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Upgrading Cracking Waste to Rubber Precursors via Oxidative Dehydrogenation

Andrew Mason
University of Nebraska-Lincoln, andmason311@gmail.com

Delaney Franck
University of Nebraska - Lincoln, delaneyjbach97@gmail.com

Firdvas Nasimov
University of Nebraska-Lincoln, firdavs.nasimov@gmail.com

Lindsey Jarema
University of Nebraska - Lincoln, firdavs.nasimov@gmail.com

Gitau Wambugu
University of Nebraska - Lincoln, gtyoungstunna@gmail.com

MEMORANDUM

To: Dr. Yasar Demirel, Professor
University of Nebraska-Lincoln
Department of Chemical and Biomolecular Engineering
From: Senior Design Team 2 - Delaney Bachman, Gitau Wambugu, Lindsey Jarema, Andy Mason, and Firdavs Nasimov
Subject: Final Report of 'Upgrading Cracking Waste to Rubber Precursors via Oxidative Dehydrogenation'
Date: May 01, 2020

Dear Dr. Demirel:

The following attachment is a report titled "Upgrading Cracking Waste to Rubber Precursors via Oxidative Dehydrogenation." This project builds on existing purification methods for high purity recovery of 1,3-Butadiene. The innovation in this process is the addition of an oxidative dehydrogenation reactor to achieve a higher product yield. This report contains several sections which detail the theory and background of the existing processes, our assumptions, process design specifications, our Aspen input summary, and preliminary information regarding economic feasibility, safety, and sustainability. We appreciate that you are taking the time to review our report and we hope you see the value and innovation in this process as we do.

Sincerely,

Senior Design Team 2[1]: Delaney Bachman, Gitau Wambugu, Lindsey Jarema, Andy Mason, and Firdavs Nasimov

[1]Department of Chemical Engineering, University of Nebraska-Lincoln, Lincoln, NE

Enclosure

Upgrading Cracking Waste to Rubber Precursors via Oxidative Dehydrogenation

CHME 453
University of Nebraska-Lincoln

Team 2:
Delaney Bachman, Andy Mason, Lindsey Jarema, Gitau Wambugu, and Firdavs Nasimov

01 May 2020

Executive Summary

As the result of process changes within an ethylene cracking plant, the amount of a C4 byproduct waste stream has significantly increased (Fabiano, Nedwick 1999). A system of extractive distillation and catalytic oxidative dehydrogenation can be used to add value to this C4 waste stream by producing high purity 1,3-Butadiene, an important rubber precursor. 1,3-Butadiene is a critical component of multiple consumer goods, including automobile tires and synthetic rubber and has a steadily increasing demand, reaching 10 million metric tons in 2012 (Biddy, Scarlata, Kinchin, 2016). The simulation assumes a feed flow rate of 30,000 lb/hr of mixed low grade fuel containing the composition provided in Table 1, with outputs of 16,900 lb/hr of 99% pure 1,3-Butadiene and 10,800 lb/hr of fuel byproduct. The fuel byproduct is mixed and sold under the same low grade fuel rating the mixed feed was previously sold by.

Table 1: Feed stream component mass fractions

Component	**Mass fraction**
1,3-Butadiene	0.43
Isobutylene	0.234
1-Butene	0.124
N-Butane	0.045
Isobutane	0.05
Cis-2-Butene	0.041
Trans-2-Butene	0.053
Vinyl Acetylene	0.007
1-Butyne	0.002
Allene	0.002
Propyne	0.007
Isopentane	0.005

The strategy of increasing stream value was achieved by a series of extractive distillation columns and separators to purify the 1,3-Butadiene from the rest of the stream, while a packed bed reactor supporting a bismuth molybdate catalyst forces a side stream to undergo an oxidative dehydrogenation reaction to convert 1-butene and trans-2-butene to more 1,3-Butadiene. Additionally, an extragent is used to facilitate effective distillation and to reduce the utility cost of separating very similar components. The extragent chosen for simulation was dimethylformamide, a stable, organic solvent capable of carrying our product. As it is a dehydrogenation reaction, hydrogen gas is produced as a side product. This gas is burned in-house for energy generation in an effort to reduce energy costs for this plant addition, and is therefore not included in mass balances throughout the system. The heating and cooling utility cost for the plant

addition is 10.38 Gcal/hr and 13.55 Gcal/hr, respectively, with potential savings to 0.2843 Gcal/hr for heating utilities and 3.457 Gcal/hr to cooling utilities. The critical equipment used for this addition includes the primary rectification column which separates the light and heavy components from the fuel mixture, an extractive distillation column to purify 1,3-Butadiene, a desorption column to separate DMF from the final product, a second rectification column to remove side products and allow for reaction of 1-butene and trans-2-butene, and the previously mentioned oxidative dehydrogenation packed bed reactor. Optimizations to minimize the heating utility is done by examining the heat exchange network system, or HENS, of our simulation. Initial simulations only included nine heat exchangers to heat and cool streams to their desired temperatures. After HENS analysis, it was found that an optimal cost required 23 heat exchangers and despite the much higher initial cost of equipment, this resulted in much lower total cost when including yearly utility cost.

While this addition was thought to be a highly lucrative investment from initial market research, it was found to be a highly exhaustive process, both energy and material-wise, and far too expensive to be feasible after economic analysis. An in depth multi-criterion decision matrix is presented in Table 2.

Table 2: Multi-Criterion Decision Matrix

Economics and sustainability indicators	Weighting factor: 0-1	Selling feed as low-grade fuel	Upgrade feed to rubber precursors
Economic indicators			
Net present value NPV	1	+	-
Payback period PBP	0.85	+	-
Rate of return ROR	0.7	+	-
Economic constraint EC	0.9	-	+
Impact on employment	0.95	-	+
Impact on customers	0.6	+	+
Impact on economy	0.95	-	+
Impact on utility	0.7	+	-
Sustainability indicators			
Material intensity	0.6	+	-
Energy intensity	0.85	+	-
Environmental impact: GHG in production	0.8	-	-
Environmental impact: GHG in utilization	0.9	-	+
Toxic/waste material emissions-	0.9	+	-
Potential for technological improvements	0.7	-	+
Security/reliability	1	+	+
Political stability and legitimacy	0.85	-	+
Quality of life	0.3	-	+
Total positive score		**9**	**9**
Total minus score		**8**	**8**
Net score (positive-minus)		**1**	**1**
Weighted total score		**0.85**	**0.75**

Despite its multiple advantages in employment, expansion into a different target market, and greenhouse gas emissions, the calculated net present value (NPV) and rate of return (ROR) are simply too low to soundly back this venture. These values are illustrated in Figure 1, a cash flow diagram which shows the yearly value of the addition over a 15 year life span and 2 year construction period.

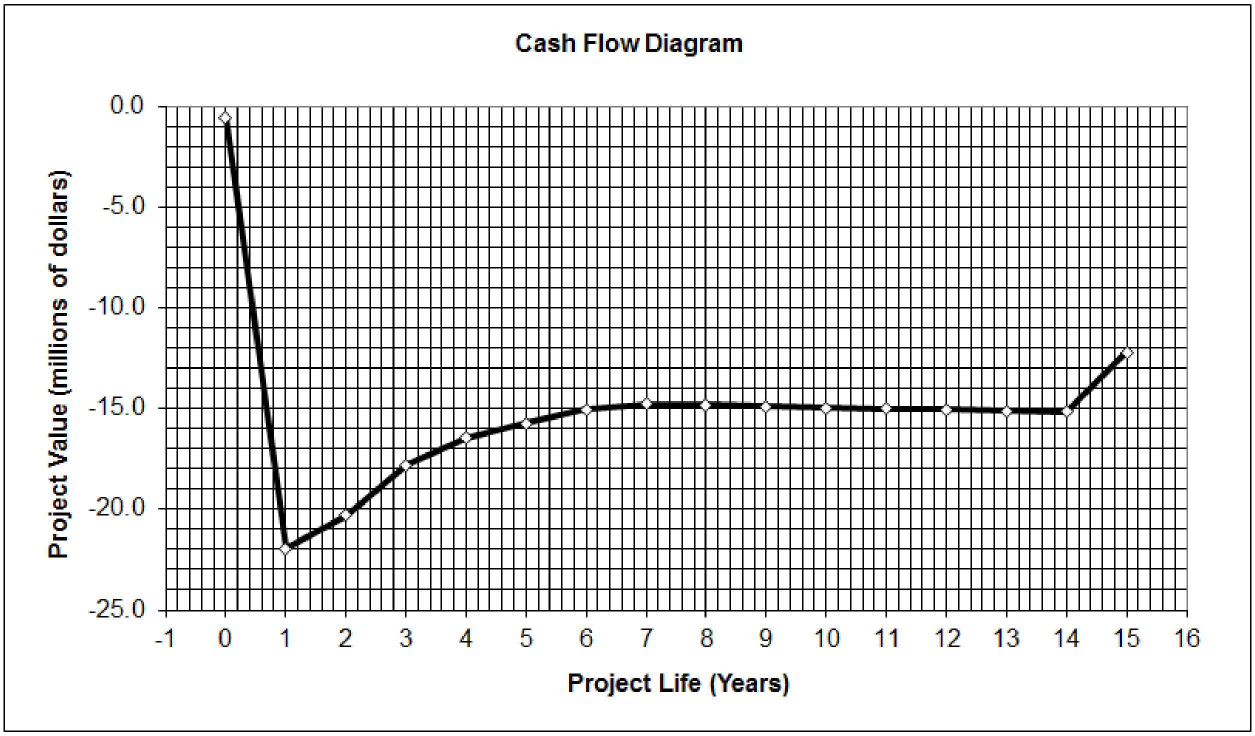

Figure 1: Cash Flow Diagram after HENS optimization

Calculation for all values presented are attached in appendices, and further examination of all topics are discussed within the following report.

Design Problem Statement

Add value to a cracking waste product stream by designing and incorporating an industrial-scale catalytic dehydrogenation reactor and separation system for more efficient production of rubber precursors (conversion of butenes to 1,3-butadiene). This cracking waste stream, consisting mainly of 4-carbon organic gases e.g. 1,3-butadiene, isobutene, 1-butene, and 2-butene (cis- and trans-), is the input of our process and has an assumed flow rate of 30,000 lb/hr. Intended product specification is 99% 1,3-Butadiene product, with any out of spec product or remaining stream components to be blended and sold at fuel value. Approximately 16,900 lb/hr of 1,3-Butadiene will be produced with 10,800 lb/hr of fuel byproduct. The process includes several separation units including extractive rectification and desorption units. The reactor is a packed bed which uses bismuth molybdate as the catalyst.

Introduction

The process of cracking, or breaking large hydrocarbon molecules into smaller hydrocarbon molecules, (Encyclopaedia Britannica, 2018) is a widely used process with worldwide familiarity bridging a number of different industries. This thermal decomposition reaction can be used to produce olefins from ethane, propane, butane, naphthas, (Fabiano, Nedwick 1999) or other large and generally flammable hydrocarbon molecules. While one particular desired product is harvested from the cracking process, a waste stream of a variety of smaller chain hydrocarbon products is also produced. In the case presented by Fabiano and Nedwick, this product stream is primarily composed of C-4 hydrocarbons, like methyl acetylene, propadiene, propane, 1,3-Butadiene, ethyl acetylene, vinyl acetylene, 1-butene, cis-2-butene, trans-2-butene, iso-butene, isobutane, and iso-pentane. This waste stream increased in volume significantly due to a change in feed to the cracking process. Because this stream was treated as waste and sold at fuel value there is room for optimization and potential to add value to this stream. The cracking process itself remains outside the scope of this focus on optimization, and only the upgrade to the waste stream will be investigated, as proposed by Fabiano and Nedwick. The largest component of the stream is 1,3-Butadiene (Butadiene), which is a building block for the industrial production of synthetic rubber (Research Nester, 2019) and rubber products like automobile tires, (Biddy, Scarlata, Kinchin, 2016) paper coatings on everyday consumer products (Mallard Creek Polymers, 2016), and other instances of applied polymer production. Butadiene is a ubiquitous and valuable product, and the total world consumption of Butadiene in 2012 was around 10 million metric tons (Biddy, Scarlata, Kinchin, 2016). Because of a worldwide trend in cracking processes using lighter feedstocks due to an abundance of shale gas, less Butadiene is produced from cracking processes relative to the ethylene being produced, but the demand for Butadiene has remained largely unchanged. For this reason, it is prudent to recover Butadiene from the given waste stream so that it can be used to produce synthetic rubbers and other products rather than being burned as fuel. Our intended product purity is decided to be 99%. The remaining streams created by the separation of Butadiene will be blended and sold at fuel value, the way the original waste stream was.

The feed stream to our proposed separation process is composed of a mixture of C-4 compounds previously described. This mixture is given to be 30,000 lb/hr leaving the cracking process, a scaled down rate from that proposed by Fabiano & Nedwick (1999). We assumed the stream to have a temperature of 200°C leaving the cracking process (Sadrameli, 2016) at a pressure of 1 atm. The composition of the stream is assumed to be 12,900 lb/hr 1,3-Butadiene, 7,020 lb/hr of iso-butene, 3,720 lb/hr of 1-butene, 1,590 lb/hr trans-2-butene, 1,230 lb/hr cis-2-butene, 1,500 lb/hr iso-butane, 1,350 lb/hr n-butane, 150 lb/hr iso-pentane, 210 lb/hr methyl acetylene, 210 lb/hr vinyl acetylene, 60 lb/hr propadiene, and 60 lb/hr ethyl acetylene, components also proposed by Fabiano & Nedwick (1999). We also assumed the composition was to remain constant, as well as assuming that there was to be no fluctuations in feed stream composition, as the cracking process upstream of the designed recovery unit is out of scope of this project.

Assumptions

There were a variety of assumptions used in the design of the Butadiene recovery system. Each assumption may fell into one of the following categories:

Thermodynamic behaviors

To select physical property methods in Aspen, the manual by Aspen Technology (2001) was consulted for differentiating the best methods for each unit in the system. Ultimately, one method proved to be useful for each primary unit in the system:

Peng-Robinson-Boston-Mathias Method

We used the Peng-Robinson-Boston-Mathias (PR-BM) method to simulate the operation of each of the primary unit operations in the overall process, i.e. Column 1, Column 2, Column 3, the Reactor, and the Desorption system consisting of three additional columns. This method is often recommended for processes related to or involving gas-processing and petrochemical applications, like refineries (Aspen Technology, 2001). The PR-BM method is also suggested for polar or mildly polar mixtures (Aspen Technology, 2001). Examples of polar mixtures are hydrocarbons and light gases, such as carbon dioxide, hydrogen sulfide, and hydrogen (Aspen Technology, 2001). Using the PR-BM property method, we obtained reasonable results at all working temperatures and pressures, and the results are accurate in the region near the critical point of the mixture (Aspen Technology, 2001). There are other physical property methods that could potentially be used for the modeling of the reactor because they also can accommodate high pressures and temperatures, and mixtures close to their critical points. These methods include Benedict-Webb-Rubin-Starling (BWRS), Benedict-Webb-Rubin-Lee-Starling (BWR-LS), Lee-Kesler-Plöcker (LK-PLOCK), and Redlich-Kwong-Soave-Boston-Mathias (RKS-BM) (Aspen Technology, 2001).

