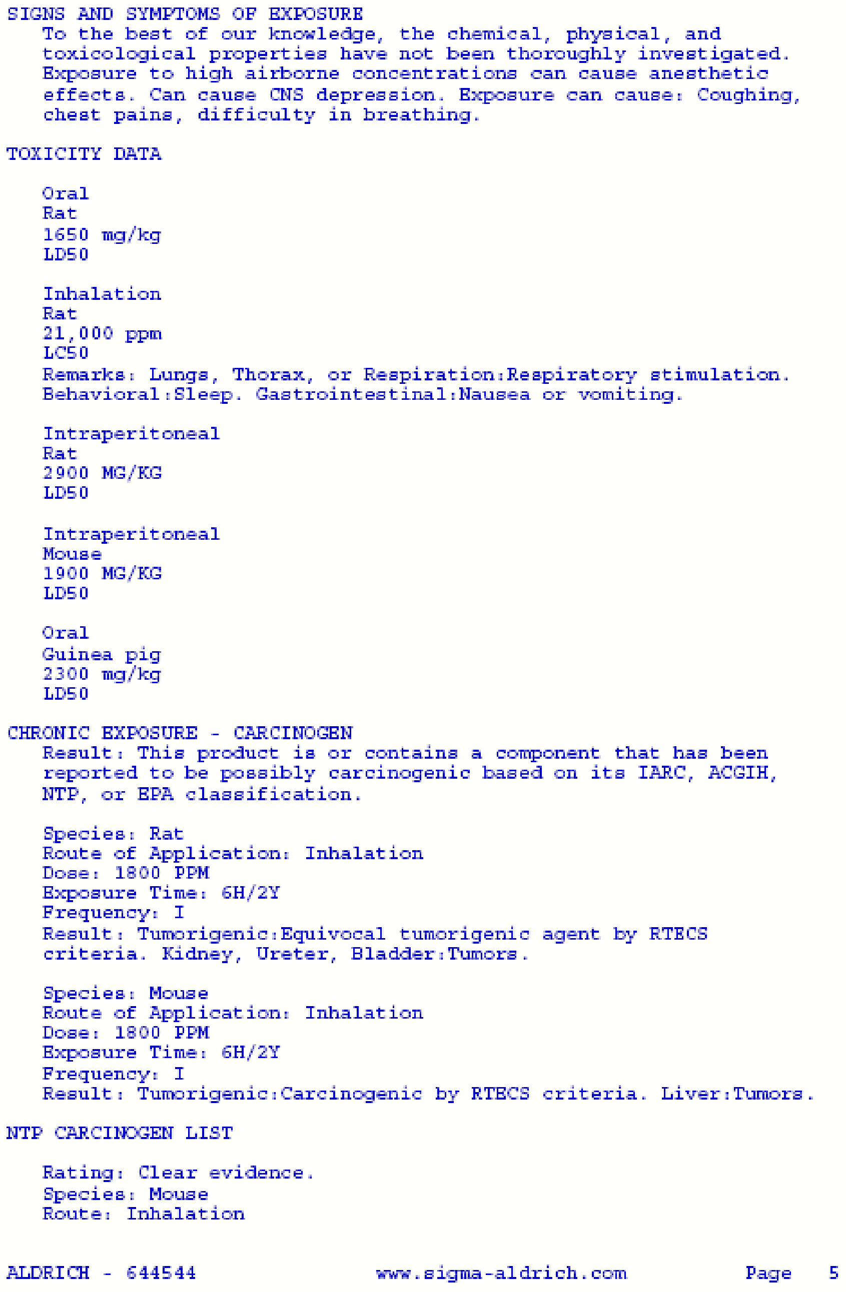
HAZARDOUS DECOMPOSITION PRODUCTS
Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

HAZARDOUS POLYMERIZATION
Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE
Skin Contact: May cause skin irritation.
Skin Absorption: May be harmful if absorbed through the skin.
Eye Contact: Causes eye irritation.
Inhalation: Material is irritating to mucous membranes and upper respiratory tract. May be harmful if inhaled.
Ingestion: May be harmful if swallowed.

TARGET ORGAN(S) OR SYSTEM(S)
Liver. Central nervous system. Kidneys.



SIGNS AND SYMPTOMS OF EXPOSURE
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Exposure to high airborne concentrations can cause anesthetic effects. Can cause CNS depression. Exposure can cause: Coughing, chest pains, difficulty in breathing.

TOXICITY DATA

Oral
Rat
1650 mg/kg
LD50

Inhalation
Rat
21,000 ppm
LC50
Remarks: Lungs, Thorax, or Respiration:Respiratory stimulation. Behavioral:Sleep. Gastrointestinal:Nausea or vomiting.

Intraperitoneal
Rat
2900 MG/KG
LD50

Intraperitoneal
Mouse
1900 MG/KG
LD50

Oral
Guinea pig
2300 mg/kg
LD50

CHRONIC EXPOSURE - CARCINOGEN
Result: This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH, NTP, or EPA classification.

Species: Rat
Route of Application: Inhalation
Dose: 1800 PPM
Exposure Time: 6H/2Y
Frequency: I
Result: Tumorigenic:Equivocal tumorigenic agent by RTECS criteria. Kidney, Ureter, Bladder:Tumors.

Species: Mouse
Route of Application: Inhalation
Dose: 1800 PPM
Exposure Time: 6H/2Y
Frequency: I
Result: Tumorigenic:Carcinogenic by RTECS criteria. Liver:Tumors.

NTP CARCINOGEN LIST

Rating: Clear evidence.
Species: Mouse
Route: Inhalation

CHRONIC EXPOSURE - TERATOGEN

Species: Rat
Dose: 5000 PPM/6H
Route of Application: Inhalation
Exposure Time: (6-19D PREG)
Result: Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

CHRONIC EXPOSURE - REPRODUCTIVE HAZARD

Species: Mouse
Dose: 1800 PPM/6H
Route of Application: Inhalation
Exposure Time: (6-17D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

Section 12 - Ecological Information

ACUTE ECOTOXICITY TESTS

Test Type: LC50 Fish
Species: Pimephales promelas (Fathead minnow)
Time: 96 h
Value: 2,160 mg/l

Test Type: EC50 Daphnia
Species: Daphnia magna
Time: 24 h
Value: 5,930 mg/l

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT

Proper Shipping Name: Tetrahydrofuran
UN#: 2056
Class: 3
Packing Group: Packing Group II
Hazard Label: Flammable liquid
PIH: Not PIH

IATA

Proper Shipping Name: Tetrahydrofuran
IATA UN Number: 2056
Hazard Class: 3
Packing Group: II

Section 15 - Regulatory Information

EU DIRECTIVES CLASSIFICATION

Symbol of Danger: F-Xi

Indication of Danger: Highly Flammable. Irritant.
R: 11-19-36/37
Risk Statements: Highly flammable. May form explosive peroxides. Irritating to eyes and respiratory system.
S: 16-29-33
Safety Statements: Keep away from sources of ignition - no smoking. Do not empty into drains. Take precautionary measures against static discharges.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Flammable (USA) Highly Flammable (EU). Irritant.
Risk Statements: May form explosive peroxides. Irritating to eyes and respiratory system.
Safety Statements: Keep away from sources of ignition - no smoking. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Do not empty into drains. Take precautionary measures against static discharges. Wear suitable protective clothing.
US Statements: Possible Carcinogen (US). Target organ(s): Liver. Nerves.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: No
TSCA INVENTORY ITEM: Yes

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: No

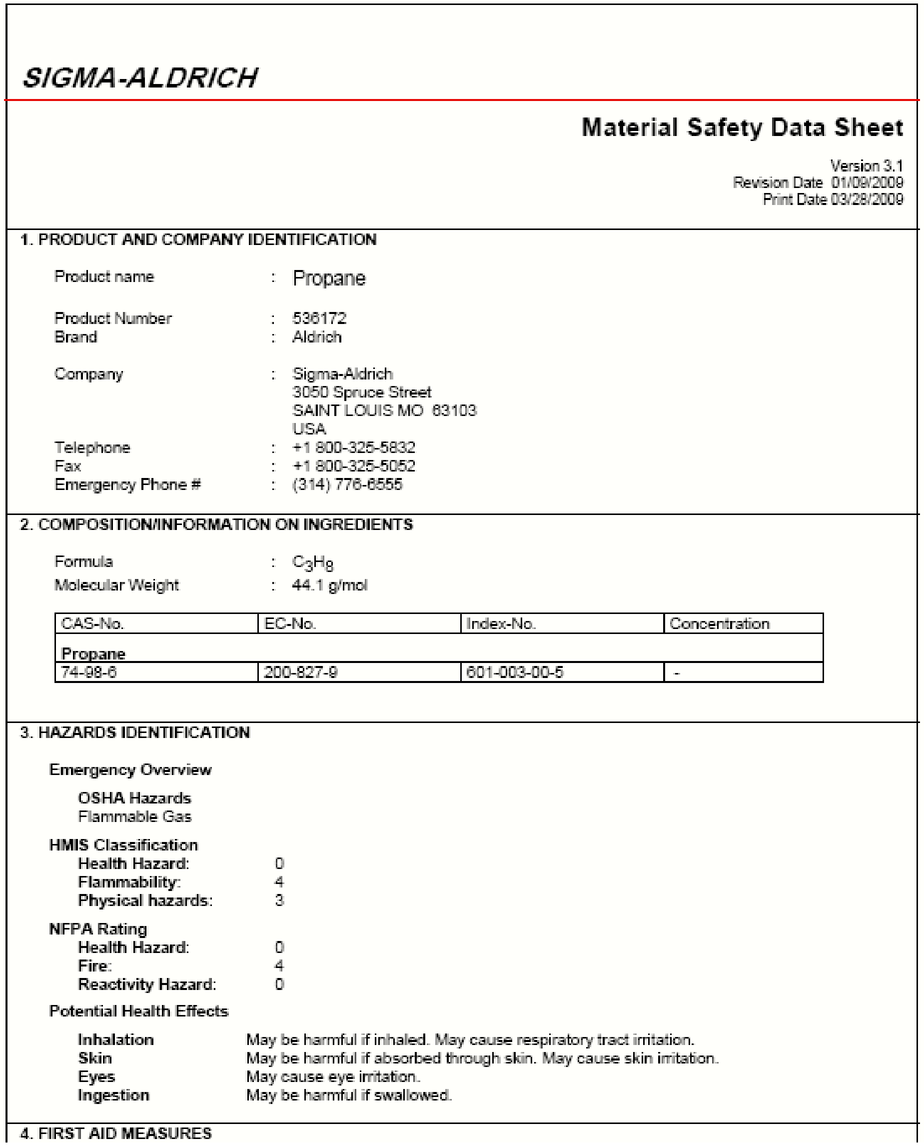
Section 16 - Other Information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

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 Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.



SIGMA-ALDRICH

Material Safety Data Sheet

Version 3.1
Revision Date 01/09/2009
Print Date 03/28/2009

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Propane

Product Number : 536172
Brand : Aldrich

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA
Telephone : +1 800-325-5832
Fax : +1 800-325-5052
Emergency Phone # : (314) 776-6555

2. COMPOSITION/INFORMATION ON INGREDIENTS

Formula : C_3H_8
Molecular Weight : 44.1 g/mol

CAS-No.	EC-No.	Index-No.	Concentration
Propane			
74-98-6	200-827-9	601-003-00-5	-

3. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Flammable Gas

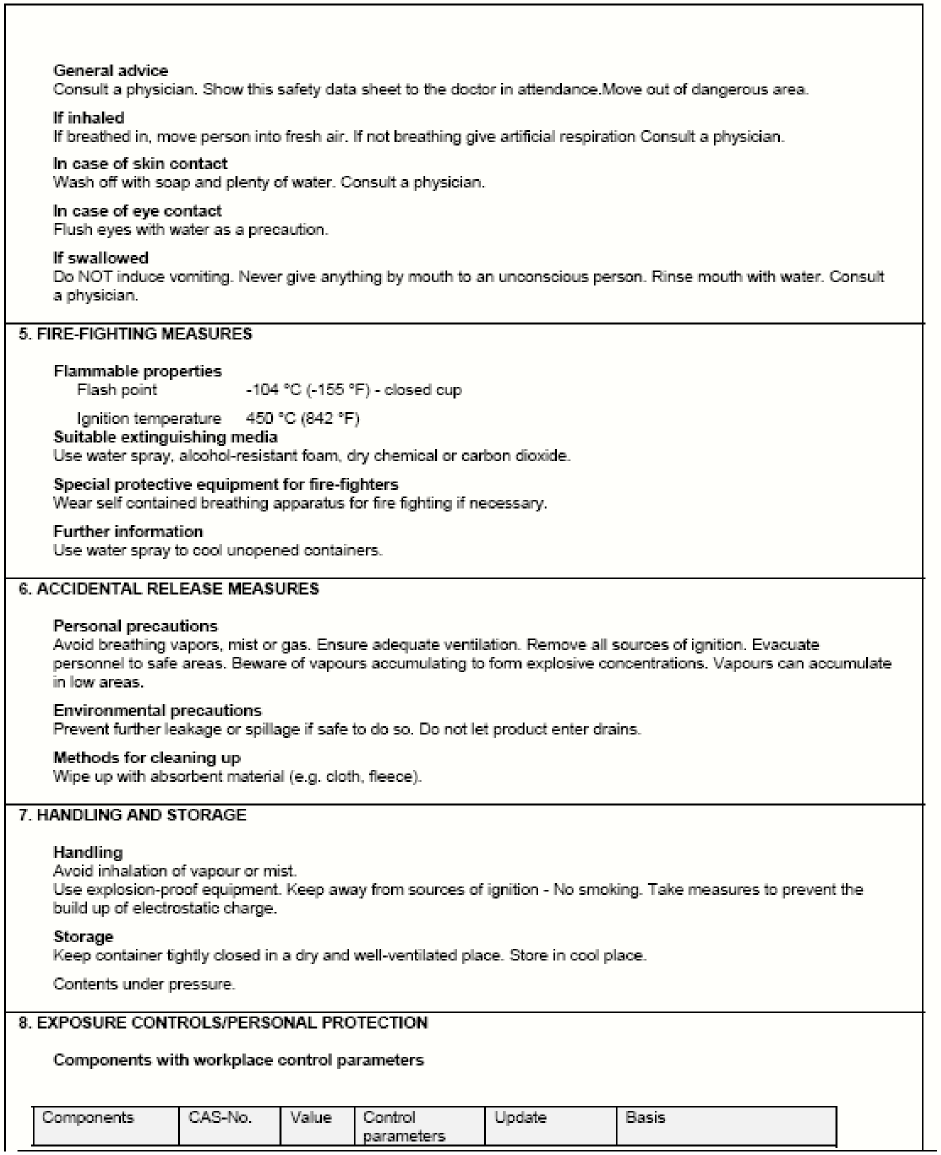
HMIS Classification
Health Hazard: 0
Flammability: 4
Physical hazards: 3

NFPA Rating
Health Hazard: 0
Fire: 4
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.

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
Flush eyes with water as a precaution.

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

5. FIRE-FIGHTING MEASURES

Flammable properties
Flash point -104 °C (-155 °F) - closed cup

Ignition temperature 450 °C (842 °F)

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

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

Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
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.

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

Methods for cleaning up
Wipe up with absorbent material (e.g. cloth, fleece).

7. HANDLING AND STORAGE

Handling
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.

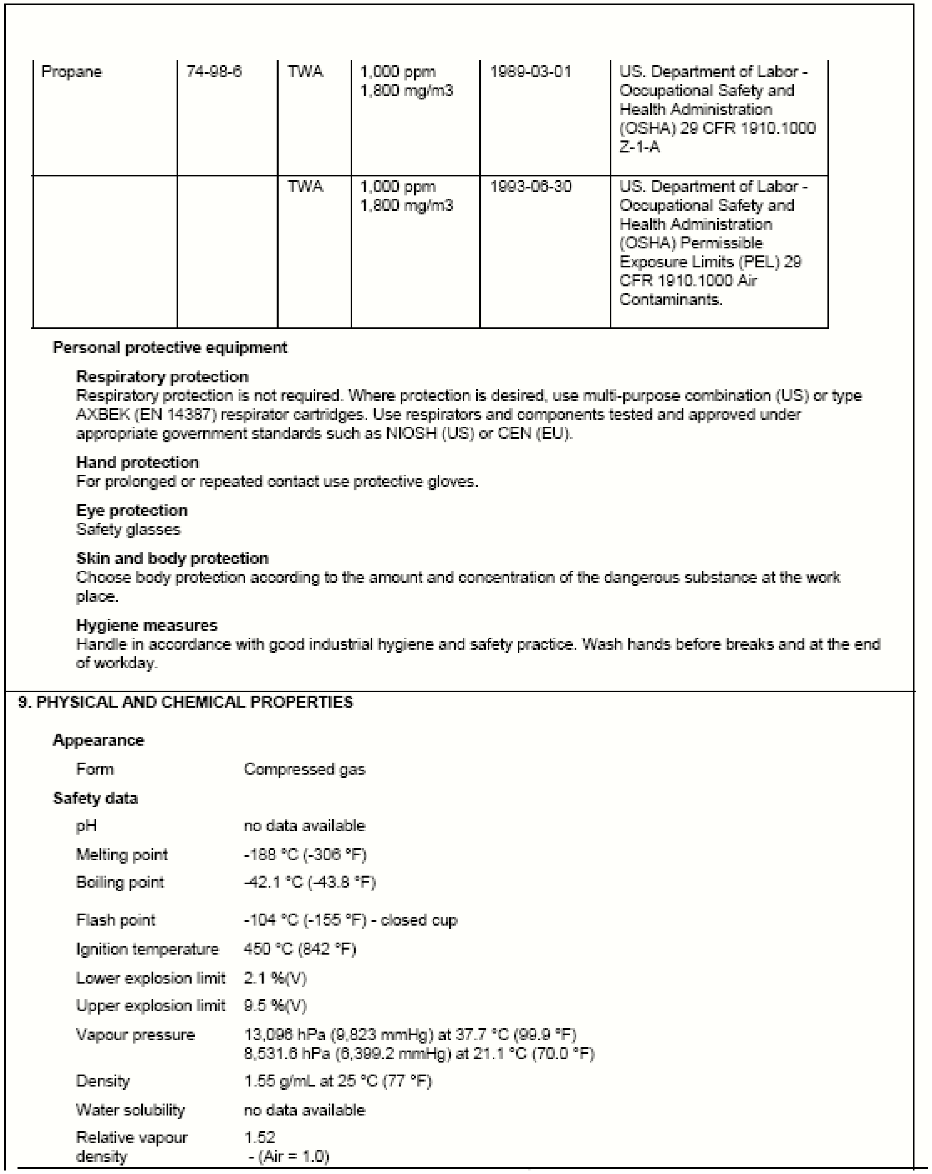
Storage
Keep container tightly closed in a dry and well-ventilated place. Store in cool place.

Contents under pressure.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Update	Basis



Propane	74-98-6	TWA	1,000 ppm 1,800 mg/m3	1989-03-01	US. Department of Labor - Occupational Safety and Health Administration (OSHA) 29 CFR 1910.1000 Z-1-A
		TWA	1,000 ppm 1,800 mg/m3	1993-06-30	US. Department of Labor - Occupational Safety and Health Administration (OSHA) Permissible Exposure Limits (PEL) 29 CFR 1910.1000 Air Contaminants.

Personal protective equipment

Respiratory protection
Respiratory protection is not required. Where protection is desired, use multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Hand protection
For prolonged or repeated contact use protective gloves.

Eye protection
Safety glasses

Skin and body protection
Choose body protection according to the amount and concentration of the dangerous substance at the work place.

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

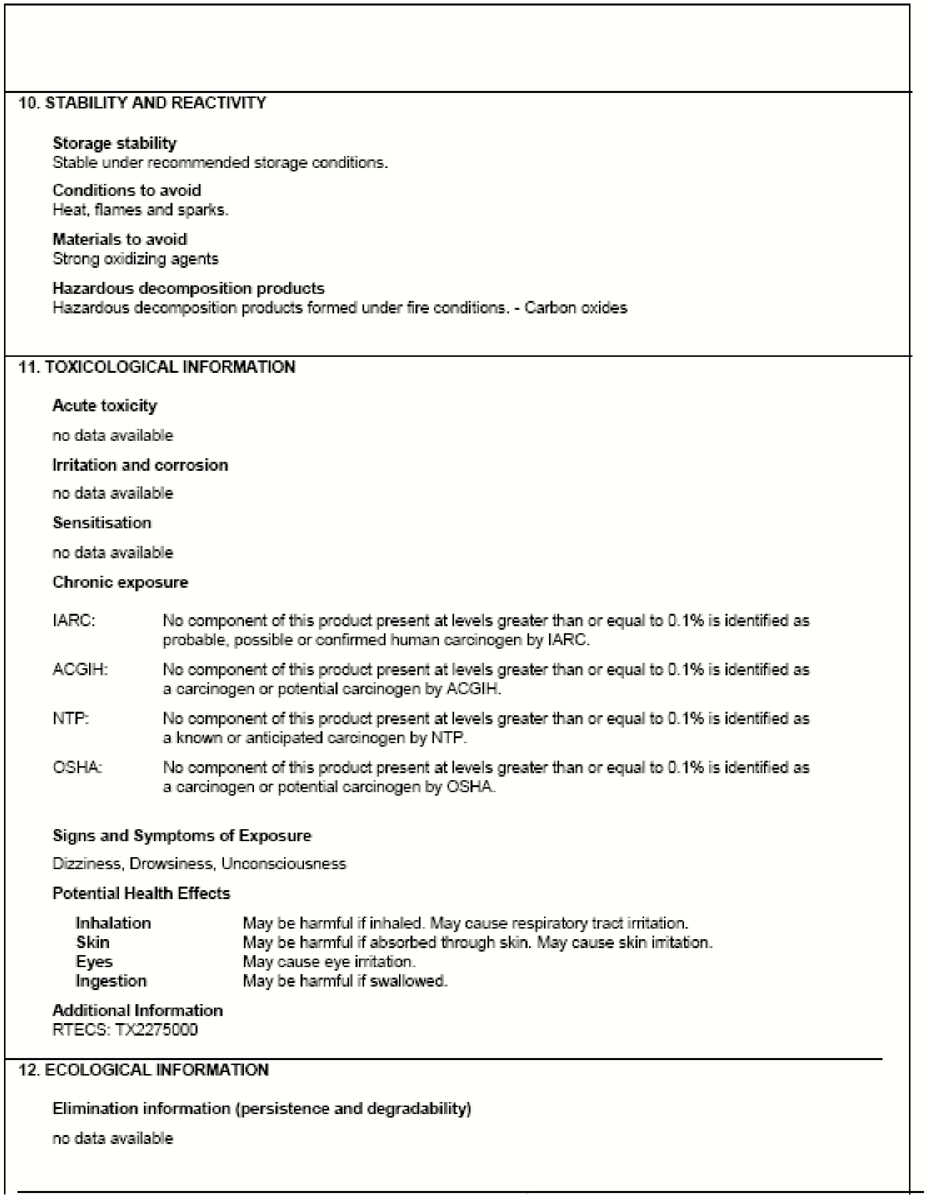
9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	Compressed gas

Safety data

pH	no data available
Melting point	-188 °C (-306 °F)
Boiling point	-42.1 °C (-43.8 °F)
Flash point	-104 °C (-155 °F) - closed cup
Ignition temperature	450 °C (842 °F)
Lower explosion limit	2.1 %(V)
Upper explosion limit	9.5 %(V)
Vapour pressure	13,096 hPa (9,823 mmHg) at 37.7 °C (99.9 °F) 8,531.6 hPa (6,399.2 mmHg) at 21.1 °C (70.0 °F)
Density	1.55 g/mL at 25 °C (77 °F)
Water solubility	no data available
Relative vapour density	1.52 - (Air = 1.0)



10. STABILITY AND REACTIVITY

Storage stability
Stable under recommended storage conditions.

Conditions to avoid
Heat, flames and sparks.

Materials to avoid
Strong oxidizing agents

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

11. TOXICOLOGICAL INFORMATION

Acute toxicity

no data available

Irritation and corrosion

no data available

Sensitisation

no data available

Chronic exposure

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.

Signs and Symptoms of Exposure

Dizziness, Drowsiness, Unconsciousness

Potential Health Effects

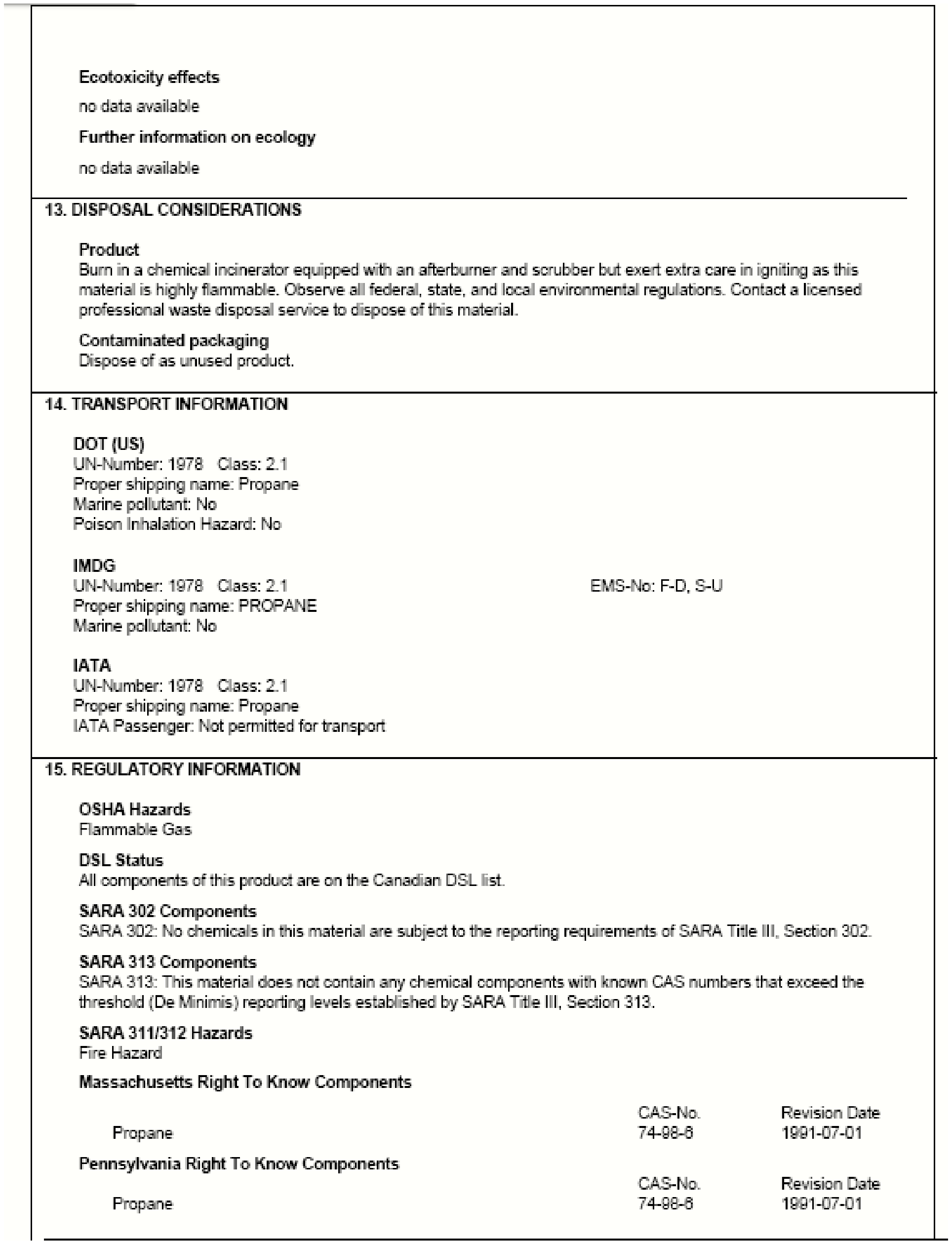
Inhalation	May be harmful if inhaled. May cause respiratory tract irritation.
Skin	May be harmful if absorbed through skin. May cause skin irritation.
Eyes	May cause eye irritation.
Ingestion	May be harmful if swallowed.

Additional Information
RTECS: TX2275000

12. ECOLOGICAL INFORMATION

Elimination information (persistence and degradability)

no data available



Ecotoxicity effects

no data available

Further information on ecology

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. Observe all federal, state, and local environmental regulations. 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: 1978 Class: 2.1
Proper shipping name: Propane
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN-Number: 1978 Class: 2.1 EMS-No: F-D, S-U
Proper shipping name: PROPANE
Marine pollutant: No

IATA
UN-Number: 1978 Class: 2.1
Proper shipping name: Propane
IATA Passenger: Not permitted for transport

15. REGULATORY INFORMATION

OSHA Hazards

Flammable Gas

DSL Status

All components of this product are on the Canadian DSL list.

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

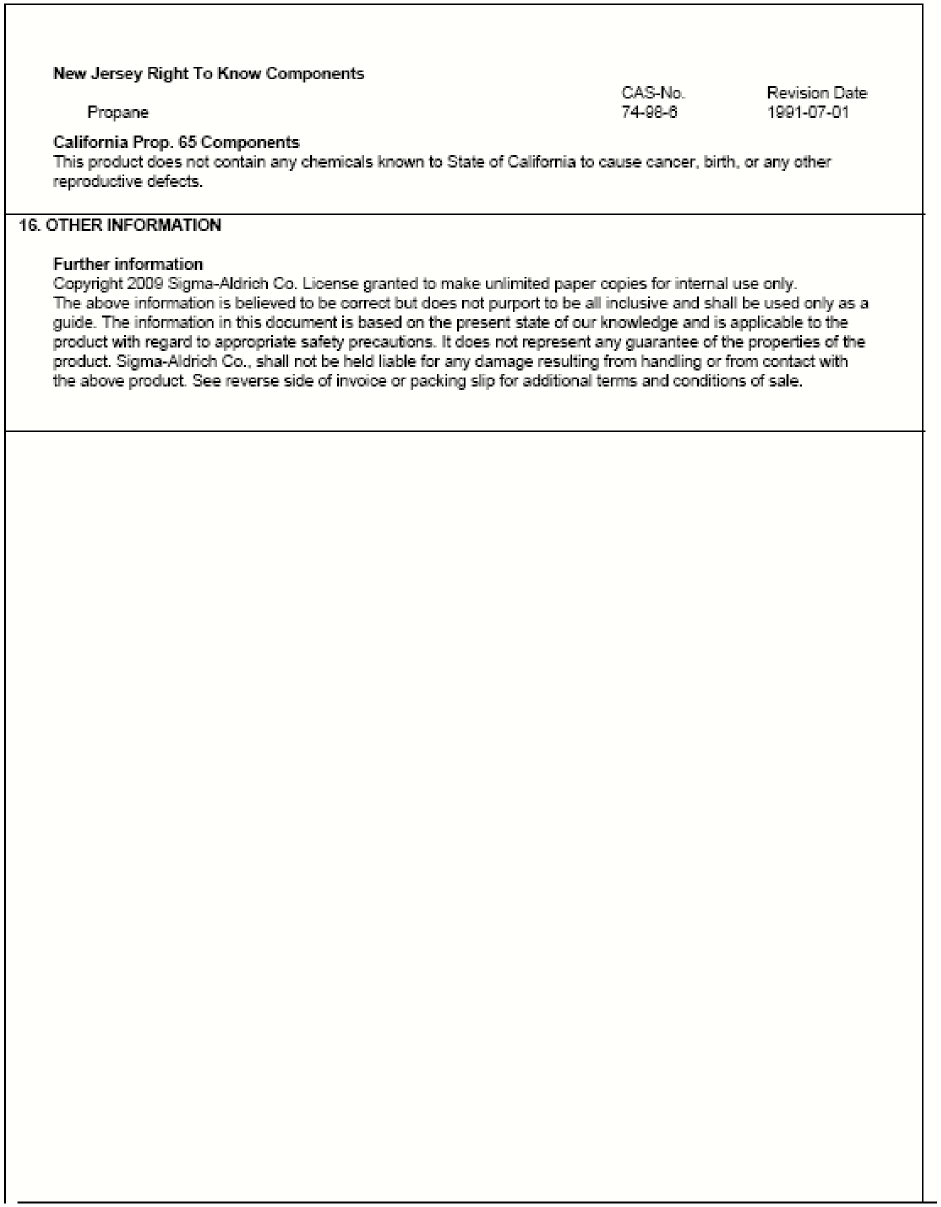
Fire Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Propane	74-98-6	1991-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Propane	74-98-6	1991-07-01



New Jersey Right To Know Components

	CAS-No.	Revision Date
Propane	74-98-6	1991-07-01

California Prop. 65 Components

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

16. OTHER INFORMATION

Further information

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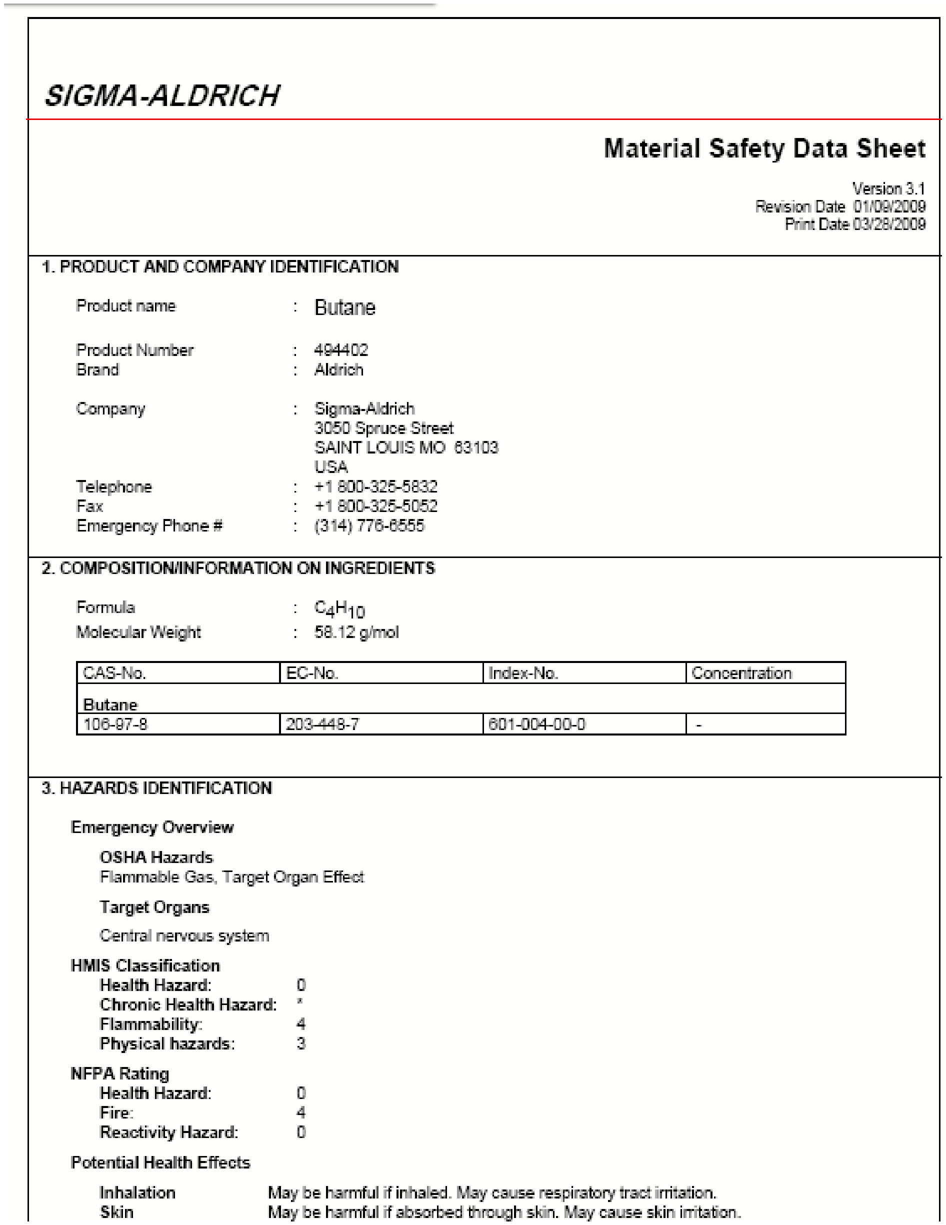
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent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



SIGMA-ALDRICH

Material Safety Data Sheet

Version 3.1
Revision Date 01/09/2009
Print Date 03/28/2009

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Butane

Product Number : 494402
Brand : Aldrich

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA
Telephone : +1 800-325-5832
Fax : +1 800-325-5052
Emergency Phone # : (314) 776-6555

2. COMPOSITION/INFORMATION ON INGREDIENTS

Formula : C_4H_{10}
Molecular Weight : 58.12 g/mol

CAS-No.	EC-No.	Index-No.	Concentration
Butane			
106-97-8	203-448-7	601-004-00-0	-

3. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Flammable Gas, Target Organ Effect

Target Organs

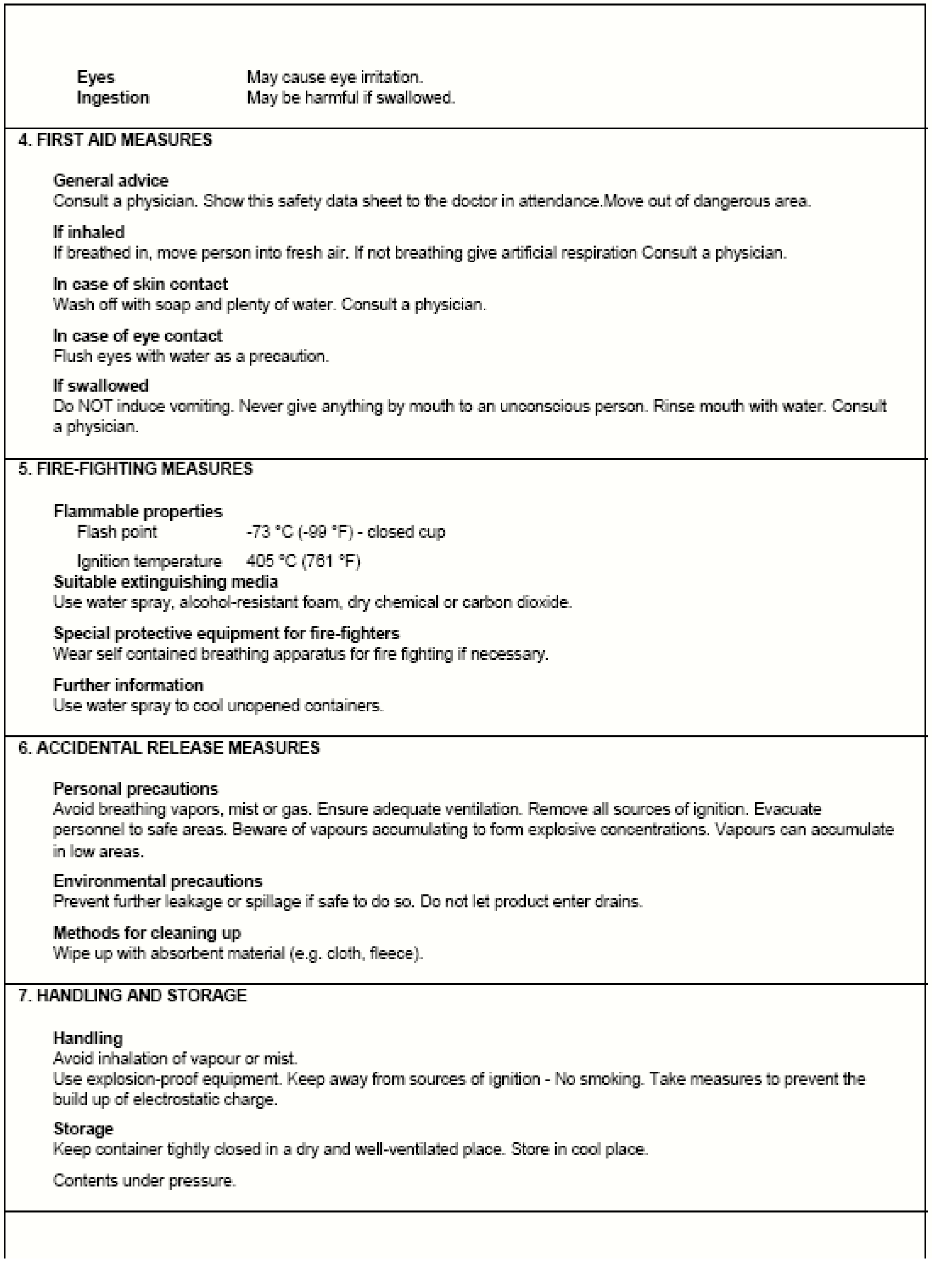
Central nervous system

HMIS Classification
Health Hazard: 0
Chronic Health Hazard: *
Flammability: 4
Physical hazards: 3

NFPA Rating
Health Hazard: 0
Fire: 4
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.