Financial calculations

For completing financial calculations, we used assumptions relating to the validity of our resource documents as well as generally accepted estimations for financial parameters and industrial demand. We assumed, for example, that given a corrected CPI factor for a current year, as well as correct specs for the piece of equipment, that the CAPCOST document will yield to us an accurate and usable price for the equipment. In these calculations, a CEPCI value of 596 from November 2019 was used. Moreover, the life of the project was assumed to be 15 years with a 7% interest rate and 35% taxation, which is taken from historical data on petrochemical process plants (Hillebrand, 2011) and heuristics (Demirel).

To calculate approximately the cost of the catalyst used in the process, a figure for which there is no industrial standard, an estimation was used for the parameters thought to contribute most to the cost. The bare cost of the chemicals was calculated using the quantities (Hartmanova, et. al, 2009) and prices for those chemicals from the chemical supply company Sigma Aldrich. The build material for all components is assumed to be carbon steel. These calculations are available in Appendix A-4 for consideration.

Operating conditions

We assumed the entire system to be operating at steady-state based on the aforementioned assumptions, to increase ease of calculations. Additionally, some operating conditions were assumed for each piece of equipment in the process and are discussed in detail in the *Results* section of this report.

Results

Process Description

The process of separating and upgrading a cracking waste stream to rubber precursors, namely 1,3-Butadiene, includes rectification, extractive distillation, and an oxidative dehydrogenation reaction.

Block Flow Diagram (BFD)

The block flow diagram for high purity 1,3-Butadiene production can be found in Figure 2. There are five main process units involved in the purification and upgrade of a primarily C4 cracking waste product stream. First, rectification is employed to separate C3 and C5 hydrocarbons such as propyne and isopentane. The Main C4 stream then goes through an extractive rectification column using dimethylformamide (DMF) as the extragent. The desorption and purification step is necessary to recover the DMF to be recycled and purify the 1,3-Butadiene to 99%. The extractive rectification column's distillate stream includes mainly 1-Butene, 2-Butenes (cis- and trans-), isobutylene, and 1,3-Butadiene. Another rectification column is used to remove isobutylene and traces of N-butane and isobutane. This stream can be sold at fuel value. The reactor involves an oxidative dehydrogenation reaction which converts 1-Butene and Trans-2-butene to 1,3-Butadiene. Bismuth molybdate is used as the catalyst. Hydrogen gas (H_2) is produced as a side product from the reaction and is assumed to be used elsewhere in the plant since this process is considered an extension of an existing refinery as stated in the design problem statement. The reaction mixture is then recycled back to the extractive rectification column to recover more 1,3-Butadiene.

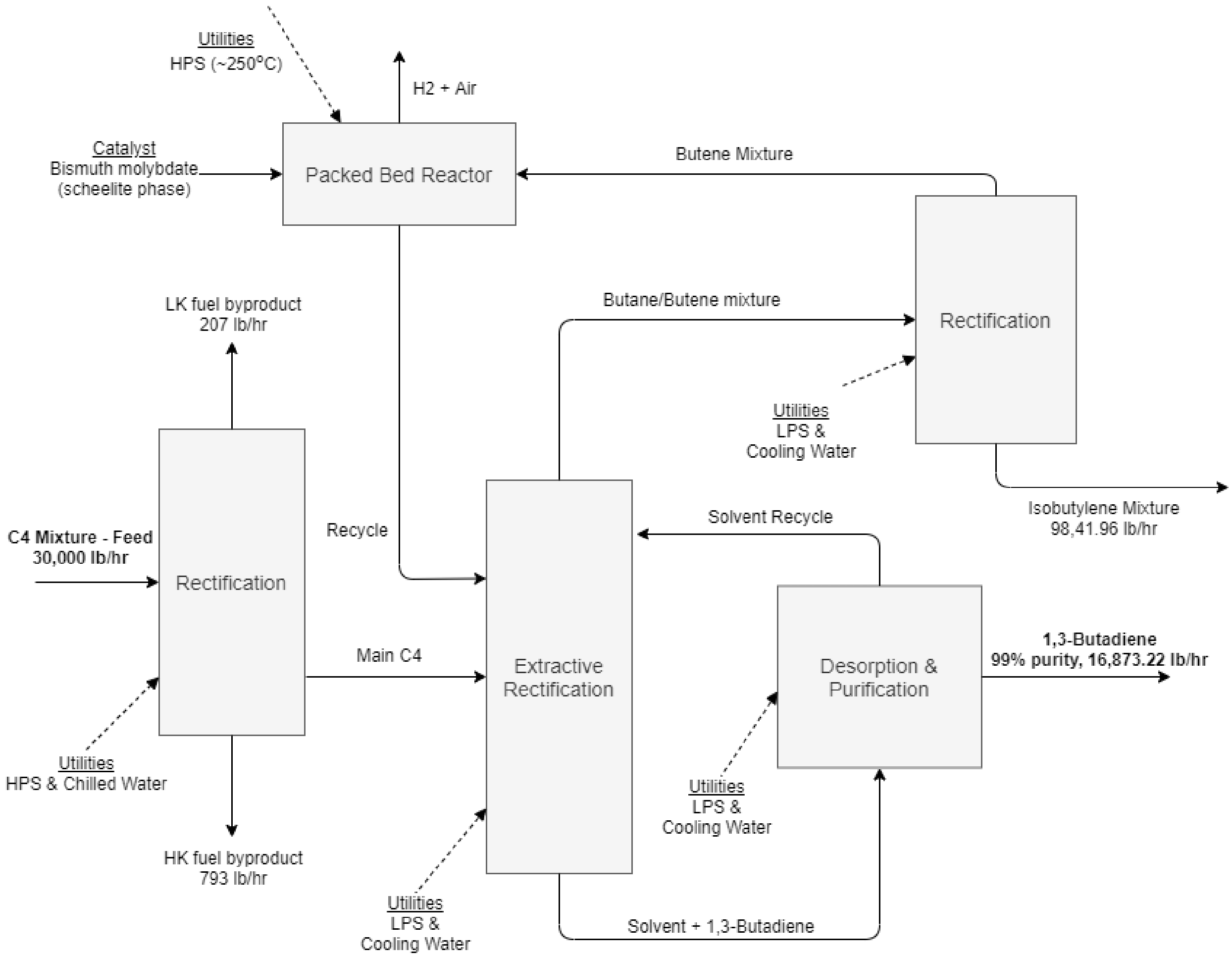

Figure 2: Block Flow Diagram

A feed flow rate of 30,000 lb/hr is assumed for this process. A product flow rate of 16,873 lb/hr of >99% 1,3-Butadiene is expected. The other byproduct flow rates can be found in the BFD. The utilities used in the process include cooling water, chilled water, low pressure steam, high pressure steam, and electricity. The specific assumptions associated with these utilities will be discussed later in the report.

Process Flow Diagram (PFD)

A detailed process flow diagram of the process was created using Aspen Plus V11 and is shown in Figure 3.

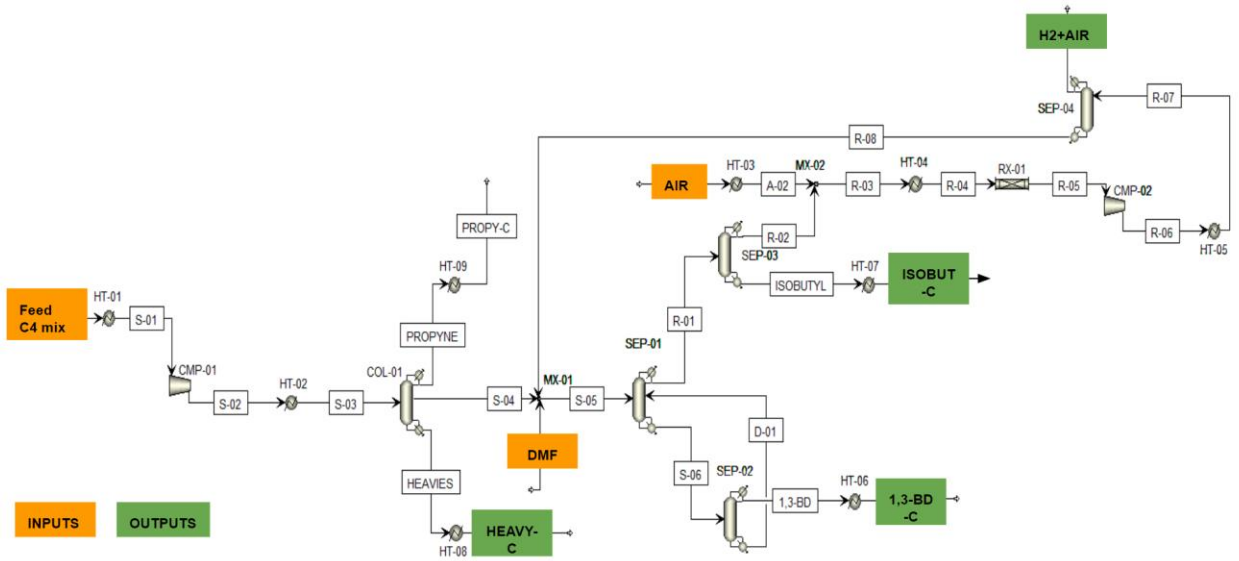

Figure 3: Overall Process Flow Diagram

In order to better understand the process, the PFD is broken into two subsections for clarity and discussion. The first section of the PFD is shown in Figure 4.

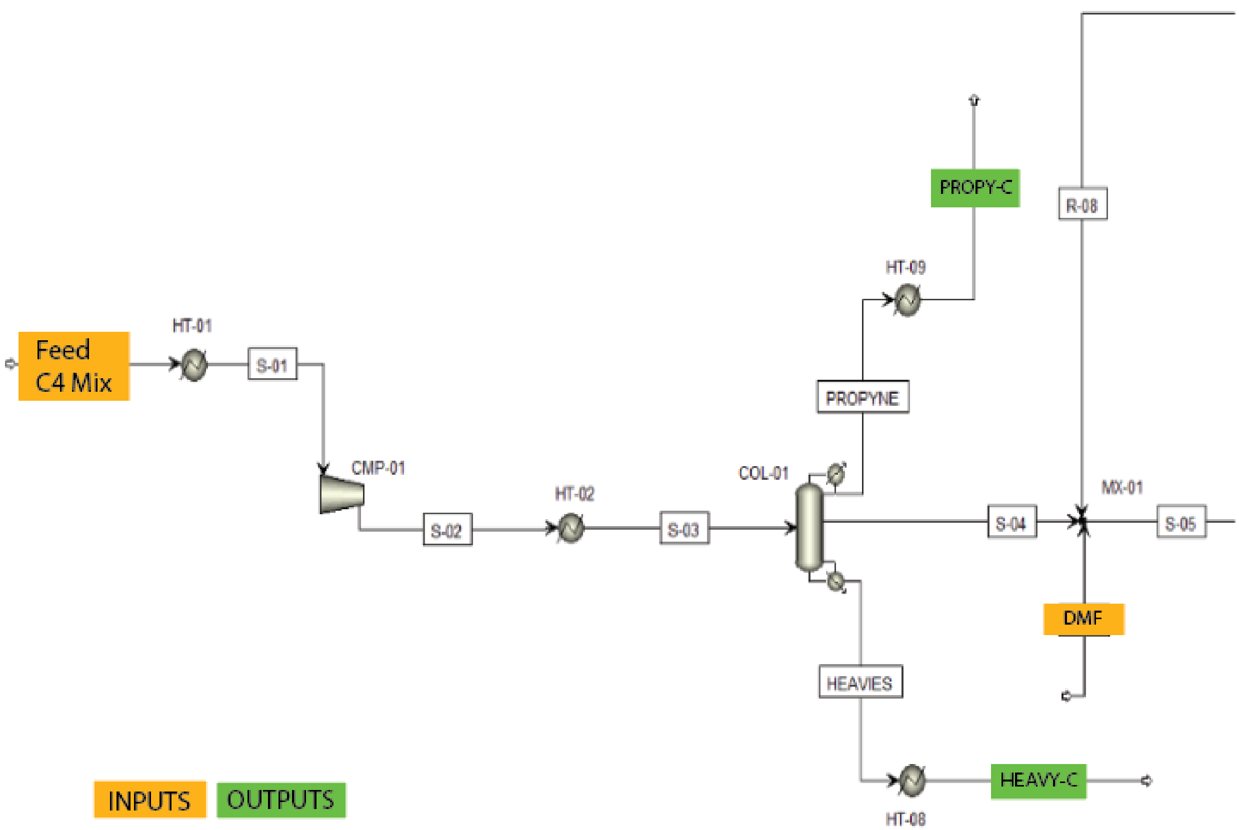

Figure 4: Initial purification step of PFD enlarged for clarity.

The first section of the PFD includes four heat exchangers, a compressor, a mixer, and the first rectification column. HT-01 is used to cool the incoming feed from 150ºC to 55ºC before pressuring the feed in the isentropic compressor, CMP-01, from 1 atm to 5.5 atm. The feed is then cooled again from 127ºC to 48ºC before entering COL-01. The distillate from COL-01, which is mostly methyl acetylene, is then heated to 25ºC in HT-09 for storage. The bottoms from COL-01, which is mostly isopentane and 2-butenes, is then cooled to 25ºC in HT-08 for storage. Stream S-04, which is mostly C4 hydrocarbons including the desired 1,3-Butadiene, is taken from tray 42 and is then mixed with the extragent, DMF, and the recycle stream in MX-01 before going into the extractive distillation column.

To further elaborate on COL-01, we designed it to have 75 total stages, with a total condenser and kettle reboiler. We assumed the feed to COL-01 to match the stream properties given in the prompt by Fabiano & Nedwick (1999), with the total stream set to a mass flow rate of 30,000 pounds per hour. This feed stream composition of chemicals and their respective mass fractions is 1,3-Butadiene (0.43), Isobutylene (0.234), 1-Butene (0.124), N-Butane (0.045), Isobutane (0.05), Cis-2-Butene (0.041), Trans-2-Butene (0.053), Vinyl Acetylene (also called Butenyne) (0.007), 1-Butyne (also called ethyl acetylene) (0.002), Allene (0.002), Propyne (0.007), and Isopentane (0.005). These values are tabulated in Table 3.

Table 3: Feed stream component mass fractions

Component	**Mass fraction**
1,3-Butadiene	0.43
Isobutylene	0.234
1-Butene	0.124
N-Butane	0.045
Isobutane	0.05
Cis-2-Butene	0.041
Trans-2-Butene	0.053
Vinyl Acetylene	0.007
1-Butyne	0.002
Allene	0.002
Propyne	0.007
Isopentane	0.005

The feed stream entered on stage 26 of the column. Using design specifications, the optimum reboiler duty was found to be 4922 kW and the optimum distillate flow rate was found to be 207 lb/hr. This was done to specify recoveries of methyl acetylene in the distillate and isopentane in the bottoms to 0.7 on a mole basis.

The second section of the PFD is shown in Figure 5.

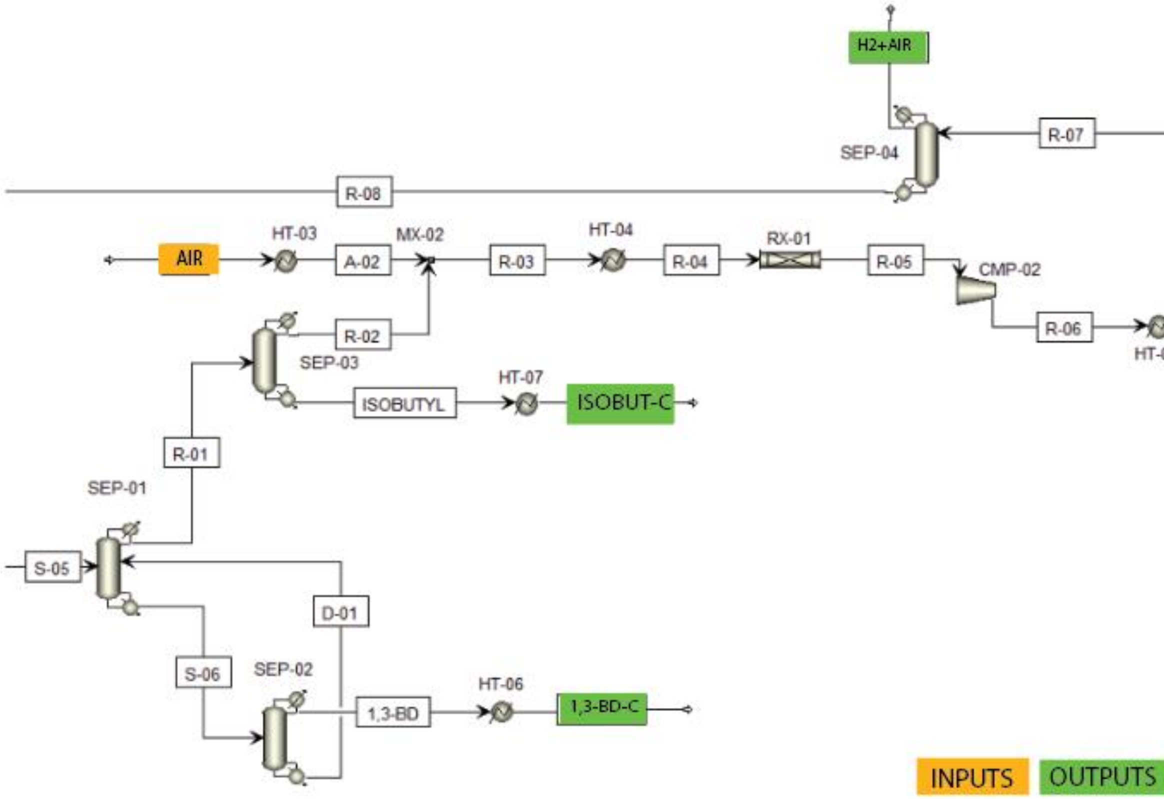

Figure 5: Reactor and final purification steps of PFD enlarged for clarity.

The second section of the PFD starts with stream S-05 entering SEP-01 which is the extractive distillation column. Due to technical difficulties encountered when modeling the extractive distillation column on Aspen Plus, the use of a separator was employed to simulate the column. The expected purities were input based on literature values (Pavlov et. al., 2011). We are also able to estimate the column size based on this literature. We assumed SEP-01 to have 150 stages with a total condenser and kettle reboiler. SEP-01 operates at a pressure of 5.5 atm. The distillate mass flow rate is 74170.9 lb/hr which is then further separated in SEP-03 to remove isobutylene and butanes. SEP-03, although modeled using a separator unit is Aspen, is a rectification column with 20 trays as seen in literature. It operates at 5.5 atm and has a bottoms flow rate of 9841.96 lb/hr. The bottoms product is then cooled to 25ºC in HT-07 for storage. This product is sold as fuel. The SEP-03 distillate flow rate is 62474.4 lb/hr and consists of 1-Butene, 2-Butenes, and 1,3-Butadiene. This stream is then mixed in MX-02 with 29170.8 lb/hr of air which was heated to 200ºC in HT-03. The mixture is then heated further to 250ºC in HT-04 before entering the reactor. The reactor will be described in detail in the following section of this report. The reaction products are then repressurized to 5.5 atm in CMP-02 and then cooled to 48ºC in HT-05. SEP-04 is a separation unit which removes the hydrogen gas produced during the reaction and air. The hydrocarbon mixture is then recycled back and mixed with the feed in MX-01 before entering SEP-01.

The bottoms of SEP-01 primarily contains the extragent, DMF, and 1,3-Butadiene. The flow rate of this stream, S-06, is 100,528 lb/hr and feeds into SEP-02. Again, due to technical difficulties with Aspen simulation, this desorption column was modeled as a separation unit with specified recoveries as seen in literature (Pavlov et. al., 2011). For cost estimates, the column was assumed to have 65 trays, a total condenser, and kettle reboiler. The bottoms product, containing the extragent, is recycled back to SEP-02. The distillate from SEP-02 meets the 1,3-butadiene product specifications of >99% purity.

Reactor

We designed the reactor to be a tube bundle reactor in accordance with the design recommendations provided in US Patent No. 7,034,195 B2 (2006), U.S. Patent No. 8,524,156 B2 (2013), and industry standards (Altoona Pipe & Steel, 2020; Archtoolbox, 2018; Colburn, n.d.; Engineering ToolBox, 2004; Ferguson Enterprises, 2020a, 2020b; Project materials, 2017; The ProcessPiping, n.d.). The reactor tubes were assumed to be schedule 40 carbon steel tubes, 21 ft in length with a nominal pipe size (NPS) of 2 inches (Altoona Pipe & Steel, 2020; Archtoolbox, 2018; Colburn, n.d.; Engineering ToolBox, 2004; Ferguson Enterprises, 2020a, 2020b; Project materials, 2017; The ProcessPiping, n.d.; U.S. Patent No. 8,524,156 B2, 2013). This style of tubing was chosen as it is readily available for purchase, eliminating the need for custom reactor tubes. The small NPS also acts to bolster heat transfer between the heating medium and tube contents as heat transfer through the reactor walls is very difficult for large diameters (Zobel et. al., 2011). Zobel et. al. (2011) also suggested that a more homogeneous void fraction distribution could be obtained if a wave-like orthogonal structure were to be applied to the tubing walls. However, we forwent this suggestion to avoid the increased costs associated with custom tubing; we believed that the homogeneity of the void fraction could be adequately ensured by careful packing of the reactor tubes. It must be stated that the inner tube diameter, referred to henceforth as tube diameter (D), for NPS 2 inches is equivalent to 52.5 mm, which is slightly larger than the maximum tube diameter specified in the U.S. Patent No. 8,524,156 B2 (2013). This divergence from the U.S. Patent No. 8,524,156 B2 (2013) tube diameter recommendation solely was because tubes with an exact inner diameter of 50 mm are not the industrial norm, and would therefore require custom ordering. We feel that the 2.5 mm difference in tube diameter is not large enough to warrant custom reactor tubes, hence why we assumed 2 inches NPS tubing instead.

We determined the number of reactor tubes required to achieve a 1-butene conversion of 0.996 to be 135 tubes. A sensitivity analysis was attempted to determine the required number of reactor tubes but yielded inconsistent results, making it unreliable. Again, we diverged from the U.S. Patent No. 8,524,156 B2 (2013) minimum tube number recommendation of 1,000 tubes as it would have resulted in an oversized reactor and thus incurred additional costs. Of the 135 reactor tubes, thirty were selected as thermometer tubes to measure the axial and radial reactor temperature at various points (U.S. Patent No. 8,524,156 B2, 2013). Thermometer tubes are reactor tubes filled with the reactor catalyst where the temperature is measured along the flow path in the catalyst bed by thermocouples (U.S. Patent No. 8,524,156 B2, 2013). These thermometer tubes would, in industrial practice, enable us to monitor the progression of the reactions within the reactor, further enhancing the process safety and potential for the reactor operator to optimize the reactor's performance based on real-time data e.g. decrease the heating duty input if the registered reactor temperatures are higher than required (U.S. Patent No. 8,524,156 B2, 2013). We assumed that there was a protective tube in the radial center of each thermometer tube, held in place by the reactor catalyst and helical spring spacers (U.S. Patent No. 8,524,156 B2, 2013). The protective tubes were constructed of carbon steel and were 21 ft in length, with an outer diameter of 3.2 mm and wall thickness of 0.2 mm (U.S. Patent No. 8,524,156 B2, 2013). Seven type K thermocouples were spaced 3 ft apart in each protective tube, starting from the end of the protective tube - these thermocouples measured the reactor temperature inside the thermometer tubes (REOTEMP Instrument Corporation, 2011; U.S. Patent No. 8,524,156 B2, 2013).

We set the reactor temperature constant to 250ºC in line with the recommendations provided in US Patent No. 7,034,195 B2 (2006). This temperature was the minimum temperature recommended by the patent, so running the reactor at the temperature allowed us to minimize the reactor's utility cost. We also opted for the lower reactor temperature to minimize sintering, and thus deactivation, of the chosen reactor catalyst, bismuth molybdate. Sintering, as defined by Worstell (2014a), is the agglomeration of catalytically active surface metal atoms due to high temperatures, resulting in their d-orbitals rearranging and becoming catalytically inactive. Schuh et. al. (2015) observed catalyst deactivation for varying bismuth molybdate system (Bi-Mo-O) catalysts at temperatures above 440 °C probably due to sintering and decreased specific surface area. Since sintering is primarily temperature-dependent, the specified reactor temperature of 250ºC greatly reduced the likelihood of this occurring within our reactor (Worstell, 2014a). Le (2018) also suggested that the sublimation of molybdenum from the bismuth molybdate catalyst may play a minor role in the deactivation process, so lower reactor temperatures reduced the prevalence of inside the reactor.

We set the initial reactor feed pressure to 1 atm and assumed that pressure drop across the reactor, ΔP, was negligible. The oxygen:trans-2-butene reactor feed mixture ratio was set at 15:10 to satisfy the oxygen requirement highlighted by our MATLAB predictive model, included in Appendix A-7. Sugiyama et. al (2017) concluded that oxygen-poor conditions within a reactor results in increased catalyst deactivation of bismuth molybdate, our chosen catalyst. This reduction in catalyst performance was noted to be due to increased coking over the catalyst surface and lattice oxygen in the catalyst moving from the bulk to the surface in order to maintain Mo_6^+ on the surface of the catalyst (Sugiyama et. al, 2017). Thus, the oxygen:trans-2-butene ratio was chosen to minimize coke formation and lattice oxygen migration.

We assumed that the tube bundle reactor annulus was constructed of carbon steel and rated for 45 bars gauge pressure (barg). We also assumed that the tube bundle reactor was well-insulated, making any heat loss negligible. We picked high-pressure steam at 41 barg and 254ºC as the heating utility. The heating utility cost was determined from the Aspen simulation calculated reactor heat duty and can be found in Appendix A-6. A summary of the reactor design parameters is presented below in Table 4.

Table 4: A summary of the reactor tube bundle design parameters.

Reactor parameter	**Specifications**

Reactor tubes	**Number required:** 135 (30 would also serve as thermometer tubes) **Length:** 21 ft **NPS:** 2 inches **Schedule:** 40 **Material of Construction (MOC):** Carbon steel
Protective tubes	**Number required:** 30 **Length:** 21 ft **Outer diameter:** 3.2 mm **Wall thickness:** 0.2 mm **MOC:** Carbon steel
Type K thermocouples	**Number required:** 210
Helical spacing springs	**Number required:** Per user discretion
Annulus	**MOC:** Carbon steel **Pressure rating:** 45 barg
Operating conditions	**Reactor temperature**: 250ºC **Reactor pressure:** 1 atm **Heat loss:** negligible **Pressure drop (ΔP):** 0 atm **Oxygen:trans-2-butene reactor feed mixture ratio:** 15:10
Heating utility (high-pressure steam)	**Temperature:** 254ºC **Pressure:** 41 barg

Catalyst: Bismuth molybdate

As mentioned above, we selected bismuth molybdate, scheelite (ɑ) phase, as our catalyst for the oxidative dehydrogenation of 1-butene and trans-2-butene to 1,3-butadiene, as per the recommendation in US Patent No. 7,034,195 B2 (2006) to use Mo-Bi-O alloy oxide systems. The scheelite phase of bismuth molybdate has been reported to be stable in a large temperature range between room temperature and 650°C, according to Le (2018). Furthermore, Le (2018) further stated that later-generation molybdate-based catalysts are almost indestructible and can easily withstand inadvertent plant upsets, including severe reductions. The lifetime for bismuth molybdate catalysts has also been reported to range between 3 to 5 years for the oxidative dehydrogenation of propene (Dittmer et. al., 2014). Additionally, Zhai et. al. (2015) documented that bismuth molybdate had a larger rate constant at temperatures lower than 633 K when compared to bismuth vanadate and a bismuth-vanadium-molybdenum-oxide hybrid. We believe that all these factors justify our choice of bismuth molybdate, scheelite phase, as a suitable catalyst for the oxidative dehydrogenation.

We selected the Raschig ring for our pellet geometry based on the suggestions for pellet geometry made in US 7,034,195 B2 (2006), and by Afandizadeh & Foumeny (2001). We felt that the Raschig ring geometry maximized catalyst performance per unit mass catalyst as it has the largest catalytic surface area to volume ratio when compared to spheres of equal volume and solid cylinders of equal height and outer diameter (Afandizadeh & Foumeny, 2001). This is an important consideration when optimizing reactor performance as the catalysis of reactions normally takes place on the catalyst surface, so a larger catalytic surface area to volume ratio results in increased process profitability.

We chose a pellet outer diameter, d_o, of 4 mm to correspond to a tube diameter to equivalent pellet spherical diameter ratio, D/d_{ps}, greater than 10 - our D/d_{ps} was 12.4. This D/d_{ps} ensured that the fluid flow velocity profile was flat across the catalyst mass (Worstell, 2014b). The pellet height to pellet outer diameter ratio, h/d_o, was chosen to be 1.25 in accordance with the optimum design range provided by Afandizadeh & Foumeny (2001). The pellet inner diameter to pellet outer diameter ratio, d_i/d_o, was chosen to be 0.6 in accordance with the optimum design range provided by Afandizadeh & Foumeny (2001). Detailed calculations of d_{ps} can be found in Appendix A-3. A summary of the catalyst pellet geometric properties is presented below as Table 5.