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
Flush eyes with water as a precaution.

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

5. FIRE-FIGHTING MEASURES

Flammable properties
Flash point -73 °C (-99 °F) - closed cup

Ignition temperature 405 °C (761 °F)

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

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

Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
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.

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

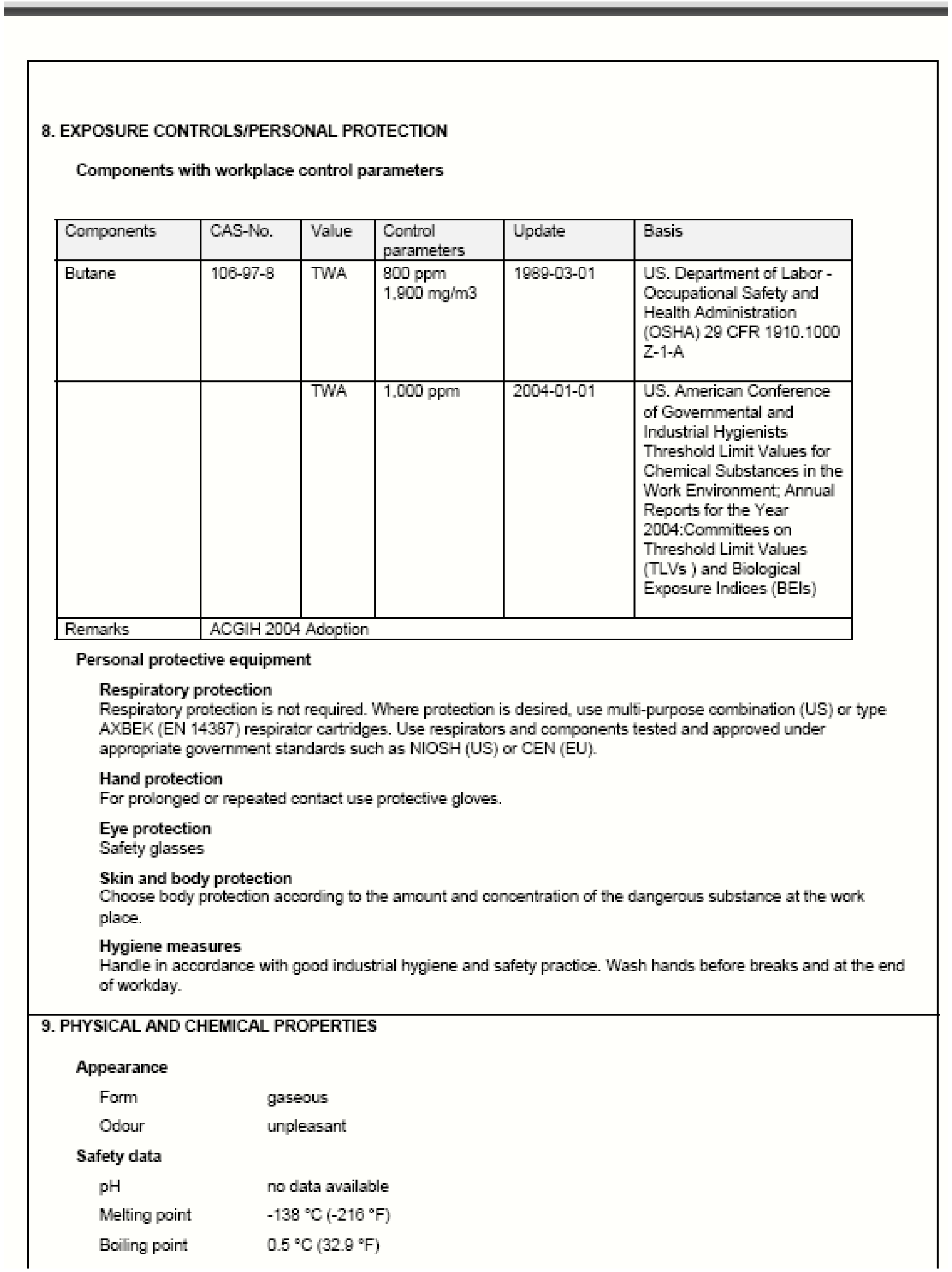
Methods for cleaning up
Wipe up with absorbent material (e.g. cloth, fleece).

7. HANDLING AND STORAGE

Handling
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.

Storage
Keep container tightly closed in a dry and well-ventilated place. Store in cool place.

Contents under pressure.



8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Update	Basis
Butane	106-97-8	TWA	800 ppm 1,900 mg/m3	1989-03-01	US. Department of Labor - Occupational Safety and Health Administration (OSHA) 29 CFR 1910.1000 Z-1-A
		TWA	1,000 ppm	2004-01-01	US. American Conference of Governmental and Industrial Hygienists Threshold Limit Values for Chemical Substances in the Work Environment; Annual Reports for the Year 2004:Committees on Threshold Limit Values (TLVs) and Biological Exposure Indices (BEIs)
Remarks	ACGIH 2004 Adoption				

Personal protective equipment

Respiratory protection
Respiratory protection is not required. Where protection is desired, use multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Hand protection
For prolonged or repeated contact use protective gloves.

Eye protection
Safety glasses

Skin and body protection
Choose body protection according to the amount and concentration of the dangerous substance at the work place.

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

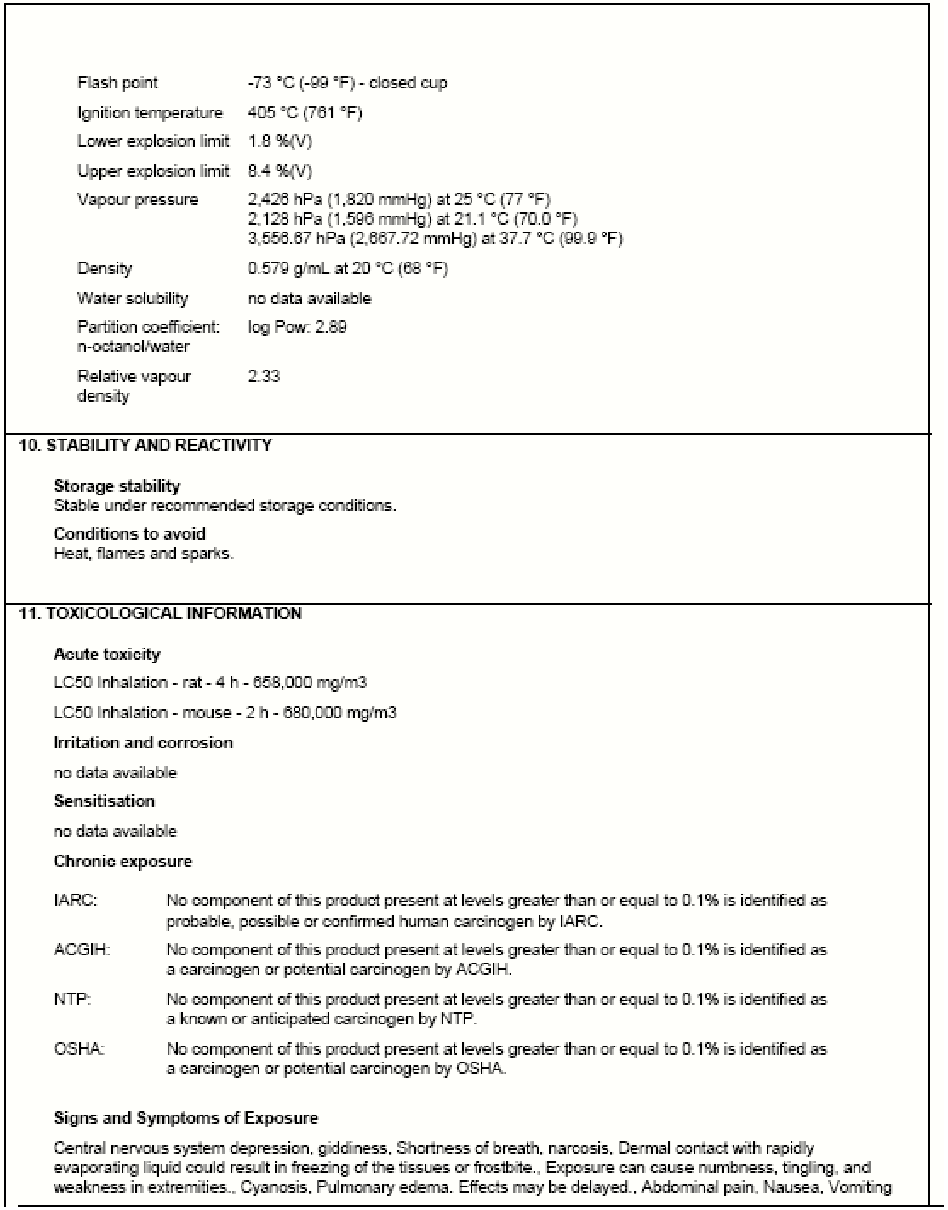
9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	gaseous
Odour	unpleasant

Safety data

pH	no data available
Melting point	-138 °C (-216 °F)
Boiling point	0.5 °C (32.9 °F)



Flash point	-73 °C (-99 °F) - closed cup
Ignition temperature	405 °C (761 °F)
Lower explosion limit	1.8 %(V)
Upper explosion limit	8.4 %(V)
Vapour pressure	2,426 hPa (1,820 mmHg) at 25 °C (77 °F) 2,128 hPa (1,596 mmHg) at 21.1 °C (70.0 °F) 3,556.67 hPa (2,667.72 mmHg) at 37.7 °C (99.9 °F)
Density	0.579 g/mL at 20 °C (68 °F)
Water solubility	no data available
Partition coefficient: n-octanol/water	log Pow: 2.89
Relative vapour density	2.33

10. STABILITY AND REACTIVITY

Storage stability
Stable under recommended storage conditions.

Conditions to avoid
Heat, flames and sparks.

11. TOXICOLOGICAL INFORMATION

Acute toxicity

LC50 Inhalation - rat - 4 h - 658,000 mg/m3

LC50 Inhalation - mouse - 2 h - 680,000 mg/m3

Irritation and corrosion

no data available

Sensitisation

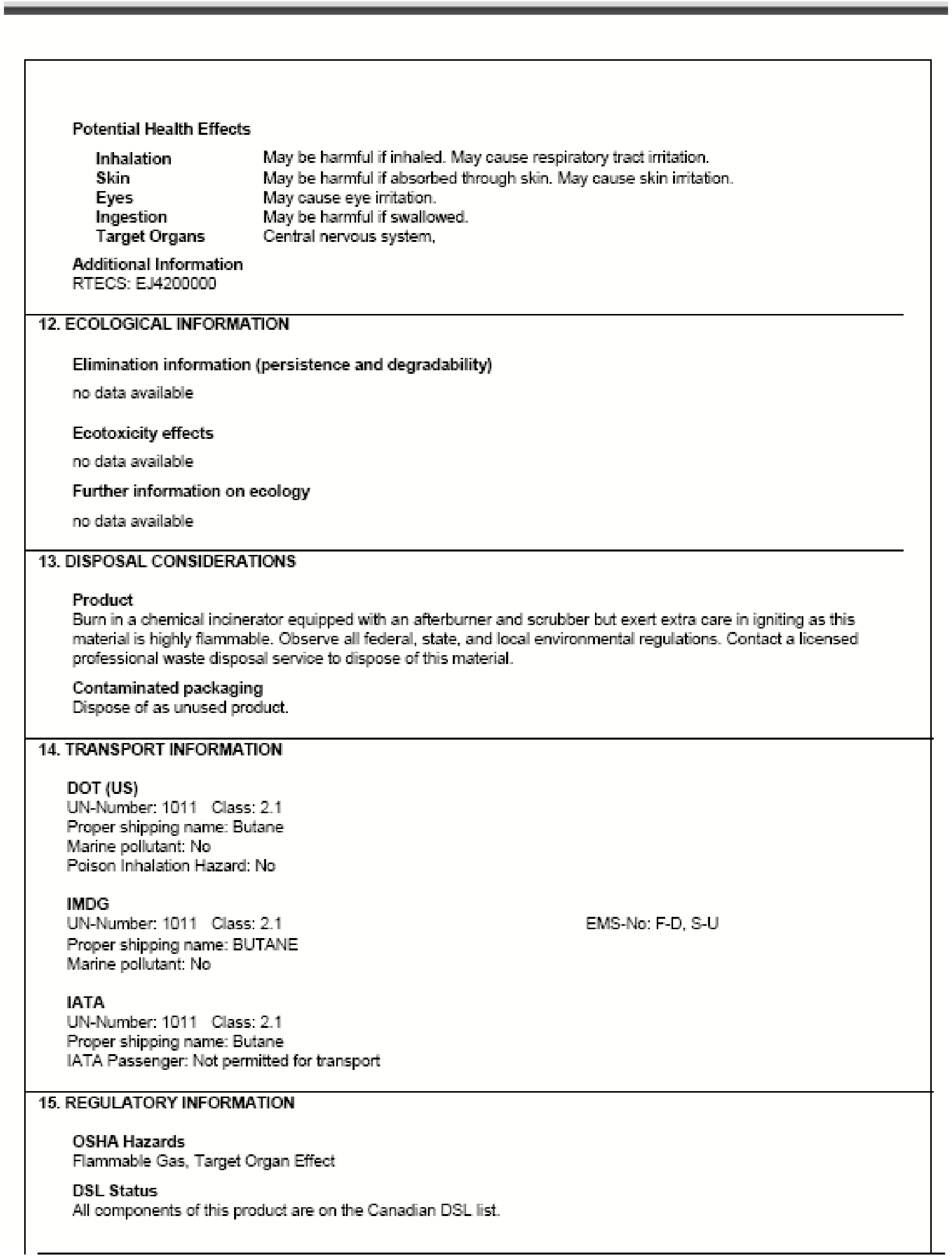
no data available

Chronic exposure

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.

Signs and Symptoms of Exposure

Central nervous system depression, giddiness, Shortness of breath, narcosis, Dermal contact with rapidly evaporating liquid could result in freezing of the tissues or frostbite., Exposure can cause numbness, tingling, and weakness in extremities., Cyanosis, Pulmonary edema. Effects may be delayed., Abdominal pain, Nausea, Vomiting



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.
Target Organs	Central nervous system,

Additional Information
RTECS: EJ4200000

12. ECOLOGICAL INFORMATION

Elimination information (persistence and degradability)

no data available

Ecotoxicity effects

no data available

Further information on ecology

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. Observe all federal, state, and local environmental regulations. 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: 1011 Class: 2.1
Proper shipping name: Butane
Marine pollutant: No
Poison Inhalation Hazard: No

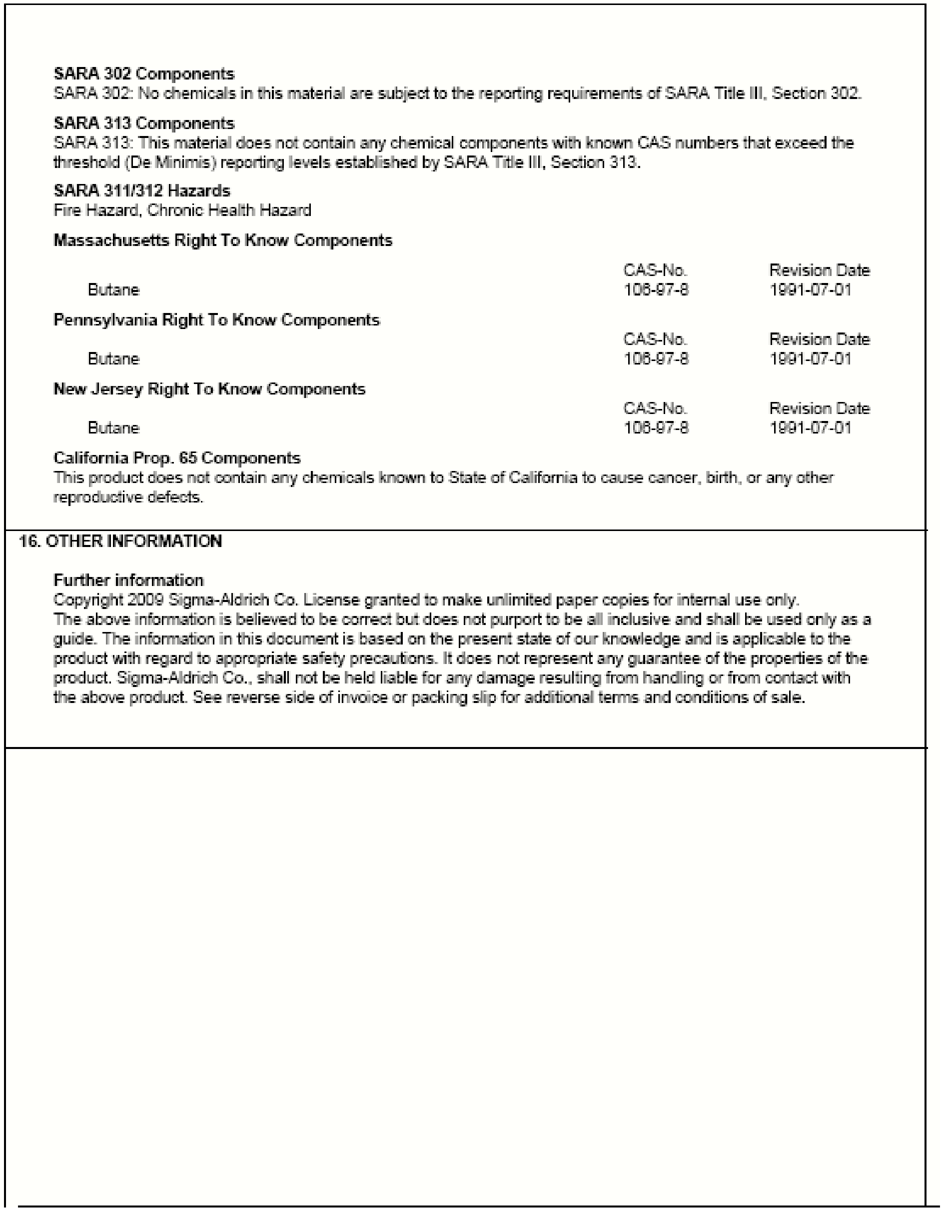
IMDG
UN-Number: 1011 Class: 2.1 EMS-No: F-D, S-U
Proper shipping name: BUTANE
Marine pollutant: No

IATA
UN-Number: 1011 Class: 2.1
Proper shipping name: Butane
IATA Passenger: Not permitted for transport

15. REGULATORY INFORMATION

OSHA Hazards
Flammable Gas, Target Organ Effect

DSL Status
All components of this product are on the Canadian DSL list.



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, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Butane	106-97-8	1991-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Butane	106-97-8	1991-07-01

New Jersey Right To Know Components

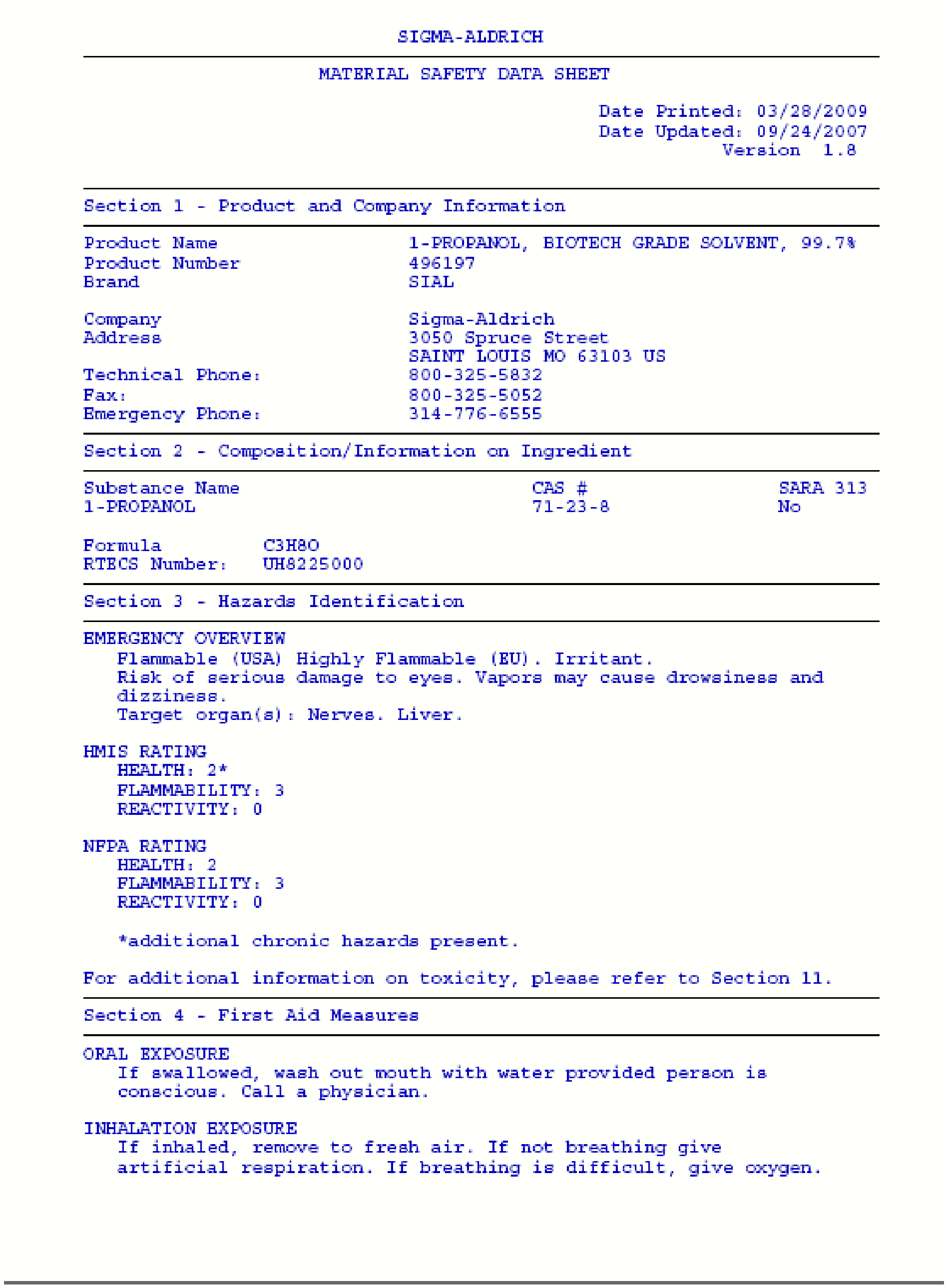
	CAS-No.	Revision Date
Butane	106-97-8	1991-07-01

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

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 Co., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.



SIGMA-ALDRICH

MATERIAL SAFETY DATA SHEET

Date Printed: 03/28/2009
Date Updated: 09/24/2007
Version 1.8

Section 1 - Product and Company Information

Product Name	1-PROPANOL, BIOTECH GRADE SOLVENT, 99.7%
Product Number	496197
Brand	SIAL
Company	Sigma-Aldrich
Address	3050 Spruce Street SAINT LOUIS MO 63103 US
Technical Phone:	800-325-5832
Fax:	800-325-5052
Emergency Phone:	314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
1-PROPANOL	71-23-8	No

Formula C3H8O
RTECS Number: UH8225000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Flammable (USA) Highly Flammable (EU). Irritant.
Risk of serious damage to eyes. Vapors may cause drowsiness and dizziness.
Target organ(s): Nerves. Liver.

HMIS RATING
HEALTH: 2*
FLAMMABILITY: 3
REACTIVITY: 0

NFPA RATING
HEALTH: 2
FLAMMABILITY: 3
REACTIVITY: 0

*additional chronic hazards present.

For additional information on toxicity, please refer to Section 11.

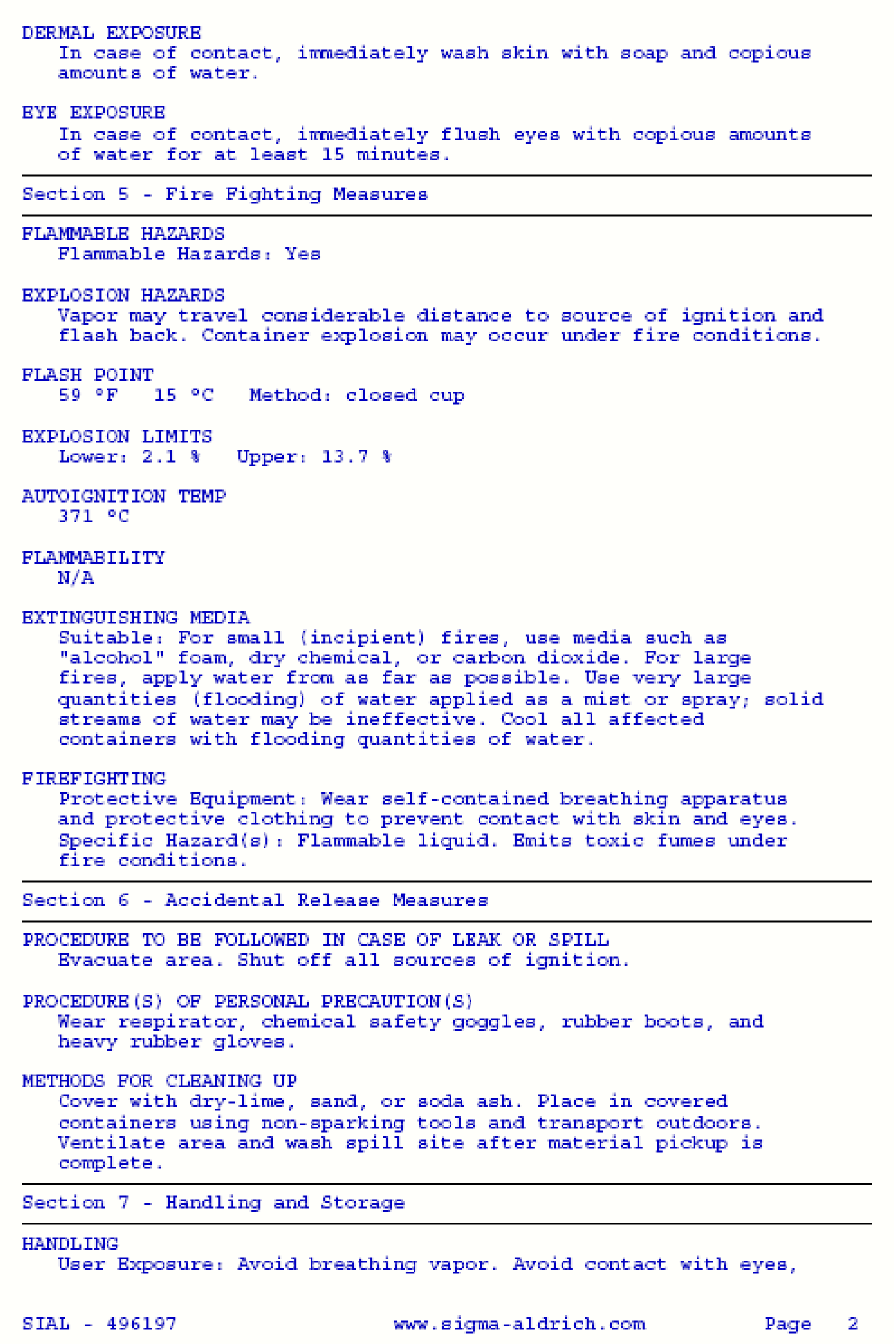
Section 4 - First Aid Measures

ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.



DERMAL EXPOSURE

In case of contact, immediately wash skin with soap and copious amounts of water.

EYE EXPOSURE

In case of contact, immediately flush eyes with copious amounts of water for at least 15 minutes.

Section 5 - Fire Fighting Measures

FLAMMABLE HAZARDS

Flammable Hazards: Yes

EXPLOSION HAZARDS

Vapor may travel considerable distance to source of ignition and flash back. Container explosion may occur under fire conditions.

FLASH POINT

59 °F 15 °C Method: closed cup

EXPLOSION LIMITS

Lower: 2.1 % Upper: 13.7 %

AUTOIGNITION TEMP

371 °C

FLAMMABILITY

N/A

EXTINGUISHING MEDIA

Suitable: 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.

FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Flammable liquid. Emits toxic fumes under fire conditions.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL

Evacuate area. Shut off all sources of ignition.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear respirator, chemical safety goggles, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP

Cover with dry-lime, sand, or soda ash. Place in covered containers using non-sparking tools and transport outdoors. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING

User Exposure: Avoid breathing vapor. Avoid contact with eyes,

SIAL - 496197 www.sigma-aldrich.com Page 2 skin, and clothing. Avoid prolonged or repeated exposure.

STORAGE
Suitable: Keep container closed. Keep away from heat, sparks, and open flame.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS
Safety shower and eye bath. Use nonsparking tools. Mechanical exhaust required.

PERSONAL PROTECTIVE EQUIPMENT
Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). 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.
Hand: Compatible chemical-resistant gloves.
Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES
Wash thoroughly after handling. Wash contaminated clothing before reuse.

EXPOSURE LIMITS

Country	Source	Type	Value
Poland		NDS	200 MG/M3
Poland		NDSCh	600 MG/M3
Poland		NDSP	-
USA	OSHA.	STEL	250 ppm
USA	OSHA.	TWA	200 ppm

Section 9 - Physical/Chemical Properties

Appearance   Physical State: Clear liquid
              Color: Colorless

Property	Value	At Temperature or Pressure
Molecular Weight	60.1 AMU	
pH	8.5	20 °C Concentration: 200 g/l
BP/BP Range	97 °C	760 mmHg
MP/MP Range	- 127.0 °C	
Freezing Point	N/A	
Vapor Pressure	14.9 mmHg	20 °C
Vapor Density	2.1 g/l	
Saturated Vapor Conc.	N/A	
SG/Density	0.8 g/cm3	
Bulk Density	N/A	
Odor Threshold	2.6 ppm	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	1	
Viscosity	2 Pas	
Surface Tension	N/A	
Partition Coefficient	Log Kow: 0.250 - 0.3	
	40	
Decomposition Temp.	N/A	
Flash Point	59 °F 15 °C	Method: closed cup
Explosion Limits	Lower: 2.1 % Upper: 13.7 %	
Flammability	N/A	
Autoignition Temp	371 °C	
Refractive Index	1.384	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	Solubility in Water:Complete	

N/A = not available

Section 10 - Stability and Reactivity

STABILITY
Stable: Stable.
Materials to Avoid: Strong oxidizing agents.

HAZARDOUS DECOMPOSITION PRODUCTS
Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

HAZARDOUS POLYMERIZATION
Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE
Skin Contact: May cause skin irritation.
Skin Absorption: May be harmful if absorbed through the skin.
Eye Contact: Causes severe eye irritation.
Inhalation: May be harmful if inhaled. Material may be irritating to mucous membranes and upper respiratory tract.
Ingestion: May be harmful if swallowed.

SENSITIZATION
Sensitization: Will not occur

TARGET ORGAN(S) OR SYSTEM(S)
Nerves. Liver.

SIGNS AND SYMPTOMS OF EXPOSURE
Can cause CNS depression. Prolonged exposure can cause: Narcotic effect. Drying, cracking, or irritation of the skin.

TOXICITY DATA
Oral
Rat
1,870 mg/kg
LD50
Oral
Mouse
4,500 mg/kg
LD50
Oral
Rat
8,038 mg/kg
LD50
1 HR.
Inhalation
Rat

20,000 ppm
LC50
Skin
Rabbit
4,000 mg/kg
LC50

IRRITATION DATA

Skin
Rabbit
Remarks: Mild irritation effect
Eyes
Rabbit
Remarks: Moderate irritation effect
Eyes
Rabbit
Remarks: Severe irritation effect

Skin
Rabbit
500 mg
Remarks: Open irritation test

Eyes
Rabbit
20 mg
24H
Remarks: Moderate irritation effect

CHRONIC EXPOSURE - CARCINOGEN

Species: Rat
Route of Application: Oral
Dose: 4
Exposure Time: 4 DAYS
Frequency: 1/ day
Species: Mouse
Route of Application: Inhalation
Exposure Time: 95 HR
Frequency: 7874 ppm

Species: Rat
Route of Application: Oral
Dose: 50 GM/KG
Exposure Time: 81W
Frequency: I
Result: Blood:Leukemia Liver:Tumors. Tumorigenic:Carcinogenic by RTECS criteria.

Species: Rat
Route of Application: Subcutaneous
Dose: 6 GM/KG
Exposure Time: 95W
Frequency: I
Result: Blood:Leukemia Liver:Tumors. Tumorigenic:Carcinogenic by RTECS criteria.

CHRONIC EXPOSURE - TERATOGEN

Species: Rat
Dose: 7000 PPM/7H
Route of Application: Inhalation
Exposure Time: (1-19D PREG)
Result: Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

CHRONIC EXPOSURE - REPRODUCTIVE HAZARD

Species: Rat
Dose: 7000 PPM/7H
Route of Application: Inhalation
Exposure Time: (6W MALE)
Result: Effects on Fertility: Male fertility index (e.g., # males impregnating females per # males exposed to fertile nonpregnant females).

Species: Rat
Dose: 10000 PPM/7H
Route of Application: Inhalation
Exposure Time: (1-19D PREG)
Result: Specific Developmental Abnormalities: Musculoskeletal system. Effects on Embryo or Fetus: Fetal death. Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

Section 12 - Ecological Information

No data available.

PHYSICAL PROPERTIES AFFECTING ECOTOXICITY

COD: 1.4 %
BOD: < 2 %
BOD after 5 Days: 1.43 - 1.6 %

ACUTE ECOTOXICITY TESTS

Test Type: LC50 Fish
Species: Pimephales promelas (Fathead minnow)
Time: 96 h
Value: 1,000 mg/l

Test Type: EC50 Daphnia
Species: Daphnia magna
Time: 48 h
Value: 3,642 mg/l

Test Type: LC50 Fish
Species: Carassius auratus (Goldfish)
Time: 24 h
Value: 5,000 mg/l

Test Type: LC50 Fish
Species: other fish
Time: 48 h
Value: 4,320.0 - 4,560.0 mg/l

Test Type: LC50 Fish
Species: Leuciscus idus
Time: 48 h
Value: > 4,000 mg/l

ELIMINATION

Elimination: > 60 %

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT

Proper Shipping Name: n-Propanol [or] Propyl alcohol, normal
UN#: 1274
Class: 3
Packing Group: Packing Group II
Hazard Label: Flammable liquid
PIH: Not PIH

IATA

Proper Shipping Name: n-Propanol
IATA UN Number: 1274
Hazard Class: 3
Packing Group: II

Section 15 - Regulatory Information

EU DIRECTIVES CLASSIFICATION

Symbol of Danger: F-Xi
Indication of Danger: Highly Flammable. Irritant.
R: 11-41-67
Risk Statements: Highly flammable. Risk of serious damage to eyes. Vapors may cause drowsiness and dizziness.
S: 7-16-24-26-39
Safety Statements: Keep container tightly closed. Keep away from sources of ignition - no smoking. Avoid contact with skin. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear eye/face protection.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Flammable (USA) Highly Flammable (EU). Irritant.
Risk Statements: Risk of serious damage to eyes. Vapors may cause drowsiness and dizziness.
Safety Statements: Keep container tightly closed. Keep away from sources of ignition - no smoking. Avoid contact with skin. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear eye/face protection.
US Statements: Target organ(s): Nerves. Liver.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: No

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: No

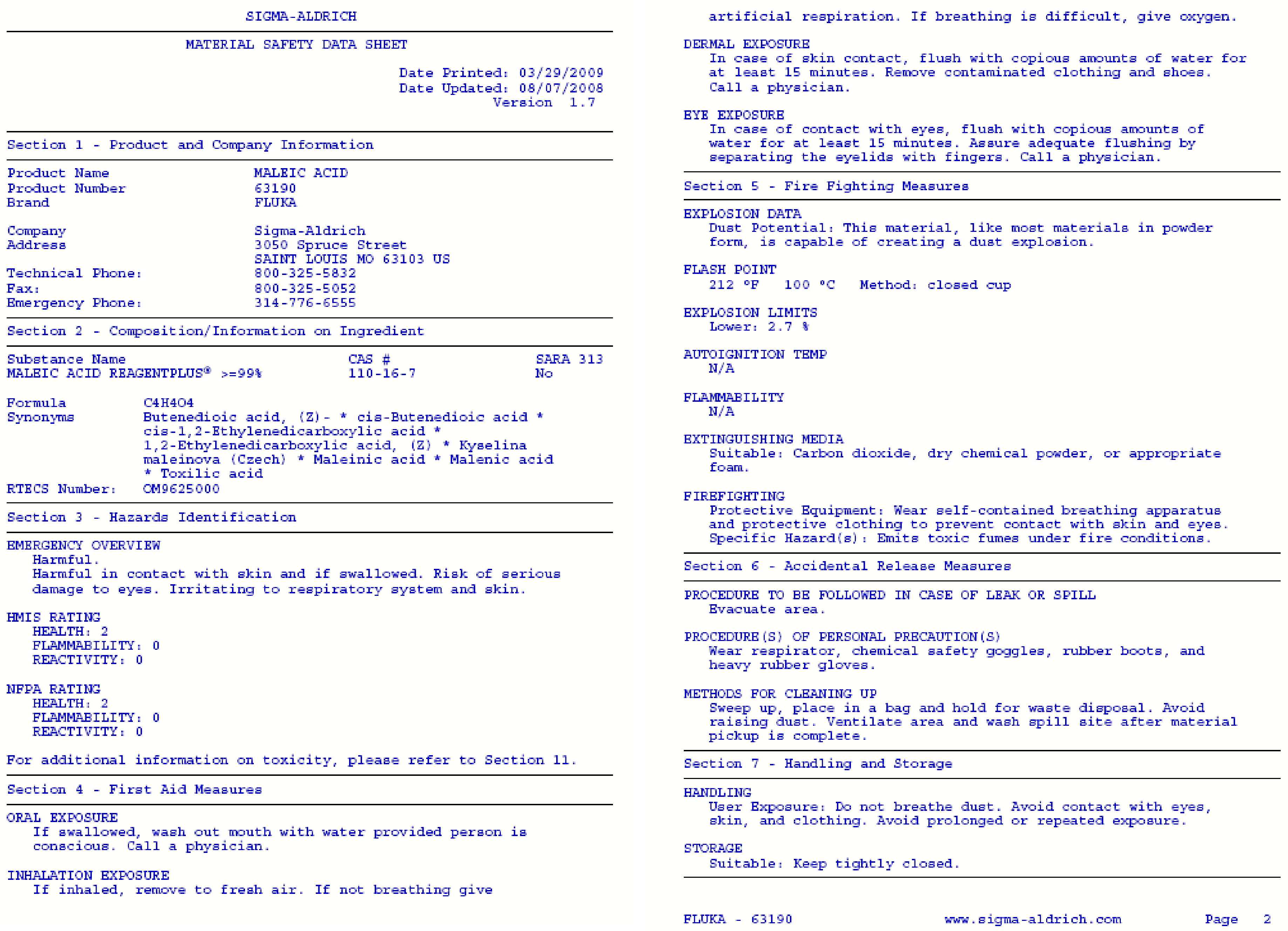
Section 16 - Other Information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

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 Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.



SIGMA-ALDRICH

MATERIAL SAFETY DATA SHEET

Date Printed: 03/29/2009
Date Updated: 08/07/2008
Version 1.7

Section 1 - Product and Company Information

Product Name	MALEIC ACID
Product Number	63190
Brand	FLUKA
Company	Sigma-Aldrich
Address	3050 Spruce Street SAINT LOUIS MO 63103 US
Technical Phone:	800-325-5832
Fax:	800-325-5052
Emergency Phone:	314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
MALEIC ACID REAGENTPLUS® >=99%	110-16-7	No

Formula	$C_4H_4O_4$
Synonyms	Butenedioic acid, (Z)- * cis-Butenedioic acid * cis-1,2-Ethylenedicarboxylic acid * 1,2-Ethylenedicarboxylic acid, (Z) * Kyselina maleinova (Czech) * Maleinic acid * Malenic acid * Toxilic acid
RTECS Number:	OM9625000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW
Harmful.
Harmful in contact with skin and if swallowed. Risk of serious damage to eyes. Irritating to respiratory system and skin.

HMIS RATING
HEALTH: 2
FLAMMABILITY: 0
REACTIVITY: 0

NFPA RATING
HEALTH: 2
FLAMMABILITY: 0
REACTIVITY: 0

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE
If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE
If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE
In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

EYE EXPOSURE
In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

Section 5 - Fire Fighting Measures

EXPLOSION DATA
Dust Potential: This material, like most materials in powder form, is capable of creating a dust explosion.

FLASH POINT
212 °F 100 °C Method: closed cup

EXPLOSION LIMITS
Lower: 2.7 %

AUTOIGNITION TEMP
N/A

FLAMMABILITY
N/A

EXTINGUISHING MEDIA
Suitable: Carbon dioxide, dry chemical powder, or appropriate foam.

FIREFIGHTING
Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Emits toxic fumes under fire conditions.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL
Evacuate area.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)
Wear respirator, chemical safety goggles, rubber boots, and heavy rubber gloves.

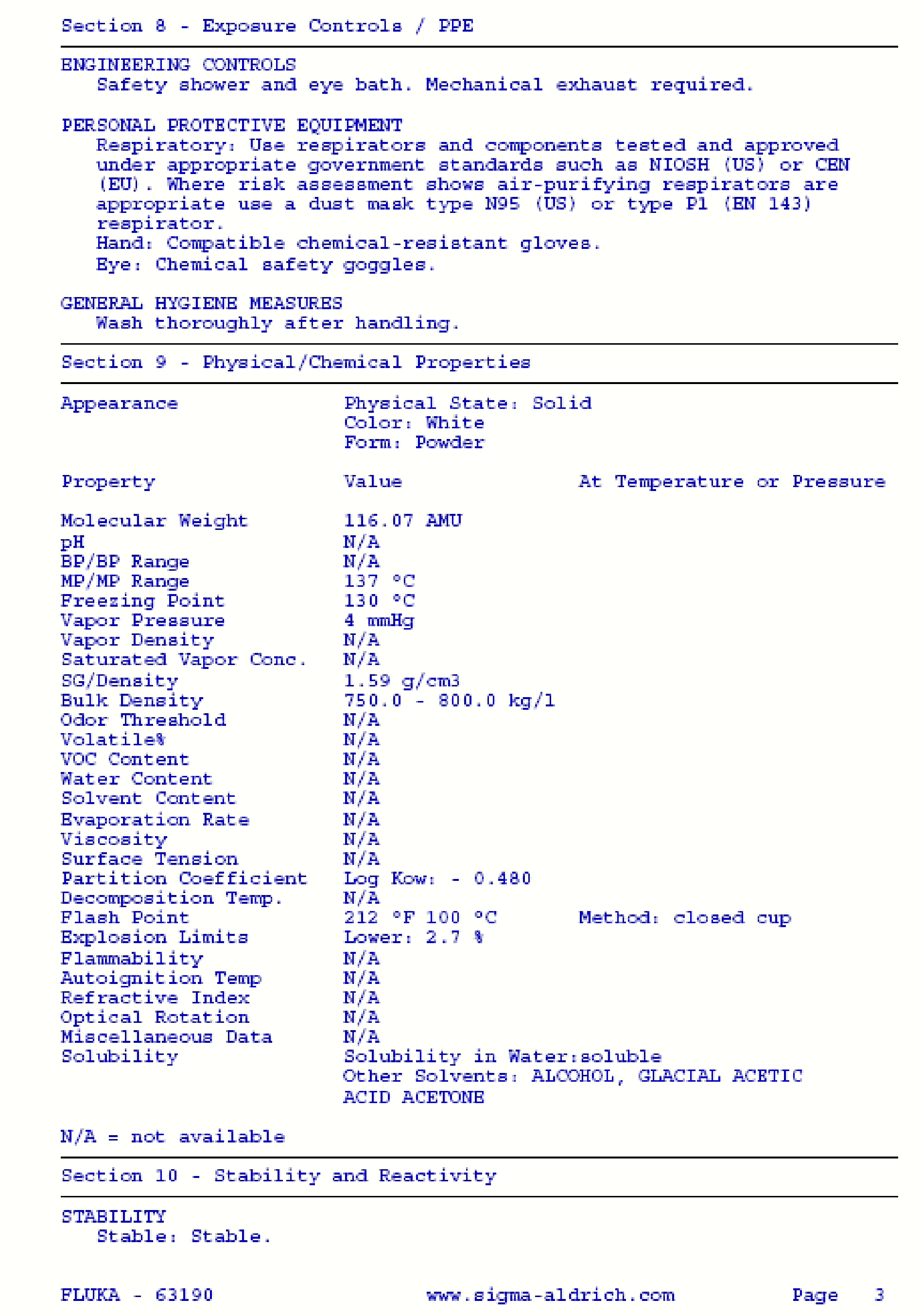
METHODS FOR CLEANING UP
Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING
User Exposure: Do not breathe dust. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

STORAGE
Suitable: Keep tightly closed.

FLUKA - 63190 www.sigma-aldrich.com Page 2



Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS
Safety shower and eye bath. Mechanical exhaust required.

PERSONAL PROTECTIVE EQUIPMENT
Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a dust mask type N95 (US) or type P1 (EN 143) respirator.
Hand: Compatible chemical-resistant gloves.
Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES
Wash thoroughly after handling.

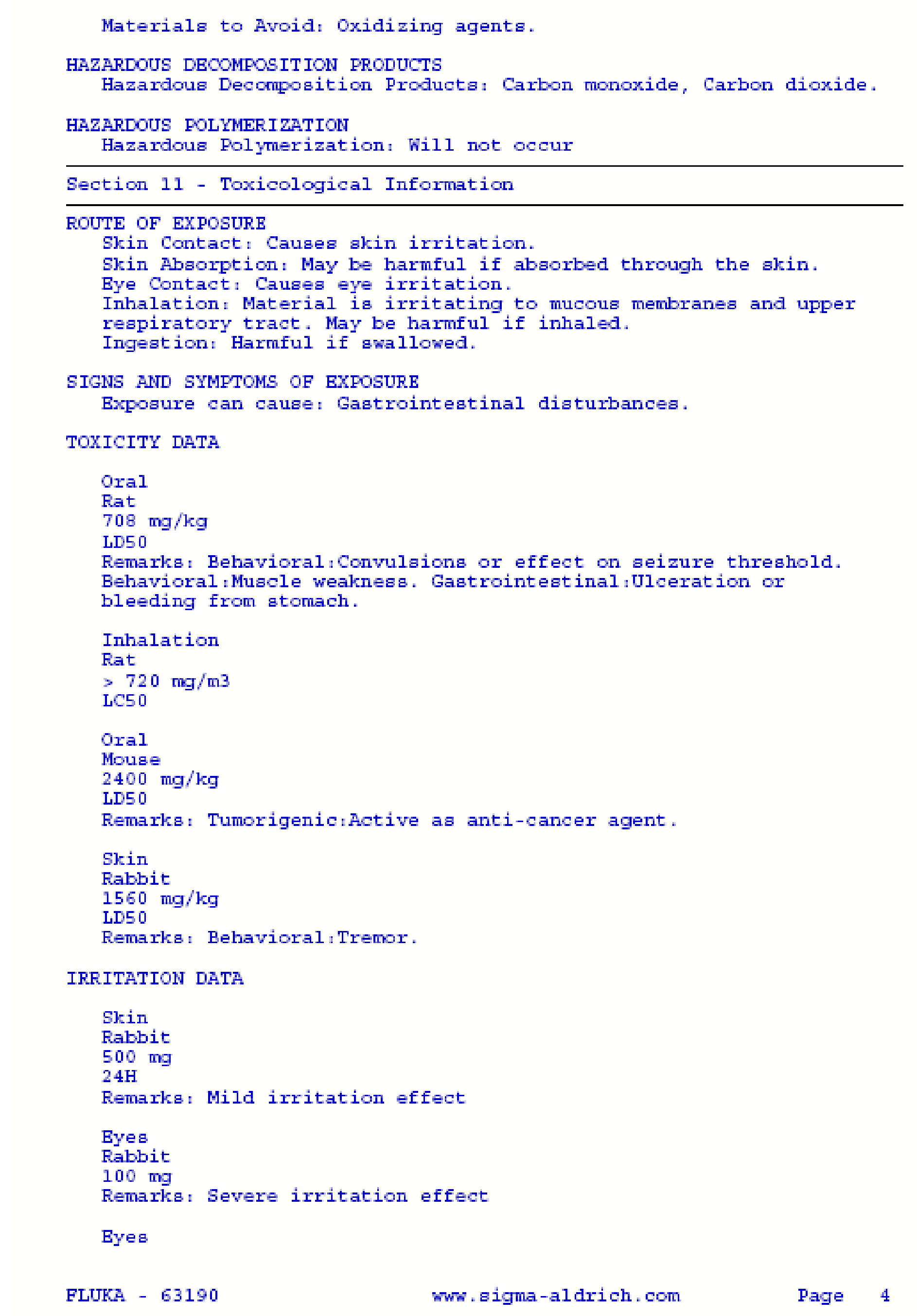
Section 9 - Physical/Chemical Properties

Appearance	Physical State: Solid Color: White Form: Powder	
Property	**Value**	**At Temperature or Pressure**
Molecular Weight	116.07 AMU	
pH	N/A	
BP/BP Range	N/A	
MP/MP Range	137 °C	
Freezing Point	130 °C	
Vapor Pressure	4 mmHg	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
SG/Density	1.59 g/cm3	
Bulk Density	750.0 - 800.0 kg/l	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	Log Kow: - 0.480	
Decomposition Temp.	N/A	
Flash Point	212 °F 100 °C	Method: closed cup
Explosion Limits	Lower: 2.7 %	
Flammability	N/A	
Autoignition Temp	N/A	
Refractive Index	N/A	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	Solubility in Water:soluble Other Solvents: ALCOHOL, GLACIAL ACETIC ACID ACETONE	

N/A = not available

Section 10 - Stability and Reactivity

STABILITY
Stable: Stable.



Materials to Avoid: Oxidizing agents.

HAZARDOUS DECOMPOSITION PRODUCTS
Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

HAZARDOUS POLYMERIZATION
Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE
Skin Contact: Causes skin irritation.
Skin Absorption: May be harmful if absorbed through the skin.
Eye Contact: Causes eye irritation.
Inhalation: Material is irritating to mucous membranes and upper respiratory tract. May be harmful if inhaled.
Ingestion: Harmful if swallowed.

SIGNS AND SYMPTOMS OF EXPOSURE
Exposure can cause: Gastrointestinal disturbances.

TOXICITY DATA

Oral
Rat
708 mg/kg
LD50
Remarks: Behavioral:Convulsions or effect on seizure threshold. Behavioral:Muscle weakness. Gastrointestinal:Ulceration or bleeding from stomach.

Inhalation
Rat
> 720 mg/m3
LC50

Oral
Mouse
2400 mg/kg
LD50
Remarks: Tumorigenic:Active as anti-cancer agent.

Skin
Rabbit
1560 mg/kg
LD50
Remarks: Behavioral:Tremor.

IRRITATION DATA

Skin
Rabbit
500 mg
24H
Remarks: Mild irritation effect

Eyes
Rabbit
100 mg
Remarks: Severe irritation effect

Eyes

Rabbit
1 %
2M
Remarks: Severe irritation effect

CHRONIC EXPOSURE - MUTAGEN

Species: Human
Dose: 20 MMOL/L
Cell Type: fibroblast
Mutation test: DNA inhibition

Section 12 - Ecological Information

ACUTE ECOTOXICITY TESTS

Test Type: EC50 Daphnia
Species: Daphnia magna
Time: 48 h
Value: 160.0 - 400.0 mg/l

Test Type: EC100 Daphnia
Species: Daphnia magna
Time: 24 h
Value: 200 mg/l

Test Type: LC50 Fish
Species: Pimephales promelas (Fathead minnow)
Time: 96 h
Value: 5 mg/l

Test Type: LC50 Fish
Species: Leuciscus idus
Value: 106 mg/l

Test Type: LC0 Fish
Species: Lepomis macrochirus (Bluegill)
Time: 96 h
Value: > 300 mg/l

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT

Proper Shipping Name: None
Non-Hazardous for Transport: This substance is considered to be non-hazardous for transport.

IATA

Non-Hazardous for Air Transport: Non-hazardous for air transport.

Section 15 - Regulatory Information

EU DIRECTIVES CLASSIFICATION

Symbol of Danger: Xn
Indication of Danger: Harmful.
R: 22-36/37/38
Risk Statements: Harmful if swallowed. Irritating to eyes, respiratory system and skin.
S: 26-28-37
Safety Statements: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. After contact with skin, wash immediately with plenty of soap-suds. Wear suitable gloves.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Harmful.
Risk Statements: Harmful in contact with skin and if swallowed. Risk of serious damage to eyes. Irritating to respiratory system and skin.
Safety Statements: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Take off immediately all contaminated clothing. Wear suitable protective clothing, gloves, and eye/face protection. Keep container tightly closed in a cool place.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: No
TSCA INVENTORY ITEM: Yes

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: No

Section 16 - Other Information

DISCLAIMER

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WARRANTY

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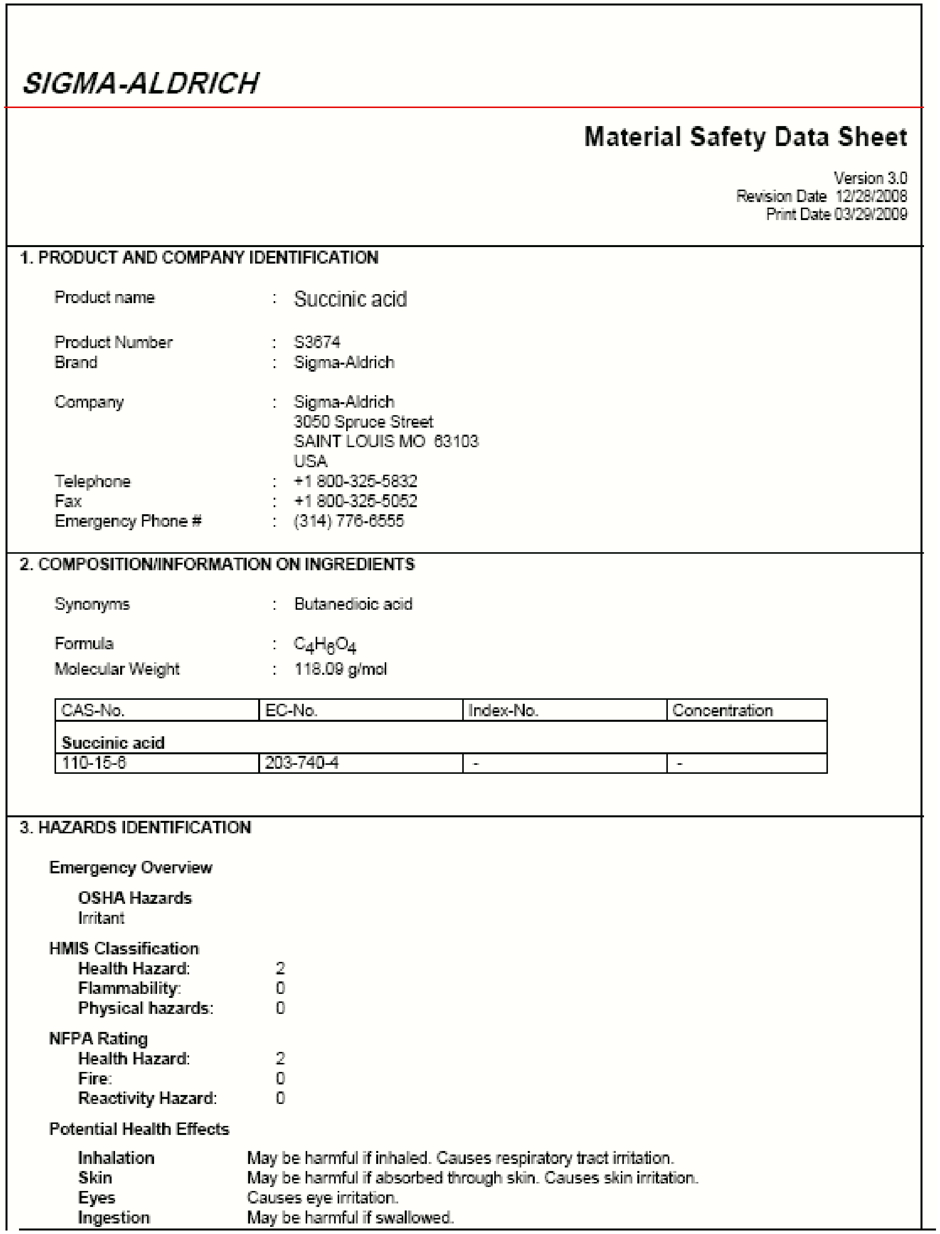


SIGMA-ALDRICH

Material Safety Data Sheet

Version 3.0
Revision Date 12/28/2008
Print Date 03/29/2009

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Succinic acid

Product Number : S3674
Brand : Sigma-Aldrich

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA
Telephone : +1 800-325-5832
Fax : +1 800-325-5052
Emergency Phone # : (314) 776-6555

2. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : Butanedioic acid

Formula : $C_4H_6O_4$
Molecular Weight : 118.09 g/mol

CAS-No.	EC-No.	Index-No.	Concentration
Succinic acid			
110-15-6	203-740-4	-	-

3. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Irritant

HMIS Classification

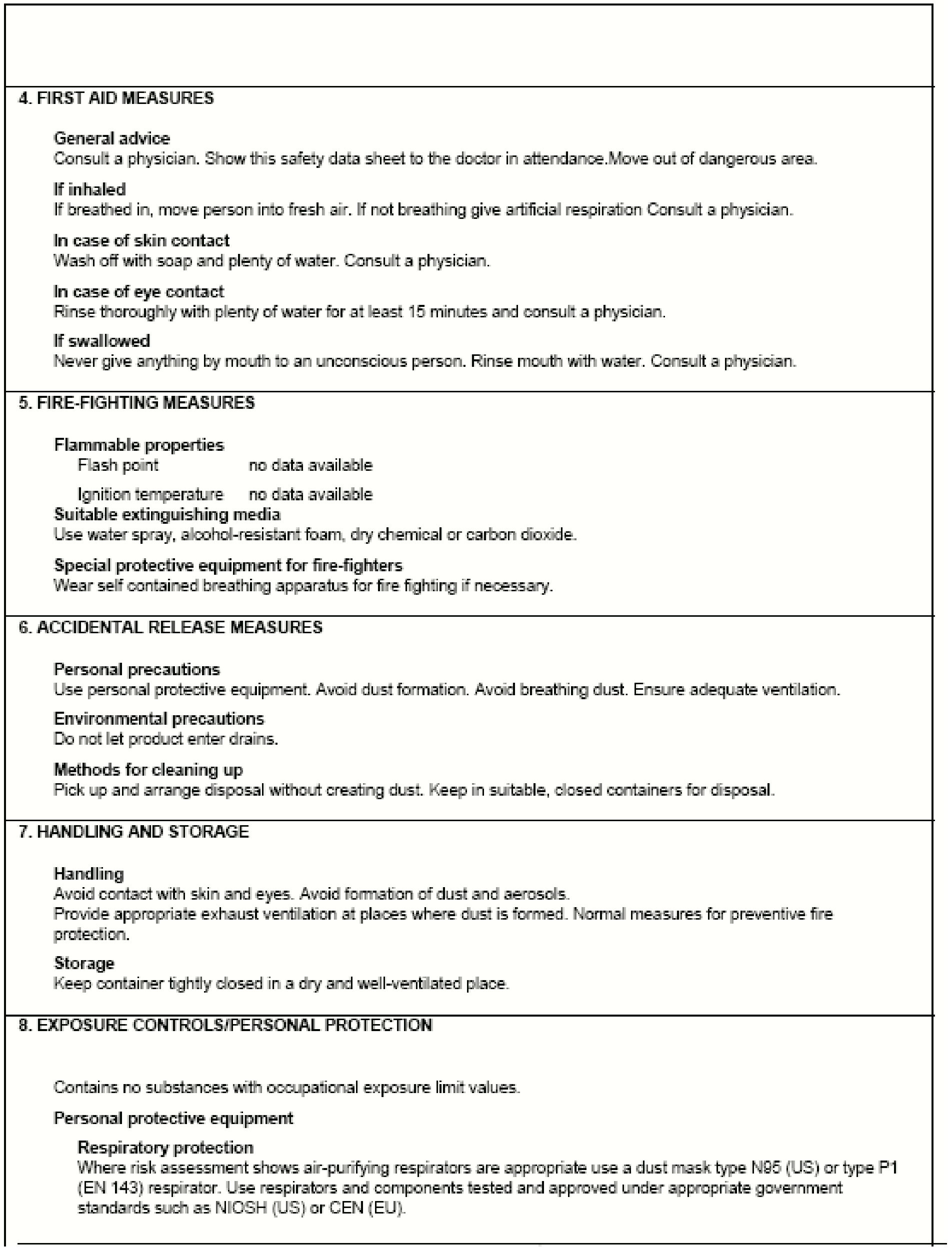
Health Hazard:	2
Flammability:	0
Physical hazards:	0

NFPA Rating

Health Hazard:	2
Fire:	0
Reactivity Hazard:	0

Potential Health Effects

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



4. FIRST AID MEASURES

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

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

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

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

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

5. FIRE-FIGHTING MEASURES

Flammable properties

Flash point	no data available
Ignition temperature	no data available

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

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

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid dust formation. Avoid breathing dust. Ensure adequate ventilation.

Environmental precautions
Do not let product enter drains.

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

7. HANDLING AND STORAGE

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.

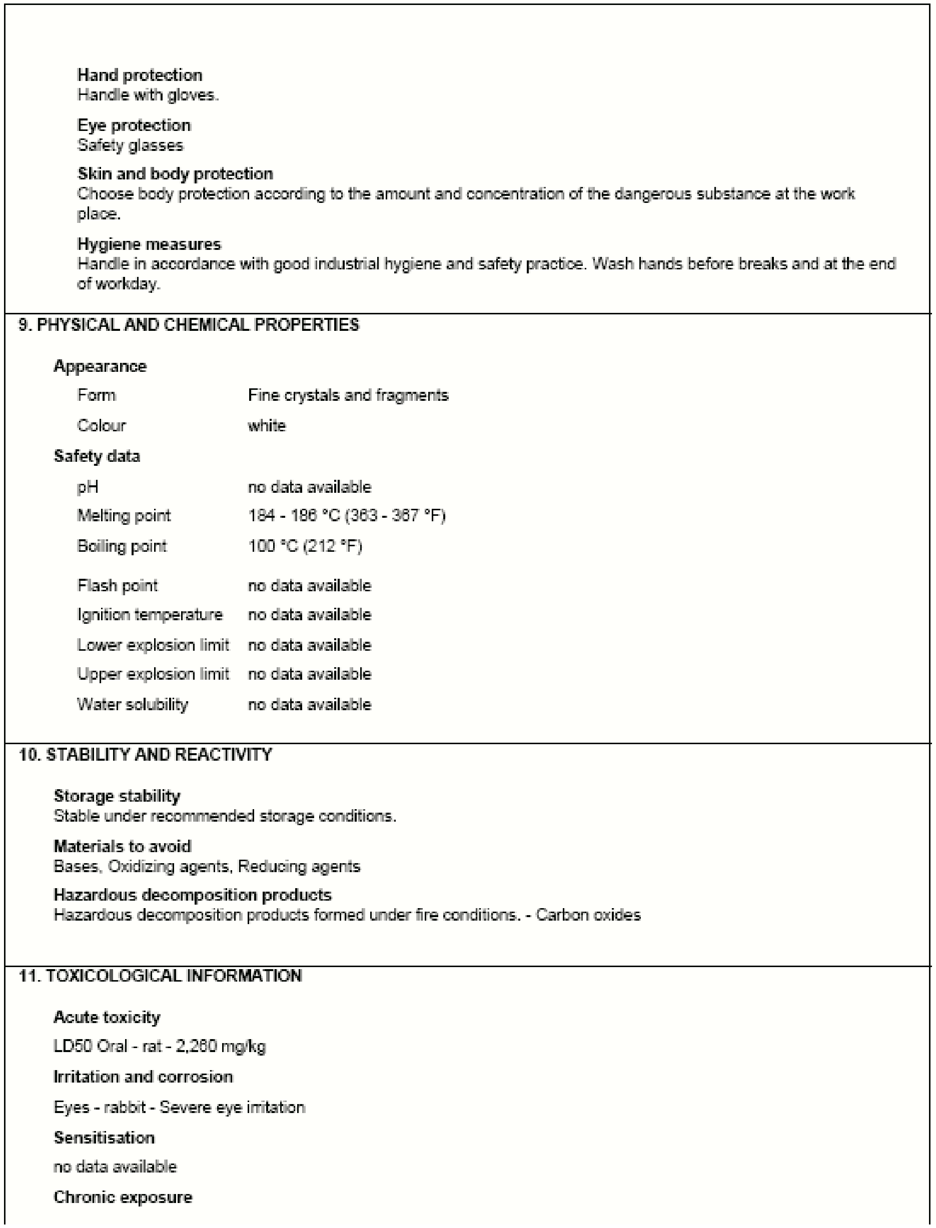
Storage
Keep container tightly closed in a dry and well-ventilated place.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a dust mask type N95 (US) or type P1 (EN 143) respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).



Hand protection
Handle with gloves.

Eye protection
Safety glasses

Skin and body protection
Choose body protection according to the amount and concentration of the dangerous substance at the work place.

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	Fine crystals and fragments
Colour	white

Safety data

pH	no data available
Melting point	184 - 186 °C (363 - 367 °F)
Boiling point	100 °C (212 °F)
Flash point	no data available
Ignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Water solubility	no data available

10. STABILITY AND REACTIVITY

Storage stability
Stable under recommended storage conditions.

Materials to avoid
Bases, Oxidizing agents, Reducing agents

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

11. TOXICOLOGICAL INFORMATION

Acute toxicity

LD50 Oral - rat - 2,260 mg/kg

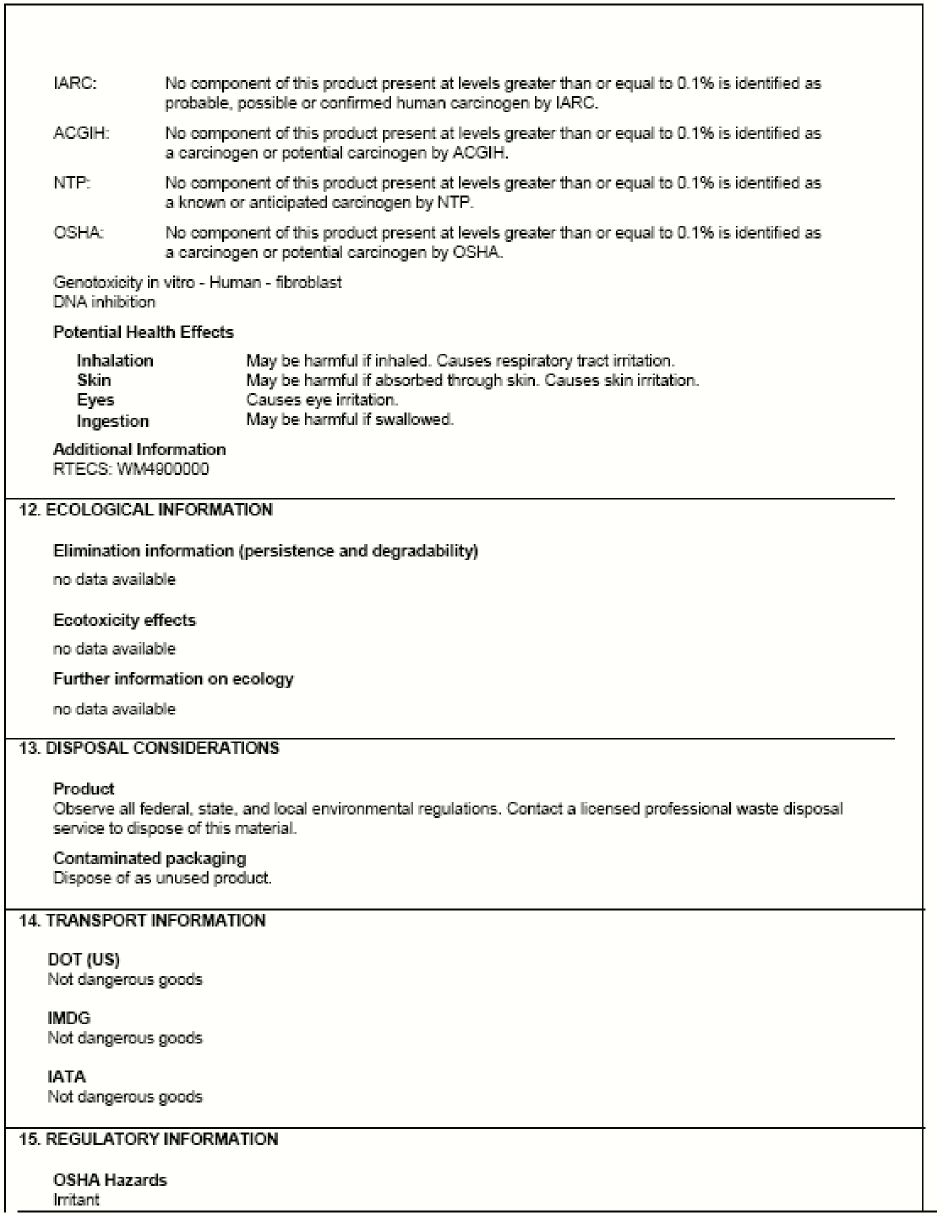
Irritation and corrosion

Eyes - rabbit - Severe eye irritation

Sensitisation

no data available

Chronic exposure



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.

Genotoxicity in vitro - Human - fibroblast
DNA inhibition

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.

Additional Information
RTECS: WM4900000

12. ECOLOGICAL INFORMATION

Elimination information (persistence and degradability)

no data available

Ecotoxicity effects

no data available

Further information on ecology

no data available

13. DISPOSAL CONSIDERATIONS

Product
Observe all federal, state, and local environmental regulations. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

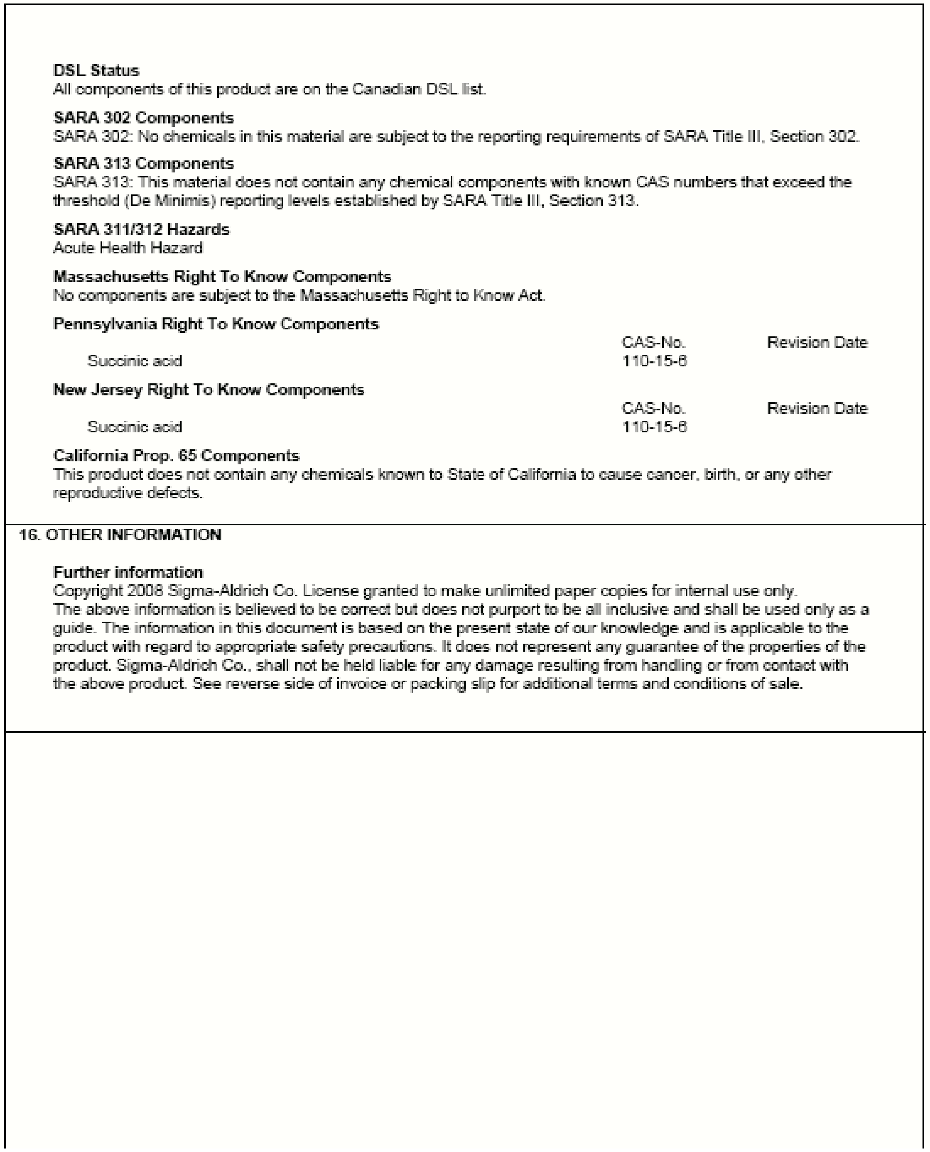
DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

OSHA Hazards
Irritant



DSL Status
All components of this product are on the Canadian DSL list.

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

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

SARA 311/312 Hazards
Acute Health Hazard

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
Succinic acid	110-15-6	

New Jersey Right To Know Components

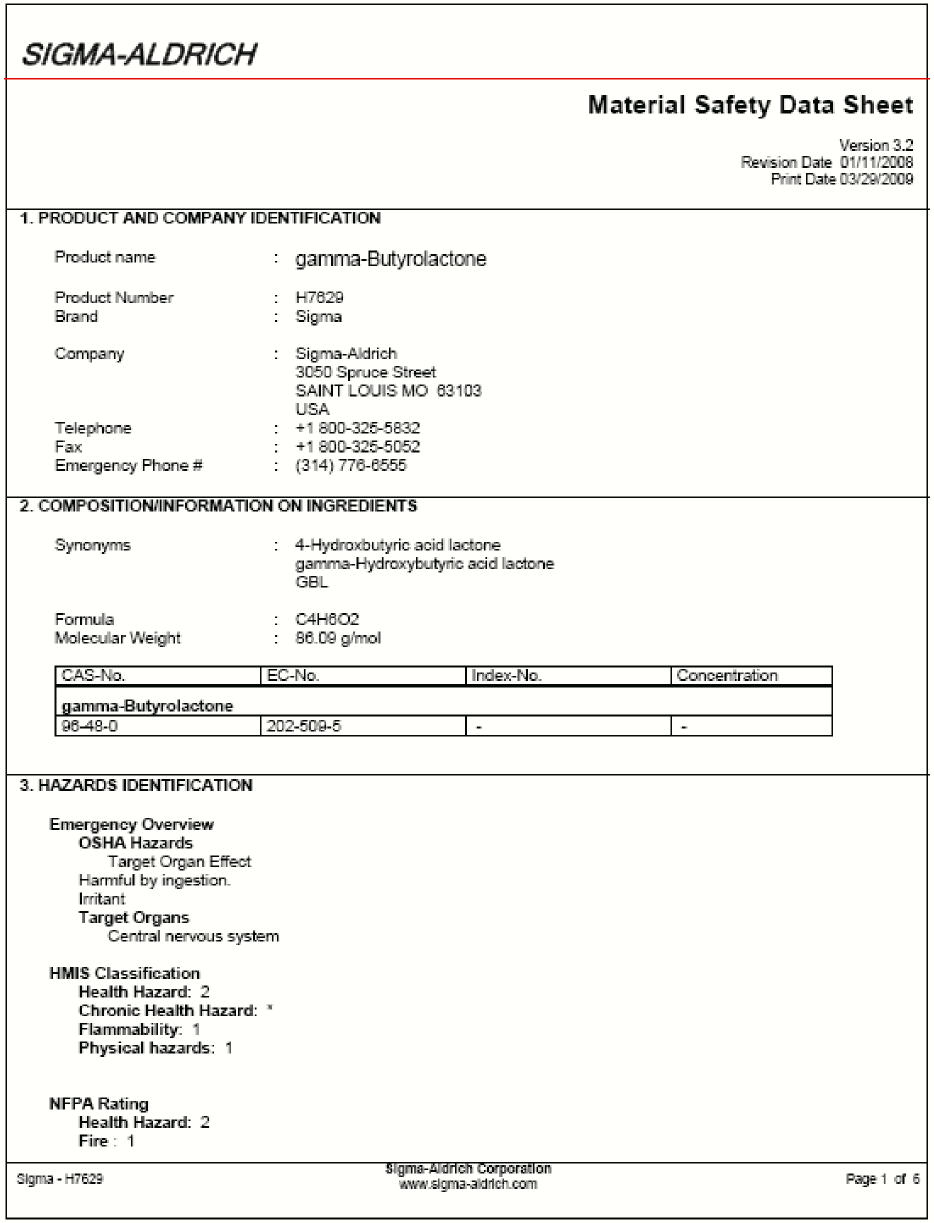
	CAS-No.	Revision Date
Succinic acid	110-15-6	

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

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 Co., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.