Table 5: A summary of the catalyst pellet geometric properties.

Geometric property	**Value**
Pellet outer diameter, d_o	4 mm
Pellet height to pellet outer diameter ratio, h/do	1.25
Pellet inner diameter to pellet outer diameter ratio, d_i/d_o	0.6
Tube diameter to equivalent pellet spherical diameter ratio, D/d_{ps}	12.4

We assumed that the reactor tubes were filled using the patented ‘snow storm filling’ method described by Afandizadeh & Foumeny (2001), paired with effective mechanical vibration being applied as the bed is being formed, to establish uniform dispersion of the catalyst during packing. In the patented ‘snow storm filling’ method, the packing material is passed over staggered wires or wire meshes so that the fall of the particles is interrupted before the particles reach the bed face (Afandizadeh & Foumeny, 2001). The uniform distribution of catalyst validated our generalization of homogeneous reaction conditions inside the reactor tubes as the orientation of the catalyst pellets inside the reactor tubes can greatly affect the progression of the reaction and production costs, according to Chutichairattanaphum et. al. (2019). This validated generalization, in turn, greatly improved the reliability of the results generated by the Aspen simulation and MATLAB model. Moreover, the 'snow storm filling' method produces consistent results, making it favorable to employ in the tube bundle reactor (Afandizadeh & Foumeny, 2001).

Reaction mechanism and rate

The reaction mechanisms for the oxidative dehydrogenation of 1-butene and trans-2-butene are thought to follow a Mars-van Krevelen mechanism, where the alkene is adsorbed onto the catalyst surface, activated by the abstraction of the α hydrogen to the double bond to produce an allylic intermediate into which reacts via the inserted lattice oxygen to form the desired products (Park & Shin, 2015; Zhai et. al, 2015). The reduced catalyst is then reoxidized by a supply of gaseous oxygen, hence why oxygen (or air) is fed into the reactor (Park & Shin, 2015; Zhai et. al, 2015). A diagram of the proposed reaction mechanism by Zhai et. al (2015) for the oxidative dehydrogenation of 1-butene to 1,3-butadiene over bismuth molybdate, scheelite phase, is presented below as Figure 6. The rate equations for the oxidative dehydrogenation of 1-butene and trans-2-butene are included in Appendix A-4. We assumed that rate equations for the isomerizations of 1-butene and trans-2-butene were identical to those for the oxidative dehydrogenation reactions, aside for the rate constants, included in Appendix A-4. In the Aspen simulation, the oxygen concentration term is omitted as Aspen does not allow the user to input a spectator chemical species into a rate equation i.e. the oxygen is not included in the final products.

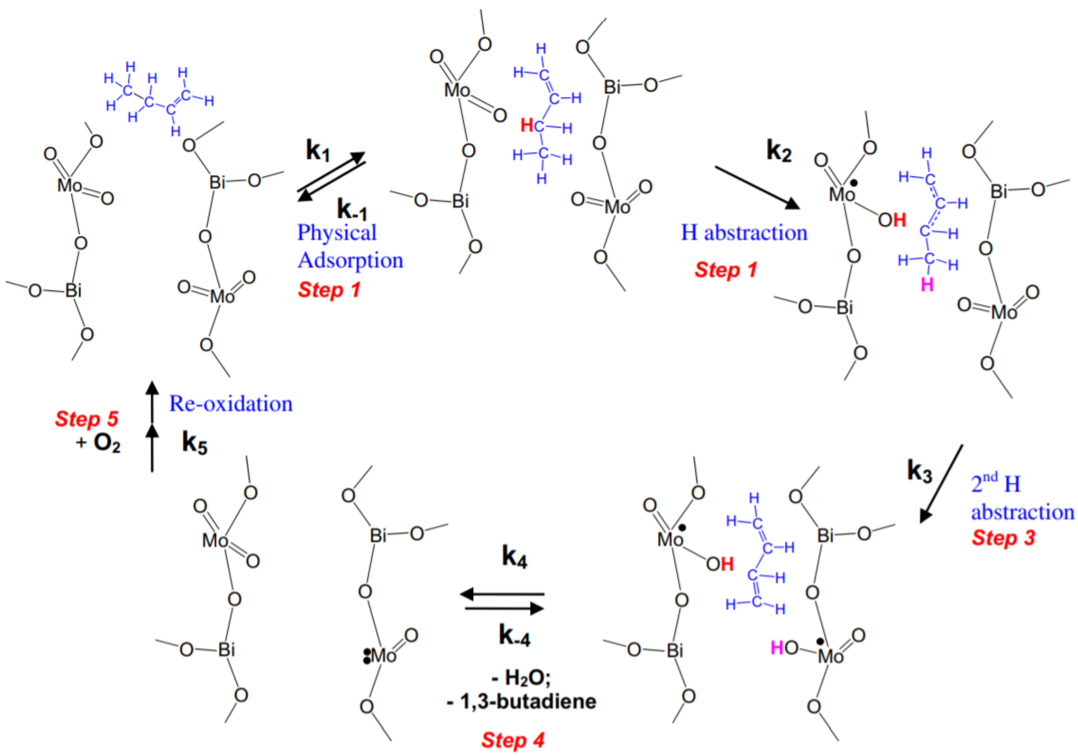

Figure 6: A diagram of the proposed reaction mechanism by Zhai et. al (2015) for the oxidative dehydrogenation of 1-butene to 1,3-butadiene over bismuth molybdate, scheelite phase.

We obtained experimental rate constants for the oxidative dehydrogenation of 1-butene and trans-2-butene from Zhai et. al. (2015). At 625 K, the experimental rate constants for the oxidative dehydrogenation of 1-butene and trans-2-butene were read to be 0.0001585 s^{-1} and 0.00001474 s^{-1}

respectively (Zhai et. al, 2015). We scaled these rate constants to calculate the reaction rates in kmol/hr and used them to determine the number of reactor tubes required to attain a 0.996 conversion of 1-butene entering the reactor, as well the steam mass flow rate to satisfy the calculated reactor heat duty. Calculations for the scaling of the rate constants can be found in Appendix A-4. The calculated reactor heat duty is 3.8961 GJ/hr

When scaling the rate constants, we assumed that the rate constants were proportional to the mass of catalyst used. We assumed the original catalyst mass used by Zhai et. al. (2015) was 125 mg, an average of the catalyst mass range used during their experiments; the new catalyst mass was assumed to be 1 kg. It would have been more appropriate to use the surface area of the catalyst to scale up the rate constants as the reactions occur on the catalyst surface. However, the surface area of the experimental catalyst was not provided by Zhai et. al. (2015) and would have been tedious to calculate for the masses generated by the Aspen simulation and MATLAB models. Thus, using the mass as a scaling factor provided a simpler means to scale the rate constant as a larger mass should normally correspond to a larger surface area. We also assumed that the original rate constant resulted in a reaction rate with units of mol/s, so we modified the original rate constants to output reaction rates in kmol/hr. For the Aspen Plus simulation, the rate constants were additionally multiplied with the assumed bismuth molybdate bulk density of 1,640 kg/m^3, which was taken to be an average of the bulk density for molybdenum oxide (1,570 kg/m^3) and molybdite powder (1,710 kg/m^3) (Binmaster, n.d.). This additional scaling enabled us to model the tube bundle reactor as a plug flow reactor in the Aspen simulation, simplifying our process flow diagram immensely. At 625 K, the scaled experimental rate constants used in the MATLAB models for the oxidative dehydrogenation of 1-butene and trans-2-butene were 4.56 hr^{-1} and 0.42 hr^{-1} respectively; the scaled experimental rate constants used in the Aspen simulation for the oxidative dehydrogenation of 1-butene and trans-2-butene were 7,486.27 hr^{-1} and 696.20 hr^{-1} respectively.

Zhai et. al. (2015) determined the experimental activation energies for the oxidative dehydrogenation of 1-butene and trans-2-butene, which were 9.2 kcal/mol and 17.4 kcal/mol respectively. For the isomerization reactions, we assumed that the rate constants were proportional to the experimental product selectivities provided by Zhai et. al. (2015) and that the isomerization activation energies were identical to those for the oxidative dehydrogenation. The bismuth molybdate, scheelite phase, experimental product selectivities for 1-butene were read to be 0.8 for 1,3-butadiene, 0.125 for cis-2-butene, and 0.075 for trans-2-butene (Zhai et. al., 2015). The bismuth molybdate, scheelite phase, experimental product selectivities for trans-2-butene were read to be 0.5 for 1,3-butadiene, 0.25 for cis-2-butene, and 0.25 for 1-butene (Zhai et. al., 2015). A summary of the original experimental rate constants at 625 K, experimental activation energies, experimental product selectivities, and scaled experimental rate constants at 625 K are presented below in Tables 6a - d.

Table 6a: The original experimental reaction rate constants for the oxidative dehydrogenation of 1-butene and trans-2-butene (Zhai et. al., 2015).

Chemical species	**Rate constant (s^{-1})**

1-butene	0.0001585
Trans-2-butene	0.00001474

Table 6b: The experimental activation energies for the oxidative dehydrogenation of 1-butene and trans-2-butene (Zhai et. al., 2015).

Chemical species	**Activation energy (kcal/mol)**
1-butene	9.2
Trans-2-butene	17.4

Table 6c: The experimental product selectivities for the oxidative dehydrogenation of 1-butene and trans-2-butene (Zhai et. al., 2015).

Chemical species	**Product selectivity**
1-butene	**1,3-butadiene:** 0.8 **Cis-2-butene:** 0.125 **Trans-2-butene:** 0.075
Trans-2-butene	**1,3-butadiene:** 0.5 **Cis-2-butene:** 0.25 **1-butene:** 0.25

Table 6d: The scaled experimental rate constants for the oxidative dehydrogenation of 1-butene and trans-2-butene used in the Aspen simulation.

Chemical species	**Rate constant (hr^{-1})**
1-butene	7,486.27
Trans-2-butene	696.20

Catalyst procurement and disposal

We assumed that the bismuth molybdate catalyst was purchased wholesale from a local distributor at a calculated cost of $369.69 per kg of catalyst. Calculations used to determine the cost of the catalyst can be found in Appendix A-4.

The tube bundle reactor operating conditions were selected to minimize processes contributing towards catalyst deactivation, as mentioned above, especially coke formation which Zhao et. al. (2017) stated as the common reason for the deactivation of dehydrogenation catalysts. The catalyst was also assumed to have been periodically regenerated via combustion to get rid of any potential coking, further extending the catalyst's lifetime (Worstell, 2014a). Thus, we assumed that our catalyst lifetime was 5 years, based on Dittmer et. al. (2014) catalyst's performance. After 5 years, the catalyst was sent for recycling by an external party at an assumed cost of $600 per short ton to recover the exotic metals bismuth and molybdenum, an estimate quote provided by Scott Fischer, a representative for ACI Industries Ltd. (Personal communication, April 27th, 2020).

Thermodynamic Model

As described in assumptions, the thermodynamic model of choice we used was the Peng-Robinson-Boston-Mathius (PR-BM) method. We used this method for all equipment included in the simulation.

Stream Tables

Aspen is able to generate stream tables for a simulated process. The tables we include in this report are specifically showing the mass flow rate in lb/hr of the components in each respective unit. A complete list of stream tables for the simulated process are included in Appendix A-6, as a part of the full Aspen report we generated for our process. The tables included in this report are the most characteristic units of our process: the first column, the reactor, and the final separator.

In this first column of the simulation, the feed stream goes through an initial separation. In this 75 stage RADFRAC column, the lightest components of the mixed C-4 feed stream are separated. The propyne rich stream leaves this column as distillate, and the lower half (and largest) product stream retains almost all of the desired 1,3-Butadiene, which will continue to be refined and separated throughout the process. A much smaller product stream leaving from the lowest stage is the "heavy" stream. This is composed mainly of isopentane and cis- and trans-2-Butenes. Table 7 below shows the stream table Aspen results for the Column 1 block.

Table 7: Column 1 stream table

	Units	S-03	HEAVIES	PROPYNE	S-04
− MIXED Substream					
Phase		Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	48	59.9706	20.3663	48.3678
Pressure	bar	5.57288	5.57288	5.57288	5.57288
Molar Enthalpy	kcal/mol	4.16077	-1.65105	39.8617	3.9771
Mass Enthalpy	kcal/kg	75.3317	-28.7817	994.905	71.8849
+ Mole Flows	**kmol/hr**	**246.372**	**6.2704**	**2.34346**	**237.758**
− Mass Flows	**lb/hr**	**30000**	**793.003**	**206.997**	**29000**
1,3-BD	lb/hr	12900	14.0315	2.5356e-05	12886
ISOBUTYL	lb/hr	7020	1.5588	0.000239762	7018.44
1-BUTENE	lb/hr	3720	0.972309	0.0001061	3719.03
N-BUTANE	lb/hr	1350	26.4554	4.38319e-07	1323.54
ISOBUTAN	lb/hr	1500	0.00575552	0.0169198	1499.98
CIS-2B	lb/hr	1230	400.294	3.50861e-09	829.707
TRANS-2B	lb/hr	1590	148.298	4.8702e-08	1441.7
BUTENYNE	lb/hr	210	69.0056	4.81987e-10	140.995
1-BUTYNE	lb/hr	60	27.3796	4.49033e-12	32.6204
PROPANE	lb/hr	0	0	0	0
ALLENE	lb/hr	60	5.06993e-16	59.9801	0.0199218
PROPYNE	lb/hr	210	2.36713e-10	147	63
ISOPENT	lb/hr	150	105.002	8.2595e-18	44.9984
DMF	lb/hr	0	0	0	0
H2	lb/hr	0	0	0	0
AIR	lb/hr	0	0	0	0
WATER	lb/hr	0	0	0	0

In the oxidative dehydrogenation reactor block, 1-butene is converted to 1,3-butadiene over a catalyst. The catalyst used in this reaction is bismuth molybdate, in the sheelite phase, as elaborated in the *Reactor* section of this report. This tube bundle reactor is one of the most essential units, and the most innovative, of the entire butadiene recovery and upgrade process because it allows us to increase our yield of 1,3-butadiene through not only separation from the stream, but introduces the ability to convert one of the waste components into butadiene, our profitable product. Table 8 below shows the stream table Aspen results for the reactor block.

Table 8: Oxidative dehydrogenation reactor stream table

	Units	R-04	R-05
− MIXED Substream			
Phase		Vapor Phase	Vapor Phase
Temperature	C	250	250
Pressure	bar	1.01325	1.01325
Molar Vapor Fraction		1	1
Molar Liquid Fraction		0	0
Molar Enthalpy	kcal/mol	2.81277	3.65303
Mass Enthalpy	kcal/kg	65.1018	87.4877
+ Mole Flows	**kmol/hr**	**962.132**	**995.563**
− Mass Flows	**lb/hr**	**91645.1**	**91645.1**
1,3-BD	lb/hr	102.482	4089.11
ISOBUTYL	lb/hr	0	0
1-BUTENE	lb/hr	3733.7	14.9413
N-BUTANE	lb/hr	0	0
ISOBUTAN	lb/hr	0	0
CIS-2B	lb/hr	50781.2	51712.2
TRANS-2B	lb/hr	7856.95	6509.52
BUTENYNE	lb/hr	0	0
1-BUTYNE	lb/hr	0	0
PROPANE	lb/hr	0	0
ALLENE	lb/hr	0	0
PROPYNE	lb/hr	0	0
ISOPENT	lb/hr	0	0
DMF	lb/hr	0	0
H2	lb/hr	0	148.573
AIR	lb/hr	29170.8	29170.8
WATER	lb/hr	0	0

The final separation block (SEP-02) is the final separation stage, the distillate of which is the final product of >99% purity butadiene. The bottoms product of this column is mostly DMF. Table 9 below shows the stream table Aspen results for the final separation block.

Table 9: Final separator (SEP-02) stream table

	Units	S-06	1,3-BD	D-01
− MIXED Substream				
Phase		Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	46.2387	46.2387	46.2387
Pressure	bar	5.57288	5.57288	5.57288
Molar Enthalpy	kcal/mol	-28.4316	21.6023	-41.5876
Mass Enthalpy	kcal/kg	-426.478	399.364	-594.574
+ Mole Flows	**kmol/hr**	**683.989**	**141.493**	**524.999**
− Mass Flows	**lb/hr**	**100528**	**16873.2**	**80956.3**
1,3-BD	lb/hr	16873.2	16873.2	0
ISOBUTYL	lb/hr	70.8933	0	70.8935
1-BUTENE	lb/hr	0	0	0
N-BUTANE	lb/hr	0	0	0
ISOBUTAN	lb/hr	0	0	0
CIS-2B	lb/hr	0	0	0
TRANS-2B	lb/hr	0	0	0
BUTENYNE	lb/hr	4366.68	0	4225.69
1-BUTYNE	lb/hr	1010.27	0	977.654
PROPANE	lb/hr	0	0	0
ALLENE	lb/hr	0.61699	0	0.597068
PROPYNE	lb/hr	1951.15	0	1888.15
ISOPENT	lb/hr	1393.63	0	1348.63
DMF	lb/hr	74861.9	0	72444.7
H2	lb/hr	0	0	0
AIR	lb/hr	0	0	0
WATER	lb/hr	0	0	0

Mass and Energy Balances

In designing the chemical separation process outlined in this report, it is important to consider the mass and energy input, output, generation, and accumulation terms of the system. For this report, the overall flow sheet balance is considered. Specific mass and energy balances for blocks in the system can be viewed in Appendix C. The overall flow sheet balance is shown below in Table 10.

Table 10: Aspen results for the overall flow sheet balance.

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
CONVENTIONAL COMPONENTS				
(KMOL/HR)				
1,3-BD	108.175	141.610	33.4304	-0.373664E-04
ISOBUTYL	56.7521	56.7521	0.00000	0.448382E-07
1-BUTENE	30.0738	0.786133E-02	-30.0637	0.726528E-04
N-BUTANE	10.5353	10.5353	0.00000	0.157212E-07
ISOBUTAN	11.7059	11.7059	0.00000	0.671793E-07
CIS-2B	9.94374	3.23611	7.52648	1.43146
TRANS-2B	12.8541	1.19889	-10.8931	0.592867E-01
BUTENYNE	1.82915	0.601055	0.00000	0.671402
1-BUTYNE	0.503138	0.229595	0.00000	0.543673
PROPANE	0.00000	0.00000	0.00000	0.00000
ALLENE	0.679289	0.679063	0.00000	0.332061E-03
PROPYNE	2.37751	1.66426	0.00000	0.300000
ISOPENT	0.943016	0.660123	0.00000	0.299988
DMF	15.0000	0.00000	0.00000	1.00000
H2	0.00000	33.4304	33.4304	0.00000
AIR	453.702	457.037	0.00000	-0.729756E-02
WATER	0.00000	0.00000	0.00000	0.00000
TOTAL BALANCE				
MOLE(KMOL/HR)	715.074	719.348	33.4304	0.405309E-01
MASS(KG/HR)	27839.3	25870.4		0.707218E-01
ENTHALPY(GCAL/HR)	1.97357	1.81546		0.801155E-01

As seen in the table above, a total of 715.074 kmol/hr or 27839.3 kg/hr and 1.97357 gcal/hr is input into the process. The figure also shows that 33.4304 kmol/hr were generated in the reactor. Adding the overall input and generation flow rates together and subtracting the output flow rate results in the relative difference of 0.405E-01 for the kmol/hr mole balance. This minimal discrepancy in flow rates shows that there is little accumulation in the system and that the mass balance closes. Table 10 also displays the difference in the amount of enthalpy input and taken out by the process, which is 0.801155E-01 Gcal/hr. This small difference shows there is little accumulation of heat energy in the system and that the energy balance closes.

Equipment List

The complete list of equipment required for the proposed process can be found in Table 11. The material of construction for all equipment is carbon steel.

Table 11: List of equipment used for the upgrade of a cracking waste stream to rubber precursors

Compressors	
CMP-01	Feed compressor
CMP-02	Reactor products compressor
Exchangers	
HT-01	Feed cooler
HT-02	Compressed feed cooler
HT-03	Air heater
HT-04	Reactor feed preheater
HT-05	Reactor product cooler
HT-06	1,3-Butadiene product cooler
HT-07	Isobutylene mixture cooler
HT-08	Isopentane and 2-Butenes cooler
HT-09	Propyne mixture heater
Mixers	
MX-01	Feed, recycle, and extragent mixer
MX-02	Air and reactor feed mixer

Reactor	
RX-01	Oxidative Dehydrogenation packed bed reactor
Storage Vessels	
TK-01	Compressed feed storage vessel
TK-02	DMF storage vessel
TK-03	1,3-Butadiene product storage vessel
TK-04	Isobutylene mixture storage vessel
TK-05	Isopentane and 2-Butenes storage vessel
TK-06	Propyne mixture storage vessel
Towers	
COL-01	First rectification column
SEP-01	Extractive distillation column
SEP-02	Desorption column
SEP-03	Second rectification column
SEP-04	Air and H2 separator

Utilities

We included five different utilities in the simulation: chilled water, cooling water, electricity, high-pressure steam, and low-pressure steam. While it is understood that any given unit in a process will likely use a combination of utilities, for example, a column will likely use steam, electricity, chilled water, and potentially others, each was assigned a primary utility or combination for the sake of calculation of cost and utility usage for the utilities that is most relevant and characteristic of each respective unit.

Chilled water

We used chilled water in several coolers and the condenser of COL-01. The assumed energy price of the chilled water was $0.40/GJ with an inlet temperature we assumed of 3°C and an outlet temperature of 8°C. We used a utility side film coefficient for energy analysis was 0.0135 GJ/hr-sqm-C. The estimated duty of this utility in a column is 17.7048 GJ/hr bringing the calculated cost to $7.08 /hr.

Cooling water

We used cooling water in various unit operations in the simulation including coolers and separators. We assumed the cooling water to have an energy price of 0.3609 $/GJ, and once again we specified the inlet and outlet conditions, this time to be 15 °C at the inlet and 25°C at the outlet. The same utility side film coefficient for energy analysis was used as for chilled water, 0.0135 GJ/hr-sqm-C. The estimated total duty for all units summed is 45.288 GJ/hr, bringing the total cost to $16.34 /hr.

Electricity

We used electricity as the primary utility in both compressors in our simulation. We assumed the cost of electricity to have a purchase price of 0.06117 $/kWhr (Demirel, 2019). The calculated duty of the electricity for both units totals 13.74 GJ/hr, bringing the cost of electricity for these units to $233.392 /hr

High-pressure steam

We used high-pressure steam in two heaters, the reactor, and the column reboiler. We assumed the energy price of steam to be 18.05 $/GJ, as well as specifying inlet and outlet conditions. We specified the inlet temperature to be 254 °C, and the outlet temperature to be 244°C. We used a utility side film coefficient for energy analysis of 0.0216 GJ/hr-sqm-C. These combine to yield a duty of 44.299 GJ/hr which yields a combined cost of around $798.31 /hr.

Low-pressure steam

We used low-pressure steam in one heater and two separators. We used an energy price of 14.32 $/GJ for low-pressure steam, and assumed inlet temperature to be 160°C and outlet temperature to be 150°C. We specified the utility side film coefficient for energy analysis to be 0.0216 GJ/hr-sqm-C. For the three separators and heater HT-03, the combined duty we simulated is 0.952 GJ/hr which brings the total utility cost for low pressure steam to be $13.63 /hr.

Design Calculations (Equipment Sizing)

In order to determine the fixed capital investment necessary for this project, each piece of equipment was sized and priced using CAPCOST with a CEPCI value of 596 from November of 2019. A summary of equipment with their associated purchase costs and bare module costs can be found in Table 12. The total equipment bare module cost, not including storage vessels, is $29,674,400. The material of construction for all equipment was assumed to be carbon steel. Heat exchanger areas, compressor power, and column internals for COL-01 were determined by Aspen. The column dimensions for the four separators were estimated using values from literature (Pavlov et. al., 2011).

Table 12: Estimated equipment costs of compressors, heat exchangers, towers, and storage tanks using CAPCOST with a CEPCI of 596.

Compressors	Compressor Type	Power (kilowatts)	# Spares	MOC	Purchased Equipment Cost	Bare Module Cost
CMP-01	Centrifugal	510	1	Carbon Steel	$ 498,000	$ 1,360,000
CMP-02	Centrifugal	1730	0	Carbon Steel	$ 1,240,000	$ 3,400,000

Exchangers	Exchanger Type	Shell Pressure (barg)	Tube Pressure (barg)	MOC	Area (square meters)	Purchased Equipment Cost	Bare Module Cost
RX-01	Fixed, Sheet, or U-Tube	45	2	Carbon Steel / Carbon Steel	6.13	$ 23,000	$ 83,000
HT-01	Floating Head	2	2	Carbon Steel / Carbon Steel	279	$ 67,900	$ 223,000
HT-02	Fixed, Sheet, or U-Tube	2	6.5	Carbon Steel / Carbon Steel	141	$ 40,300	$ 133,000
HT-03	Fixed, Sheet, or U-Tube	2	45	Carbon Steel / Carbon Steel	850	$ 104,000	$ 350,000
HT-04	Fixed, Sheet, or U-Tube	2	45	Carbon Steel / Carbon Steel	8740	$ 1,020,000	$ 3,440,000
HT-05	Floating Head	2	6.5	Carbon Steel / Carbon Steel	770	$ 161,000	$ 530,000
HT-06	Double Pipe		6.5	Carbon Steel / Carbon Steel	3.66	$ 4,580	$ 15,100
HT-07	Double Pipe		6.5	Carbon Steel / Carbon Steel	2.35	$ 4,130	$ 13,600
HT-08	Double Pipe		6.5	Carbon Steel / Carbon Steel	1	$ 3,320	$ 10,900
HT-09	Double Pipe		6.5	Carbon Steel / Carbon Steel	0.5	$ 3,320	$ 10,900
Condenser	Floating Head	2	6.5	Carbon Steel / Carbon Steel	162	$ 48,200	$ 159,000
Reboiler	Fixed, Sheet, or U-Tube	6.5	45	Carbon Steel / Carbon Steel	13.2	$ 23,300	$ 83,900

Towers	Tower Description	Height (meters)	Diameter (meters)	Tower MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost
COL-01	73 Carbon Steel Sieve Trays	62.1	1.69	Carbon Steel		6	$ 322,000	$ 938,000
SEP-01	150 Carbon Steel Sieve Trays	125	4	Carbon Steel		6.5	$ 3,560,000	$ 14,400,000
SEP-02	65 Carbon Steel Sieve Trays	55.7	3	Carbon Steel		6.5	$ 809,000	$ 2,990,000
SEP-03	20 Carbon Steel Sieve Trays	19.2	2	Carbon Steel		6.5	$ 127,000	$ 434,000
SEP-04	35 Carbon Steel Sieve Trays	31.4	2.5	Carbon Steel		6.5	$ 311,000	$ 1,100,000
						Total Bare Module Cost		$ 29,674,400

Storage Vessels

In order to account for any interruptions in production or temporary pauses, storage tanks were used to temporarily hold all entering and exiting streams. Based upon potential safety hazards, it was determined that one week's supply of each stream was an acceptable volume to hold. Since the proposed process is an extension of an existing plant, storing more than one week's supply of feed is unnecessary. It is assumed that if the feed storage vessel is necessary, the container will hold the cooled and compressed feed, or stream S-03. Thus, the necessary tank volume is based upon the compressed stream flow rate. From these calculated volumes, the dimensions of the tanks were calculated using Heuristics 7 (Demirel) and are shown in Table 13. Moreover, the material of construction for all of the tanks was determined to be carbon steel as indicated in Heuristics 7.

Table 13: Volumetric requirements and dimensions of storage tanks

Stream	Press (atm)	Flow Rate (m^3/hr)	Tank Volume for One Week (m^3)	Tank Diameter (m)	Tank Height (m)
Feed (TK-01)	5.5	23.1531	3889.7208	25	24.9
DMF (TK-02)	5	1.61311	271.00248	10	10.8
1,3-BD (TK-03)	5	12.0051	2016.8568	20	20.2
Isobutyl (TK-04)	5	7.33542	1232.35056	17	17.1
Heavies (TK-05)	5	0.562217	94.452456	7	7.7
Propyne (TK-06)	5	9.57901	1609.27368	18	19.9

Storage vessel costs were also determined using CAPCOST and a CEPCI value of 596 from November 2019. A summary of purchased costs and bare module costs for the storage vessels can be found in Table 14.

Table 14: Estimated costs of storage vessels using CAPCOST with a CEPCI of 596.

Storage Tanks	Tank Type	Volume (cubic meters)	Tank MOC	Pressure (bargs)	Diameter (meters)	Height (meters)	Purchased Equipment Cost	Bare Module Cost
TK-01	Fixed Roof	3890	Carbon Steel	5.57	25	24.9	$ 291,000	$ 320,000
TK-02	Fixed Roof	272	Carbon Steel	5.06	10	10.8	$ 82,500	$ 90,800
TK-03	Fixed Roof	2020	Carbon Steel	5.06	20	20.2	$ 196,000	$ 216,000
TK-04	Fixed Roof	1240	Carbon Steel	5.06	17	17.1	$ 151,000	$ 167,000
TK-05	Fixed Roof	95	Carbon Steel	5.06	7	7.7	$ 64,100	$ 70,500
TK-06	Fixed Roof	1610	Carbon Steel	5.06	18	19.9	$ 173,000	$ 191,000
							Total Bare Module Cost	$ 1,055,300

The total bare module cost for the storage vessels is $1,055,300. This results in a total bare module cost of $30,729,700 for all equipment and vessels for the project.