SIGMA-ALDRICH

Material Safety Data Sheet

Version 3.2
Revision Date 01/11/2008
Print Date 03/29/2009

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : gamma-Butyrolactone

Product Number : H7629
Brand : Sigma

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA
Telephone : +1 800-325-5832
Fax : +1 800-325-5052
Emergency Phone # : (314) 776-6555

2. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : 4-Hydroxbutyric acid lactone
gamma-Hydroxybutyric acid lactone
GBL

Formula : $C_4H_6O_2$
Molecular Weight : 86.09 g/mol

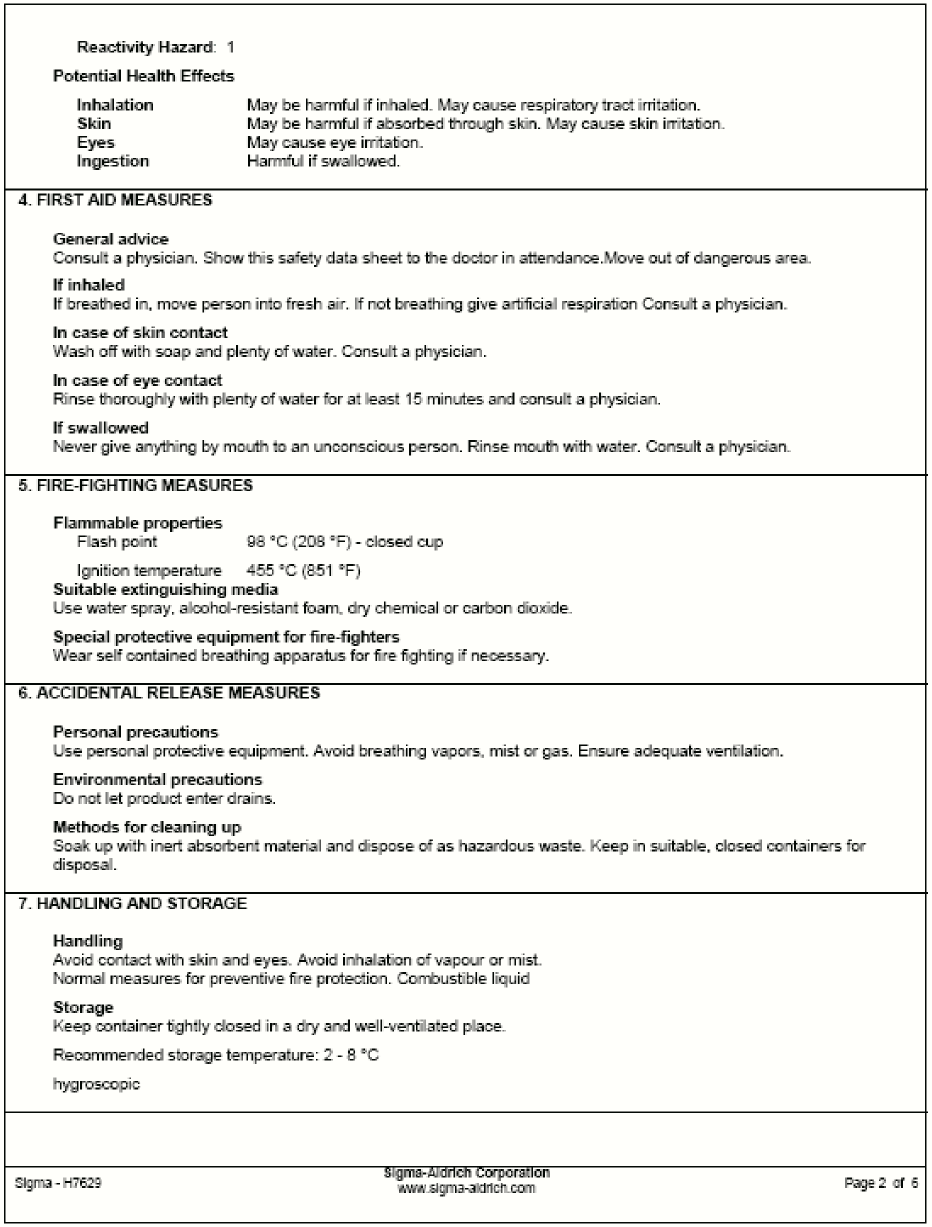
CAS-No.	EC-No.	Index-No.	Concentration
gamma-Butyrolactone			
96-48-0	202-509-5	-	-

3. HAZARDS IDENTIFICATION

Emergency Overview
OSHA Hazards
Target Organ Effect
Harmful by ingestion.
Irritant
Target Organs
Central nervous system

HMIS Classification
Health Hazard: 2
Chronic Health Hazard: *
Flammability: 1
Physical hazards: 1

NFPA Rating
Health Hazard: 2
Fire : 1



Reactivity Hazard: 1

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	Harmful if swallowed.

4. FIRST AID MEASURES

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

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

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

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

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

5. FIRE-FIGHTING MEASURES

Flammable properties

Flash point	98 °C (208 °F) - closed cup
Ignition temperature	455 °C (851 °F)

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

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

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation.

Environmental precautions
Do not let product enter drains.

Methods for cleaning up
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

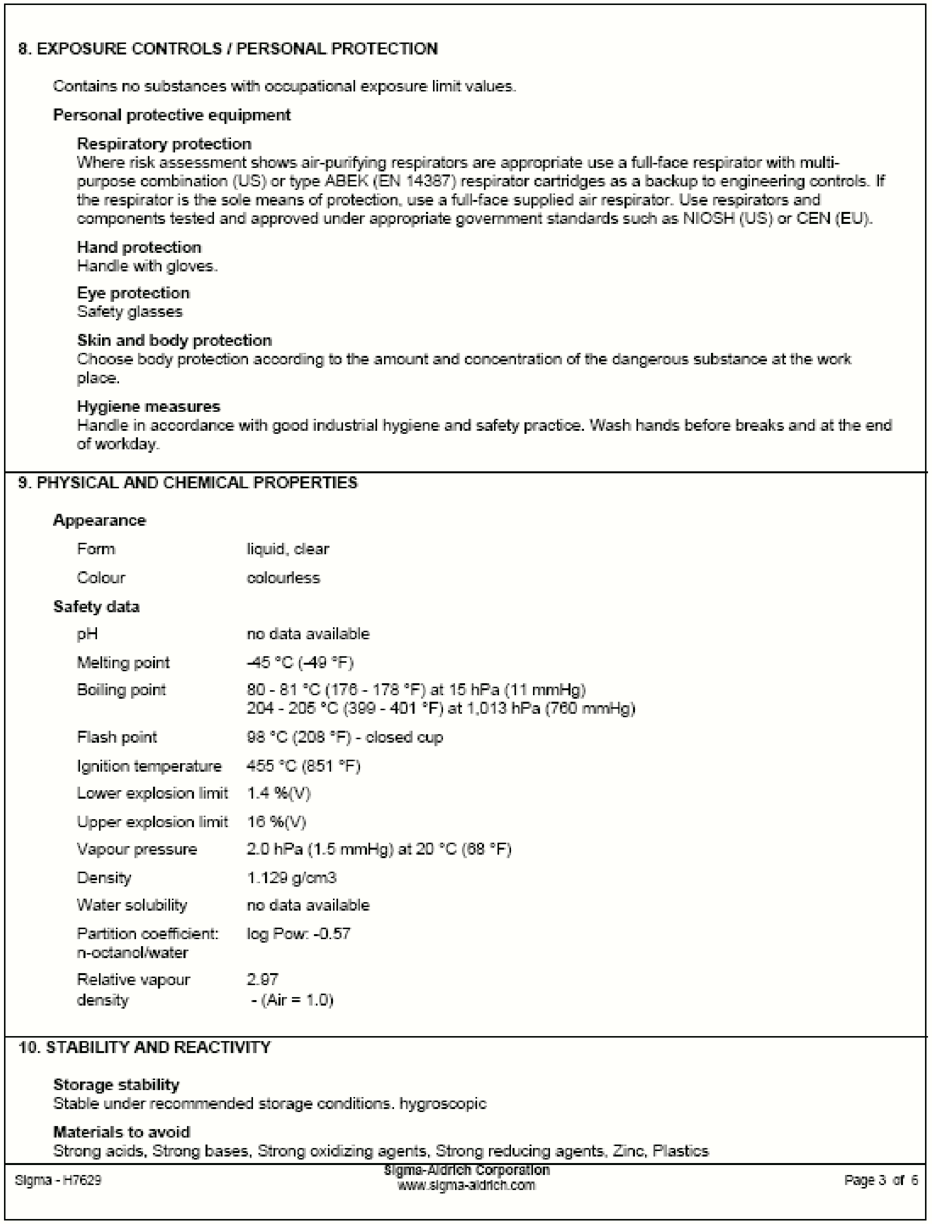
7. HANDLING AND STORAGE

Handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Normal measures for preventive fire protection. Combustible liquid

Storage
Keep container tightly closed in a dry and well-ventilated place.

Recommended storage temperature: 2 - 8 °C

hygroscopic



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.

Eye protection
Safety glasses

Skin and body protection
Choose body protection according to the amount and concentration of the dangerous substance at the work place.

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	liquid, clear
Colour	colourless

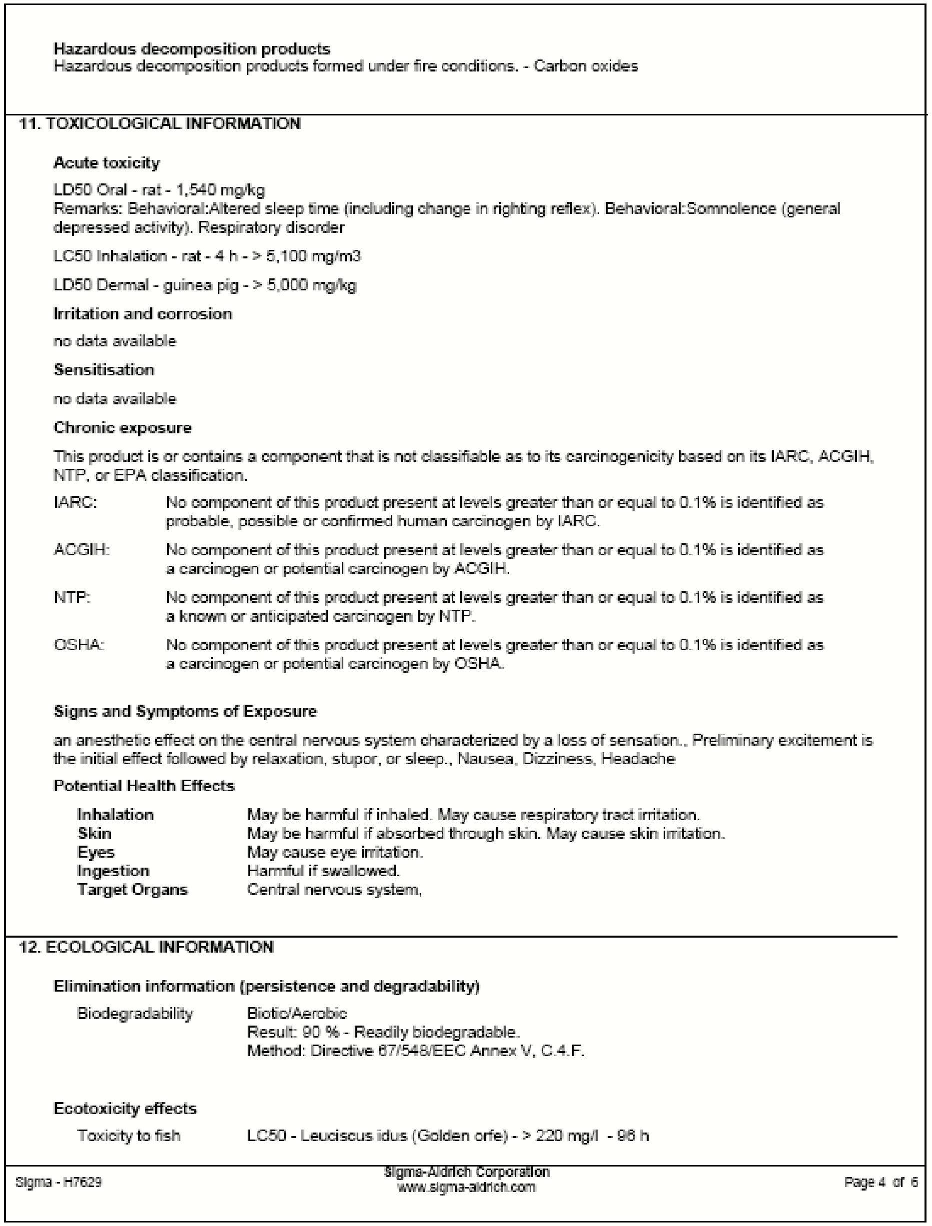
Safety data

pH	no data available
Melting point	-45 °C (-49 °F)
Boiling point	80 - 81 °C (176 - 178 °F) at 15 hPa (11 mmHg) 204 - 205 °C (399 - 401 °F) at 1,013 hPa (760 mmHg)
Flash point	98 °C (208 °F) - closed cup
Ignition temperature	455 °C (851 °F)
Lower explosion limit	1.4 %(V)
Upper explosion limit	16 %(V)
Vapour pressure	2.0 hPa (1.5 mmHg) at 20 °C (68 °F)
Density	1.129 g/cm3
Water solubility	no data available
Partition coefficient: n-octanol/water	log Pow: -0.57
Relative vapour density	2.97 - (Air = 1.0)

10. STABILITY AND REACTIVITY

Storage stability
Stable under recommended storage conditions. hygroscopic

Materials to avoid
Strong acids, Strong bases, Strong oxidizing agents, Strong reducing agents, Zinc, Plastics



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

11. TOXICOLOGICAL INFORMATION

Acute toxicity

LD50 Oral - rat - 1,540 mg/kg
Remarks: Behavioral:Altered sleep time (including change in righting reflex). Behavioral:Somnolence (general depressed activity). Respiratory disorder

LC50 Inhalation - rat - 4 h - > 5,100 mg/m3

LD50 Dermal - guinea pig - > 5,000 mg/kg

Irritation and corrosion

no data available

Sensitisation

no data available

Chronic exposure

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

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.

Signs and Symptoms of Exposure

an anesthetic effect on the central nervous system characterized by a loss of sensation., Preliminary excitement is the initial effect followed by relaxation, stupor, or sleep., Nausea, Dizziness, Headache

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	Harmful if swallowed.
Target Organs	Central nervous system,

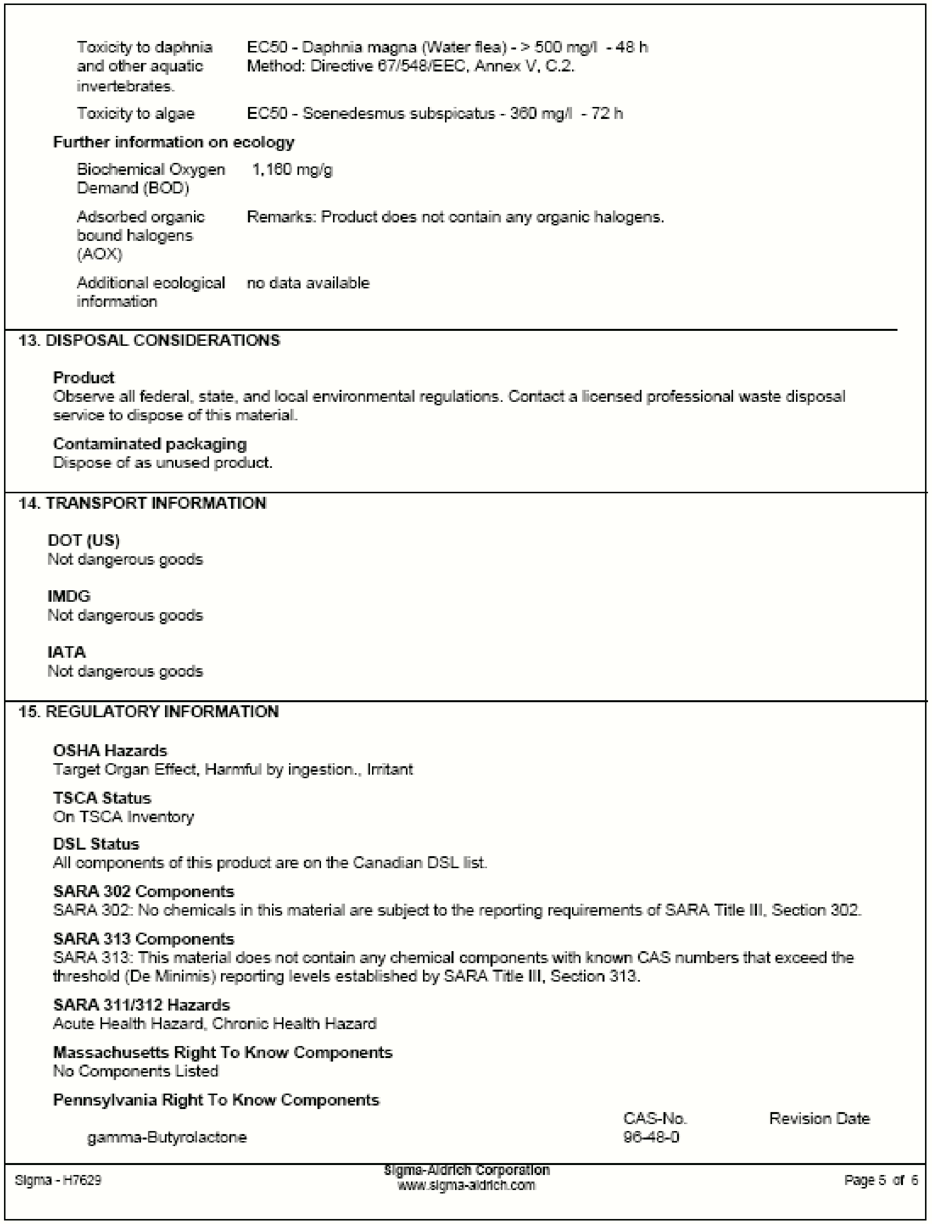
12. ECOLOGICAL INFORMATION

Elimination information (persistence and degradability)

Biodegradability	Biotic/Aerobic Result: 90 % - Readily biodegradable. Method: Directive 67/548/EEC Annex V, C.4.F.

Ecotoxicity effects

Toxicity to fish	LC50 - Leuciscus idus (Golden orfe) - > 220 mg/l - 96 h



Toxicity to daphnia and other aquatic invertebrates.	EC50 - Daphnia magna (Water flea) - > 500 mg/l - 48 h Method: Directive 67/548/EEC, Annex V, C.2.
Toxicity to algae	EC50 - Scenedesmus subspicatus - 360 mg/l - 72 h

Further information on ecology

Biochemical Oxygen Demand (BOD)	1,160 mg/g
Adsorbed organic bound halogens (AOX)	Remarks: Product does not contain any organic halogens.
Additional ecological information	no data available

13. DISPOSAL CONSIDERATIONS

Product
Observe all federal, state, and local environmental regulations. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

OSHA Hazards
Target Organ Effect, Harmful by ingestion., Irritant

TSCA Status
On TSCA Inventory

DSL Status
All components of this product are on the Canadian DSL list.

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

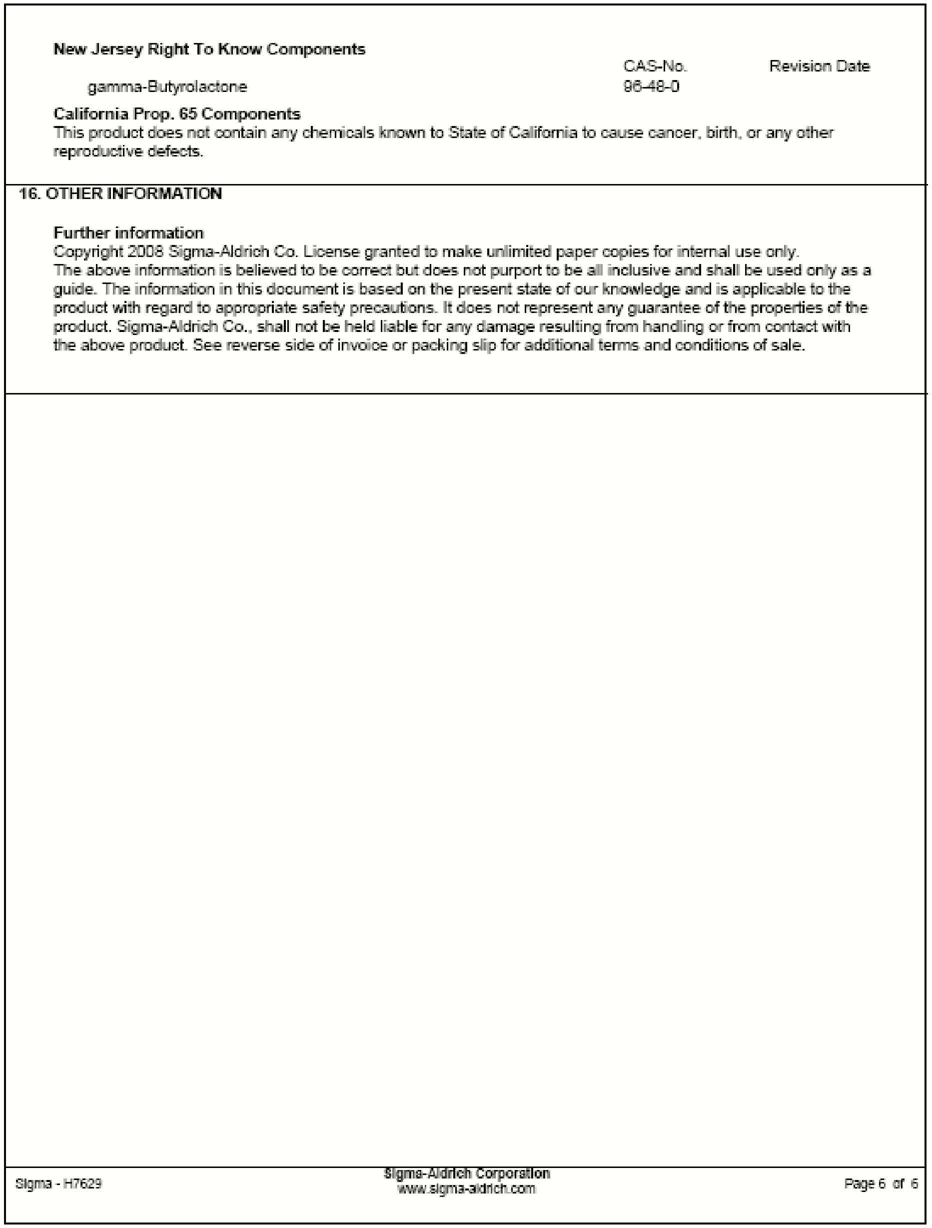
SARA 313 Components
SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

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

Massachusetts Right To Know Components
No Components Listed

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
gamma-Butyrolactone	96-48-0	



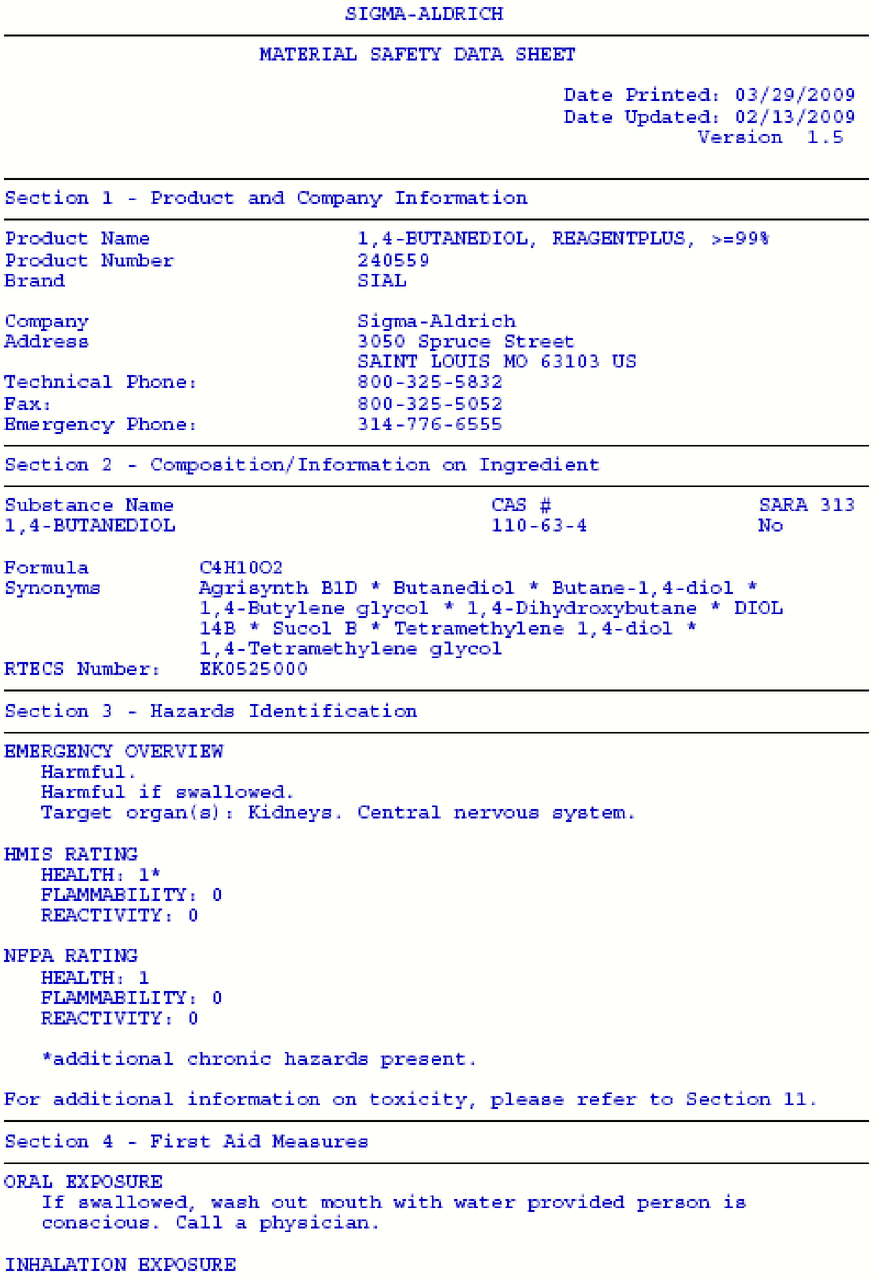
New Jersey Right To Know Components

	CAS-No.	Revision Date
gamma-Butyrolactone	96-48-0	

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

16. OTHER INFORMATION

Further information
Copyright 2008 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.
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 Co., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.



SIGMA-ALDRICH

MATERIAL SAFETY DATA SHEET

Date Printed: 03/29/2009
Date Updated: 02/13/2009
Version 1.5

Section 1 - Product and Company Information

Product Name	1,4-BUTANEDIOL, REAGENTPLUS, >=99%
Product Number	240559
Brand	SIAL
Company	Sigma-Aldrich
Address	3050 Spruce Street SAINT LOUIS MO 63103 US
Technical Phone:	800-325-5832
Fax:	800-325-5052
Emergency Phone:	314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
1,4-BUTANEDIOL	110-63-4	No

Formula	$C_4H_{10}O_2$
Synonyms	Agrisynth B1D * Butanediol * Butane-1,4-diol * 1,4-Butylene glycol * 1,4-Dihydroxybutane * DIOL 14B * Sucol B * Tetramethylene 1,4-diol * 1,4-Tetramethylene glycol
RTECS Number:	EK0525000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW
Harmful.
Harmful if swallowed.
Target organ(s): Kidneys. Central nervous system.

HMIS RATING
HEALTH: 1*
FLAMMABILITY: 0
REACTIVITY: 0

NFPA RATING
HEALTH: 1
FLAMMABILITY: 0
REACTIVITY: 0

*additional chronic hazards present.

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE
If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE

In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

EYE EXPOSURE

In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

Section 5 - Fire Fighting Measures

FLASH POINT

273.2 °F   134 °C   Method: closed cup

AUTOIGNITION TEMP

370 °C

FLAMMABILITY

N/A

EXTINGUISHING MEDIA

Suitable: Carbon dioxide, dry chemical powder, or appropriate foam. Water spray.

FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Emits toxic fumes under fire conditions.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL

Evacuate area.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP

Absorb on sand or vermiculite and place in closed containers for disposal. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING

User Exposure: Avoid prolonged or repeated exposure. Do not breathe vapor. Avoid contact with eyes, skin, and clothing.

STORAGE

Suitable: Keep tightly closed.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS

Safety shower and eye bath. Mechanical exhaust required.

PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). 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.
Hand: Compatible chemical-resistant gloves.
Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES

Wash thoroughly after handling.

Section 9 - Physical/Chemical Properties

Appearance	Physical State: Liquid	
Property	Value	At Temperature or Pressure
Molecular Weight	90.12 AMU	
pH	N/A	
BP/BP Range	120.0 - 122.0 °C	10 mmHg
MP/MP Range	19 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	3.1 g/l	
Saturated Vapor Conc.	N/A	
SG/Density	1.014 g/cm3	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	N/A	
Decomposition Temp.	N/A	
Flash Point	273.2 °F 134 °C	Method: closed cup
Explosion Limits	N/A	
Flammability	N/A	
Autoignition Temp	370 °C	
Refractive Index	1.446	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

N/A = not available

Section 10 - Stability and Reactivity

STABILITY

Stable: Stable.
Materials to Avoid: Strong oxidizing agents, Acid chlorides, Acid anhydrides, Reducing agents.

HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE

Skin Contact: May cause skin irritation.
Skin Absorption: May be harmful if absorbed through the skin.
Eye Contact: May cause eye irritation.
Inhalation: Material may be irritating to mucous membranes and upper respiratory tract. May be harmful if inhaled.
Ingestion: Harmful if swallowed.

TARGET ORGAN(S) OR SYSTEM(S)

Kidneys. Central nervous system.

SIGNS AND SYMPTOMS OF EXPOSURE

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

TOXICITY DATA

Rectal
Man
429 MG/KG
LDLO

Oral
Rat
1525 mg/kg
LD50
Remarks: Behavioral:Somnolence (general depressed activity). Behavioral:Altered sleep time (including change in righting reflex). Blood:Other changes.

Intraperitoneal
Rat
1070 MG/KG
LD50

Oral
Mouse
2062 mg/kg
LD50
Remarks: Behavioral:Somnolence (general depressed activity). Behavioral:Altered sleep time (including change in righting reflex). Blood:Other changes.

Intraperitoneal
Mouse
1650 MG/KG
LD50

Oral
Rabbit
2531 mg/kg
LD50
Remarks: Behavioral:Somnolence (general depressed activity). Behavioral:Altered sleep time (including change in righting reflex). Blood:Other changes.

Oral
Guinea pig
1200 mg/kg

LD50
Remarks: Behavioral:Altered sleep time (including change in righting reflex). Behavioral:Somnolence (general depressed activity). Blood:Other changes.

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT

Proper Shipping Name: None
Non-Hazardous for Transport: This substance is considered to be non-hazardous for transport.

IATA

Non-Hazardous for Air Transport: Non-hazardous for air transport.

Section 15 - Regulatory Information

EU ADDITIONAL CLASSIFICATION

Symbol of Danger: Xn
Indication of Danger: Harmful.
R: 22
Risk Statements: Harmful if swallowed.
S: 36
Safety Statements: Wear suitable protective clothing.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Harmful.
Risk Statements: Harmful if swallowed.
Safety Statements: Wear suitable protective clothing.
US Statements: Target organ(s): Kidneys. Central nervous system.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: No
TSCA INVENTORY ITEM: Yes

CANADA REGULATORY INFORMATION

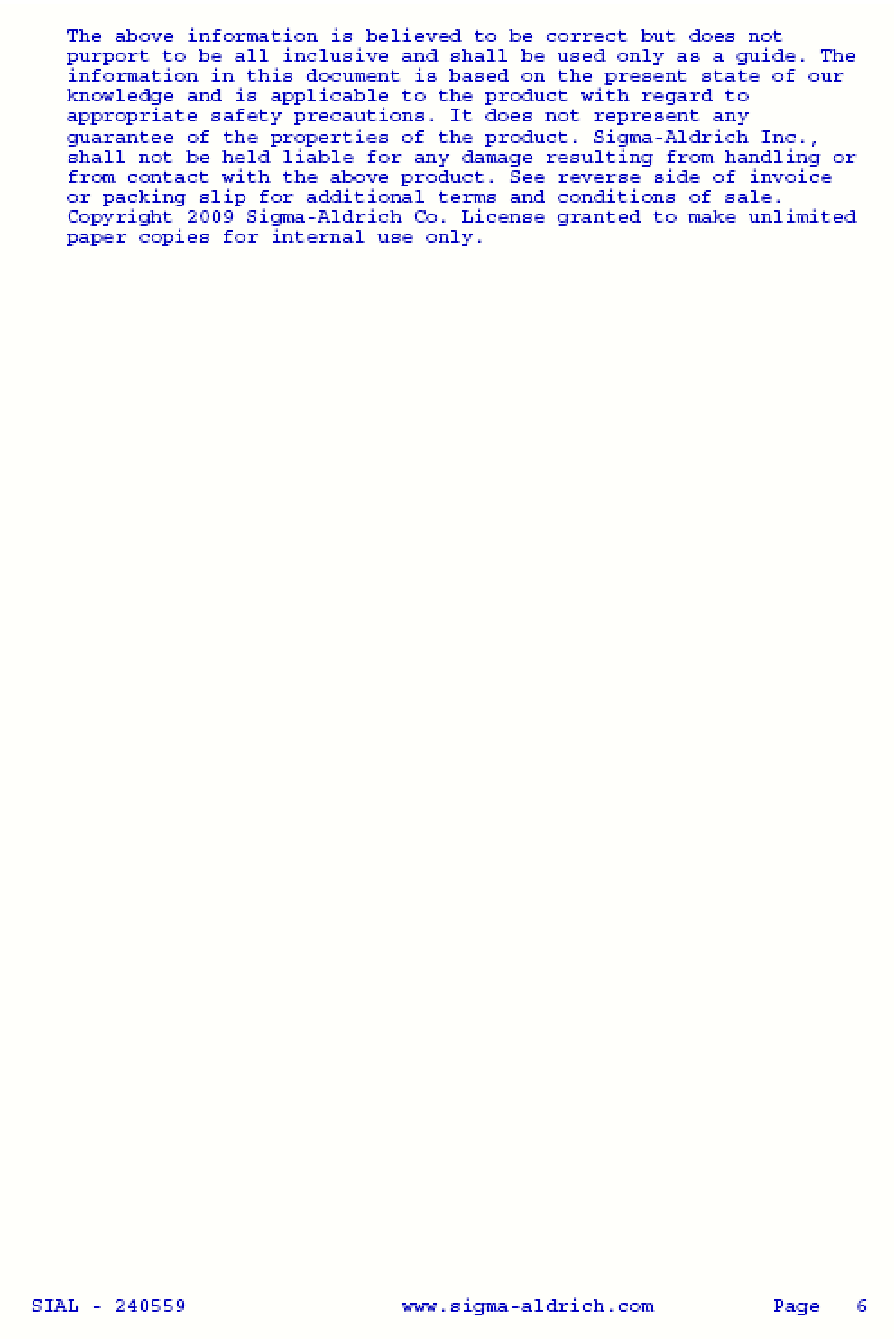
WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: No

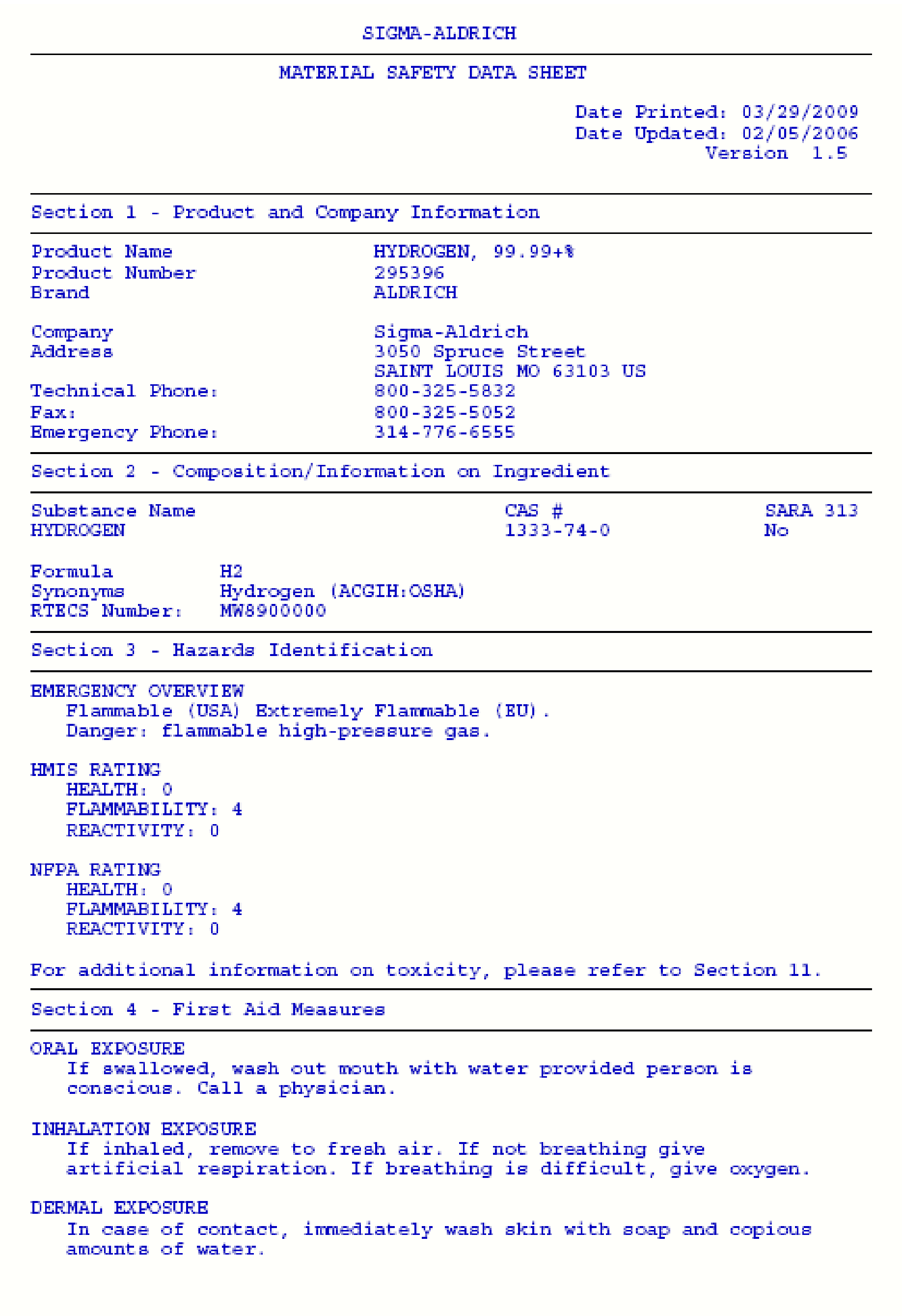
Section 16 - Other Information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY





SIGMA-ALDRICH

MATERIAL SAFETY DATA SHEET

Date Printed: 03/29/2009
Date Updated: 02/05/2006
Version 1.5

Section 1 - Product and Company Information

Product Name	HYDROGEN, 99.99+%
Product Number	295396
Brand	ALDRICH
Company	Sigma-Aldrich
Address	3050 Spruce Street SAINT LOUIS MO 63103 US
Technical Phone:	800-325-5832
Fax:	800-325-5052
Emergency Phone:	314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
HYDROGEN	1333-74-0	No

Formula	H2
Synonyms	Hydrogen (ACGIH:OSHA)
RTECS Number:	MW8900000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW
Flammable (USA) Extremely Flammable (EU).
Danger: flammable high-pressure gas.