Simulations

Aspen Plus V11 was utilized for all simulations of the proposed process. The final simulation was completed with a few warnings but no errors. Due to the complex nature of the system including 15 units, convergence is near impossible to achieve without warnings.

Optimization

There is significant room for improvement and optimization, especially when it comes to utility usage and carbon emissions. Figure 7 shows the potential energy savings and CO_2 emission reduction as generated by Aspen Plus for our process.

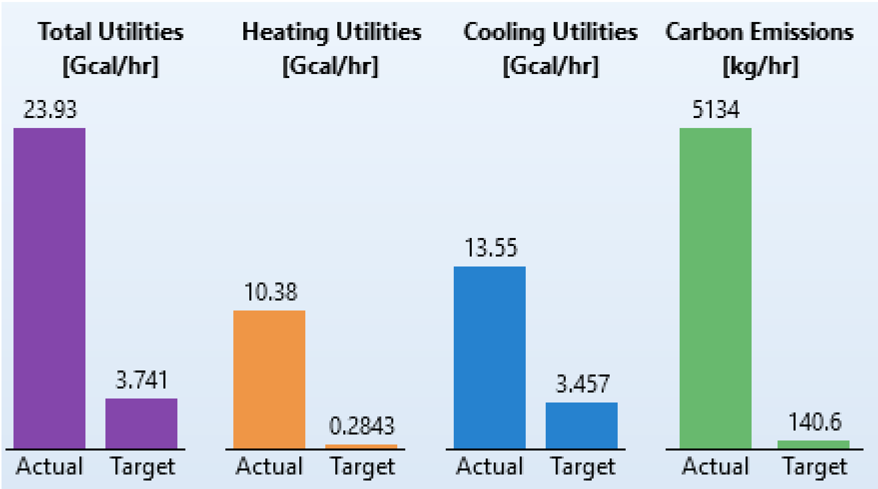

Figure 7: Aspen generated potential energy savings and CO_2 emission reduction summary bar graph

Similarly, the specific values for available saving and the % of Actual can be found in Table 15.

Table 15: Aspen generated potential energy savings and CO_2 emission reduction summary table

Summary Table

	Actual	Target	Available Savings	% of Actual
Total Utilities [Gcal/hr]	23.93	3.741	20.19	84.37
Heating Utilities [Gcal/hr]	10.38	0.2843	10.10	97.26
Cooling Utilities [Gcal/hr]	13.55	3.457	10.09	74.49
Carbon Emissions [kg/hr]	5134	140.6	4993.00	97.26

The detailed utility usage summary for the process before optimization can be found in Table 16. The total hot utility cost is $6,725,024/year but has a 97.83% potential reduction. The total cold utility cost is $136,550 and has a 73.5% potential reduction.

Table 16: Detailed utility usage information prior to optimization.

	Energy			Greenhouse Gases			Energy Cost Savings		ΔTmin [C]	Status
	Current [Gcal/hr]	Target [Gcal/hr]	Saving Potential [Gcal/hr]	Current [kg/hr]	Target [kg/hr]	Reduction Potential [kg/hr]	$/Yr	%		
HPS	10.37	0	10.37	5129	0	5129	6,868,872	100.00	10.0	
LPS	0.01063	0.2843	-0.2737	5.256	140.6	-135.4	-143,848	-2,575.75	10.0	
Total Hot Utilities	**10.38**	**0.2843**	**10.1**	**5134**	**140.6**	**4993**	**6,725,024**	**97.83**		
CHILL-W	4.382	2.406	1.976	0	0	0	29,010	45.10	10.0	
CW	9.17	1.051	8.119	0	0	0	107,540	88.54	10.0	
Total Cold Utilities	**13.55**	**3.457**	**10.1**	**0**	**0**	**0**	**136,550**	**73.50**		

Details about the proposed heat exchanger network system (HENS) proposed to optimize energy usage and emissions can be found in the sustainability analysis section of this report.

Flowsheeting Options - Calculator block

We employed a calculator block dubbed "AIRFLOW" to calculate the required molar flow rate of air, and thus oxygen, into the tube bundle reactor to maintain aerobic conditions within the reactor tubes. The aerobic conditions within the reactor further legitimize our assumptions of the five-year catalyst lifetime by reducing the prevalence of coking on the catalyst surface, as well as satisfies the oxygen demand calculated by our MATLAB models in the *Reactor tube internal profiles* section. We determined that the minimum oxygen:trans-2-butene molar flow rate ratio was 15:10, so we scripted our FORTRAN equation accordingly, as shown below in Appendix A-5. Our initial guess for the air molar flow rate was 1 kmol/hr, the calculated air molar flow rate was 453.702 kmol/hr based on the trans-2-butene flow rate of 63.5183 kmol/hr. This air molar flow rate would correspond to an oxygen molar flow rate of 95.28 kmol/hr, which is exactly 1.5 times larger than the trans-2-butene molar flow rate. Thus, our calculator block operated as expected. A summary of the AIRFLOW calculator block results from the Aspen simulation is presented below as Table 17.

Table 17: A summary of the AIRFLOW calculator block results.

Main Flowsheet | **AIRFLOW - Results**

Summary | Define Variable | Status

Variable	Value read	Value written	Units
AIRFLOW	306.446	453.702	KMOL/HR
TRN2BF	63.5183		KMOL/HR

N-Q Curve

In order to make an N-Q Curve for COL-01, three design specifications for each stream leaving the column were necessary. These design specifications are described in detail in the following *Design Specifications* section. The NQ curve calculations are based on equilibrium stages. For COL-01, we specified upper and lower limits for the number of stages to be 27 and 75 respectively. We chose Q_{reb}-Q_{cond} as the objective function. Unfortunately, convergence was not achieved for the N-Q Curve optimization on COL-01. This is likely due to the complexity of having three product streams, rather than two in a typical column.

Design Specifications

We chose design specifications for COL-01 to reasonably maximize the separation of propyne and isopentane from the initial process feed stream without incurring sizable utility costs for the column. This is because a large reboiler duty would be required for better separation of the two mentioned components, both of which are of low monetary value. In accordance with this criteria, we chose a mole recovery fraction of 0.7 for propyne in the distillate stream PROPYNE and a mole recovery fraction of 0.7 for isopentane in the bottoms stream HEAVIES. The final design specification, necessary for N-Q Curve optimization, was to specify a mole recovery of 0.999 for 1,3-Butadiene in the primary product stream S-04. A summary of the design specification results is presented below as Table 18.

Table 18: A summary of the design specification results.

ID	Description	Type	Units	Target Value	Calculated Value	Error
1	Mole recovery, 0.7	Mole-Recov		0.7	0.700332	-0.000332212
2	Mole recovery, 0.7	Mole-Recov		0.7	0.699994	5.66242e-06
3	Mole recovery, 0.999	Mole-Recov		0.999	0.998923	7.69433e-05

Pinch Analysis

Pinch analysis is used to minimize utility usage as previously discussed in the optimization section of this report. Figure 8 shows the composite curve for the process with a selected minimum temperature difference of 10^{o}C.

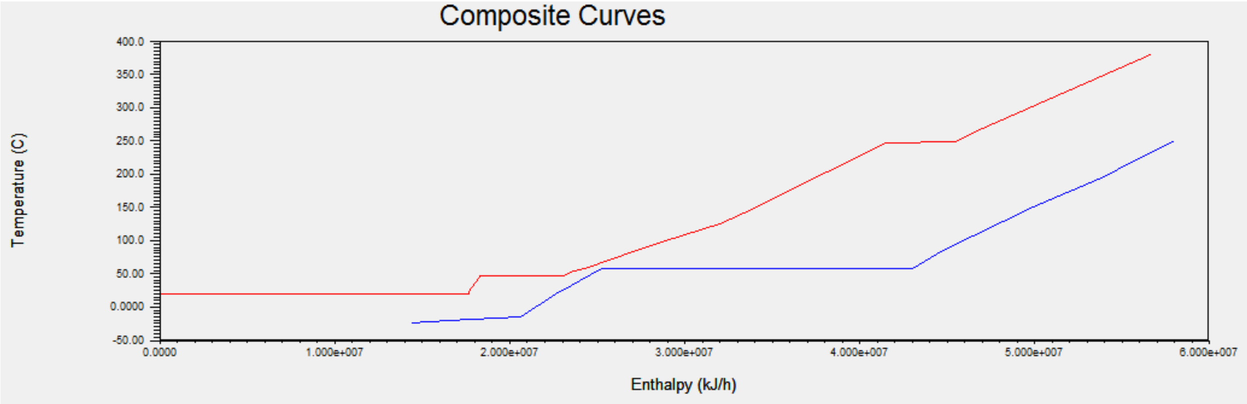

Figure 8: Composite curve for ΔT_{min} = 10ºC

Similarly, Figure 9 shows the grand composite curve for the system.

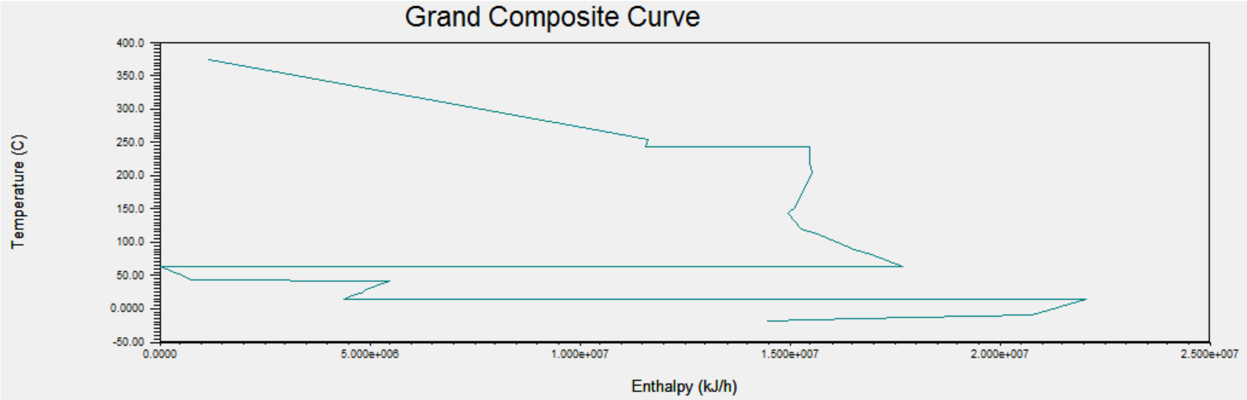

Figure 9: Grand composite curve for ΔT_{min} = 10ºC

Details regarding the selected heat exchanger network system is outlined in the following sustainability section of the report.

Column Internals

We designed and specified the column internals for COL-01 in the Aspen simulation to determine the required tray spacing, tray diameter, and column height. Aspen Plus generated estimates for our column internals through an initial simulation run. These estimates were then used to further specify parameters to calculate the column internals. The column stage section CS-1 was specified to be between stages 2 and 7 with an interactive sizing mode to determine the tray diameter. Sieve trays were selected as the tray type inside the column, with one pass on each tray. These specifications can be found in greater detail in Appendix A-5. The total tray section height for COL-01 was calculated to be 59.1008 m, with the tray spacing set to 0.8096 m to prevent weeping from occuring inside the column. The sieve tray diameter was calculated to be 1.69433 m. The total residence time in the column was calculated to be 0.0352273 hr. The pressure drop across the trays was calculated to be 0.535639 bar. The head loss across the trays (the hot liquid height) was calculated to be 9129.98 mm. A summary of the calculated column internals and the limiting conditions within COL-01 are presented below as Tables 19 and 20.

Table 19: A summary of the column internals generated in COL-01 by Aspen Plus.

Summary | By Tray | Messages

Name: CS-1   Status: Active

Property	Value	Units
Section starting stage	2	
Section ending stage	74	
Calculation Mode	Sizing	
Tray type	SIEVE	
Number of passes	1	
Tray spacing	0.8096	meter
Section diameter	1.69433	meter
Section height	59.1008	meter
Section pressure drop	0.535639	bar
Section head loss (Hot liquid height)	9129.98	mm
Trays with weeping	None	
Section residence time	0.0352273	hr

Table 20: A summary of the limiting column internal conditions in COL-01.

Limiting conditions

Property	Value	Units	Tray	Location
Maximum % jet flood	80.0007		40	
Maximum % downcomer backup (aerated)	38.0348		40	
Maximum downcomer loading	479.754	cum/hr/sqm	40	Side
Maximum % downcomer choke flood	80		40	Side
Maximum weir loading	88.795	cum/hr-meter	40	Side
Maximum aerated height over weir	0.252386	meter	40	
Maximum % approach to system limit	56.4622		40	
Maximum Cs based on bubbling area	0.0906141	m/sec	40	

Reactor tube internal profiles

After running the Aspen simulation, we used the properties of the feed stream entering the reactor i.e. the overall stream molar flow rate and the stream component molar fractions, as well the number of reactor tubes inside the reactor to determine the approximate mass of catalyst in each reactor tube. The catalyst mass inside each reactor tube was then multiplied by the number of reactor tubes to deduce the total mass of catalyst required in the reactor. The equations used to deduce the catalyst mass in each reactor tube can be found in Appendix A-3, while the MATLAB script can be found in Appendix A-7b and A-7c. The MATLAB differential equation solver *ode45* was utilized to solve the numerous differential equations in Appendix A-3. The conversion achieved by the Aspen simulation reactor was 0.996. This conversion corresponded to a catalyst mass of 3.547 kg per reactor tube in the '*conversion*' script results, henceforth referred to as MATLAB model results. With 135 reactor tubes, the total required reactor catalyst mass equated to 478.8 kg for the tube bundle reactor. The catalyst mass per a catalyst tube and total reactor catalyst mass are presented below in Table 21.

Table 21: A summary of the catalyst mass required to achieve a 0.996 conversion in the MATLAB model.

Number of reactor tubes	**Required catalyst mass (kg)**
1	3.547
135	478.8

A summary of the MATLAB model results is presented below as Figures 10 and 11. Figure 10 is a visual representation of the conversion of 1-butene along a single reactor tube. Figure 11 is a visual representation of the molar flow profiles of 1-butene, oxygen, 1,3-butadiene, and hydrogen along a single reactor tube. Trans-2-butene and cis-2-butene were omitted from Figure 15 as their molr flow profiles were relatively constant through the reactor tube.

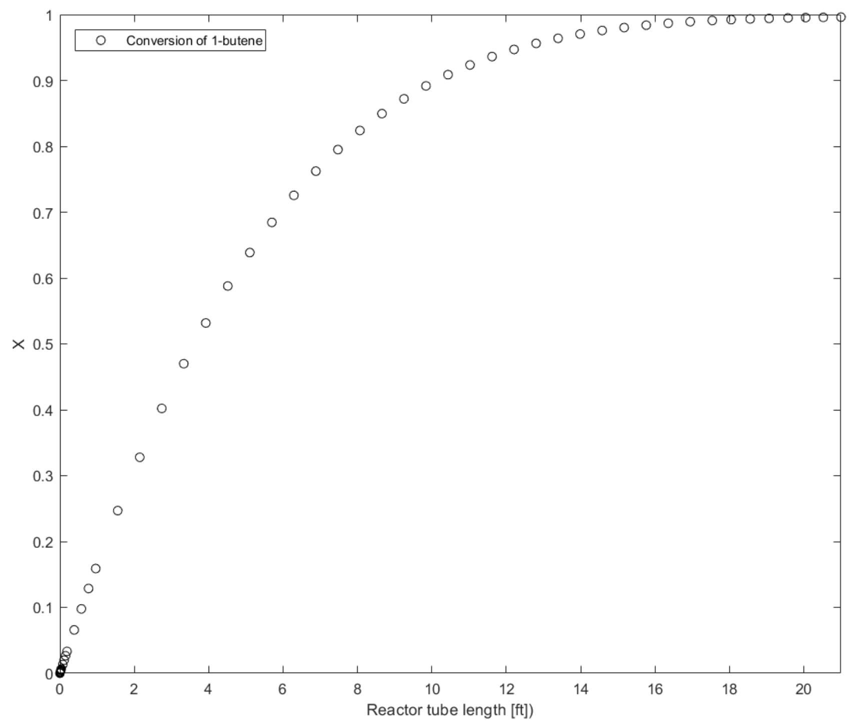

Figure 10: The conversion of 1-butene along a single reactor tube.

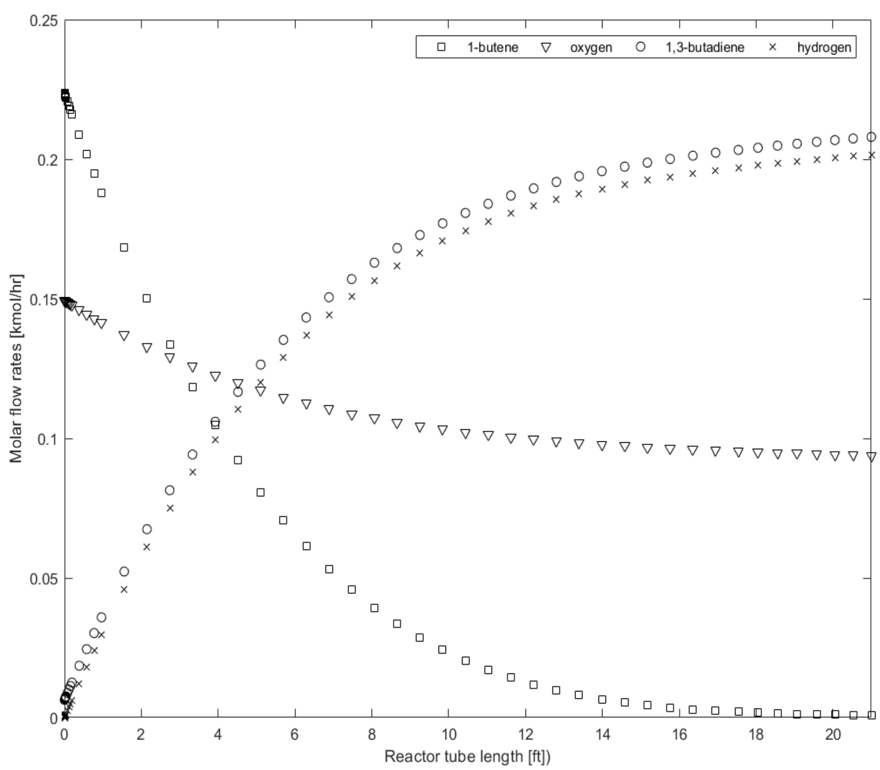

Figure 11: The molar flow profiles of 1-butene, oxygen, 1,3-butadiene, and hydrogen along a single reactor tube.

As highlighted above in Figure 11, conditions inside the reactor tube are relatively aerobic as the oxygen molar flow rate remains above 0.05 kmol/hr through the entire length of the reactor tube length. Thus, the selected oxygen:trans-2-butene molar flow rate ratio is proven appropriate and our assumption of a 5-year catalyst lifetime further validated.

Safety

HAZOP Analysis

We performed a hazard and operability (HAZOP) study on the catalytic reactor in the system, as we assumed this unit to have the largest potential for hazards. The second portion of the HAZOP analysis was performed on the heater immediately preceding the reactor. Each of these analyses includes the unit itself (RX-01 and HT-04) as well as incoming and outgoing streams from each unit. This is not to say that other units, particularly columns are far less risky, as we would recommend for future study that a HAZOP analysis be performed on every unit in the system before breaking ground on a project such as this. It is particularly crucial that time is taken to develop standard operating procedures (SOP's) and that operators are trained with the expectation that they perform job hazard analysis (JHA) before performing particularly high risk tasks. To ensure that the staff of a plant do not become complacent with the processes at hand, we recommend that such a HAZOP study be reviewed for equipment in the plant at regular intervals to ensure that changes to the process are considered and updated, and new observations are incorporated. We performed the HAZOP study using the HAZOPtimizer tool provided to us, run via Microsoft Excel. The detailed HAZOP analysis can be found in Appendix A-8. In the HAZOP of the reactor and heater (including input and output streams of each), we identified risks as summarized in Table 22.

Table 22: Quantity of potential hazard conditions identified, sorted by risk-rank level

Risk-rank level	Number Identified
A	0
B	0
C	11
D	20

A guide to the risk-ranking system we used is shown below. This guide shows the subsequent risk-rank level for a given risk and is a function of likelihood and consequence. Figure 12 and Table 23 are taken directly from the HAZOPtimizer excel sheet program.

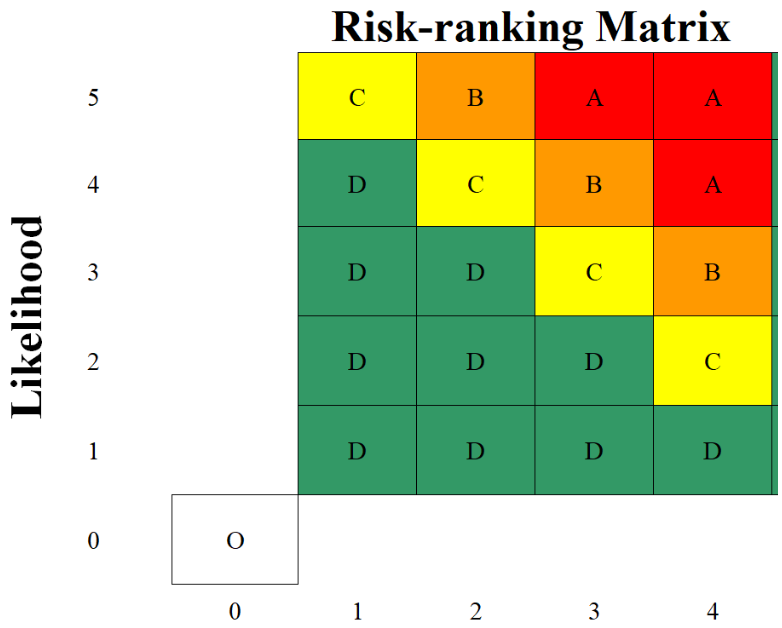

Figure 12: Risk-ranking matrix diagram from HAZOPtimizer excel program, Likelihood vs Consequence

While Figure 12 indicates the possible hazard risk-ranking levels for any given combination of likelihood and consequence, hazards from all levels were not observed in our HAZOP analysis. For the HAZOP analysis of both the reactor and the heater, the distribution of risk-ranking levels for the identified potential hazards is shown in Figure 13.

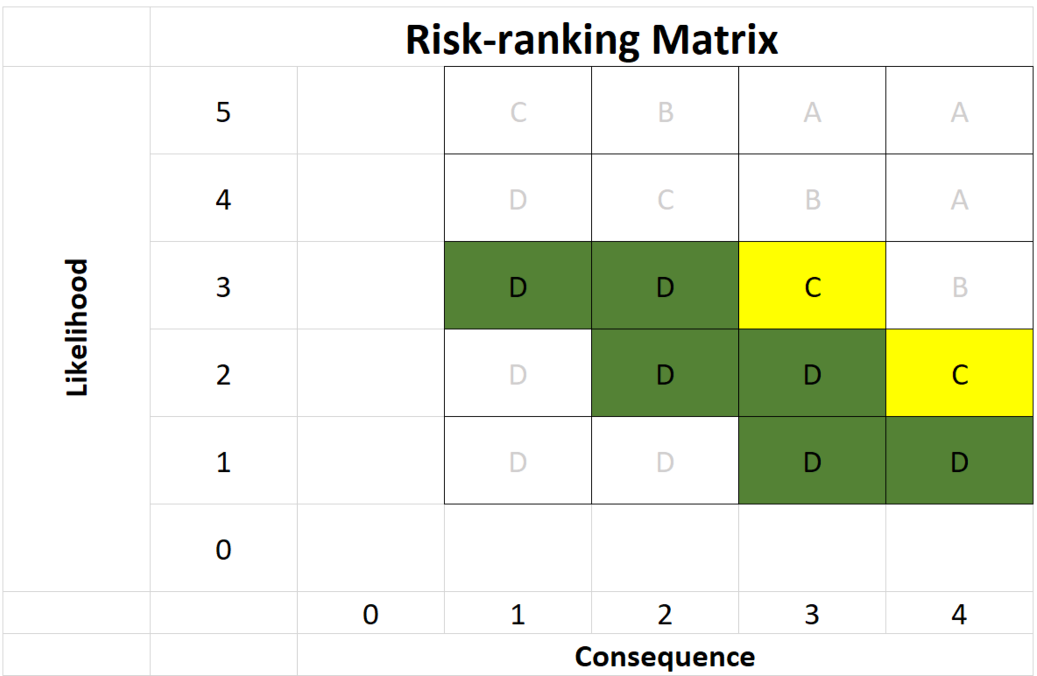

Figure 13: Observed hazard levels from HAZOPtimizer study of RX-01 and HT-04

An additional key for the risk-ranking matrix is shown below, to give context for each rating of likelihood or consequence used in the risk-ranking determination for each evaluated deviation in the catalytic reactor.

Table 23: Key for risk-ranking diagram

Risk Ranking Consequence and Frequency Ranges

Consequence Range	Safety Consequence Criteria	
5	Optional	
4	One or more onsite or offsite fatalities	
3	Disabling injury	
2	Lost workday injury	
1	Recordable injury	
Likelihood Range	**Event Frequency**	**Impact Frequency**
5	$>10^{-1}$/yr	$>10^{-2}$/yr
4	10^{-1} to 10^{-2}/yr	10^{-2} to 10^{-3}/yr
3	10^{-2} to 10^{-3}/yr	10^{-3} to 10^{-4}/yr
2	10^{-3} to 10^{-4}/yr	10^{-4} to 10^{-5}/yr
1	$<10^{-4}$	$<10^{-5}$

This key illuminates the quantitative basis behind the seemingly qualitative assignment of risk-level in a HAZOP analysis. The frequency of event and impact as well as the safety consequence criteria can be estimated using this quantitative basis before qualitatively assessing the risks relative to standards, statistics, and one another.

Process Safety

To ensure the safety of workers and operators in proximity to the operations, it is important to use recognized and industrially accepted practices when designing, installing, and operating our system. With this, workers will be required to self-report potential accidents and dangers and follow the near-miss system when reporting. We will also enforce industry standard rules for oil refineries such as: conduct gas tests regularly, verify isolation from the operational processes before beginning working on the plant, obtain authorization before entering confined spaces, obtain authorization before disabling safety-critical equipment, no smoking or use of inhibitory substances while at the plant, and use personal protective equipment whenever applicable.

Chemical Safety

A Safety Data Sheet (SDS) is available for each of the chemicals used in the waste stream upgrade process. Each sheet details physical properties of relevant chemicals as well as critical safety information. Though various aspects of chemical safety are covered in this section, the SDS sheets for each chemical include greater detail and should be referenced for more specific quantitative information. These SDS sheets can be found in the Appendices of this report.

1,3-Butadiene, which makes up the largest fraction of components in the stream, is a chemical that carries quite a few risks to safety if not handled properly. In addition to the hazards of the chemical that begin to take the form of fire safety risks, there are serious health hazards, such as being a carcinogen and carrying the potential to cause genetic defects. 1,3-Butadiene is rated a Category 1 hazard for carcinogenicity, 1B for germ cell mutagenicity, and category 4 for acute toxicity by inhalation (Airgas, n.d.).

Fire Safety

All chemicals in the waste stream used to feed the butadiene extraction process are flammable gases, which can form explosive mixtures in air or explode when heated. For this reason, it is important that the installed system is inspected for structural integrity on a routine basis to prevent and quickly catch leaks in the system that could lead to loss of containment and the formation of a flammable vapor cloud. It is also important that the National Fire Protection Association (NFPA) guidelines for best practice should be followed in every aspect of the installation and operation of a system that contains these flammable components. While the NFPA codes applicable to this process are only one of many resources for the inherently safer design of a system of explosive chemicals, it will be consulted as the primary source of information on best practice for the purpose of this report and a general overview.

NFPA Code 67 details a Guide on Explosion Protection for Gaseous Mixtures in Pipe Systems. While this code should not limit all of the regulations and codes that are to be referenced while building and operating a system such as this, it will serve as a basis for incorporating some of the key elements that will allow for the creation of an inherently safer design. One method of detonation prevention discussed is interting the environment, in this case, the piping carrying the combustible gases, with a non-combustible vapor such as nitrogen, to keep the fuel concentration from existing between the lower and upper explosive limits (LEL and UEL respectively) (NFPA 67, 2019) . In addition to the piping of the systems being potential candidates for being interted, NFPA code 67 section 6.1.2.3 details that interting is “Typical processes for which inerting is used are confined reactors, mixers, ovens, storage tanks, and vent collection headers.” (NFPA 67, 2019). Because of this, it is recommended that other units in the process such as the distillation columns or reactors may want to be inerted, at least upon startup to prevent explosive hazards.

In addition to recommending ways to prevent the detonation of flammable gases, NFPA recommends a few specific methods of inherently safer design that can help to isolate parts of the plant, should a detonation, deflagration, or other fire-related hazard occur. One way is to ensure that pipelines and units of the plant can be isolated in the event of an emergency using passive intervention systems such as flow actuated float valves, explosion diverters, deflagration and detonation arresters, hydraulic flame arresters, and liquid seals-- all of which are suitable for gases (NFPA 67, 2019). It is recommended that such an isolation device is incorporated at regular intervals throughout the plant on flammable lines.