HMIS RATING
HEALTH: 0
FLAMMABILITY: 4
REACTIVITY: 0

NFPA RATING
HEALTH: 0
FLAMMABILITY: 4
REACTIVITY: 0

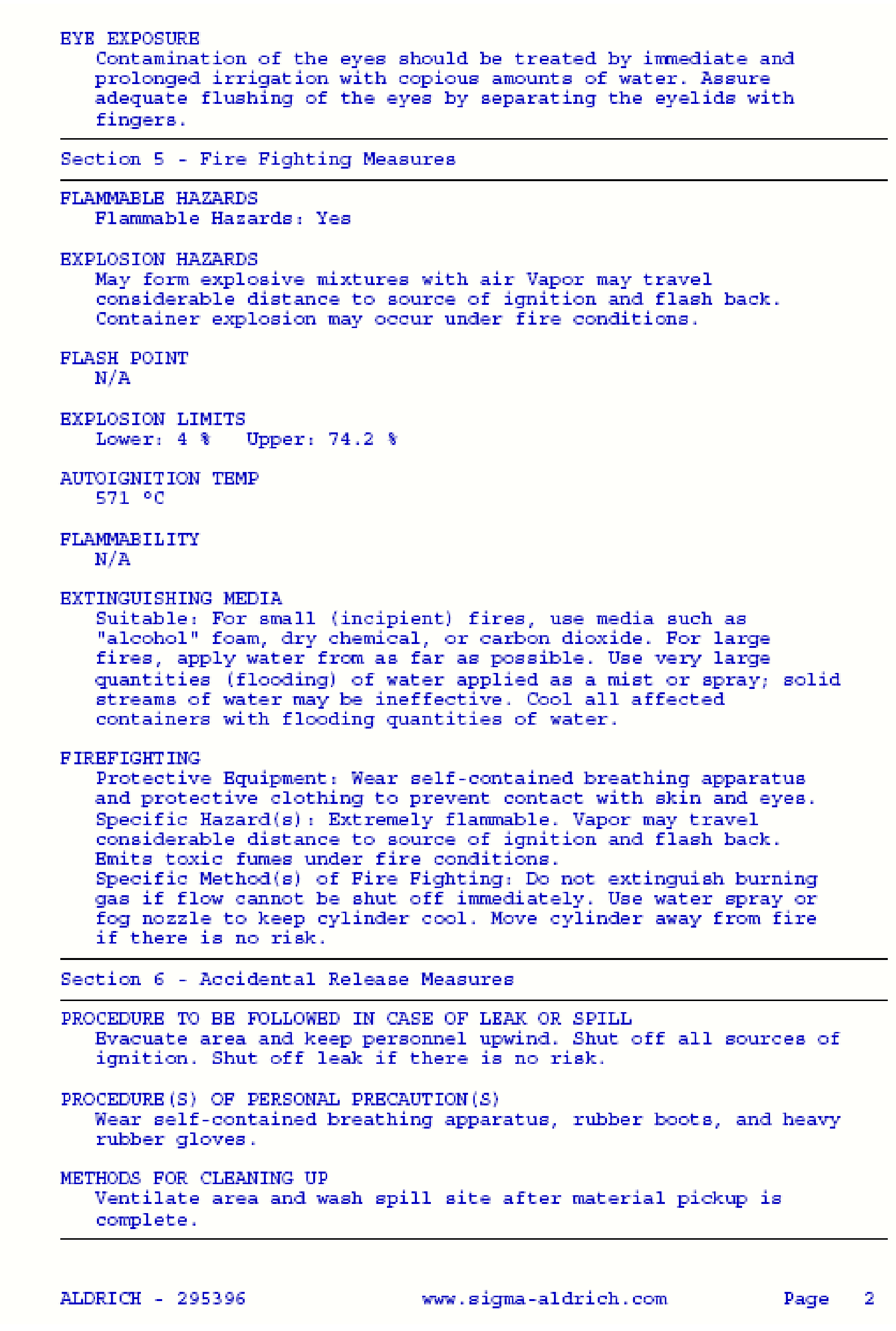
For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE
If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE
If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE
In case of contact, immediately wash skin with soap and copious amounts of water.



EYE EXPOSURE

Contamination of the eyes should be treated by immediate and prolonged irrigation with copious amounts of water. Assure adequate flushing of the eyes by separating the eyelids with fingers.

Section 5 - Fire Fighting Measures

FLAMMABLE HAZARDS

Flammable Hazards: Yes

EXPLOSION HAZARDS

May form explosive mixtures with air Vapor may travel considerable distance to source of ignition and flash back. Container explosion may occur under fire conditions.

FLASH POINT

N/A

EXPLOSION LIMITS

Lower: 4 %   Upper: 74.2 %

AUTOIGNITION TEMP

571 °C

FLAMMABILITY

N/A

EXTINGUISHING MEDIA

Suitable: 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.

FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Extremely flammable. Vapor may travel considerable distance to source of ignition and flash back. Emits toxic fumes under fire conditions.
Specific Method(s) of Fire Fighting: Do not extinguish burning gas if flow cannot be shut off immediately. Use water spray or fog nozzle to keep cylinder cool. Move cylinder away from fire if there is no risk.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL

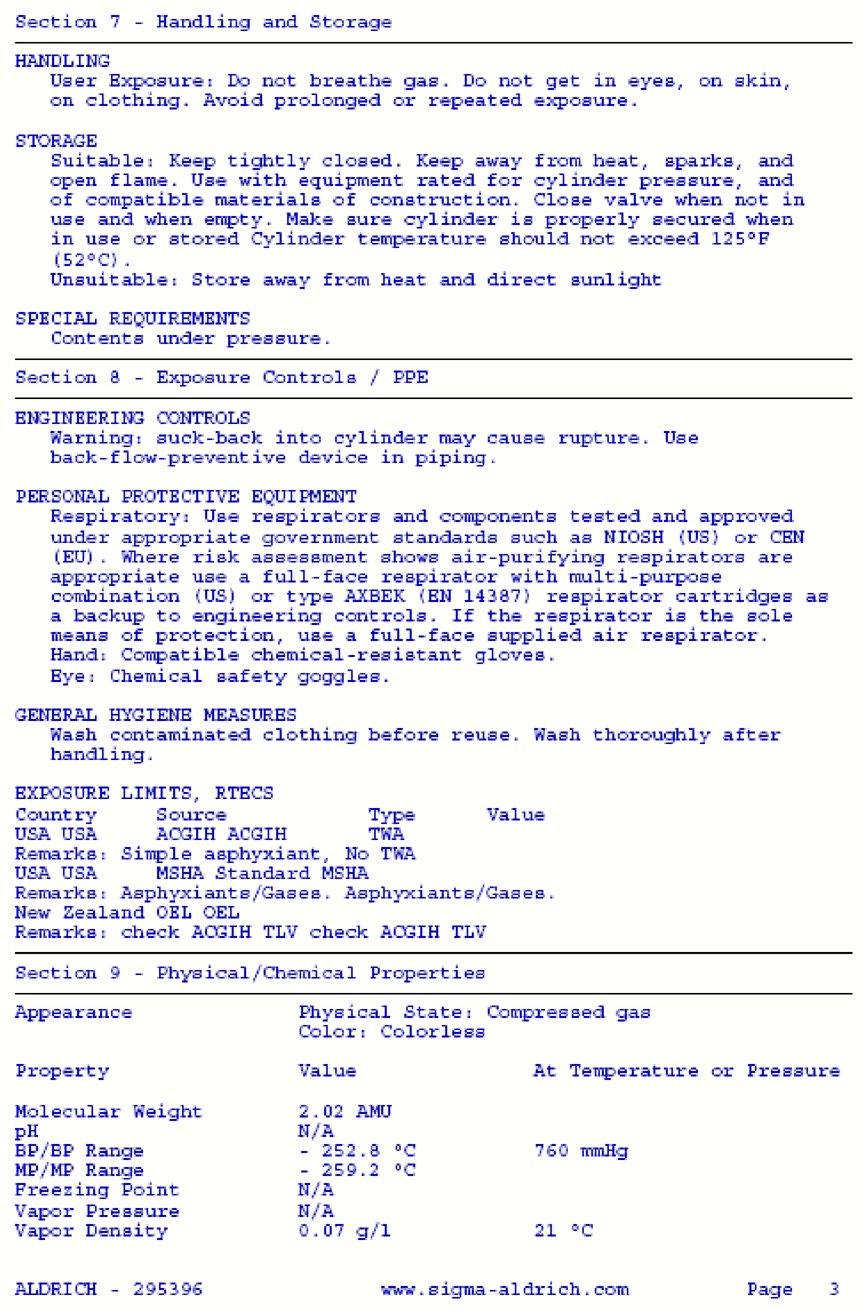
Evacuate area and keep personnel upwind. Shut off all sources of ignition. Shut off leak if there is no risk.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP

Ventilate area and wash spill site after material pickup is complete.



Section 7 - Handling and Storage

HANDLING

User Exposure: Do not breathe gas. Do not get in eyes, on skin, on clothing. Avoid prolonged or repeated exposure.

STORAGE

Suitable: Keep tightly closed. Keep away from heat, sparks, and open flame. Use with equipment rated for cylinder pressure, and of compatible materials of construction. Close valve when not in use and when empty. Make sure cylinder is properly secured when in use or stored Cylinder temperature should not exceed 125°F (52°C).
Unsuitable: Store away from heat and direct sunlight

SPECIAL REQUIREMENTS

Contents under pressure.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS

Warning: suck-back into cylinder may cause rupture. Use back-flow-preventive device in piping.

PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (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.
Hand: Compatible chemical-resistant gloves.
Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES

Wash contaminated clothing before reuse. Wash thoroughly after handling.

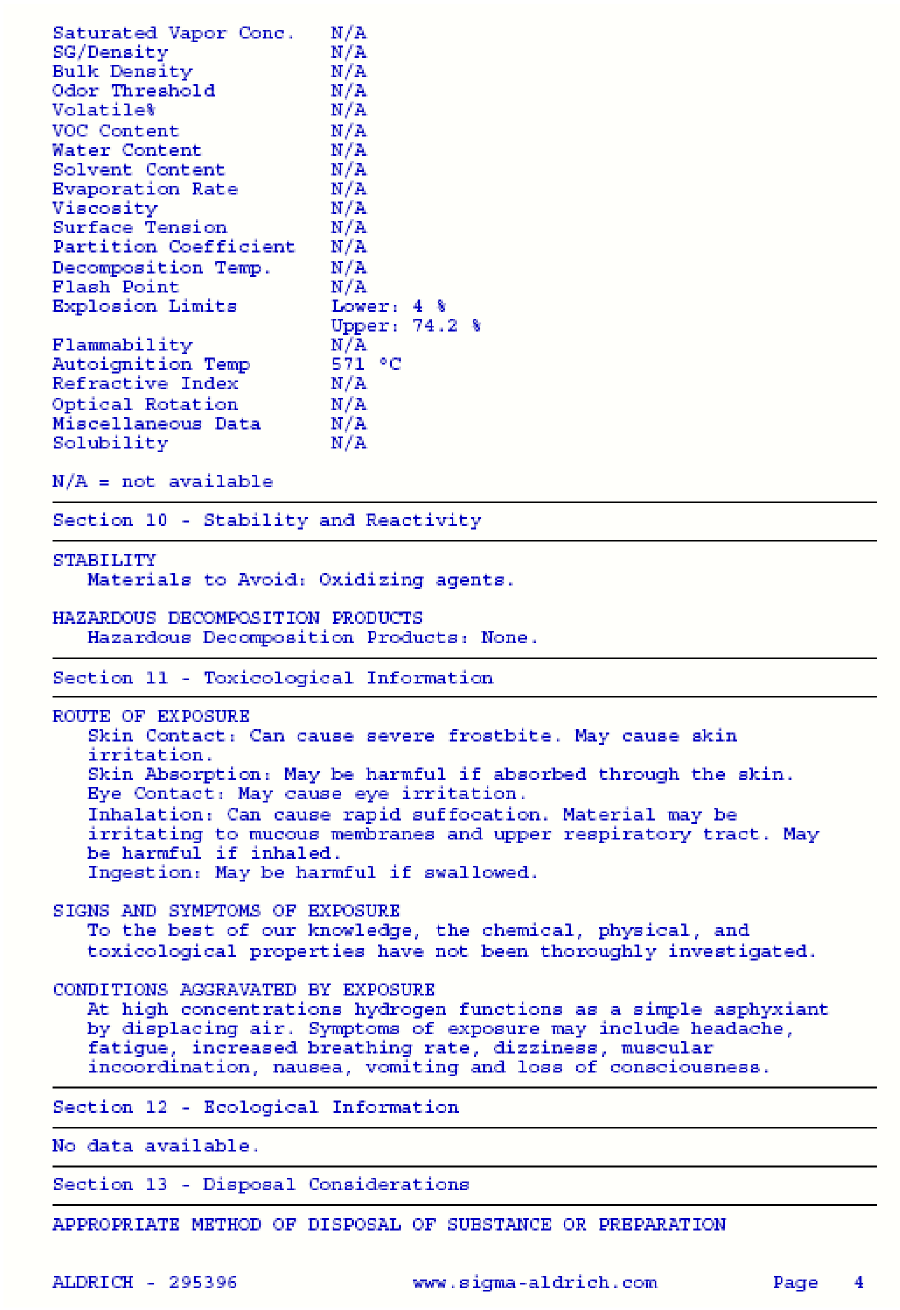
EXPOSURE LIMITS, RTECS

Country	Source	Type	Value
USA USA	ACGIH ACGIH	TWA	
Remarks: Simple asphyxiant, No TWA			
USA USA	MSHA Standard MSHA		
Remarks: Asphyxiants/Gases. Asphyxiants/Gases.			
New Zealand OEL OEL			
Remarks: check ACGIH TLV check ACGIH TLV			

Section 9 - Physical/Chemical Properties

Appearance — Physical State: Compressed gas
Color: Colorless

Property	Value	At Temperature or Pressure
Molecular Weight	2.02 AMU	
pH	N/A	
BP/BP Range	- 252.8 °C	760 mmHg
MP/MP Range	- 259.2 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	0.07 g/l	21 °C



Saturated Vapor Conc.	N/A
SG/Density	N/A
Bulk Density	N/A
Odor Threshold	N/A
Volatile%	N/A
VOC Content	N/A
Water Content	N/A
Solvent Content	N/A
Evaporation Rate	N/A
Viscosity	N/A
Surface Tension	N/A
Partition Coefficient	N/A
Decomposition Temp.	N/A
Flash Point	N/A
Explosion Limits	Lower: 4 % Upper: 74.2 %
Flammability	N/A
Autoignition Temp	571 °C
Refractive Index	N/A
Optical Rotation	N/A
Miscellaneous Data	N/A
Solubility	N/A

N/A = not available

Section 10 - Stability and Reactivity

STABILITY
Materials to Avoid: Oxidizing agents.

HAZARDOUS DECOMPOSITION PRODUCTS
Hazardous Decomposition Products: None.

Section 11 - Toxicological Information

ROUTE OF EXPOSURE
Skin Contact: Can cause severe frostbite. May cause skin irritation.
Skin Absorption: May be harmful if absorbed through the skin.
Eye Contact: May cause eye irritation.
Inhalation: Can cause rapid suffocation. Material may be irritating to mucous membranes and upper respiratory tract. May be harmful if inhaled.
Ingestion: May be harmful if swallowed.

SIGNS AND SYMPTOMS OF EXPOSURE
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

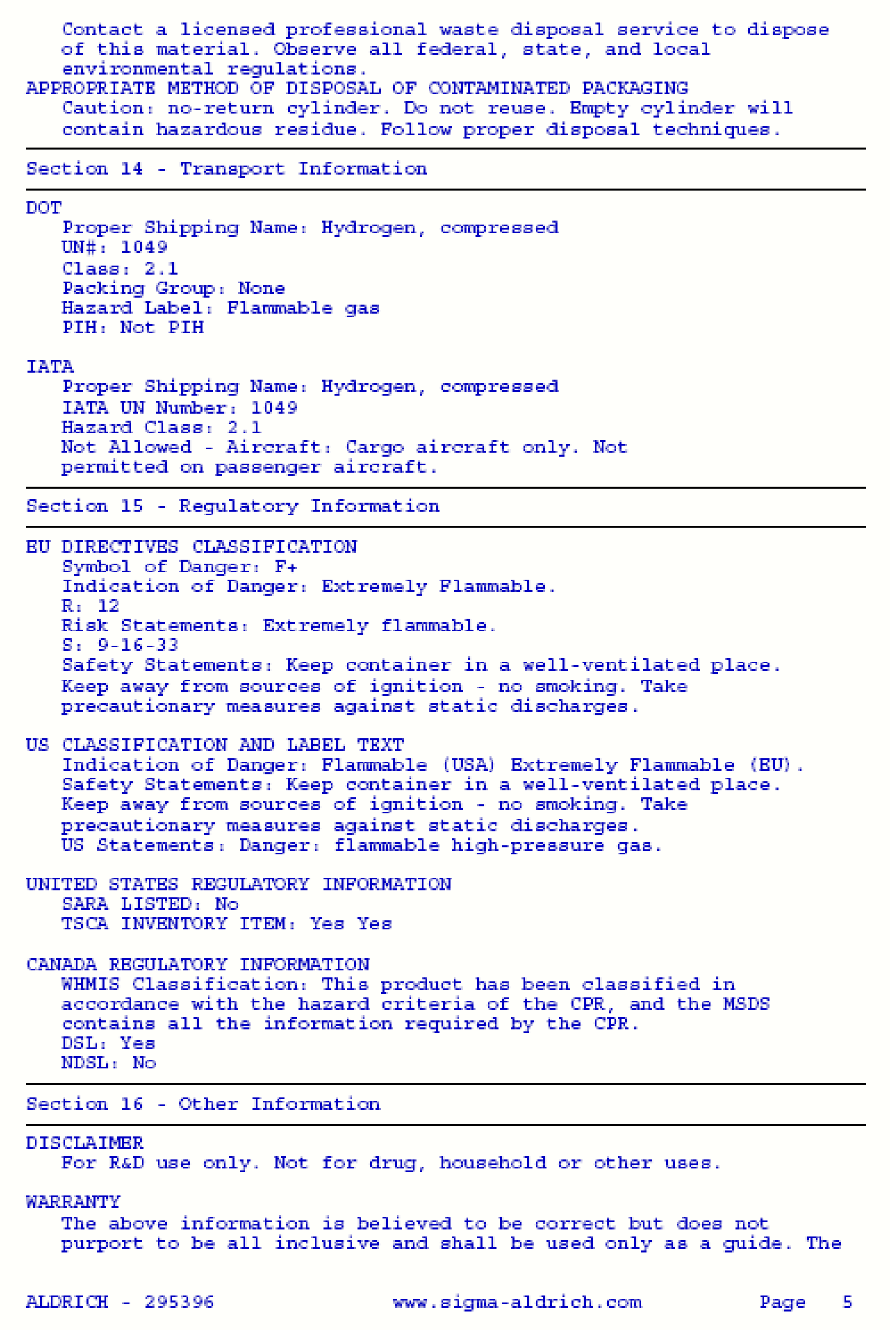
CONDITIONS AGGRAVATED BY EXPOSURE
At high concentrations hydrogen functions as a simple asphyxiant by displacing air. Symptoms of exposure may include headache, fatigue, increased breathing rate, dizziness, muscular incoordination, nausea, vomiting and loss of consciousness.

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION



Contact a licensed professional waste disposal service to dispose of this material. Observe all federal, state, and local environmental regulations.

APPROPRIATE METHOD OF DISPOSAL OF CONTAMINATED PACKAGING
Caution: no-return cylinder. Do not reuse. Empty cylinder will contain hazardous residue. Follow proper disposal techniques.

Section 14 - Transport Information

DOT
Proper Shipping Name: Hydrogen, compressed
UN#: 1049
Class: 2.1
Packing Group: None
Hazard Label: Flammable gas
PIH: Not PIH

IATA
Proper Shipping Name: Hydrogen, compressed
IATA UN Number: 1049
Hazard Class: 2.1
Not Allowed - Aircraft: Cargo aircraft only. Not permitted on passenger aircraft.

Section 15 - Regulatory Information

EU DIRECTIVES CLASSIFICATION
Symbol of Danger: F+
Indication of Danger: Extremely Flammable.
R: 12
Risk Statements: Extremely flammable.
S: 9-16-33
Safety Statements: Keep container in a well-ventilated place. Keep away from sources of ignition - no smoking. Take precautionary measures against static discharges.

US CLASSIFICATION AND LABEL TEXT
Indication of Danger: Flammable (USA) Extremely Flammable (EU).
Safety Statements: Keep container in a well-ventilated place. Keep away from sources of ignition - no smoking. Take precautionary measures against static discharges.
US Statements: Danger: flammable high-pressure gas.

UNITED STATES REGULATORY INFORMATION
SARA LISTED: No
TSCA INVENTORY ITEM: Yes Yes

CANADA REGULATORY INFORMATION
WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: No

Section 16 - Other Information

DISCLAIMER
For R&D use only. Not for drug, household or other uses.

WARRANTY
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 Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.

SIGMA-ALDRICH

MATERIAL SAFETY DATA SHEET

Date Printed: 03/29/2009
Date Updated: 02/28/2006
Version 1.4

Section 1 - Product and Company Information

Product Name	DOWTHERM(R) A
Product Number	44570
Brand	ALDRICH
Company	Sigma-Aldrich
Address	3050 Spruce Street SAINT LOUIS MO 63103 US
Technical Phone:	800-325-5832
Fax:	800-325-5052
Emergency Phone:	314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #		SARA 313
DOWTHERM(R) A	8004-13-5		Yes

Ingredient Name	CAS #	Percent	SARA 313
BIPHENYL	92-52-4	26.5	Yes
DIPHENYL ETHER (DIPHENYL OXIDE)	101-84-8	73.5	No

Section 3 - Hazards Identification

EMERGENCY OVERVIEW
Irritant. Dangerous for the environment.
Irritating to eyes, respiratory system and skin. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
Target organ(s): Kidneys. Liver.

HMIS RATING
HEALTH: 2*
FLAMMABILITY: 0
REACTIVITY: 0

NFPA RATING
HEALTH: 2
FLAMMABILITY: 0
REACTIVITY: 0

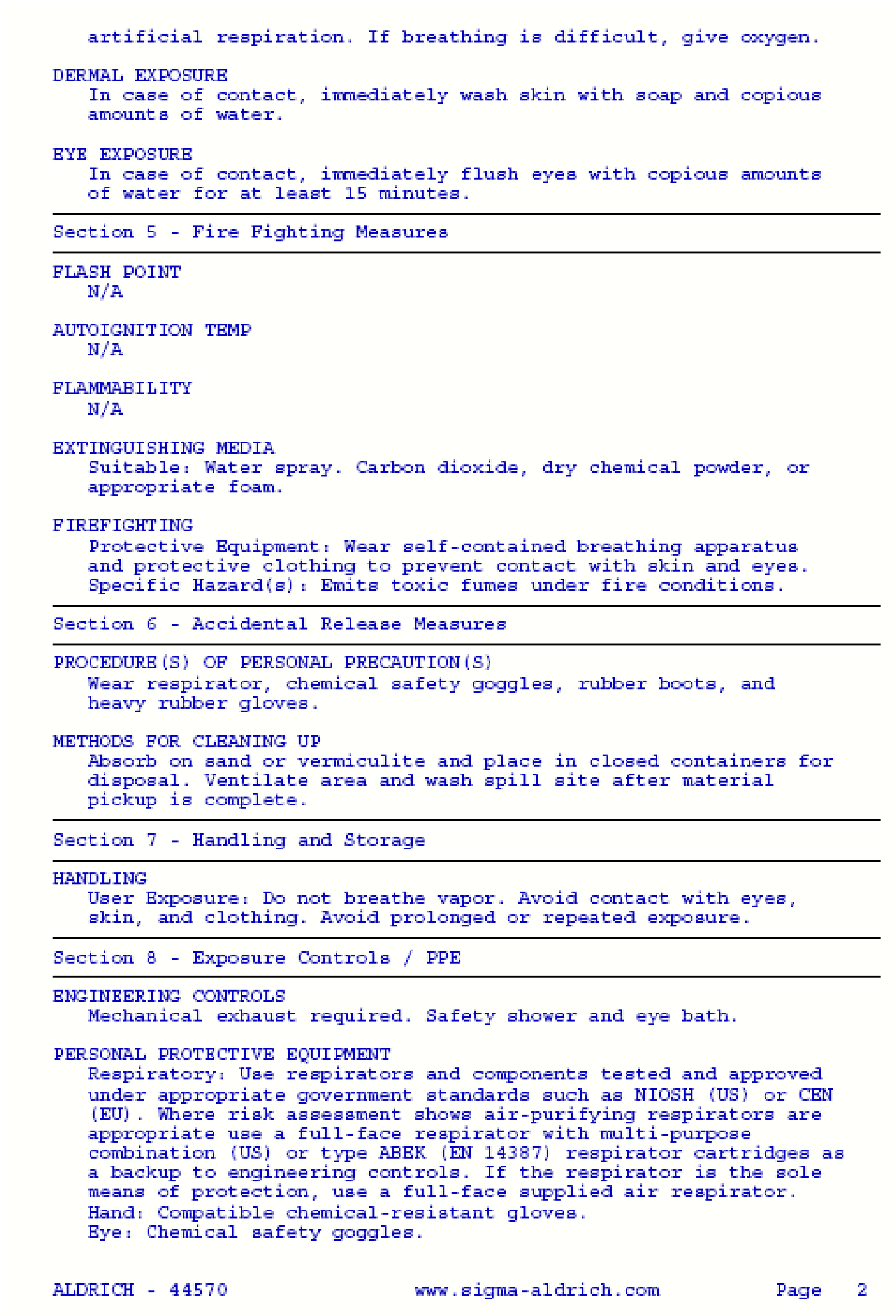
*additional chronic hazards present.

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE
If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE
If inhaled, remove to fresh air. If not breathing give



artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE

In case of contact, immediately wash skin with soap and copious amounts of water.

EYE EXPOSURE

In case of contact, immediately flush eyes with copious amounts of water for at least 15 minutes.

Section 5 - Fire Fighting Measures

FLASH POINT

N/A

AUTOIGNITION TEMP

N/A

FLAMMABILITY

N/A

EXTINGUISHING MEDIA

Suitable: Water spray. Carbon dioxide, dry chemical powder, or appropriate foam.

FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Emits toxic fumes under fire conditions.

Section 6 - Accidental Release Measures

PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear respirator, chemical safety goggles, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP

Absorb on sand or vermiculite and place in closed containers for disposal. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING

User Exposure: Do not breathe vapor. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

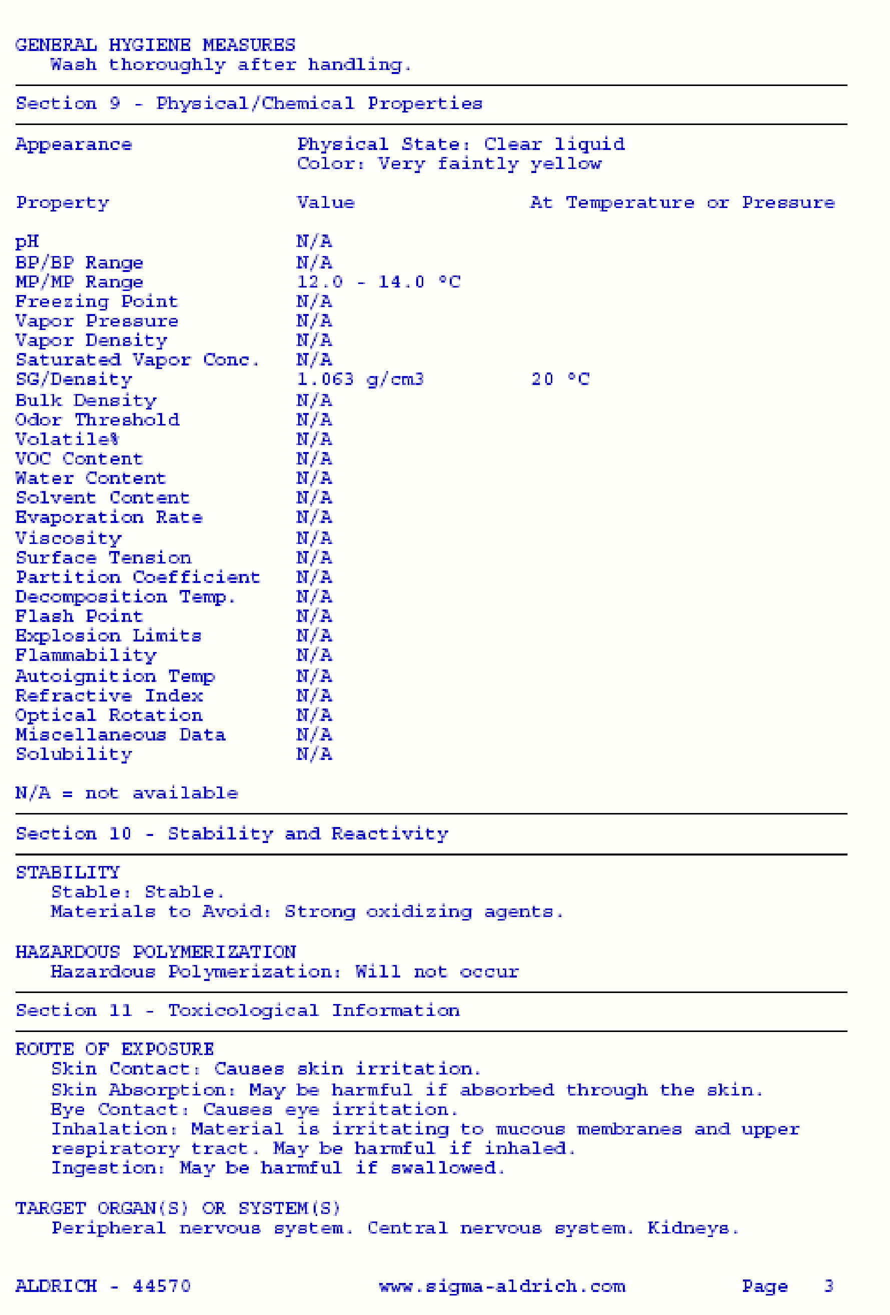
Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS

Mechanical exhaust required. Safety shower and eye bath.

PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). 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.
Hand: Compatible chemical-resistant gloves.
Eye: Chemical safety goggles.



GENERAL HYGIENE MEASURES

Wash thoroughly after handling.

Section 9 - Physical/Chemical Properties

Appearance	Physical State: Clear liquid Color: Very faintly yellow	
Property	Value	At Temperature or Pressure
pH	N/A	
BP/BP Range	N/A	
MP/MP Range	12.0 - 14.0 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
SG/Density	1.063 g/cm3	20 °C
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	N/A	
Decomposition Temp.	N/A	
Flash Point	N/A	
Explosion Limits	N/A	
Flammability	N/A	
Autoignition Temp	N/A	
Refractive Index	N/A	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

N/A = not available

Section 10 - Stability and Reactivity

STABILITY

Stable: Stable.
Materials to Avoid: Strong oxidizing agents.

HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE

Skin Contact: Causes skin irritation.
Skin Absorption: May be harmful if absorbed through the skin.
Eye Contact: Causes eye irritation.
Inhalation: Material is irritating to mucous membranes and upper respiratory tract. May be harmful if inhaled.
Ingestion: May be harmful if swallowed.

TARGET ORGAN(S) OR SYSTEM(S)

Peripheral nervous system. Central nervous system. Kidneys.

Liver. Spleen. Thyroid.

SIGNS AND SYMPTOMS OF EXPOSURE

Prolonged exposure can cause: Gastrointestinal disturbances. Dermatitis. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

CONDITIONS AGGRAVATED BY EXPOSURE

May cause nervous system disturbances.

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Bury in a landfill site approved for the disposal of chemical and hazardous wastes. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT

Proper Shipping Name: Environmentally hazardous substances, liquid, n.o.s.
UN#: 3082
Class: 9
Packing Group: Packing Group III
Hazard Label: Class 9
PIH: Not PIH

IATA

Proper Shipping Name: Environmentally hazardous substance, liquid, n.o.s.
IATA UN Number: 3082
Hazard Class: 9
Packing Group: III

Section 15 - Regulatory Information

EU ADDITIONAL CLASSIFICATION

Symbol of Danger: Xi-N
Indication of Danger: Irritant. Dangerous for the environment.
R: 36/37/38-50/53
Risk Statements: Irritating to eyes, respiratory system and skin. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
S: 26-60-61
Safety Statements: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. This material and its container must be disposed of as hazardous waste. Avoid release to the environment. Refer to special instructions/safety data sheets.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Irritant. Dangerous for the environment.
Risk Statements: Irritating to eyes, respiratory system and skin. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
Safety Statements: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. This material and its container must be disposed of as hazardous waste. Avoid release to the environment. Refer to special instructions/safety data sheets.
US Statements: Target organ(s): Kidneys. Liver.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: Yes
NOTES: This product is or contains a component that is subject to SARA313 reporting requirements.

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: No

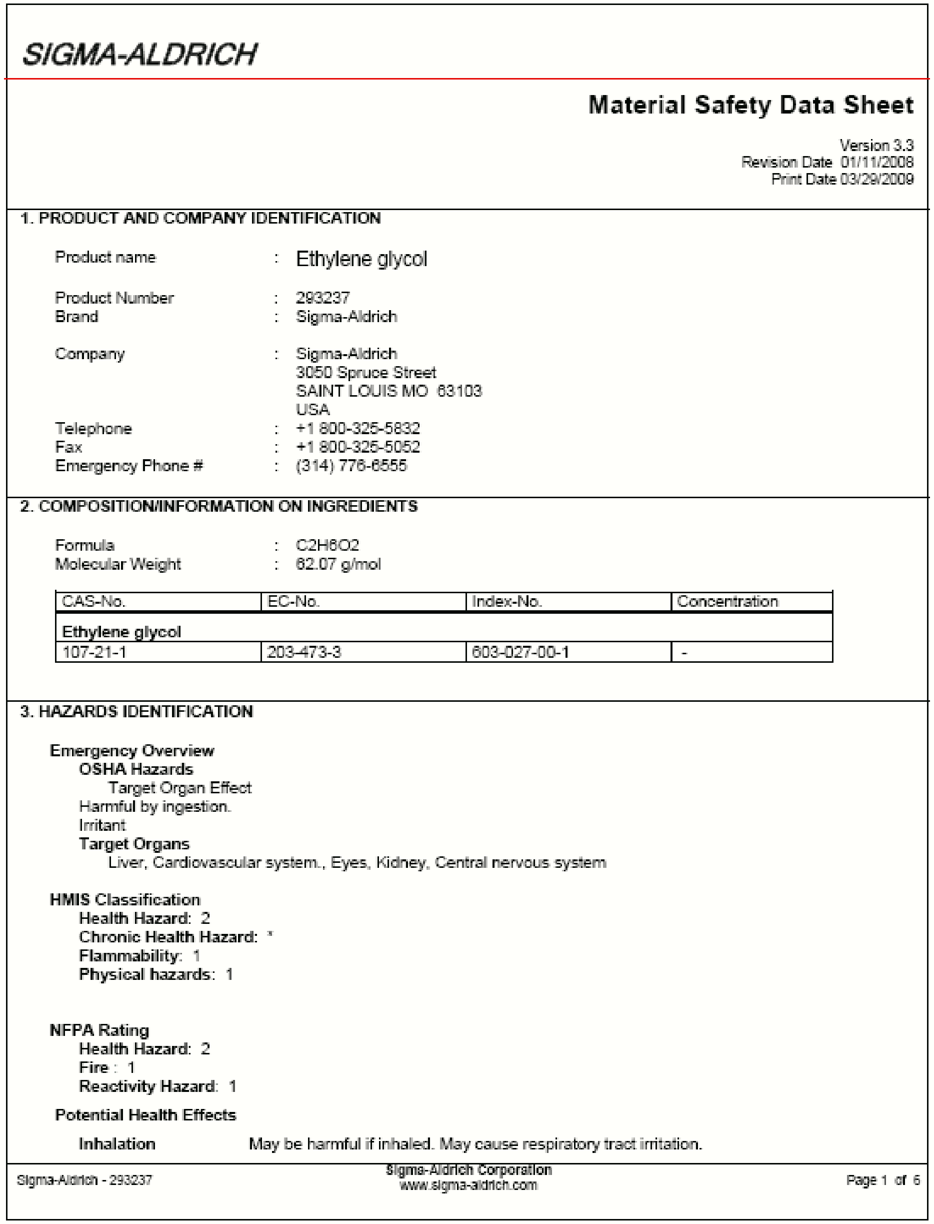
Section 16 - Other Information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

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 Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.



SIGMA-ALDRICH

Material Safety Data Sheet

Version 3.3
Revision Date 01/11/2008
Print Date 03/29/2009

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	: Ethylene glycol
Product Number	: 293237
Brand	: Sigma-Aldrich
Company	: Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	: +1 800-325-5832
Fax	: +1 800-325-5052
Emergency Phone #	: (314) 776-6555

2. COMPOSITION/INFORMATION ON INGREDIENTS

Formula : $C_2H_6O_2$
Molecular Weight : 62.07 g/mol

CAS-No.	EC-No.	Index-No.	Concentration
Ethylene glycol			
107-21-1	203-473-3	603-027-00-1	-

3. HAZARDS IDENTIFICATION

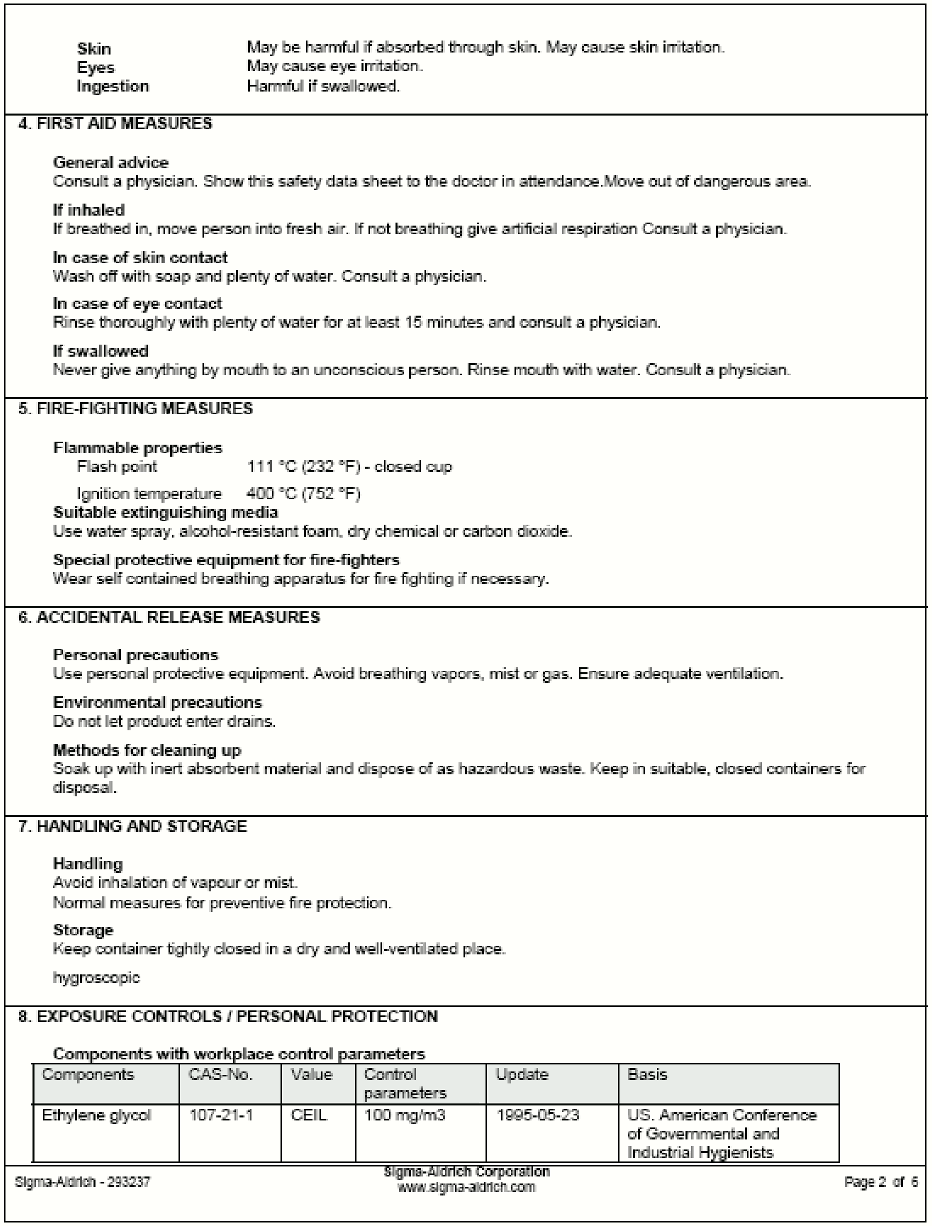
Emergency Overview
OSHA Hazards
Target Organ Effect
Harmful by ingestion.
Irritant
Target Organs
Liver, Cardiovascular system., Eyes, Kidney, Central nervous system

HMIS Classification
Health Hazard: 2
Chronic Health Hazard: *
Flammability: 1
Physical hazards: 1

NFPA Rating
Health Hazard: 2
Fire : 1
Reactivity Hazard: 1

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	Harmful if swallowed.

4. FIRST AID MEASURES

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

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

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

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

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

5. FIRE-FIGHTING MEASURES

Flammable properties

Flash point	111 °C (232 °F) - closed cup
Ignition temperature	400 °C (752 °F)

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

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

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation.

Environmental precautions
Do not let product enter drains.

Methods for cleaning up
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

7. HANDLING AND STORAGE

Handling
Avoid inhalation of vapour or mist.
Normal measures for preventive fire protection.

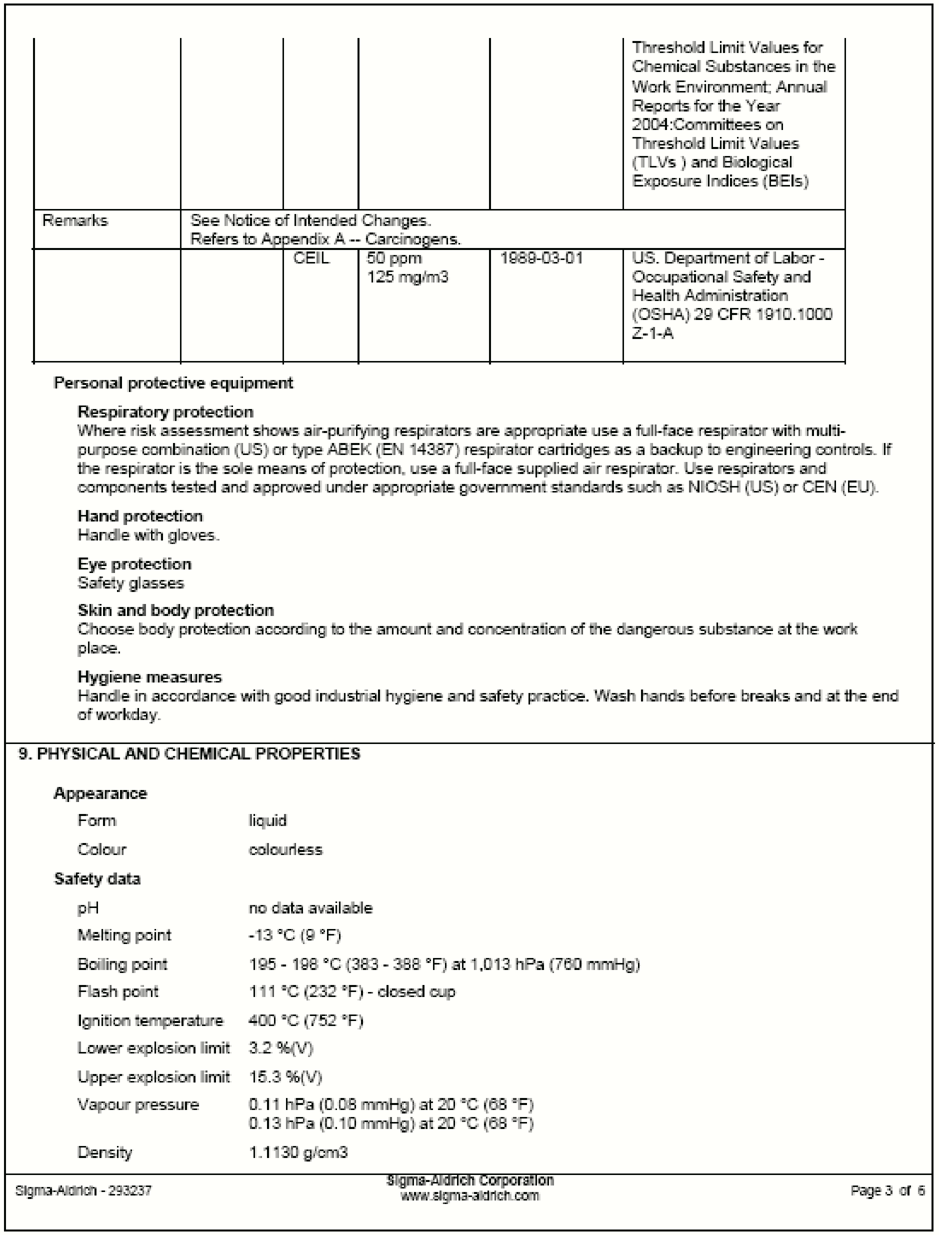
Storage
Keep container tightly closed in a dry and well-ventilated place.

hygroscopic

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Update	Basis
Ethylene glycol	107-21-1	CEIL	100 mg/m3	1995-05-23	US. American Conference of Governmental and Industrial Hygienists



					Threshold Limit Values for Chemical Substances in the Work Environment; Annual Reports for the Year 2004:Committees on Threshold Limit Values (TLVs) and Biological Exposure Indices (BEIs)
Remarks	See Notice of Intended Changes. Refers to Appendix A -- Carcinogens.				
		CEIL	50 ppm 125 mg/m3	1989-03-01	US. Department of Labor - Occupational Safety and Health Administration (OSHA) 29 CFR 1910.1000 Z-1-A

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.

Eye protection
Safety glasses

Skin and body protection
Choose body protection according to the amount and concentration of the dangerous substance at the work place.

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

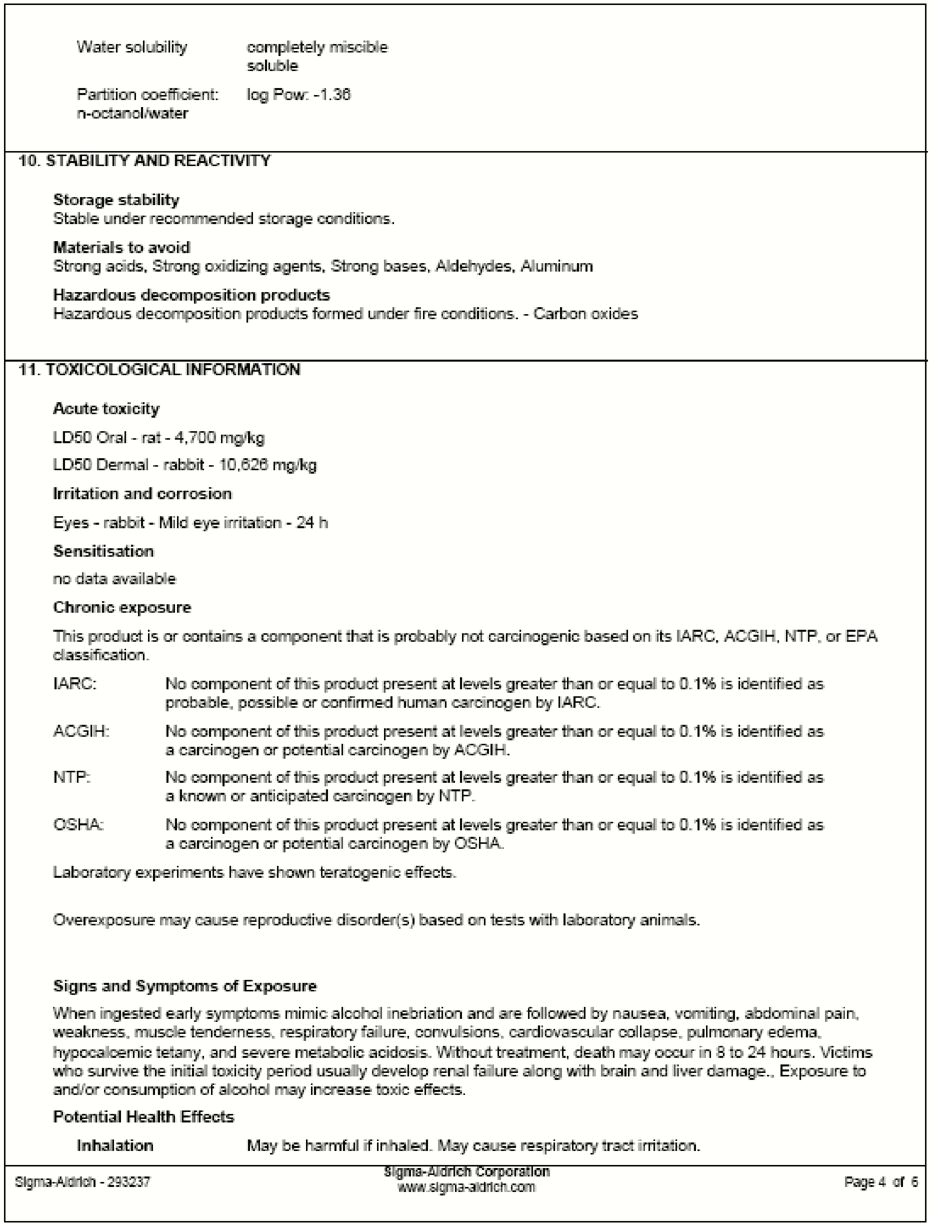
9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	liquid
Colour	colourless

Safety data

pH	no data available
Melting point	-13 °C (9 °F)
Boiling point	195 - 198 °C (383 - 388 °F) at 1,013 hPa (760 mmHg)
Flash point	111 °C (232 °F) - closed cup
Ignition temperature	400 °C (752 °F)
Lower explosion limit	3.2 %(V)
Upper explosion limit	15.3 %(V)
Vapour pressure	0.11 hPa (0.08 mmHg) at 20 °C (68 °F) 0.13 hPa (0.10 mmHg) at 20 °C (68 °F)
Density	1.1130 g/cm3



Water solubility	completely miscible soluble
Partition coefficient: n-octanol/water	log Pow: -1.38

10. STABILITY AND REACTIVITY

Storage stability
Stable under recommended storage conditions.

Materials to avoid
Strong acids, Strong oxidizing agents, Strong bases, Aldehydes, Aluminum

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

11. TOXICOLOGICAL INFORMATION

Acute toxicity

LD50 Oral - rat - 4,700 mg/kg

LD50 Dermal - rabbit - 10,626 mg/kg

Irritation and corrosion

Eyes - rabbit - Mild eye irritation - 24 h

Sensitisation

no data available

Chronic exposure

This product is or contains a component that is probably not carcinogenic based on its IARC, ACGIH, NTP, or EPA classification.

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.

Laboratory experiments have shown teratogenic effects.

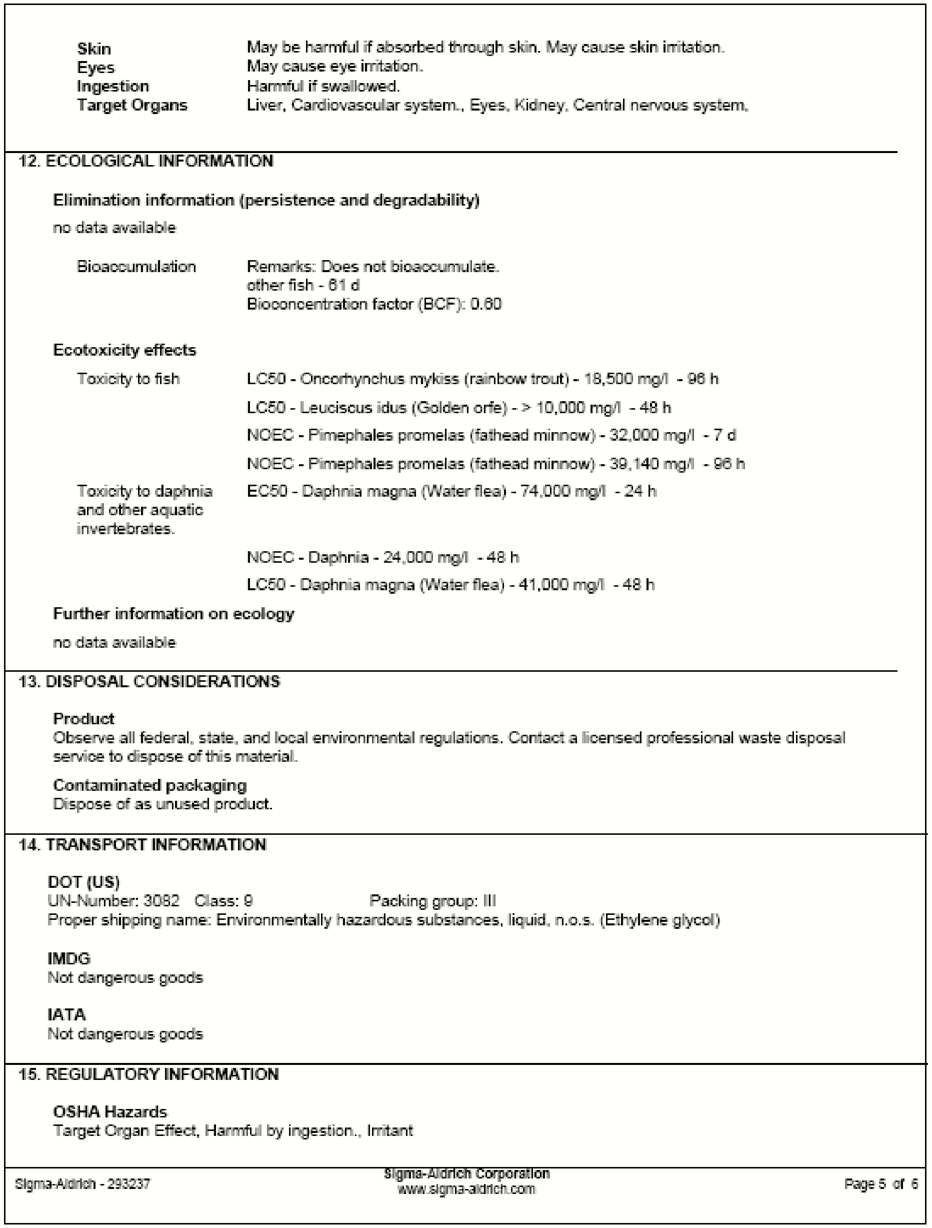
Overexposure may cause reproductive disorder(s) based on tests with laboratory animals.

Signs and Symptoms of Exposure

When ingested early symptoms mimic alcohol inebriation and are followed by nausea, vomiting, abdominal pain, weakness, muscle tenderness, respiratory failure, convulsions, cardiovascular collapse, pulmonary edema, hypocalcemic tetany, and severe metabolic acidosis. Without treatment, death may occur in 8 to 24 hours. Victims who survive the initial toxicity period usually develop renal failure along with brain and liver damage., Exposure to and/or consumption of alcohol may increase toxic effects.

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	Harmful if swallowed.
Target Organs	Liver, Cardiovascular system., Eyes, Kidney, Central nervous system,

12. ECOLOGICAL INFORMATION

Elimination information (persistence and degradability)

no data available

Bioaccumulation	Remarks: Does not bioaccumulate. other fish - 61 d Bioconcentration factor (BCF): 0.60

Ecotoxicity effects

Toxicity to fish	LC50 - Oncorhynchus mykiss (rainbow trout) - 18,500 mg/l - 96 h
	LC50 - Leuciscus idus (Golden orfe) - > 10,000 mg/l - 48 h
	NOEC - Pimephales promelas (fathead minnow) - 32,000 mg/l - 7 d
	NOEC - Pimephales promelas (fathead minnow) - 39,140 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates.	EC50 - Daphnia magna (Water flea) - 74,000 mg/l - 24 h
	NOEC - Daphnia - 24,000 mg/l - 48 h
	LC50 - Daphnia magna (Water flea) - 41,000 mg/l - 48 h

Further information on ecology

no data available

13. DISPOSAL CONSIDERATIONS

Product
Observe all federal, state, and local environmental regulations. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

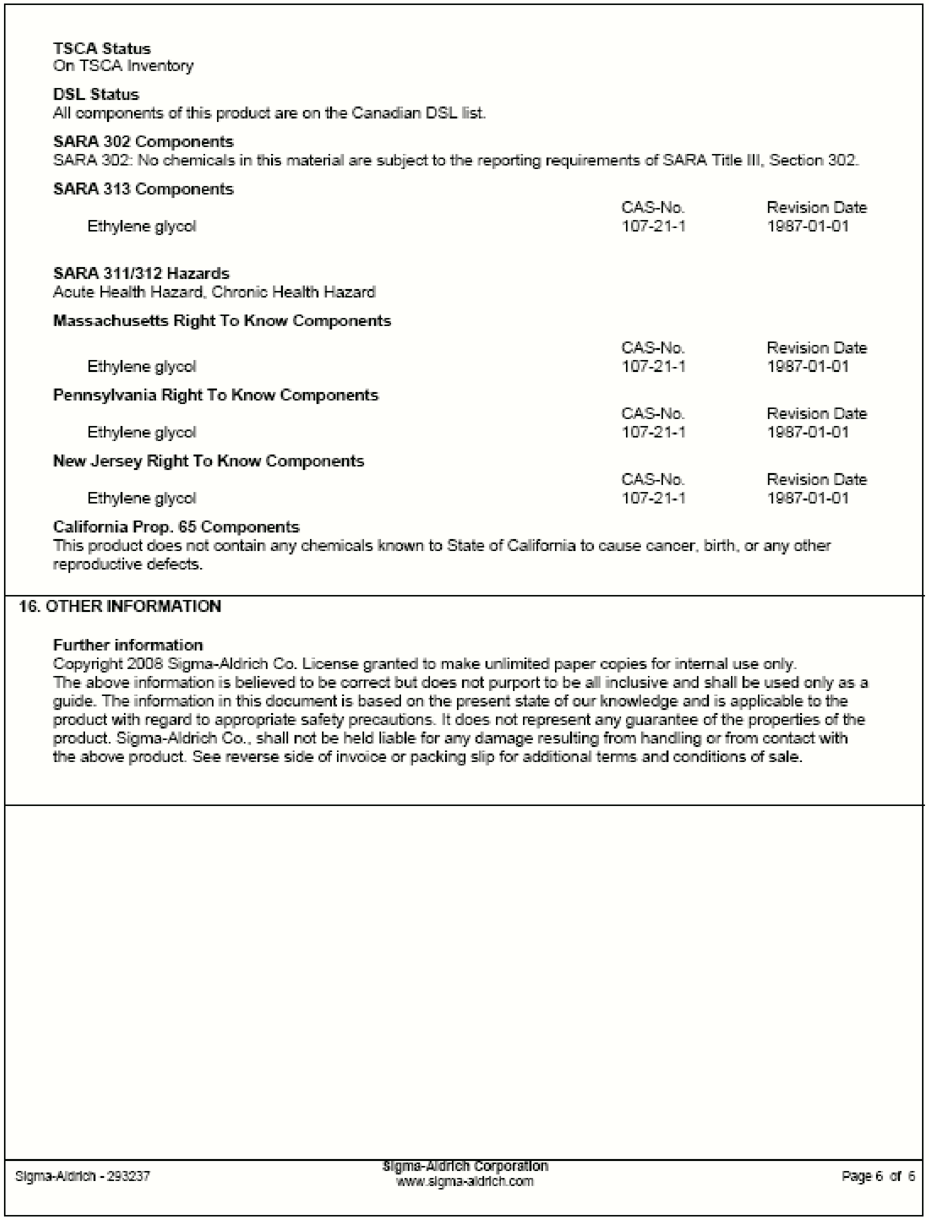
DOT (US)
UN-Number: 3082 Class: 9 Packing group: III
Proper shipping name: Environmentally hazardous substances, liquid, n.o.s. (Ethylene glycol)

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

OSHA Hazards
Target Organ Effect, Harmful by ingestion., Irritant



TSCA Status
On TSCA Inventory

DSL Status
All components of this product are on the Canadian DSL list.

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

	CAS-No.	Revision Date
Ethylene glycol	107-21-1	1987-01-01

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

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Ethylene glycol	107-21-1	1987-01-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Ethylene glycol	107-21-1	1987-01-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Ethylene glycol	107-21-1	1987-01-01

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

16. OTHER INFORMATION

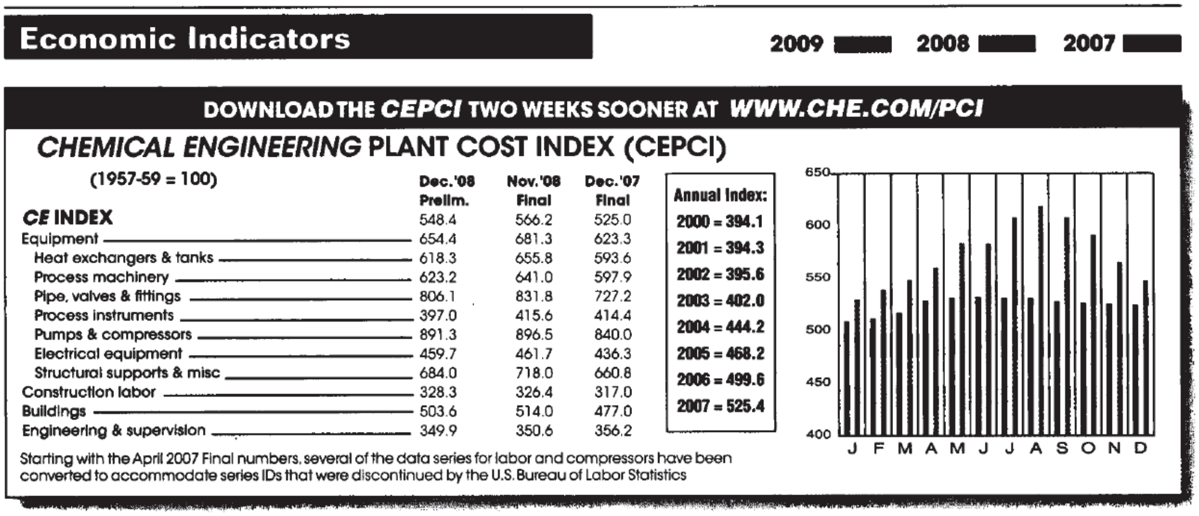
Further information

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 Co., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.

A.5 Relevant Data and Articles

Economic Indicators:

CE Index from Issue 116, Volume 3 of *Chemical Engineering* released March 2009. (Chemical Engineering, 2009)



Economic Indicators

DOWNLOAD THE *CEPCI* TWO WEEKS SOONER AT *WWW.CHE.COM/PCI*

CHEMICAL ENGINEERING PLANT COST INDEX (CEPCI)

(1957-59 = 100)

	Dec.'08 Prelim.	Nov.'08 Final	Dec.'07 Final
***CE* INDEX**	548.4	566.2	525.0
Equipment	654.4	681.3	623.3
Heat exchangers & tanks	618.3	655.8	593.6
Process machinery	623.2	641.0	597.9
Pipe, valves & fittings	806.1	831.8	727.2
Process instruments	397.0	415.6	414.4
Pumps & compressors	891.3	896.5	840.0
Electrical equipment	459.7	461.7	436.3
Structural supports & misc	684.0	718.0	660.8
Construction labor	328.3	326.4	317.0
Buildings	503.6	514.0	477.0
Engineering & supervision	349.9	350.6	356.2

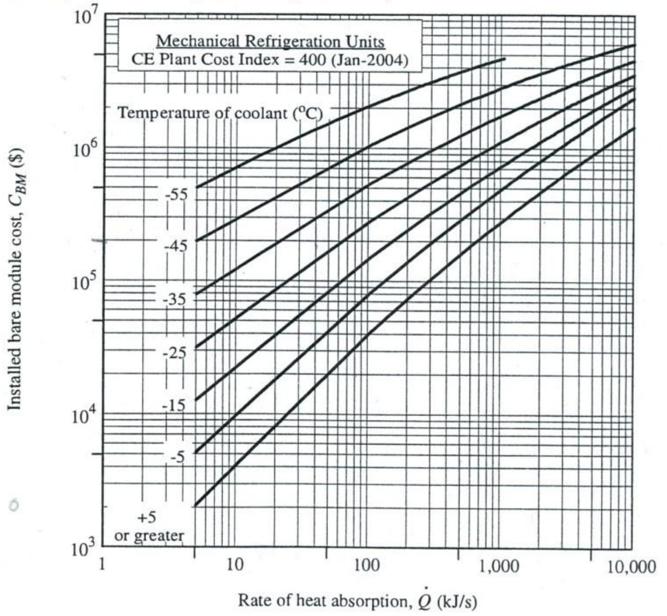
Annual Index:
2000 = 394.1
2001 = 394.3
2002 = 395.6
2003 = 402.0
2004 = 444.2
2005 = 468.2
2006 = 499.6
2007 = 525.4

Starting with the April 2007 Final numbers, several of the data series for labor and compressors have been converted to accommodate series IDs that were discontinued by the U.S. Bureau of Labor Statistics

Air-Cooled Refrigeration Unit Bare Module Cost:

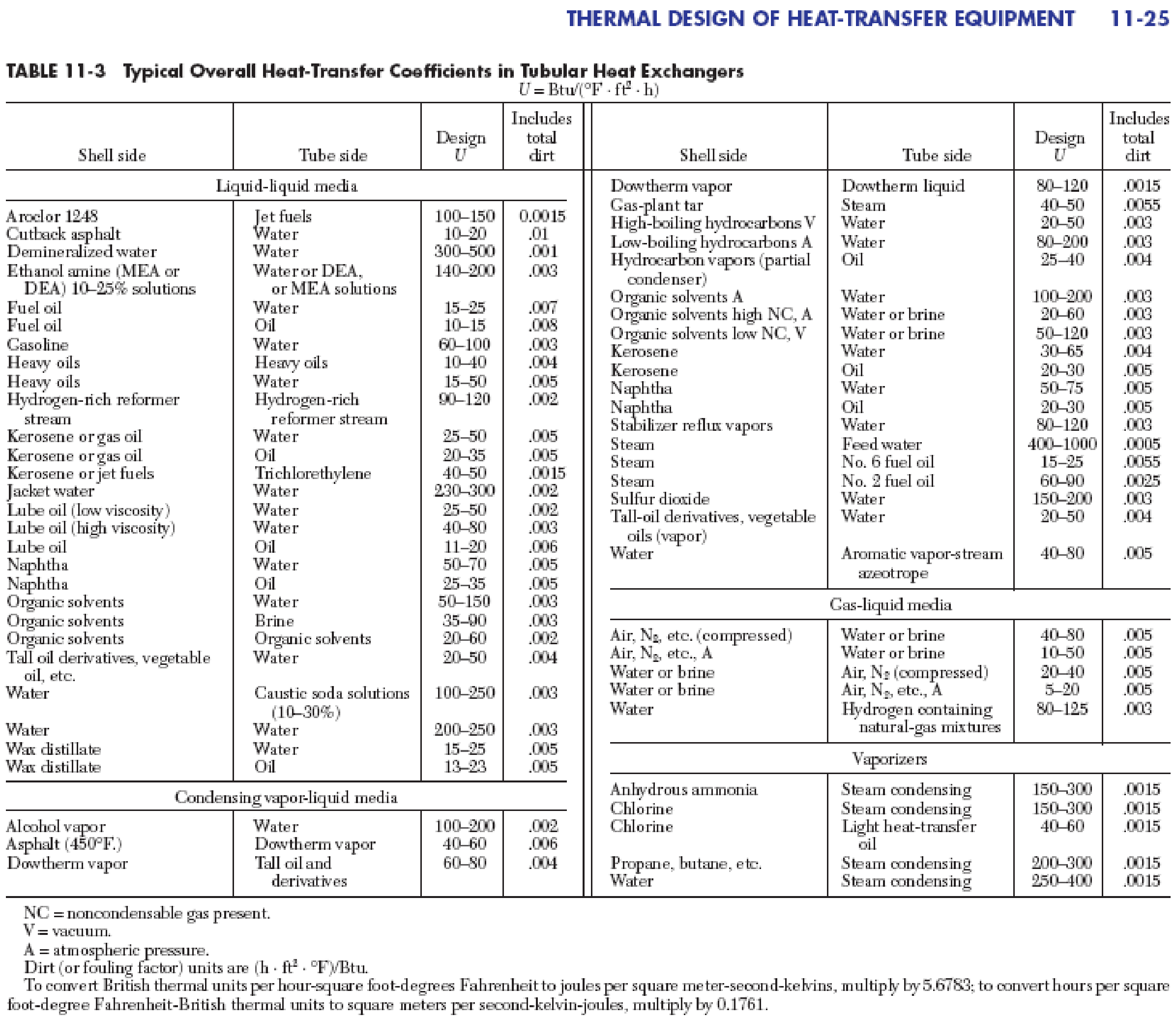
C_{BM} for air-cooled, mechanical refrigeration unit from *Chemical Engineering Process Design Economics, a Practical Guide*, *2nd Edition* (Ulrich & Vasudevem, 2004)

FIGURE 5.11 Bare module cost for air-cooled mechanical refrigeration units, complete except for the absorptive heat exchanger, which is part of main process module.



Typical Overall Heat Transfer Coefficients for Shell-and-Tube Heat Exchangers:

U from *Perry's Chemical Engineers' Handbook*, 7th Edition, page 1059. (Perry, 1999)



THERMAL DESIGN OF HEAT-TRANSFER EQUIPMENT 11-25

TABLE 11-3 Typical Overall Heat-Transfer Coefficients in Tubular Heat Exchangers

$U = \text{Btu}/(°\text{F} \cdot \text{ft}^2 \cdot \text{h})$

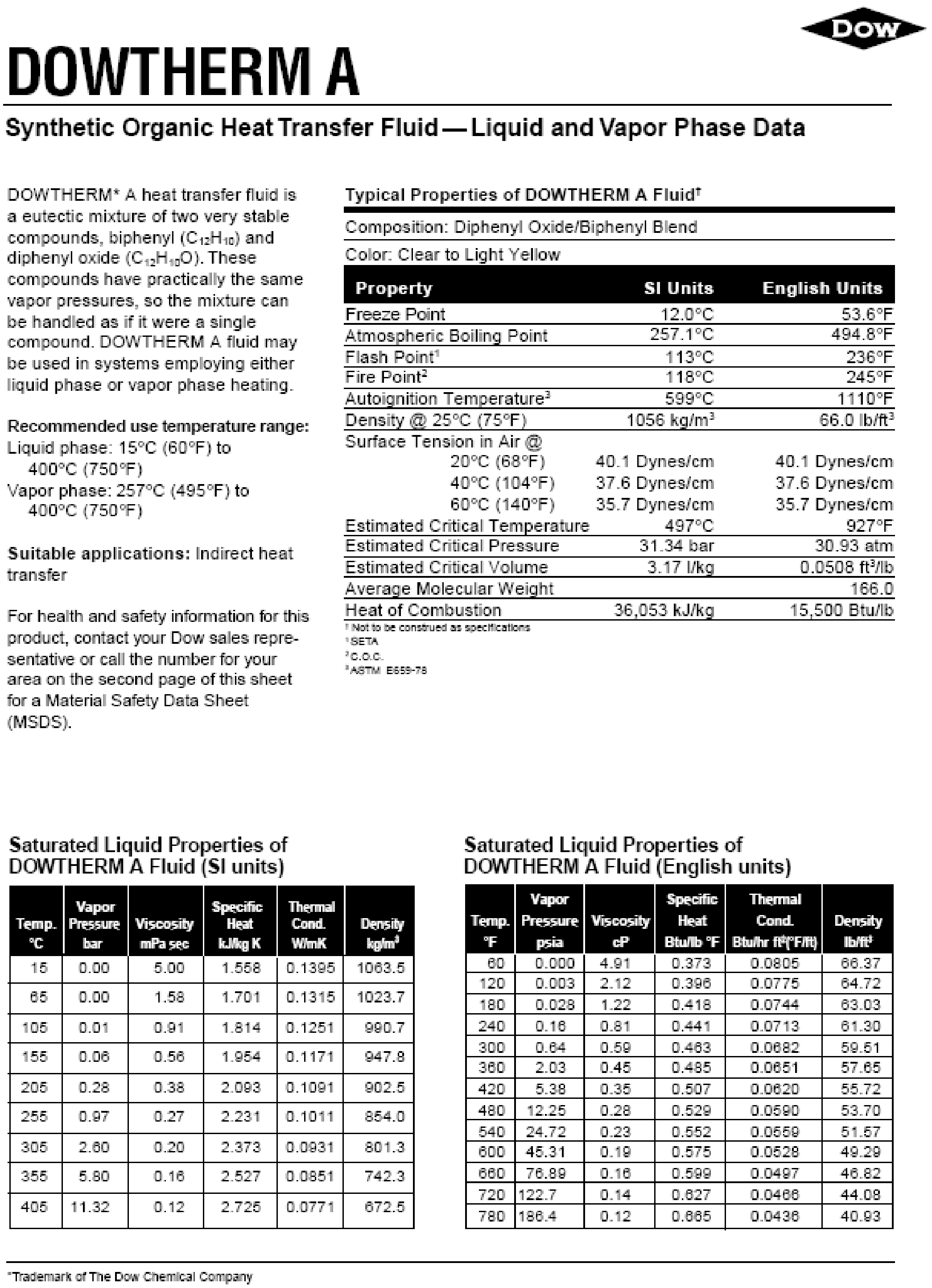
Shell side	Tube side	Design U	Includes total dirt
Liquid-liquid media			
Aroclor 1248	Jet fuels	100–150	0.0015
Cutback asphalt	Water	10–20	.01
Demineralized water	Water	300–500	.001
Ethanol amine (MEA or DEA) 10–25% solutions	Water or DEA, or MEA solutions	140–200	.003
Fuel oil	Water	15–25	.007
Fuel oil	Oil	10–15	.008
Gasoline	Water	60–100	.003
Heavy oils	Heavy oils	10–40	.004
Heavy oils	Water	15–50	.005
Hydrogen-rich reformer stream	Hydrogen-rich reformer stream	90–120	.002
Kerosene or gas oil	Water	25–50	.005
Kerosene or gas oil	Oil	20–35	.005
Kerosene or jet fuels	Trichlorethylene	40–50	.0015
Jacket water	Water	230–300	.002
Lube oil (low viscosity)	Water	25–50	.002
Lube oil (high viscosity)	Water	40–80	.003
Lube oil	Oil	11–20	.006
Naphtha	Water	50–70	.005
Naphtha	Oil	25–35	.005
Organic solvents	Water	50–150	.003
Organic solvents	Brine	35–90	.003
Organic solvents	Organic solvents	20–60	.002
Tall oil derivatives, vegetable oil, etc.	Water	20–50	.004
Water	Caustic soda solutions (10–30%)	100–250	.003
Water	Water	200–250	.003
Wax distillate	Water	15–25	.005
Wax distillate	Oil	13–23	.005
Condensing vapor-liquid media			
Alcohol vapor	Water	100–200	.002
Asphalt (450°F.)	Dowtherm vapor	40–60	.006
Dowtherm vapor	Tall oil and derivatives	60–80	.004
Dowtherm vapor	Dowtherm liquid	80–120	.0015
Gas-plant tar	Steam	40–50	.0055
High-boiling hydrocarbons V	Water	20–50	.003
Low-boiling hydrocarbons A	Water	80–200	.003
Hydrocarbon vapors (partial condenser)	Oil	25–40	.004
Organic solvents A	Water	100–200	.003
Organic solvents high NC, A	Water or brine	20–60	.003
Organic solvents low NC, V	Water or brine	50–120	.003
Kerosene	Water	30–65	.004
Kerosene	Oil	20–30	.005
Naphtha	Water	50–75	.005
Naphtha	Oil	20–30	.005
Stabilizer reflux vapors	Water	80–120	.003
Steam	Feed water	400–1000	.0005
Steam	No. 6 fuel oil	15–25	.0055
Steam	No. 2 fuel oil	60–90	.0025
Sulfur dioxide	Water	150–200	.003
Tall-oil derivatives, vegetable oils (vapor)	Water	20–50	.004
Water	Aromatic vapor-stream azeotrope	40–80	.005
Gas-liquid media			
Air, N_2, etc. (compressed)	Water or brine	40–80	.005
Air, N_2, etc., A	Water or brine	10–50	.005
Water or brine	Air, N_2 (compressed)	20–40	.005
Water or brine	Air, N_2, etc., A	5–20	.005
Water	Hydrogen containing natural-gas mixtures	80–125	.003
Vaporizers			
Anhydrous ammonia	Steam condensing	150–300	.0015
Chlorine	Steam condensing	150–300	.0015
Chlorine	Light heat-transfer oil	40–60	.0015
Propane, butane, etc.	Steam condensing	200–300	.0015
Water	Steam condensing	250–400	.0015

NC = noncondensable gas present.
V = vacuum.
A = atmospheric pressure.
Dirt (or fouling factor) units are $(\text{h} \cdot \text{ft}^2 \cdot °\text{F})/\text{Btu}$.

To convert British thermal units per hour-square foot-degrees Fahrenheit to joules per square meter-second-kelvins, multiply by 5.6783; to convert hours per square foot-degree Fahrenheit-British thermal units to square meters per second-kelvin-joules, multiply by 0.1761.

Thermophysical Data for Dowtherm A and Dowtherm SR-1:

Costs from Dow Chemical Company website, pulled on March 31, 2009. (Dow Chemical Company, 2009)



DOWTHERM A

Synthetic Organic Heat Transfer Fluid — Liquid and Vapor Phase Data

DOWTHERM* A heat transfer fluid is a eutectic mixture of two very stable compounds, biphenyl ($C_{12}H_{10}$) and diphenyl oxide ($C_{12}H_{10}O$). These compounds have practically the same vapor pressures, so the mixture can be handled as if it were a single compound. DOWTHERM A fluid may be used in systems employing either liquid phase or vapor phase heating.

Recommended use temperature range:
Liquid phase: 15°C (60°F) to 400°C (750°F)
Vapor phase: 257°C (495°F) to 400°C (750°F)

Suitable applications: Indirect heat transfer

For health and safety information for this product, contact your Dow sales representative or call the number for your area on the second page of this sheet for a Material Safety Data Sheet (MSDS).

Typical Properties of DOWTHERM A Fluid†

Composition: Diphenyl Oxide/Biphenyl Blend

Color: Clear to Light Yellow

Property	SI Units	English Units
Freeze Point	12.0°C	53.6°F
Atmospheric Boiling Point	257.1°C	494.8°F
Flash Point[1]	113°C	236°F
Fire Point[2]	118°C	245°F
Autoignition Temperature[3]	599°C	1110°F
Density @ 25°C (75°F)	1056 kg/m³	66.0 lb/ft³
Surface Tension in Air @		
20°C (68°F)	40.1 Dynes/cm	40.1 Dynes/cm
40°C (104°F)	37.6 Dynes/cm	37.6 Dynes/cm
60°C (140°F)	35.7 Dynes/cm	35.7 Dynes/cm
Estimated Critical Temperature	497°C	927°F
Estimated Critical Pressure	31.34 bar	30.93 atm
Estimated Critical Volume	3.17 l/kg	0.0508 ft³/lb
Average Molecular Weight		166.0
Heat of Combustion	36,053 kJ/kg	15,500 Btu/lb

† Not to be construed as specifications
[1] SETA
[2] C.O.C.
[3] ASTM E659-78

Saturated Liquid Properties of DOWTHERM A Fluid (SI units)

Temp. °C	Vapor Pressure bar	Viscosity mPa sec	Specific Heat kJ/kg K	Thermal Cond. W/mK	Density kg/m³
15	0.00	5.00	1.558	0.1395	1063.5
65	0.00	1.58	1.701	0.1315	1023.7
105	0.01	0.91	1.814	0.1251	990.7
155	0.06	0.56	1.954	0.1171	947.8
205	0.28	0.38	2.093	0.1091	902.5
255	0.97	0.27	2.231	0.1011	854.0
305	2.60	0.20	2.373	0.0931	801.3
355	5.80	0.16	2.527	0.0851	742.3
405	11.32	0.12	2.725	0.0771	672.5

Saturated Liquid Properties of DOWTHERM A Fluid (English units)

Temp. °F	Vapor Pressure psia	Viscosity cP	Specific Heat Btu/lb °F	Thermal Cond. Btu/hr ft²(°F/ft)	Density lb/ft³
60	0.000	4.91	0.373	0.0805	66.37
120	0.003	2.12	0.396	0.0775	64.72
180	0.028	1.22	0.418	0.0744	63.03
240	0.16	0.81	0.441	0.0713	61.30
300	0.64	0.59	0.463	0.0682	59.51
360	2.03	0.45	0.485	0.0651	57.65
420	5.38	0.35	0.507	0.0620	55.72
480	12.25	0.28	0.529	0.0590	53.70
540	24.72	0.23	0.552	0.0559	51.57
600	45.31	0.19	0.575	0.0528	49.29
660	76.89	0.16	0.599	0.0497	46.82
720	122.7	0.14	0.627	0.0466	44.08
780	186.4	0.12	0.665	0.0436	40.93

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*Trademark of The Dow Chemical Company

Product Information

DOWTHERM SR-1

Inhibited Ethylene Glycol-based Heat Transfer Fluid

DOWTHERM* SR-1 heat transfer fluid is a formulation of 95.5 weight percent ethylene glycol and a specially designed package of industrial corrosion inhibitors. The fluid is dyed fluorescent pink for leak detection purposes. Solutions in water provide freeze protection to below -50°C (-60°F) and burst protection to below -73°C (-100°F).

Recommended use temperature range: -50°C (-60°F) to 120°C (250°F).

Suitable applications: closed-loop, water-based HVAC, process heating and cooling, food industry applications within temperature range

For health and safety information for this product, contact your Dow sales representative or call the number for your area on the second page of this sheet for a Material Safety Data Sheet (MSDS).

Typical Concentrations of DOWTHERM SR-1 Fluid Required to Provide Freeze and Burst Protection at Various Temperatures

Temperature °C	(°F)	Percent DOWTHERM SR-1 Fluid Concentration Required: For Freeze Protection Volume %	For Burst Protection Volume %
-7	(20)	16.8	11.5
-12	(10)	26.2	17.8
-18	(0)	34.6	23.1
-23	(-10)	40.9	27.3
-29	(-20)	46.1	31.4
-34	(-30)	50.3	31.4
-40	(-40)	54.5	31.4
-46	(-50)	58.7	31.4
-51	(-60)	62.9	31.4

NOTE: These figures are examples only and may not be appropriate to your situation. Generally, for an extended margin of protection, you should select a temperature in this table that is at least 3°C (5°F) lower than the expected lowest ambient temperature. Inhibitor levels should be adjusted for solutions of less than 30% glycol. Contact Dow for information on specific cases or further assistance.

ATTENTION: These are typical numbers only and are not to be regarded as specifications. As use conditions are not within its control, Dow does not guarantee results from use of the information or products herein; and gives no warranty, express or implied.

Typical Freezing and Boiling Points of DOWTHERM SR-1 Fluid[†]

Wt. % Ethylene Glycol	Vol. % Ethylene Glycol	Wt. % DOWTHERM SR-1	Vol. % DOWTHERM SR-1	Freezing Point °C	(°F)	Boiling Point °C @ 101 kPa	(°F @ 760 mmHG)	Degree Brix[††]	Refractive Index 22°C (72°F)
0.0	0.0	0.0	0.0	0	(32.0)	100.0	(212)	0.0	1.3328
5.0	4.4	5.2	4.6	-1.4	(29.4)	100.6	(213)	3.8	1.3378
10.0	8.9	10.5	9.3	-3.2	(26.2)	101.1	(214)	6.8	1.3428
15.0	13.6	15.7	14.2	-5.4	(22.2)	101.7	(215)	9.9	1.3478
20.0	18.1	20.9	19.0	-7.8	(17.9)	102.2	(216)	13.0	1.3530
25.0	22.9	26.2	24.0	-10.7	(12.7)	103.3	(218)	16.1	1.3582
30.0	27.7	31.4	29.0	-14.1	(6.7)	104.4	(220)	19.2	1.3635
35.0	32.6	36.6	34.1	-17.9	(-0.2)	105.0	(221)	22.3	1.3688
40.0	37.5	41.9	39.3	-22.3	(-8.1)	105.6	(222)	25.3	1.3741
45.0	42.5	47.1	44.5	-27.5	(-17.5)	106.7	(224)	28.3	1.3796
50.0	47.6	52.4	49.8	-33.8	(-28.9)	107.2	(225)	31.2	1.3849
55.0	52.7	57.6	55.2	-41.1	(-42.0)	108.3	(227)	33.9	1.3900
60.0	57.8	62.8	60.5	-48.3	(-54.9)	110.0	(230)	36.6	1.3952
65.0	62.8	68.0	65.8	a		112.8	(235)	39.1	1.4003
70.0	68.3	73.3	71.5	a		116.7	(242)	41.7	1.4055
75.0	73.6	78.5	77.1	a		120.0	(248)	44.2	1.4107
80.0	78.9	83.8	82.6	-46.8	(-52.2)	123.9	(255)	46.6	1.4159
85.0	84.3	89.0	88.3	-36.9	(-34.5)	133.9	(273)	49.0	1.4208
90.0	89.7	94.2	93.9	-29.8	(-21.6)	140.6	(285)	51.2	1.4255
95.0	95.0	99.5	99.5	-19.4	(-3.0)	158.3	(317)	53.2	1.4300

[†] Typical properties, not to be construed as specifications.

[††] Degree Brix is a measure of the sugar concentration in a fluid and is important in fermentation and syrups applications. Although there is no sugar present in DOWTHERM heat transfer fluids, the glycol affects the refractive index of the fluid in a similar fashion.

[a] Freezing points are below -50°C (-60°F).

NOTE: Generally, for an extended margin of protection, you should select a temperature in this table that is at least 3°C (5°F) lower than the expected lowest ambient temperature. Inhibitor levels should be adjusted for solutions of less than 30% glycol. Contact Dow for information on specific cases or further assistance.

DOWTHERM SR-1
Inhibited Ethylene Glycol-based Heat Transfer Fluid

Typical Properties[†] of DOWTHERM SR-1 Fluid

	DOWTHERM SR-1 Heat Transfer Fluid
Composition (% by weight)	
Ethylene Glycol	95.5
Performance Additives	4.5
Color	Fluorescent Pink
Specific Gravity 25/25° (77/77°F)	1.1250–1.1350
pH of Solution (50% glycol)	9.0–10.5
Reserve Alkalinity (min.)	12.0 ml

[†] Typical properties, not to be construed as specifications. Complete sales specifications are available on request.

Saturation Properties of DOWTHERM SR-1 Fluid at 30% Ethylene Glycol Concentration by Volume

Temp. °C	(°F)	Specific Heat kJ/(kg)(K)	(Btu/lb°F)	Density kg/m³	(lb/ft³)	Therm. Cond. W/mK	[Btu/hr ft² (°F/ft)]	Viscosity mPa·s	(cps)
-10	(14)	3.562	(0.851)	1055.47	(65.89)	0.4154	(0.2400)	6.1788	(6.18)
10	(50)	3.619	(0.865)	1049.91	(65.54)	0.4420	(0.2554)	2.9482	(2.95)
40	(104)	3.704	(0.885)	1037.92	(64.80)	0.4731	(0.2733)	1.3398	(1.34)
65	(149)	3.775	(0.902)	1024.59	(63.96)	0.4909	(0.2836)	0.8246	(0.82)
90	(194)	3.846	(0.919)	1008.20	(62.94)	0.5015	(0.2897)	0.5599	(0.56)
120	(248)	3.931	(0.939)	984.53	(61.46)	0.5044	(0.2915)	0.3846	(0.38)

Saturation Properties of DOWTHERM SR-1 Fluid at 40% Ethylene Glycol Concentration by Volume

Temp. °C	(°F)	Specific Heat kJ/(kg)(K)	(Btu/lb°F)	Density kg/m³	(lb/ft³)	Therm. Cond. W/mK	[Btu/hr ft² (°F/ft)]	Viscosity mPa·s	(cps)
-20	(-4)	3.336	(0.797)	1073.23	(67.00)	0.3707	(0.2142)	15.7533	(15.75)
10	(50)	3.436	(0.821)	1064.73	(66.47)	0.4053	(0.2342)	4.0451	(4.05)
40	(104)	3.537	(0.845)	1051.85	(65.66)	0.4312	(0.2491)	1.7731	(1.77)
65	(149)	3.621	(0.865)	1037.76	(64.79)	0.4462	(0.2578)	1.0646	(1.06)
90	(194)	3.705	(0.885)	1020.63	(63.72)	0.4552	(0.2630)	0.7013	(0.70)
120	(248)	3.805	(0.909)	996.06	(62.18)	0.4582	(0.2647)	0.4614	(0.46)

Saturation Properties of DOWTHERM SR-1 Fluid at 50% Ethylene Glycol Concentration by Volume

Temp. °C	(°F)	Specific Heat kJ/(kg)(K)	(Btu/lb°F)	Density kg/m³	(lb/ft³)	Therm. Cond. W/mK	[Btu/hr ft² (°F/ft)]	Viscosity mPa·s	(cps)
-30	(-22)	3.090	(0.739)	1090.31	(68.07)	0.3333	(0.1926)	43.9970	(44.00)
-20	(-4)	3.129	(0.748)	1088.15	(67.93)	0.3442	(0.1989)	22.0816	(22.08)
10	(50)	3.245	(0.776)	1078.72	(67.34)	0.3724	(0.2152)	5.5071	(5.51)
40	(104)	3.361	(0.803)	1064.91	(66.48)	0.3937	(0.2275)	2.2567	(2.26)
65	(149)	3.457	(0.826)	1050.05	(65.55)	0.4062	(0.2347)	1.2936	(1.29)
90	(194)	3.554	(0.849)	1032.15	(64.44)	0.4139	(0.2391)	0.8227	(0.82)
120	(248)	3.670	(0.877)	1006.66	(62.84)	0.4168	(0.2408)	0.5252	(0.53)

For further information, call...

In the United States and Canada: 1-800-447-4369 • FAX: 1-989-832-1465
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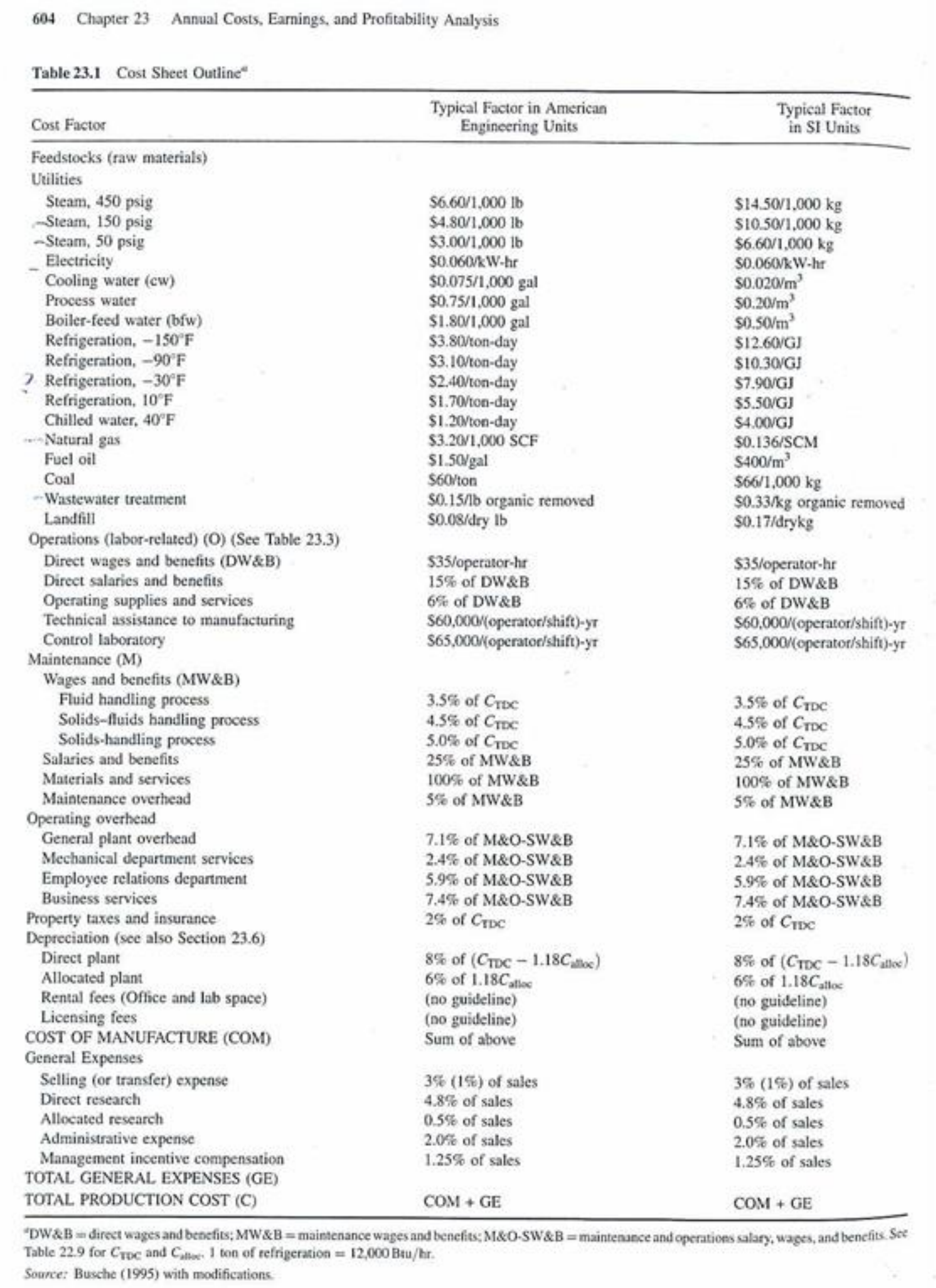
Estimated Utility Costs:

Costs from *Product and Process Design Principles*, 3rd Edition, page 604. (Seider, Seader, Lewin, & Widagdo, 2009)



604 Chapter 23 Annual Costs, Earnings, and Profitability Analysis

Table 23.1 Cost Sheet Outline[a]

Cost Factor	Typical Factor in American Engineering Units	Typical Factor in SI Units
Feedstocks (raw materials)		
Utilities		
Steam, 450 psig	\$6.60/1,000 lb	\$14.50/1,000 kg
Steam, 150 psig	\$4.80/1,000 lb	\$10.50/1,000 kg
Steam, 50 psig	\$3.00/1,000 lb	\$6.60/1,000 kg
Electricity	\$0.060/kW-hr	\$0.060/kW-hr
Cooling water (cw)	\$0.075/1,000 gal	\$0.020/m³
Process water	\$0.75/1,000 gal	\$0.20/m³
Boiler-feed water (bfw)	\$1.80/1,000 gal	\$0.50/m³
Refrigeration, −150°F	\$3.80/ton-day	\$12.60/GJ
Refrigeration, −90°F	\$3.10/ton-day	\$10.30/GJ
Refrigeration, −30°F	\$2.40/ton-day	\$7.90/GJ
Refrigeration, 10°F	\$1.70/ton-day	\$5.50/GJ
Chilled water, 40°F	\$1.20/ton-day	\$4.00/GJ
Natural gas	\$3.20/1,000 SCF	\$0.136/SCM
Fuel oil	\$1.50/gal	\$400/m³
Coal	\$60/ton	\$66/1,000 kg
Wastewater treatment	\$0.15/lb organic removed	\$0.33/kg organic removed
Landfill	\$0.08/dry lb	\$0.17/drykg
Operations (labor-related) (O) (See Table 23.3)		
Direct wages and benefits (DW&B)	\$35/operator-hr	\$35/operator-hr
Direct salaries and benefits	15% of DW&B	15% of DW&B
Operating supplies and services	6% of DW&B	6% of DW&B
Technical assistance to manufacturing	\$60,000/(operator/shift)-yr	\$60,000/(operator/shift)-yr
Control laboratory	\$65,000/(operator/shift)-yr	\$65,000/(operator/shift)-yr
Maintenance (M)		
Wages and benefits (MW&B)		
Fluid handling process	3.5% of C_{TDC}	3.5% of C_{TDC}
Solids–fluids handling process	4.5% of C_{TDC}	4.5% of C_{TDC}
Solids-handling process	5.0% of C_{TDC}	5.0% of C_{TDC}
Salaries and benefits	25% of MW&B	25% of MW&B
Materials and services	100% of MW&B	100% of MW&B
Maintenance overhead	5% of MW&B	5% of MW&B
Operating overhead		
General plant overhead	7.1% of M&O-SW&B	7.1% of M&O-SW&B
Mechanical department services	2.4% of M&O-SW&B	2.4% of M&O-SW&B
Employee relations department	5.9% of M&O-SW&B	5.9% of M&O-SW&B
Business services	7.4% of M&O-SW&B	7.4% of M&O-SW&B
Property taxes and insurance	2% of C_{TDC}	2% of C_{TDC}
Depreciation (see also Section 23.6)		
Direct plant	8% of $(C_{TDC} - 1.18C_{alloc})$	8% of $(C_{TDC} - 1.18C_{alloc})$
Allocated plant	6% of $1.18C_{alloc}$	6% of $1.18C_{alloc}$
Rental fees (Office and lab space)	(no guideline)	(no guideline)
Licensing fees	(no guideline)	(no guideline)
COST OF MANUFACTURE (COM)	Sum of above	Sum of above
General Expenses		
Selling (or transfer) expense	3% (1%) of sales	3% (1%) of sales
Direct research	4.8% of sales	4.8% of sales
Allocated research	0.5% of sales	0.5% of sales
Administrative expense	2.0% of sales	2.0% of sales
Management incentive compensation	1.25% of sales	1.25% of sales
TOTAL GENERAL EXPENSES (GE)		
TOTAL PRODUCTION COST (C)	COM + GE	COM + GE

[a] DW&B = direct wages and benefits; MW&B = maintenance wages and benefits; M&O-SW&B = maintenance and operations salary, wages, and benefits. See Table 22.9 for C_{TDC} and C_{alloc}. 1 ton of refrigeration = 12,000 Btu/hr.

Source: Busche (1995) with modifications.

A.6 Relevant Correspondence

This section contains all relevant correspondence between the design team and our professors, industrial consultants, and industrial consultant advisor. A significant amount of information was provided to the team via email, and it is included here for the reader's reference.

Subject: **Re: Kinetics Information for Design Project**
Date: **Thu, 15 Jan 2009 16:23:46 EST [01/15/2009 04:23:46 PM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu**
Cc: **seider@seas.upenn.edu**

Hi Michael, Daniyal, Kathleen;

I'm glad you are getting an early start on this design project and you have started to look into the reactor which is likely to be the most difficult step to model in ASPEN.

The reaction does take place in a single CSTR reactor with liquid feed (maleic+H2O), liquid recycle (GBL+H2O+some intermediates) and vapor product (THF+H2+ByPr+some intermediates). The reaction of maleic to THF is a series of steps, each adding one or two H2 except for the BDO --> THF + H2O which is a ring closure. The reaction of maleic to THF actually uses five H2. The reactions all take place using Pd/Re on a carbon support catalyst. The reaction rate constants are for this catalyst.

The reaction does not occur all at once but is actually relatively slow as can be seen by the STY value of 500 lbs/hr THF/1000 lbs catalyst.

There are two major modeling problems around the reactor:

1.) the reaction kinetics: The rate is essentially independent of the organics, i.e. if the feed concentration is doubled it takes twice as long to reach the same fractional conversion to THF. The reactor was modeled in ASPEN using a FORTRAN subroutine. Current versions of ASPEN may have more flexibility/options for reaction kinetic models and we can discuss this.

2.) the energy balance: The reactor is adiabatic, the heat of reaction (along with feed temperature) must evaporate the THF, H2O and ByPr made. You need to design a control system which will do this.

This is a commercial plant and the process was modeled in the 1980's using an earlier version of ASPEN.

If you have any questions feel free to call (302) 475-1966.

I will be at UPenn next Tuesday. My train schedule gets me to campus about 11:15 so we could meet at lunch time if you want to discuss further.

Wayne Robbins

Subject: **Reactor Exit Flow**

Date: **Wed, 21 Jan 2009 09:34:35 EST [01/21/2009 09:34:35 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu**
Cc: **seider@seas.upenn.edu**

Hi Michael, Daniyal, Kathleen;

As we discussed yesterday, I am providing the reactor exit flows to help you get started on the down stream flowsheet. The flows are from a converged model run with the kinetics reactor model. All flows are in LbMol/hr.

Comp	Flow
H2O	1512
GBL	45
BDO	3
THF	184
H2	2929
CH4	35
C3H8	3
C4H10	12
PrOH	8
BuOH	11
N2	46

T=250 C, P=2000 psi, Vfrac=1

As you run the flowsheet model you will see what happens to the BuOH and PrOH. You may need to add additional unit ops to separate them from the THF.

Wayne Robbins

Subject: **Membrane Performance**

Date: **Wed, 21 Jan 2009 09:51:21 EST [01/21/2009 09:51:21 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu**
Cc: **seider@seas.upenn.edu**

Hi Michael, Daniyal, Kathleen;

Your flowsheet includes a block SEP1 to separate recycle H_2 from alkanes. You will need to find a vendor to supply the membrane but for now use the following separations:

Comp	Frac
H_2O	0.99
H_2	0.99
THF	0.125
CH_4	0.20
C_3H_8	0.125
C_4H_{10}	0.125
N_2	0.25
All others	~0

Frac is the fraction of feed thru the membrane.

Wayne Robbins

Subject: **Re: Design Project**

Date: **Thu, 29 Jan 2009 11:33:44 EST [01/29/2009 11:33:44 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu**
Cc: **SEIDER@seas.upenn.edu**

Hi Michael, Daniyal, Kathleen,

You have quite a list of questions from your Week 2 meeting. I will answer the questions on your Week 2 Word document first and then your questions contained in your EMail of 1/28/09.

1.) Reactor Design

a. If the reactions and VLE are done in separate blocks it will not properly simulate the rapid removal of the THF from the liquid phase by the excess H_2 flow. Also, the REQUIL block is for equilibrium reactions (not VLE, i.e. Vapor-Liquid Equil) and should not be used for kinetic reactions.

b. If you use the RADFRAC block you could use a REACTIONS block if the reactions were of the power law form:

Rate = k*A^m*B^n....

and then specify which stages had reactions. (Note: This method was used for earlier versions of ASPEN, current versions may incorporate the kinetics directly into the RADFRAC block.)

The actual reactions have a denominator term which may or may not be allowed in current versions of ASPEN. We wrote a FORTRAN subroutine which called the concentrations, did the rate calculations and returned the rates to the RADFRAC block.

c. If you want to use hydrogenated catalyst as a basis for reaction kinetics you need to pick two high boiling components which differ by a H_2. For the two you pick check their VLE with H_2O. High activity coefficients could cause them to go into the vapor even though they are high boilers.

d. Yes the liquid feed comes in on stage 1 (top of distl column).

e. The reactor exit composition was provided on a temporary basis to allow the downstream modeling to proceed. Its composition may vary somewhat based on your model runs. No other streams will be provided.

2.) Separation Design

a. Where/how the BuOH and PrOH are removed is part of the design problem you need to solve. There are significant activity coefficients involved and it is difficult to predict ahead of time where they will end up. Run the THF/H_2O separation and go from there.

b. I would suggest you make some VLE diagrams of the THF/H_2O separation at atmospheric pressure and at a higher pressure so you can see how the curves shift. These are very non-ideal multi component systems and you need to run rigorous distilation blocks, i.e. RADFRAC.

ci. Use two RADFRAC blocks for the pressure swing distl columns. DSTWU is a simplified estimation method and I doubt it will work for these separations.

cii. Any pair of VLE or T-x-y diagrams will be helpful in understanding the pressure swing distillation. I am sure Dr Seider's book will be very helpful.

ciii. There is nothing magical about the two pressures used. The first column is usually atmospheric pressure but the second column can vary. We used 100 psig (115 psia, 7.8 bar) and had overheads compositions of 12 - 13.5% H2O. A higher pressure (10 bar) in the second column would allow higher than 12 - 13.5% H2O in the overheads and reduce the interflow. It's your choice.

Wayne Robbins

Subject: **Re: Design Project**

Date: **Thu, 29 Jan 2009 12:09:56 EST [01/29/2009 12:09:56 PM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu**
Cc: **SEIDER@seas.upenn.edu**

Hi Michael, Daniyal, Kathleen,

Here are answers to questions in your EMail of 1/28/09.

The reactor is essentially isothermal. However, the operating temperature can be varied. Note: The reaction rate constant equations were simply centered on 250 C (523 K), the rates do vary with reactor temperature.

The b,c and d terms were used in fitting the experimental data. See the second page of the reaction kinetics Word document for an explination of their values.

Any time a molecule loses an oxygen it will show up as H2O. Also, any time a molecule loses a carbon it will show up as CH4. So a CH4 is made for each PrOH or propane made.

The H2 feed is all H2. The N2 represents the small amount of N2 brought into the system from instruments and padding. The N2 is probably too much detail for this model and you can omit it.

This was 20 years ago and I wish I had written down the units. Since the equations went directly into an ASPEN model I believe they rates are in the standard ASPEN units moles/sec/vol where vol is really in terms of catalyst wt. For the rate constant, the H2 pressure is the vapor phase partial pressure in psi. The catalyst weight was in lbs.

A rigorous reactor model may be too complex for modeling at this point in time. I can recommend some alternate solutions to simplify the problem. It would be best if we met with Dr Seider to discuss them. I will be at UPenn on Tuesday, Feb 3rd. I could come early and we meet in the late morning if this is OK.

Wayne Robbins

Subject: **Follow-up on Tuesday questions**

Date: **Wed, 4 Feb 2009 10:11:18 EST [02/04/2009 10:11:18 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu, seider@seas.upenn.edu**
Cc: **heresdanny@gmail.com, dmicha@seas.upenn.edu, lfabiano@seas.upenn.edu**

Good morning Michael, Daniyal, Kathleen,

Here are answers for some of the questions from our meeting on Tuesday.

1.) The large amount of H2 in the liquid phase and the problem with the condensers in the distillation column is probably a result of not specifying that certain components are non-condensable super critical components. These components follow Henry's Law (you can read about it in your text books) and must be specified in the INPUT file. In the old days it was entered as HENLIST but has probably been updated. ASPEN contains the Henry's constants for most components in water and since there is water in virtually every stream ASPEN should have no problems. Specify the following as Henry's components: H2, Methane, Propane, Butane

2.) There should be only a small amount of H2 going to the distillation columns. If you still have problems with the condensers on the distillation column, allow for a small purge stream by setting Vfrac at a small value or setting the condenser temperature and letting it determine the purge rate.

3.) Most chemical plants on the Gulf coast use cooling tower water (CTW) for the heat exchangers. The limiting temperature of the CTW is determined by ambient conditions. In the summer it is often 90 & 90 (90 F and 90% humidity and two steps after leaving the A/C control room you are soaking wet). These conditions determine the CTW temperature. Also, you need to keep the process side about 5 C or 10 F higher in temperature to allow for reasonable dT driving force for heat transfer.

4.) It looks like ASPEN can now handle a denominator term in the kinetics equation. The problem is that using the H2 in the liquid phase as the driving force (instead of the H2 partial pressure in the vapor phase as we did in our FORTRAN subroutine) will give you a rate that is much too slow. I suggest you set up the equations and then adjust rates so that the catalyst makes 600 STY. Note: Adjust all rates up or down together, the relative rates should stay the same.

5.) Since the by-product reactions give a certain split of alcohol and alkane I suggest you have only one by-product reaction for each species, GBL, BDO, THF. That is instead of having four reactions:
GBL -> BuOH
GBL -> Butane
GBL -> PrOH + methane
GBL -> Propane + Methane
have it be:
GBL -> m BuOH + n butane + o PrOH + p propane + (o+p)Methane
where m, n, o and p are the respective splits

6.) What happens to the BuOH and PrOH? I would suggest this approach: Set up the distillation columns you know you need, i.e. GBL/intermediates recycle column and the two pressure swing distillation columns. Get these set up and running without BuOH and PrOH in the feeds. Then add a small amount of the alcohols to the feed and see where they want to go in the system. At this point you can decide where is the best point to remove the alcohols.

Wayne Robbins

Subject: **A request and follow-up on item 5**

Date: **Thu, 5 Feb 2009 09:05:56 EST [02/05/2009 09:05:56 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu, seider@seas.upenn.edu**
Cc: **heresdanny@gmail.com, dmicha@seas.upenn.edu, lfabiano@seas.upenn.edu**

Hi Michael, Daniyal, Kathleen,

A request:

Somehow I don't have your Week 3 Questions handout. In handling all the graphs and notes we had at Tuesday's meeting I may have accidentally returned it to you. Could you please EMail a copy of your handout (in the earlier version of Word).

Follow-up on Item 5 of 2/4/09 memo:

The split between alcohol and alkane was provided but not between the two alcohols which will be determined by relative rates. I should have reduced the four reactions to two reactions:

GBL -> m BuOH + n butane
GBL -> o PrOH + p propane + (o+p) methane

and in a similar way for BDO and THF to by-products. (Note: you need to make H2O to account for the oxygens removed to make the alcohols and alkanes.)

Wayne Robbins

Subject: **THF Safety/Storage**

Date: **Thu, 5 Feb 2009 09:37:11 EST [02/05/2009 09:37:11 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu, seider@seas.upenn.edu**
Cc: **heresdanny@gmail.com, dmicha@seas.upenn.edu, lfabiano@seas.upenn.edu**

Although still early, there are a couple of important safety concerns with THF.

1.) If you look at a MSDS the THF is listed as a flamable organic solvent. If the THF is to be stored before shipment it must be kept away from oxygen/air. In the past it was stored in tanks with a N2 pad. A slight positive N2 pressure was maintained so that air would not enter. The problem with a N2 pad system is that every time the tank is filled the N2, and THF vapors, would escape.

To eliminate the THF emissions, storage tanks now use an internal floating roof design and your final project design should use this type of storage tank.

2.) THF is also a peroxidizable compound. On exposure to air it will slowly form peroxides. The peroxides normally do not cause a problem unless you try to distill the THF after they have formed. The peroxides are high boilers and will concentrate in the column bottoms. If concentrated to a sufficient level they can explode since they are shock sensative. These explosions have occured many times in labs because the THF was not properly stored.

To prevent peroxide formation a stabilizer is added to the THF product before shipment. The stabilizer is butylated hydroxy toluene (BHT). In spite of its big name BHT is actually a completely safe, common food preservative. It is even in the ASPEN data bank. If you assume the polymer plant is adjacent, i.e. within a pipeline distance, the BHT is not needed. If you assume you are shipping the THF by tank truck or tank car then BHT must be added. It is usually added by co-feeding it into the pump feeding the T/T or T/C.

Wayne Robbins

Subject: **Cooling/splitting Reactor Vapor Product**

Date: **Sun, 8 Feb 2009 20:57:01 EST [02/08/2009 08:57:01 PM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu**
Cc: **heresdanny@gmail.com, dmicha@seas.upenn.edu, lfabiano@seas.upenn.edu, seider@seas.upenn.edu**

Good evening Michael, Daniyal, Kathleen,

While talking with Kathleen about the reaction kinetics she mentioned that there are still problems with modeling the cooling and separation of the reactor vapor product. Specifying certain components as Henry components did not resolve the problems. While I did not want to give any more stream information I believe the info on our calculated splits will help. You need to get your ASPEN model to calculate this stream but here is what our earlier (late 1980's) ASPEN model calculated:

The flows are in LbMol/hr. The model had a heat exchanger to cool the reactor effluent to 40 C, with a 2 psi dP followed by a FLASH2 block with 0.2 dP and no duty.

Comp	Rx Efl	Vapor	Liquid	K value
H2O	1512	3	1509	.001
GBL	45	~0	45	~0
BDO	3	~0	3	~0
THF	184	13	171	0.4
H2	2929	2926	3	550
CH4	35	35	~0	430
C3H8	3	3	~0	380
C4H10	12	12	~0	310
PrOH	8	0.1	8	.01
BuOH	11	0.1	11	.01
Temp,C	250	40	40	

Hopefully this will help you to get the ASPEN model going. If not, let me know.

Wayne Robbins

Subject: Re: Reactor Product Vap/Liq Separation

Date: Tue, 10 Feb 2009 13:34:46 EST [02/10/2009 01:34:46 PM EDT]
From: ROBBI2WT@aol.com
To: heresdanny@gmail.com
Cc: ekat@seas.upenn.edu, dmicha@seas.upenn.edu

Hi Michael, Daniyal, Kathleen,

The recovery/still train needs a lot of work. Here is my list of what needs to be done:

1.) Have ASPEN calculate X-Y curves for THF/H2O VLE at 14.7 psia and 114.7 psia (i.e. 100 psig). Check to see that they look like the graphs I gave you last week. Older versions of ASPEN did not do well at predicting the 100 psig curve and we had to enter our own activity coefficients. Prof Fabiono says the data has been updated but have ASPEN calculate them to be sure.

2.) In a pressure swing distillation you have a "race track" back and forth between the two columns. The pressure column overheads (LIQDIS3 on your flowsheet) must go back to the atmospheric column. You must specify this as a TEAR stream and give an initial estimate of its flow. Assume it has 12 wt% H2O, balance THF for a starting composition. Also, assume atmosheric column overheads contain 6 wt% water in calculating the initial estimated flow. Use DIRECT substitution for updating this stream. The pressure swing distillation is very sensitive and the accelerated convergence techniques cause instability and actually take more iterations to close.

3.) Set atmospheric column reflux ratio at 30 to 50% of overheads and keep it fixed at the ratio you pick. ASPEN may say you can run lower but there is a practical limit of keeping the trays wetted at very low reflux flows. To simulate the way the plants run, set the reflux mass flow (not ratio) at a fixed value.

4.) Cool condensers to 40 C and let ASPEN calculate the vapor (inerts) purge.

5.) Set atmospheric column bottoms flow to water flow in LIQDIS1. Set up a SPEC-VARY to control mid column temperature at 85 C by varying bottoms flow rate. Important: See my later note about alcohols, Item 7), before you do this.

6.) Set up a SPEC-VARY in the pressure column overheads for 145 C half way between the feed tray and bottom tray.Have it vary the column overheads flow (LIQDIS3). It is important that you do item 1) first and see not only the X-Y curve but the temperature vs composition. The pressure column can also run at a relatively low reflux ratio. Set it at 30 to 50% and keep it fixed at the ratio you pick. To simulate the way the plants run, set the reflux mass flow (not ratio) at a fixed value.

7.) Run the model without alcohols in the feed until you understand how the pressure swing distillation works. You must get it to run w/o alcohols! Then add a small flow of alcohols to see where they go. Note that BuOH/H2O have VLL equilibrium at certain concentrations

8.) Waste stream contains significant THF that must be recovered.

9.) Flash should be at 40 C. The small amount of H2 in the liquid phase looks good but too much THF is going in the vapor phase.

10.) What physical properties did you use to get the splits shown in streams NONCNDSB and CONDSBL streams? Prof Fabiano mentioned using Peng-Robinson. Did you use P-R or stay with NRTL/R-K?

Wayne Robbins

Subject: Re: Reactor Product Vap/Liq Separation

Date: Tue, 10 Feb 2009 16:33:16 EST [02/10/2009 04:33:16 PM EDT]
From: ROBBI2WT@aol.com
To: heresdanny@gmail.com
Cc: ekat@seas.upenn.edu, dmicha@seas.upenn.edu

Hi Michael, Daniyal, Kathleen,

Comments on the reactor area:

Any model you use for the reactor will have vapor and liquid streams leaving it. Our model with the RADFRAC block had a bottoms liquid stream which was mixed with the feed stream and returned to the reactor. Think of it as a side draw stream from which you flash a little bit of product and then return the liquid to the reactor. However you can't return the liqud directly to the reactor, ASPEN does not like that. Take the reactor liquid product stream and mix it with the reactor MAC/H2O feed stream and feed that total stream to the reactor. Again this is going to introduce a TEAR stream in the model, i.e. the reactor liquid return stream. Converge this using DIRECT replacement. Accelerated convergence techniques do not work well when reactions occur within the loop it is trying to converge.

Once you have enough catalyst, i.e. reaction rate, to convert most of the MAC to THF the reaction can not proceed much further. The rate, i.e. amount of catalyst, needs to be enough to give the offgas composition seen in my memo of 1/21/09. Then you will have the reaction rates for the correct amount of intermediates.

For the alcohol/alkane specified splits just write the reaction to give:

0.85 BuOH + 0.15 C_4H_{10}

or

0.9 PrOH + 0.1 C_3H_8 + CH_4

for each GBL, BDO or THF reacted. Or course you need to account for any oxygens not in the alcohol or alkane as H_2O and do the H_2 balance. The equations shown as reactions 4ab, 5ab and 7ab on page 3 of your handout just need the appropriate multipliers inserted into them as shown above.

For the rate constant use (1/0.85) times the rate to BuOH and (1/0.9) for the rate to PrOH.

Wayne Robbins

Subject: Modeling suggestions

Date: Wed, 18 Feb 2009 10:29:56 EST [02/18/2009 10:29:56 AM EDT]
From: ROBBI2WT@aol.com
To: ekat@seas.upenn.edu
Cc: dmicha@seas.upenn.edu, heresdanny@gmail.com

Hi Michael, Daniyal, Kathleen,

As a follow-up on our work yesterday, here are a few reactor area suggestions:

From Dr Seider's comments I assume he will now let you use the STOIC model for the reactor if you continue to have problems with the kinetic model. Since the STOIC model converts the feed to the vapor leaving the reactor, i.e. in effect does both reaction and VLE, you will not be able to calculate the feed conditions to get the desired reactor temperature of 250 C. So here are the feed conditions:

MAC/H2O feed: 60 wt% MAC at 94 C. Assume 60 wt% feed is available at 40 C

Reactor H2 feed: Mix make-up with recycle, compress to 2040 psig and heat to 300 C. You need to decide if one or two compressors are needed, when to mix the make-up and recycle H2 and when to heat the H2.

Note 1: Recycle H2 is approximately 2.5x the make-up H2.
Note 2: Make-up H2 is equal to H2 reacted + H2 purged
Note 3: Make-up H2 is available at 20 C and 250 psi
Note 4: 2000 psi is the pressure at the top of the reactor. H2 enters at the bottom where the pressure is higher due to the height of liquid.

I will send some distillation area suggestions later today or Thursday.

Wayne Robbins

Subject: Modeling suggestions II

Date: Wed, 18 Feb 2009 16:47:09 EST [02/18/2009 04:47:09 PM EDT]
From: ROBBI2WT@aol.com
To: heresdanny@gmail.com
Cc: ekat@seas.upenn.edu, dmicha@seas.upenn.edu

Hi Michael, Daniyal, Kathleen,

Here are a few distillation area suggestions;

As we discussed yesterday, the stream currently labeled WASTE does contain a significant amount of THF which needs to be recovered. Since most of the inerts were removed by the membrane the THF, H2O, etc. should be removed by a simple flash block calculation. The vapor (i.e. H2, CH4, etc) can now go to waste. The liquid stream needs to go to the atmospheric column if it contains no intermediates (GBL, BDO) or to the GBL recovery column if it does contain GBL and BDO.

You need to add two blocks between the high pressure separator bottoms and the GBL recovery column. The first block is a low pressure separator (flash block) to remove the inerts at pressure of the GBL recovery column. This is a real unit operation. Next add a separator block to to remove the last of the non-condensables (H2, CH4, C3H8, C4H10). This is not a real unit operation but by removing the non-condensables down to 0.0 it will help stabilize the distillation columns. In reality the non-condensables are so low they should not affect operation of the real columns. Now there is no need to specify a vapor stream from the column condensers to account for the small amount of non-condensables. Also, you should not get negative (below 0) condenser temperatures.

The atmospheric column feeds should go above and below the SPEC-VARY column stage. The GBL recovery column overheads are relatively high in H2O and should go below, the pressure column return stream contains 88 wt% THF and should go above the SPEC-VARY control tray. For now specify the pressure column return flow as equal to the pressure column bottoms flow and containing 12 wt% H2O but do not connect as a TEAR stream until the model settles down.

If you look at the pressure column profile you will see there is a large decrease in vapor flow up the column above the feed trays. This decrease is due to the large amount of liquid feeds. Some plants operate with a partial condenser on the column ahead of the atmospheric column (GBL recovery column). This will give a more uniform vapor flow and also represent an energy savings since the GBL recovery column overheads do not need to be condensed and then vaporized.

Let me know how your work is going.

Wayne Robbins

Subject: Physical Properties

Date: Fri, 20 Feb 2009 10:29:32 EST [02/20/2009 10:29:32 AM EDT]
From: ROBBI2WT@aol.com
To: ekat@seas.upenn.edu
Cc: dmicha@seas.upenn.edu, heresdanny@gmail.com, lfabiano@seas.upenn.edu, SEIDER@seas.upenn.edu

Hi Michael, Daniyal, Kathleen,

Using the .INP files you gave me on Tuesday I've looked thru the physical properties and have some comments.

First I will list the physical properties from the .INP files.

DATABANKS ......

PROP-SOURCES ......

are the same in both files.

Reaction area:

```
    HENRY-COMPS HC-1 HYDROGEN METHANE PROPANE NBUTANE

    PROPERTIES NRTL-RK HENRY-COMPS=HC-1
        PROPERTIES IDEAL / NRTL / PENG-ROB

    ESTIMATE ALL
        NRTL ALL ALL UNIFAC
```

Distillation area:

```
    HENRY-COMPS HC-1 HYDROGEN

    PROPERTIES NRTL-RK
        PROPERTIES NRTL

    ESTIMATE ALL
        NRTL ALL ALL UNIFAC
```

1.) In the distillation area the Henry component is identified but not shown following the PROPERTIES NRTL-RK statement. I am not sure why ASPEN is treating the hydrogen as a non-condensable without this statement. Also, methane is a Henry's component at the temperatures in the distillation area. However, since the model is working I am reluctant to change it.

2.) In the reaction area the Henry components are identified and included in the PROPERTIES statement and should work. PROPANE and NBUTANE are Henry's components at 250 C but not at the temperatures downstream of the reactor.

3.) Did ASPEN automatically pick the alternate IDEAL / PENG-ROB data sets? PENG-ROB is a possible alternative but we don't want the IDEAL. I would take these both out of the model and use just the NRTL.

4.) I have one other thought if the reaction area still does not work. The problem may be the MAC and SAC, two components with virtually no vapor pressure. The FLASH block may have trouble converging with components of negligible vapor pressure. The stream info I provided for the distillation area has 0.0 MAC and SAC because so little leaves the reactor (it is actually << 1 mole/hr). Try adding a SEP block after the reactor to remove the MAC and SAC then try the FLASH block. This SEP block is not a real unit op but it should help resolve the physical properties question.

Wayne Robbins

Subject: Re: THF Reactor Model
Date: Sun, 22 Feb 2009 08:44:11 EST [02/22/2009 08:44:11 AM EDT]
From: ROBBI2WT@aol.com
To: ekat@seas.upenn.edu
Cc: dmicha@seas.upenn.edu, heresdanny@gmail.com, lfabiano@seas.upenn.edu, SEIDER@seas.upenn.edu

Hi Kathleen,

The results, especially the H2 split, look better with the NRTL/R-K physical properties. The significantly lower H2 in the liquid phase has probably greatly slowed the reaction rates.

Try increasing the reaction rate by increasing the catalyst amount. Keep in mind this is an adjustment because we have changed the reaction rate calculations by not using a subroutine program. The actual catalyst amount and reactor size will be determined by the STY in my initial memo and as we discussed later.

Watch the recycle stream carefully. If it just keeps increasing from iteration to iteration and does not appear to be leveling off at a constant value it probably indicates that the rates are not fast enough. In particular watch the MAC, SAC and GBL concentrations. By 30 iterations the recycle should be nearing its final value.

If the kinetic model can not be made to work fairly soon, suggest you go to the RSTOIC model so you do not get behind schedule.

Wayne Robbins

Subject: Re: THF Reactor Model
Date: Mon, 23 Feb 2009 08:22:47 -0500 [02/23/2009 08:22:47 AM EDT]
From: lfabiano@seas.upenn.edu
To: ROBBI2WT@aol.com
Cc: ekat@seas.upenn.edu, dmicha@seas.upenn.edu, heresdanny@gmail.com, SEIDER@seas.upenn.edu

Hello all:

I've already suggested to Kathleen to use RSTOIC or RYEILD two weeks ago. I feel that the reactor model is not responding to produce anywhere near what Wayne Robbins expected and knows that in practice works. Unfortunately your team will not be able to really investigate the reactor design and offer alternative operations. However at this stage of effort I'm concerned that time is not on your side.

Use the results of the reaction as stated by Mr. Robbins and go forward.

Professor Fabiano

Subject: **Re: THF Reactor Model**
Date: **Tue, 24 Feb 2009 09:55:52 -0500 [02/24/2009 09:55:52 AM EDT]**
From: **Warren D Seider <seider@seas.upenn.edu>**
To: **lfabiano@seas.upenn.edu, ROBBI2WT@aol.com**
Cc: **ekat@seas.upenn.edu, dmicha@seas.upenn.edu, heresdanny@gmail.com**

Dear Len,

I met with Katie yesterday - and we agreed that Katie would try Wayne Robbins' suggestion to increase the amount of catalyst in an attempt to obtain an acceptable production of THF. However, if not successful by our meeting today, she will use an RSTOIC model with the specifications provided by Wayne Robbins. Whether or not she is successful, today, she will begin focusing on other aspects of completing the design project, working with Daniyal and Michael. Emphasis will be shifted toward sizing the equipment, estimating costs, carrying out the profitability analysis, preparing the written report, etc.

Regards, Warren

Subject: **RE: UPenn Senior Design Question**
Date: **Wed, 25 Feb 2009 13:27:09 -0500 [02/25/2009 01:27:09 PM EDT]**
From: **Brostow,Adam A. <BROSTOAA@airproducts.com>**
To: **Padovani,Julio C. <PADOVAJC@airproducts.com>**
Cc: **Kathleen E. Wu <ekat@seas.upenn.edu>**

Julio,

Do you know somebody who could give Kathleen some information about membranes, probably technical information and cost?

Adam

-----Original Message-----
From: Kathleen E. Wu [mailto:ekat@seas.upenn.edu]
Sent: Tuesday, February 24, 2009 1:32 PM
To: Brostow,Adam A.
Subject: UPenn Senior Design Question

Dear Mr. Brostow,

My name is Kathleen Wu and we met briefly two weeks ago to discuss my senior design project on THF production at the University of Pennsylvania. You mentioned that Air Products has an excellent membrane division in St. Louis, and I was hoping you could put me in contact with someone in the division so that we may do further research for our project. I tried calling the HQ of Prism Membranes, but was not able to get through. Your help would be greatly appreciated.

Thanks!

Best,
Kathleen Wu

Subject: **ATTACHMENT OF POSSIBLE INTEREST: CBE459-001-2009A**
Date: **Wed, 25 Feb 2009 14:25:54 -0500 [02/25/2009 02:25:54 PM EDT]**
From: **Leonard Fabiano <lfabiano@seas.upenn.edu>**
To: **Undisclosed Recipients**
1 Attachment Save All
2 DRUMSIZING.xls 21 KB

Hello Students:

One student asked me last night if I could provide background on sizing flash drums. I covered the subject overview with the student. This is the type subject that I thought that I would go over at a voluntary class meeting in a message I sent several weeks ago.

To that end, I have produced an excel program that does the sizing for flash drums and or surge drums in which there is a vapor and liquid as a feed. The object is to allow as little of the liquid to be entrained in the vapor out the top as practical. One could add a mesh packing section at the top of the vessel if closer to zero liquid out with the vapor is desired. If any of you wish to go over more details you can contact me or ask for one of the voluntary night sessions. I could make the meeting on a Wednesday evening say 6 PM if anyone is interested.

The excel spreadsheet may not be pretty but it does the job and I'm pretty certain that all of you can figure out what to input.

For those groups that have distillation columns in your project it would be most useful for you to learn how to take an ASPEN PLUS output and convert it to a "real design". Whether you ask me for a meeting at night or not PLEASE REMEMBER TO HAVE THE TOP OF THE TOWER PRESSURE TO BE AT LEAST 18-20 PSIA(UNLESS IT IS OPERATING UNDER VACUUM); AND IN ALL CASES THERE IS A PRESSURE DROP ACROSS THE COLUMN SO YOU MUST INPUT THAT INTO ASPEN PLUS. TYPICAL PRESSURE DROPS ACROSS A REAL TRAY IS 5-6 mmHg and since ASPEN PLUS DEALS WITH THEORETICAL STAGES YOU MUST INCREASE THE PRESSURE DROP PER TRAY BY DIVIDING BY THE TRAY EFFICIENCY.

This is another class to show you how to make a good prediction of tray efficiency. I've also attached a guidline for tower sizing.

Professor Fabiano

Subject: **Re: THF Combined Model**
Date: **Sat, 28 Feb 2009 21:40:05 EST [02/28/2009 09:40:05 PM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu**
Cc: **dmicha@seas.upenn.edu, heresdanny@gmail.com, lfabiano@seas.upenn.edu, SEIDER@seas.upenn.edu**

Hi Michael, Daniyal, Kathleen,

Here are the answers to your questions and some suggested changes/upgrades to your flowsheet model:

1.) Your RSTOIC blocks are working correctly. There are three differences:

1a.) The model needs to have the H2 recycle returned to the reactor. This stream will return some of the alkanes to the reactor since the membrane is not 100% efficient at separating the H2 from the alkanes.

1b.) I checked again and the reactor exit flows I gave you were from an early model run which had a purge instead of a membrane in the H2 recycle loop. When we realized how much H2 we were losing to purge the alkanes we had R&D do a membrane study. With the membrane the alkane recycle flows are greatly reduced, hence your numbers.

1c.) The original MAC feed contained significant amounts of C2 and C3 acids which produced quite a bit of MeOH, EtOH, PrOH and C2H6, C3H8. When we found that the MeOH and THF produce a difficult to separate mix we decided to clean up the feed so it had only MAC and H2O. I removed the EtOH and C2H6 from the reactor exit flows. Since some PrOH and C3H8 also came from the MAC feed I left them in but my amount is definitely to high.

2.) The following blocks need to be added to your combined flowsheet:

A FLASH2 block is needed on the WASTE stream to recover the GBL, BDO, THF values. With much of the non-condensables removed by the SEP2 membrane, it should be easy to condense the GBL, BDO, THF, H2O. The liquid stream should be returned to the DIST1 column if it contains GBL and BDO or to the PSWING1 column if only THF.

A low pressure FLASH block is needed on the CONDNSBL stream to remove most of the remaining non-condensables. Keep a few psig so it can feed the DIST1 GBL recycle column.

A SEPARATOR block is needed after the low pressure FLASH block to remove all of the non-condensables. This block is not a real unit operation, but removing the last of the non-condensables will help stabilize the pressure swing columns. In any case the amount of non-condensables is small and would have minimal effect on real column operation.

Remove the VAPDIS1,2,3 vapor purge streams from all three columns. Now you can specify a subcooled reflux/distillate temperature. As long as you have a vapor purge the temperature is determined by VLE.

Consider having a partial condenser on the DIST1 GBL column and feed the vapor to the PSWING1 column. This change will give a more consistent vapor traffic in the PSWING1 column and represent a real energy savings.

3.) How to remove the alcohols is your choice. The BuOH and PrOH may or may not go down the PSWING1 column. The BuOH has a high activity coefficient in H_2O and has a higher boiling point than THF so it will probably form a concentration bulge in PSWING1. BuOH and PrOH can be separated from THF so you may want to let them follow the THF and then do a final product distillation.

BuOH/H_2O will probably not form two liquid phases in the presence of THF since each is soluble in THF. You can calculate the three component phase diagram curves in ASPEN.

Let me know how your model runs are going. See you on Tuesday.

Wayne Robbins

Subject: **Re: THF Combined Model**
Date: **Sun, 1 Mar 2009 16:01:32 EST [03/01/2009 04:01:32 PM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu**
Cc: **dmicha@seas.upenn.edu, heresdanny@gmail.com**

Hi Michael, Daniyal, Kathleen,

Good afternoon. In my previous EMail I told you to add a block on the WASTE stream to recover the GBL, BDO, THF values. I forgot about the non-condensables. This stream should go to the low pressure FLASH2 block to remove the non-condensables and continue on to the dummy SEP2 block to remove the last of the non-condensables.

I do not have plant data on the pressure swing distillation columns from the plant we built in Europe but I do have data for another plant which did a THF/H_2O separation and had only THF/H_2O in the feed, i.e. no alcohols. Here is the data:

Atmospheric column:

Top pressure: 0 psig, 14.7 psia
Column dP: 0.9 - 1.2 psi (depends on rate)
Reflux ratio: 0.45 - 0.54 reflux/ohds product
Temperatures:
  Reflux: 35 - 42 C
  Top tray: 63 - 64 C
  Mid-upper: 67 - 68 C
  Mid-lower: 75 - 80 C
  Bottom: 101 - 102 C
Ohds composition: 6.1 - 6.3 wt% H_2O

Pressure column:
Top Pressure: 88 psig, 103 psia
Column dP: 1.1 - 1.5 psi (depends on rate)
Reflux ratio: 0.72 - 0.84 reflux/ohds product
Temperatures:
  Top: 132 C
  Mid: 138 C
  Btm: 143 C
Ohds composition: 13 - 15 wt% H_2O (varied with reflux ratio)

Note: Temperatures will be slightly higher at 100 psig, 115 psia

Hope this helps you get the columns lined out.

Wayne Robbins

Subject: MATERIALS OF CONSTRUCTION GUIDE: CBE459-001-2009A
Date: Sun, 1 Mar 2009 21:24:38 -0500 [03/01/2009 09:24:38 PM EDT]
From: Leonard Fabiano <lfabiano@seas.upenn.edu>
To: Undisclosed Recipients
4 Attachments Save All

2	PAGE100.pdf	702 KB	Download in .zip Format
3	PAGE98[1].pdf	602 KB	Download in .zip Format
4	page 97.pdf	743 KB	Download in .zip Format
5	page 99.pdf	605 KB	Download in .zip Format

HELLO STUDENTS:

ATTACHED ARE FOUR PAGES ON MATERIAL OF CONSTRUCTION THAT I THINK WILL BE OF HELP TO YOU. THE PAGES COME FROM:

CHEMICAL ENGINEERING PROCESS DESIGN AND ECONOMICS;
ULRICH AND VASUDEVAN; PROCESS PUBLISHING;
2ND EDITION; 2004

PROFESSOR FABIANO

Subject: THEORETICAL STAGES vs REFLUX RATION GUIDELINES: CBE459-001-2009A
Date: Sun, 1 Mar 2009 21:37:22 -0500 [03/01/2009 09:37:22 PM EDT]
From: Leonard Fabiano <lfabiano@seas.upenn.edu>
To: Undisclosed Recipients
3 Attachments Save All

2	OPT%20RR%20KISTER[1].pdf	581 KB	Download in .zip Format
3	NvsRR%20EXPLANATION[1].pdf	524 KB	Download in .zip Format
4	NvsRR%20KISTER[1].pdf	509 KB	Download in .zip Format

HELLO STUDENTS:

ATTACHED ARE PAGES FROM HENRY KISTER'S BOOK; DISTILLATION DESIGN. THIS IS A GREAT BOOK AS IS HIS BOOK: DISTILLATION OPERATIONS. THOSE OF YOU THAT WILL BE INVOLVED IN PROCESS ENGINEERING DESIGN OR OPERATIONS THAT WILL INCLUDE DISTILLATION TOWERS SHOULD OWN THE BOOKS.

BY THE WAY IF YOU GOOGLE THE BOOKS YOU CAN SEE THE ENTIRE BOOK FOR FREE ON THE WEB.

THESE PAGES WILL PROVIDE YOU BACKGROUND ON SELECTING THE "BEST" COMBINATION OF STAGES AND REFLUX RATIO.

ON PAGE 99 THE CONVENTIONAL GUIDELINE FOR "OPTIMIZING" THIS SELECTION BY CHOOSING THE MINIMUM COST COMBINATION OF TOWER COST AND ENERGY CONSUMPTION. THIS IS A VERY INTERESTING EXCERCIZE BUT AS I AM A REAL PRACTITIONER OF THE "SCIENCE AND ART" OF DESIGNING TOWERS AND TOWER SYSTEMS I SUBMIT THAT THIS IS NOT THE BEST WAY TO MAKE THE DECISION. RATHER STABLE OPERATION IS THE BEST CHOICE WHICH CAN BE MADE WITH THE DEVELOPMENT OF THE GRAPH ON PAGE 105. THEN PAY SPECIFIC ATTENTION TO THE NEXT TO LAST PARAGRAPH ON PAGE 104 THAT DESCRIBES ONE WAY THAT IT CAN BE DEVELOPED.

I WILL BE SENDING ANOTHER E-MAIL TONIGHT ON TRAY EFFICIENCY CALCULATIONS. IF ANYONE IS INTERESTED IN LISTENING TO ME DISCUSS THESE METHODS IN DETAIL AND MY ANSWERS TO YOUR QUESTIONS THEN I WOULD BE WILLING TO MEET WITH THOSE STUDENTS ON THIS COMING WEDNESDAY EVENING AT 6 PM. YOU HAVE TO RESPOND BY MONDAY IN ORDER FOR ME TO ARRANGE A ROOM AND MAKE MY OWN SCHEDULE CHANGES.

PROFESSOR FABIANO

Subject: **HOW TO ESTIMATE TRAY EFFICIENCIES: CBE459-001-2009A**

Date: **Sun, 1 Mar 2009 22:00:15 -0500 [03/01/2009 10:00:15 PM EDT]**
From: **Leonard Fabiano <lfabiano@seas.upenn.edu>**
To: **Undisclosed Recipients**
2 Attachments Save All
2 TOWER EFF 2.xls 41 KB
3 OCONNELL%20KISTER%20BOOK[1].pdf 698 KB Download in .zip Format

HELLO AGAIN STUDENTS:

THE ATTACHED FILE ARE:

A REPRESENTATION BOTH VIA A GRAPH AND AN EQUATION FOR THE LINE ON THE GRAPH FOR THE OCONNELL CORRELATION. AS YOU CAN SEE FROM THE REFERENCE THIS DATA WAS ASSEMBLED BACK IN 1946 AND IS AS GOOD AS ANY OF THE MORE COMPLICATED METHODS (NONE OF WHICH ARE HIGHLY ACCURATE). I'VE USED IT OVER THE YEARS AS HAVE MANY PRACTICING PROCESS DESIGN ENGINEERS TO DESIGN REAL TOWERS THAT HAVE ACTUALLY WORKED FINE IN PLANTS.

THE SECOND EXCEL SPREADSHEET IS AN EXAMPLE THAT I ACTUALLY USED RECENTLY.

AGAIN, ANYONE WISHING TO DISCUSS THIS WITH ME FOR A BETTER UNDERSTANDING IS REQUESTED TO E-MAIL ME SO THAT I CAN SET UP AN HOUR OR SO THIS WEDNESDAY AT 6 PM.

PROFESSOR FABIANO

Subject: **THF/H2O VLE at 100 PSIG**

Date: **Wed, 4 Mar 2009 10:36:08 EST [03/04/2009 10:36:08 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu**
Cc: **dmicha@seas.upenn.edu, heresdanny@gmail.com**

Hi Michael, Daniyal, Kathleen,

I am addressing this EMail to all three of you but primarily to Daniyal who is doing the downstream distllation modeling.

The pressure column PSWING2 is just not separating THF and H2O nearly as well as I know it does in actual running columns at our various plants. I strongly suspect the problem is in the ASPEN calculated VLE at 100 psig (114.7 psia). In order to check this I need ASPEN to calculate the VLE for the THF/H2O binary system at 114.7 psia.

With earlier versions of ASPEN you could make a TGS (Table Generating System) run. It is not a normal flowsheet run but will calculate and tabulate the temperature, liquid and vapor compositions at a given pressure. If TGS is available please make a run for THF/H2O at 114.7 psia using the NRTL/R-K physical properties in ASPEN.

If TGS is not available, set-up a single FLASH2 block and again use the NRTL/R-K physical properties in ASPEN. Run the black several times with feeds containing 55, 60, 65, 70, 75, 80, 85, 90, 95 mole % THF in the feed. Feed a 1000 total moles and flash 1 mole, 0.001 Vfrac, so that the liquid composition after the flash is the same as what was fed. Set pressure at 114.7 psia and record the temperature and vapor mole fraction composition (to 4 signif figures) for each feed.

If you will do these runs and send the results to me as a table, I will check the calculated values vs duPont company data I have.

I know that the number of stages we specified in the PSWING2 column should give much better separation and I suspect that VLE is the problem.

Thank you,
Wayne Robbins

Subject: **Re: THF Combined Model**

Date: **Wed, 4 Mar 2009 11:20:54 EST [03/04/2009 11:20:54 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **ekat@seas.upenn.edu**
Cc: **dmicha@seas.upenn.edu, heresdanny@gmail.com**

Hi Michael, Daniyal, Kathleen,

I know you are close to a final flowsheet but here are a few recommendations:

1.) Only the recycle H_2 stream is heated. The fresh H_2 stream is compressed but not heated prior to entering the reactor. I had a wrong memory on this point.

2.) The GBL column bottoms contain too much H_2O which will eventually require more heat in the reactor. The bottoms should contain about 10 wt% or 40 mole% water. This change should not cause a change in the amount of water going to the PSWING1 column, but only reduce the amount of water recycling thru the reactor. Remember, water going to the PSWING1 column should be the total of water fed plus water made by reaction less any in purge streams. These values are not changed. I assume you are giving an estimated flow for the GBL recycle stream to the reactor. You know it contains ~ 45 mol/hr of GBL, so set the H_2O at ~ 30 mol/hr.

3.) If you keep the BuOH/H_2O column in the model this may be your chance to have a decanter to make a liquid - liquid separation. The overheads of the column will approach the azeo composition. The vapor from the top tray, after being condensed can go to a decanter. Reflux the water rich phase and take the BuOH rich phase as overhead product. Note: you will need to specify 3-phase, VLL, in the upper stages and condenser of this column. An overheads decanter can be specified within the ASPEN RADFRAC block. Normally ASPEN will make the more dense stream, in this case the H_2O rich stream, as the 2nd liquid stream but check your results.

Wayne Robbins

Subject: **Re: THF/H2O VLE at 100 PSIG**

Date: **Tue, 10 Mar 2009 10:10:42 EDT [03/10/2009 10:10:42 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **heresdanny@gmail.com**
Cc: **ekat@seas.upenn.edu, dmicha@seas.upenn.edu, lfabiano@seas.upenn.edu, SEIDER@seas.upenn.edu**

Hi Daniyal, Michael, Kathleen,

Daniyal, thank you for doing the ASPEN THF/H_2O VLE calculations at 100 psig.

As I feared, the ASPEN calculations have the vapor THF rich vs our company data. Two results are:

1.) You will need higher reflux or more stages since there is less separation between the VLE curve and the operating line.

2.) The THF/H_2O azeotrope is at 0.6588 mole frac THF which is 88.5 wt% THF, 11.5 wt% H_2O. The model will never allow you to run at 12% H_2O in the overheads. (Even at 88 psig, 103 psia, our plants were able to run at 12.5 - 13 wt% H_2O in the overheads as confirmed by lab analysis of the stream's water content and by mass balance based on flows around the column.)

The PSWING2 column bottoms product flow must be less than 1/2 of the column feed assuming you have 6 wt% water in the PSWING1 overheads.

Wayne Robbins

Note: Our company models used a custom physical properties data set provided by our thermodynamics expert. I do not know what values he used for the NRTL coefficients.

Subject: **Re: THF Combined Model**
Date: **Tue, 10 Mar 2009 10:22:21 EDT [03/10/2009 10:22:21 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **heresdanny@gmail.com**
Cc: **ekat@seas.upenn.edu, dmicha@seas.upenn.edu**

Hi Kathleen, Daniyal, Michael,

Ref.: My 3/10 memo of THF/H2O VLE

After reading your memo, my best guess as to the problem is that you are asking the model to satisfy an impossible specification. BuOH and PrOH are both high boilers compared to THF so they will concentrate in the PSWING2 column bottoms. Unless the PrOH and BuOH are sufficiently removed in the PSWING1 column bottoms you will not be able to meet the product spec in the PSWING2 column bottoms.

Please do a quick mass balance check by hand calculator and see if the PSWING2 column bottoms can meet the spec.

Couple of modeling options:

1.) Try setting the PSWING2 bottoms at a fraction of the column feed, my guess is somewhere around 46 - 48% (see ref memo).

2.) Try allowing a bit more PSWING1 bottoms flow to reduce alcohols going to PSWING2.

If still not meeting the product spec, you may need to add a column after the PSWING2 bottoms to remove the last of the alcohols.

Wayne Robbins

Subject: **Re: Membrane Sizing**
Date: **Thu, 19 Mar 2009 09:17:42 EDT [03/19/2009 09:17:42 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **dmicha@seas.upenn.edu**
Cc: **heresdanny@gmail.com, ekat@seas.upenn.edu**

Hi Michael, Daniyal, Kathleen,

I looked through my old notes on the membrane separator and found the following information on the pressure drops:

1.) The stream going through the equipment but not going through the membrane, i.e. the alkane purge stream, drops about 20 psi.

2.) The H2 recycle stream which does go through the membrane drops several hundred psi.

I recommend you go with the pressure drop calculated by Mr Histed since he has a computer program to do specific membrane calculations.

Wayne Robbins

Subject: **Re: Membrane Sizing**
Date: **Sat, 21 Mar 2009 15:41:16 EDT [03/21/2009 03:41:16 PM EDT]**
From: **ROBBI2WT@aol.com**
To: **dmicha@seas.upenn.edu**
Cc: **heresdanny@gmail.com, ekat@seas.upenn.edu**

Hi Michael, Daniyal, Kathleen,

If the membrane gets too big and expensive you might consider the following option:

Take only part of the recycle stream thru the membrane, i.e. take 80 - 85% directly back to the reactor and only 15 - 20% thru the membrane separator. The alkanes are currently quite low concentration. This flow split will effectively raise the concentration of the alkanes which will slightly reduce the H2 concentration in the reactor, but means the membrane can be significantly smaller in area.

Just an option to consider.

Wayne Robbins

Date: Tue, 24 Mar 2009 11:53:19 -0400
From: "Histed,Adam J." <HISTEDAJ@airproducts.com>
Subject: RE: Re: Membrane Sizing
To: Michael Abuschinow <dmicha@seas.upenn.edu>

Mike

I think it will be easier for you to simulate the membranes yourself. Then it will fit in nicely with your Heat and Mass Balance. Attached is a PDF file from a membrane manufacturer called Udel. They make membranes called Solvay Advanced Polymers.

In aspen, you will go into membrane block set-up and select Generic as the membrane type. We operate our membranes in Countercurrent flow. The flow model is Plug-Plug, and you'll use Partial-Pressure as your driving force. Membrane Area will be determined by a design spec. Later. Just put in 100 sqft for now.

An Aside - The inside of the membrane fibers would be considered the tube-side of the vessel. H2 Gas permeates through the membranes from the shell side to the tube side. I don't know what your understanding of membranes is, but essentially, inside the vessel there are thousands of spaghetti-like strands all bundled together. The strands are hollow inside, and that is what I mean by "tube side". The membrane bundle is really a lot like a shell and tube heat exchanger, but with thousands of tiny tubes, and the membrane is exchanging mass instead of heat. For the purpose of your simulation, your basically assuming a sheet membrane though.

In the advanced tab, you'll specify the permeability. Enter your permeabilies from the values in the PDF. In the PDF, there are a list of membrane properties, including the permeabilities of various gases. (Pg. 45 on paper...but pg. 47 in the pdf). All of your components aren't listed in the PDF, but hydrogen and methane are. Use 50% * Methane for propane, and 75% * propane for butane. Use the H2 permeability for water. Typically, larger molecules permeate slower than smaller molecules, but there are exceptions. Therefore, to be conservative, use the same permeability as methane for tetrahydrofuran. That should get you started. In Aspen, the "permeability" is actually the permeability/(membrane skin thickness). You can assume a skin thickness of 1000 angstroms. So divide the permeabilities in the PDF by 1000, and select the correct permeability units in aspen.

Under the Pressure-Drop Tab, select the Pressure you'd like your permeate at (I recommend a DP of 1000 psi for good separation). Under the heat-transfer tab, click "Membrane Operates isothermally" and select "Average Temperature" as the temp. option. Once you get results you are happy with, you can price the membrane. Assume $10 per sq. Ft. of membrane area. Also, you'll have to design a pressure vessel to go around the membrane. You can probably use pipe.

If you have any questions about membrane simulation, let me know. It will probably be easier to help you if you have an aspen deck open in front of you, so maybe just give a quick call and I'll assist you.

Regards,

Adam Histed
Air Products and Chemicals
Generated Gases - Hydrogen Membranes

Subject: **Catalyst cost**
Date: **Wed, 25 Mar 2009 10:02:46 EDT [10:02:46 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **dmicha@seas.upenn.edu**
Cc: **heresdanny@gmail.com, ekat@seas.upenn.edu**

Hi Michael,

The chemists I knew who worked on the catalyst have all retired and I have lost contact with them. We may need to make an educated guess on catalyst price. When you send your list of price questions please include the info you found yesterday on several catalyst prices, i.e. various precious metal loadings, Pd or Re, etc.

Wayne Robbins

Subject: **THF Price**
Date: **Wed, 25 Mar 2009 11:00:54 EDT [11:00:54 AM EDT]**
From: **ROBBI2WT@aol.com**
To: **dmicha@seas.upenn.edu**
Cc: **heresdanny@gmail.com, ekat@seas.upenn.edu**

Hi Michael, Daniyal, Kathleen

Here is the info on THF and Maleic prices.

I found THF prices on the internet of $2.76 - 2.80 / kg for orders of 20,000 kg or more. I talked with my friends at DuPont (now Invista) and while not saying an exact price they did confirm that the above prices are very comparable.

For Maleic use $1 / kg. This will not be a price you find on the internet but our Maleic comes from an in-house process using butane and air as raw materials.

If you would like more info on THF (product specs, MSDS, etc) you can go to the following Web site:

www.terathane.invista.com

The THF you are making is for internal consumption and for reliability of supply. The process needs economics so management knows how it is doing on cost vs buying on the open market.

The overall process is:

Butane -> Maleic -> THF -> THF polymer (TERATHANE) -> LYCRA

The big $'s are in the LYCRA sales and a reliable THF supply is critical.

TERATHANE is a registered trade name for what used to be called by its chemical name of PTMEG (Poly Tetra Methylene Ether Glycol).

Wayne Robbins

Subject: **Re: THF Price**
Date: **Thu, 26 Mar 2009 15:29:54 EDT [03/26/2009 03:29:54 PM EDT]**
From: **ROBBI2WT@aol.com**
To: **dmicha@seas.upenn.edu**
Cc: **heresdanny@gmail.com, ekat@seas.upenn.edu**
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Hi Michael, (Daniyal, Kathleen),

The info on the multi-step processes to make LYCRA was for background so you can see where the MAC to THF fits into the overall picture. Your job is to design the process to make THF and be sure that it is economically viable. You should not be concerned with any process other than MAC to THF.

I will look at the .zip file and get back to you later.

Wayne Robbins

Subject: **Re Price/Mat'l Const**
Date: **Fri, 27 Mar 2009 16:15:46 EDT [03/27/2009 04:15:46 PM EDT]**
From: **ROBBI2WT@aol.com**
To: **dmicha@seas.upenn.edu**
Cc: **heresdanny@gmail.com, ekat@seas.upenn.edu**
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Hi Michael, Daniyal, Kathleen,

I am trying to come up with an estimated cost for the catalyst. Let's buy the Re powder and have a vendor apply it to the Pd/C catalyst. There seems to be some economy of scale in purchasing larger amounts of Re and extrapolating the data (always risky) I came up with an estimated cost of $390,000 for the 189 g of Re.

I am trying for an estimate of the low Pd on C catalyst but, as you know, most price data is for 10% Pd.

Material of construction: Our lab reactors used 304SS or 316SS tubes for the reactor (not sure which). Check with Dr Seider or Prof Fabiano for their recommendation. Your choices are:

1.) Make the entire reactor of 304SS or 316SS
2.) Make the reactor of carbon steel with an interior layer of 304SS or 316SS
3.) Make the reactor of carbon steel with an interior layer of copper

Cost will determine your best option.

Wayne Robbins

Date: Fri, 27 Mar 2009 14:44:03 -0400
From: "Histed,Adam J." <HISTEDAJ@airproducts.com>
Subject: RE: Re: Membrane Sizing
To: Michael Abuschinow <dmicha@seas.upenn.edu>

Mike

The membranes are constructed of a polymer that allows gas permeation. Various blends of polysulfonate polymer are typically used for H2 applications. I have no experience with spiral wound membranes. Our membranes are hollow fiber membranes. Think of them as essentially thousands of tiny straws bound together and capped at one end. The feed stream enters the membrane housing vessel on the shell side and is dispersed through the membrane fibers. As the gas flows through the vessel, H2 permeates into the membrane fibers. H2 leaves the vessel from inside the membrane fibers (it flows out the non-capped end of the straw-like membrane fibers) while the remaining alkanes flow out of the shell side exit.

I supplied you the membrane skin thickness, not the thickness of the actual membrane fibers. If you are putting your permeability values into your aspen simulation, I think the units won't necessarily match up. The units given in the PDF are as follows:

(mm^3*m)/(m^2*mPa*day) @ stp   Therefore the mm^3/day (volumetric flow) is actually a standard volume flow, or mol flow. Keep this in mind.

You need to divide the permeability values in the PDF by the skin thickness to get a (p/l) value, which aspen calls "permeability". Anyway, without getting into un-necessary complications, divide the permeability values by the skin thickness, and then your units will match the aspen input units desired.

Example units in aspen

(Std cm^3)/(cm^2 * sec * cmHG)

If you compare the units, you'll see that the values from the PDF have an extra length property in the numerator. This length is the skin thickness. I'm relatively new to this position, and haven't taken mass transfer in a while, so I can't really explain it to you. From my understanding, I think it's a region of the membrane that is mass-transfer limited. Basically, it's a property of the polymer that affects the rate of permeability. Divide permeability values by skin thickness, convert the units and enter your calculated membrane permeability into aspen. Let me know how it works for you.

Adam Histed

Date: Mon, 6 Apr 2009 09:50:34 -0400
From: "Histed,Adam J." <HISTEDAJ@airproducts.com>
Subject: RE: Re: Membrane Sizing
To: Michael Abuschinow <dmicha@seas.upenn.edu>

Yes, I think that you're results are reasonable. That is about the same membrane area that I calculated you would require. How is your hydrogen recovery/purity?

For the purposes of your study, I think it is a good assumption that permeability is a constant across all pressures. Operating pressure does have some effect on the performance of membranes, but you can assume it is negligible.

Just for your information - For Air Products membranes, as temperature increases, the membranes become more permeable overall, so product purity suffers but recovery of H2 increases. The effect of higher or lower operating pressure is really not as important to me in designing as pressure ratios and differential pressure. Changes in pressure directly change the driving force for separation and the effect dominates permeability changes for Air Products.

The more differential pressure, the more driving force you'll have. The better the feed - permeate pressure ratio, the better your separation will be. So, if I designed a system that had a DP of 300 psi, but the feed pressure was 350 psi, the feed:permeate ratio would be 350/50 = 7. This system would have better performance than your system which has the same differential pressure (driving force), but a smaller feed to permeate pressure ratio. This can be explained because the membranes separation driving force is the partial pressure of the components.

Good luck with your project. Let me know if you have any other membrane questions.

Regards,

Adam Histed

Subject: **Re: Pd-Rh Catalyst Inquiry**
Date: **Tue, 7 Apr 2009 13:34:53 -0400 [04/07/2009 01:34:53 PM EDT]**
From: **Rick Clayton <rick.clayton@basf.com>**
To: **Kathleen E. Wu <ekat@seas.upenn.edu>**
Cc: **Glenora Ashworth <glenora.ashworth@basf.com>**
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Kathleen;

With the generic information supplied below I will provide what you may consider recovery charges for taking the spent catalyst. Glenora will then provide you with some target numbers for the fresh catalyst based on assumptions.
All this information is just to be used inside your project model and does not constitute a quotation.

Treatment charge: $2.35 per kilo of net weight of catalyst returned for metal recovery.
Refining charge: $12.00 per troy ounce of palladium returned and $58.00 per troy ounce of rhodium returned
Metal return: 98% of assayed palladium content and 96% of assayed rhodium content of prepared sample
Assay charge: $450 which covers for both metals.
Settlement time: 14 weeks from receipt of the spent catalyst at the recovery facility.
Shipment: DDU Refinery dock with all shipment charges born by shipper.

Good luck with your project.

Best regards

____
_

Rick Clayton
Chemical / Refinery Sales

Phone: 1-864-885-1253
Fax: 864-885-1374
E-Mail: rick.clayton@basf.com
Postal Address:
BASF Catalysts LLC
554 Engelhard Drive
Seneca, SC 29678
USA

Subject: **Re: Pd-Rh Catalyst Inquiry**
Date: **Tue, 7 Apr 2009 13:50:16 -0400 [04/07/2009 01:50:16 PM EDT]**
From: **Glenora Ashworth <glenora.ashworth@basf.com>**
To: **Kathleen E. Wu <ekat@seas.upenn.edu>**
Cc: **Rick Clayton <rick.clayton@basf.com>**
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Kathleen, below is a rough estimate of price for the catalyst you describe below. Price is estimated for your project, and as Rick declares, does not consitute a quotation.

Fabrication charge: 70.18/kg
Rhodium charge: 18.65/kg (based on 0.5% metal loading per kg and todays market price of $1160 per troy ounce)
Palladium charge: 3.63/kg (based on 0.5% metal loading per kg and todays market price of $226 per troy ounce)
Total price: $92.46/kg

Price is FOB, Seneca SC. For an estimate of freight charges within continental US (if needed), you may use$0 .20/KG.

____
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Glenora Ashworth
Pricing Analyst - Process Technologies
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Seneca, SC 29678

BASF - The Chemical Company

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