Maintenance of this system must also be performed in accordance with NFPA guidelines. It is recommended that explosion protection systems, like those aforementioned, should be inspected in accordance with manufacturer's requirements, but also that they should be inspected at least once a year minimum, and inspected every three months when first installed, and more frequently if significant changes to the process are made, or there are otherwise reasons to suspect that the performance of the device could be compromised sooner (NFPA 67, 2019). NFPA guidelines should be consulted when creating the JIS (Job Instruction Sheet) or SOP (Standard Operating Procedure) for any maintenance or operating jobs and tasks pertaining to the system.

Personal Safety

To ensure maximum care is taken in providing potential operators and employees of the plant with a reliably safe workplace in which the prevention of injuries and incidents is paramount, we suggest including a few additional measures be taken for the installation of such a system. One such recommendation we are choosing to include in our project is the use of industrial insulation on lines that are hot. In addition to retaining more heat in the line, such as a steam line, insulation can prevent accidental burns should an operator come into contact with the pipe surface.

Sustainability Analysis

The sustainability of the process was evaluated using a variety of tools. Among these include an energy conservation analysis and waste material management evaluation. These pillars of the sustainability analysis aided in the creation of an informed evaluation of the overall sustainability of this waste stream upgrade process.

Energy Conservation

As previously stated in the optimization section of this report, there is significant potential for reducing carbon emissions and energy costs. The Energy Analyzer tool of Aspen Plus was utilized to generate several possible heat exchanger network systems (HENS) which would minimize the utilities necessary to heat and cool process streams. Existing heat in process streams is utilized before requiring utilities such as steam and cooling water. For this process, a ΔT_{min} value of 10ºC was used to optimize the HENS. After comparing 10 recommended designs generated using Aspen Energy Analyzer, the best design was selected based on the lowest estimated total cost. The selected design is shown in Figure 14.

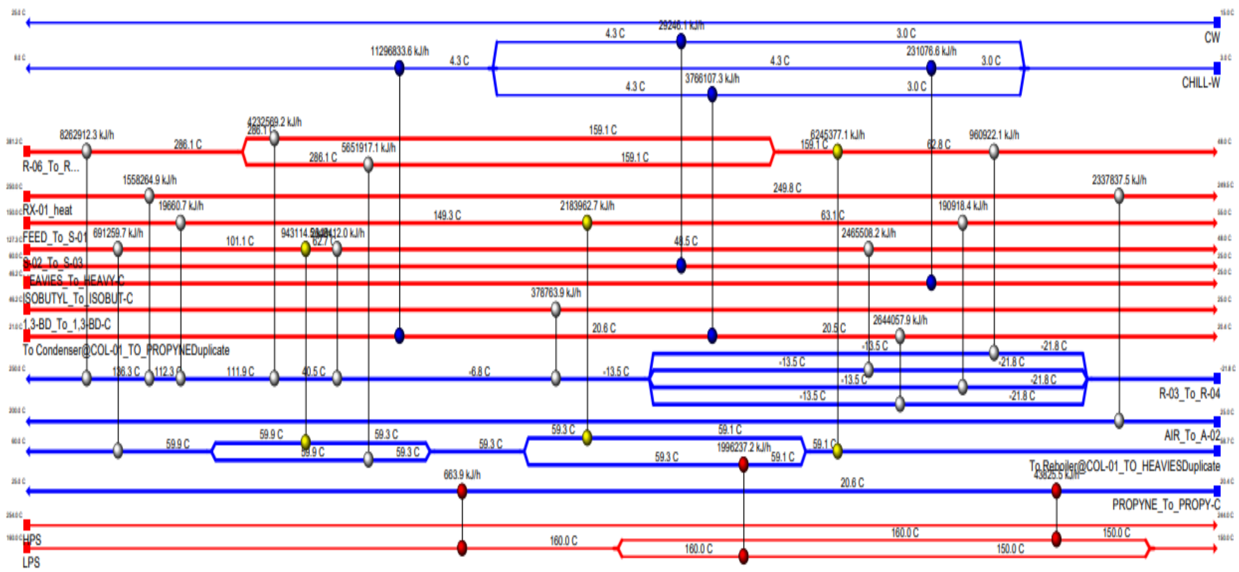

Figure 14: Selected heat exchanger network system to optimize utility costs

The respective cost indexes and network performance specifications can be found in Table 24.

Table 24: Cost indexes and network performance specifications for the selected HENS as generated using Aspen Energy Analyzer

Network Cost Indexes

	Cost Index	% of Target
Heating [Cost/s]	8.118e-003	43.56
Cooling [Cost/s]	1.703e-003	85.28
Operating [Cost/s]	9.820e-003	156.0
Capital [Cost]	2.575e+006	79.95
Total Cost [Cost/s]	3.136e-002	94.35

Network Performance

	HEN	% of Target
Heating [kJ/h]	2.041e+006	171.4
Cooling [kJ/h]	1.532e+007	105.9
Number of Units	23.00	127.8
Number of Shells	36.00	150.0
Total Area [m2]	9580	71.04

The proposed HENS includes 23 heat exchangers for a total area of 9580 square meters. In comparison, the simulated process has 9 heat exchangers, condenser, reboiler, and reactor cooler for a total area of 935 square meters. Even with the significantly higher heat exchanger area, the total cost is projected to be significantly reduced due to the amount saved from utility costs.

Greenhouse Gas Emissions

To estimate the CO_2 emissions for our process, we used Aspen's results summary for CO_2. This summary shows the net stream, utility stream, total CO_2 emissions, and even a net carbon fee or tax applicable to this process. It also breaks down which product streams have which respective flow rates and CO_2 emissions to better understand the process. For this process in particular, there are no net stream CO_2 emissions to consider, only those from utilities. This results summary table can be seen in Table 25 below.

Table 25: Aspen results summary of CO2 emissions

Hierarchy	PLANT	
Net stream CO2e	0	kg/hr
Utility CO2e	7586.96	kg/hr
Total CO2e	7586.96	kg/hr
Net carbon fee / tax	0	$/hr

Feed stream name	Flow	CO2e
	kg/hr	kg/hr
AIR	13135.1	0
DMF	1096.42	0
FEED	13607.8	0

Product stream name	Flow	CO2e
	kg/hr	kg/hr
H2+AIR	13299	0
1,3-BD-C	7653.57	0
ISOBUT-C	4464.24	0
HEAVY-C	359.7	0
PROPY-C	93.8924	0

The Aspen results summary for CO_2 emissions shown in Table 18 illustrates that while there is a total CO_2 emission of 7586.96 kg/hr from this process, 100% of that emission is from utility emissions used in the process, and none is reported as generated by the process itself. The potential for reducing CO_2 emissions is hinted at in Table 26 below.

Table 26: Aspen energy analysis

	Energy			Greenhouse Gases			Energy Cost Savings		ΔTmin [C]	Status
	Current [Gcal/hr]	Target [Gcal/hr]	Saving Potential [Gcal/hr]	Current [kg/hr]	Target [kg/hr]	Reduction Potential [kg/hr]	$/Yr	%		
HPS	10.37	0	10.37	5129	0	5129	6,868,872	100.00	10.0	
LPS	0.01063	0.2843	-0.2737	5.256	140.6	-135.4	-143,848	-2,575.75	10.0	
Total Hot Utilities	**10.38**	**0.2843**	**10.1**	**5134**	**140.6**	**4993**	**6,725,024**	**97.83**		
CHILL-W	4.382	2.406	1.976	0	0	0	29,010	45.10	10.0	
CW	9.17	1.051	8.119	0	0	0	107,540	88.54	10.0	
Total Cold Utilities	**13.55**	**3.457**	**10.1**	**0**	**0**	**0**	**136,550**	**73.50**		

This potential for greenhouse gas emissions via reduction of utility use once again shows the importance of implementing a HENS analysis, as this process has lots of potential for reduction of energy. Without the use of the HENS analysis, the calculated CO_2 from high and low pressure steam total 5143.8602 kg/hr, with over 99% of that coming from the high pressure steam in the system. With the electricity utility contributing an additional calculated 2443.11 kg/hr, the total utility CO_2 emissions come to 7586.9702 kg/hr without the HENS analysis reduction. The HENS analysis indicates in Table 17 that (with a conversion from kJ/hr and the given CO_2 emission factor in Aspen of $1.0042*10^{-4}$ kg/kJ) the CO_2 emissions from heating and cooling utilities is down to 1743.39 kg/h, which is down 77% from the original simulation and shows much promise for improvement through heat exchanger network design.

Waste Material Management

Material produced by the process that is either out of spec or is one of the few side products mentioned in this report will be collected and sold as waste fuel, at fuel value. The process described by Fabiano and Nedwick states that without this process, the waste stream we are upgrading is sold as-is at this fuel value. We made an assumption that whatever market exists for this hypothetical waste stream will continue to be available for us as an outlet for side products and out of spec products that can be collected, blended, and sold the way the waste stream was before the creation of this butadiene recovery process.

Feasibility Analysis

Several factors must be considered when determining the feasibility of a project. Safety considerations, environmental impacts, and cost are all important to consider. The safety and sustainability of this project have already been discussed. Cost is the biggest factor for most investors and will now be discussed in detail.

Cost calculations

There are many cost considerations when designing a new plant, or an addition to an existing process as is the case for this project. First, the cost and availability of raw materials must be evaluated. Table 27 shows the projected annual costs for the three main raw materials used in the process. First, the method for calculating the cost of the catalyst was described previously. The value displayed in Table 27 is an annual average since the catalyst is only replaced every five years. It also includes the cost of disposal for the catalyst. The cost of the feed is included even though it is a byproduct from ethylene cracking. The value of the feed is based on if it were sold as low-grade fuel for $194/MT (EIA.gov, n.d.). DMF, used as the extragent for extractive rectification, is recycled but must be replenished over time. Based on a price of $740/MT, the annual cost of DMF was determined and is displayed in Table 27 (China, 2020).

Table 27: Annual raw material costs

	Catalyst	**FEED**	**DMF**
Annual Cost ($/yr)	35,468	23,149,800	7,111,000

The total raw material cost is $30,296,268/year. Next, the annual revenue from the product and byproduct streams is calculated. Table 28 shows the estimated annual revenue from each of the product streams. 99% 1,3-Butadiene is the primary product with a value of $496/MT (Echemi, n.d.). The three byproduct streams, PROPYNE, HEAVIES, and ISOBUTYL are assumed to be blended and sold as a low-grade fuel with a value of $194/MT (EIA.gov, n.d.). Hydrogen gas, mixed with air, is produced in the catalytic oxidative dehydrogenation reactor. The value of hydrogen was calculated assuming that it is burned to produce electricity. This process was not included in the PFD.

Table 28: Annual revenue from product streams

	PROPYNE	HEAVIES	ISOBUTYL	H2+AIR	1,3-BD
Annual Revenue ($/yr)	159,728	611,932	7,594,677	1,351,983	33,261,755

The total annual revenue is $42,980,075/year. As stated in the assumptions, an interest rate of 7%, tax rate of 35%, and project life of 15 years is assumed. Other assumptions including cost of land, working capital, and cost of labor were made based on heuristics and can be found in Appendix A-4 (Demirel, 2019).

Discounted Cash Flow Diagrams

The process feasibility was analyzed for both before and after implementing the proposed heat exchanger network system (HENS). Figure 15 shows the cash flow diagram for the process without the recommended HENS.

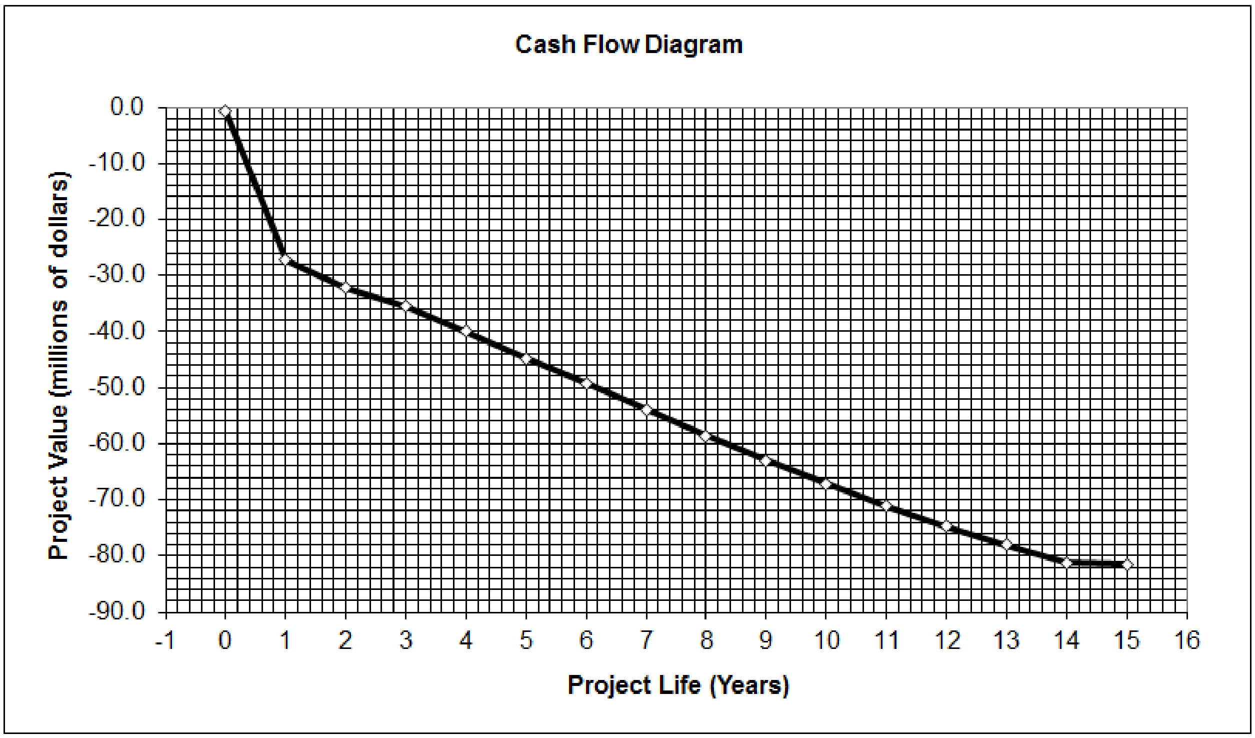

Figure 15: Cash Flow Diagram before HENS optimization

As can be seen in Figure 15, this project is highly infeasible without implementation of the HENS. An annual utility cost of $9,204,300/year is largely to blame. Figure 16 shows the cash flow diagram for the process after implementing the proposed HENS.

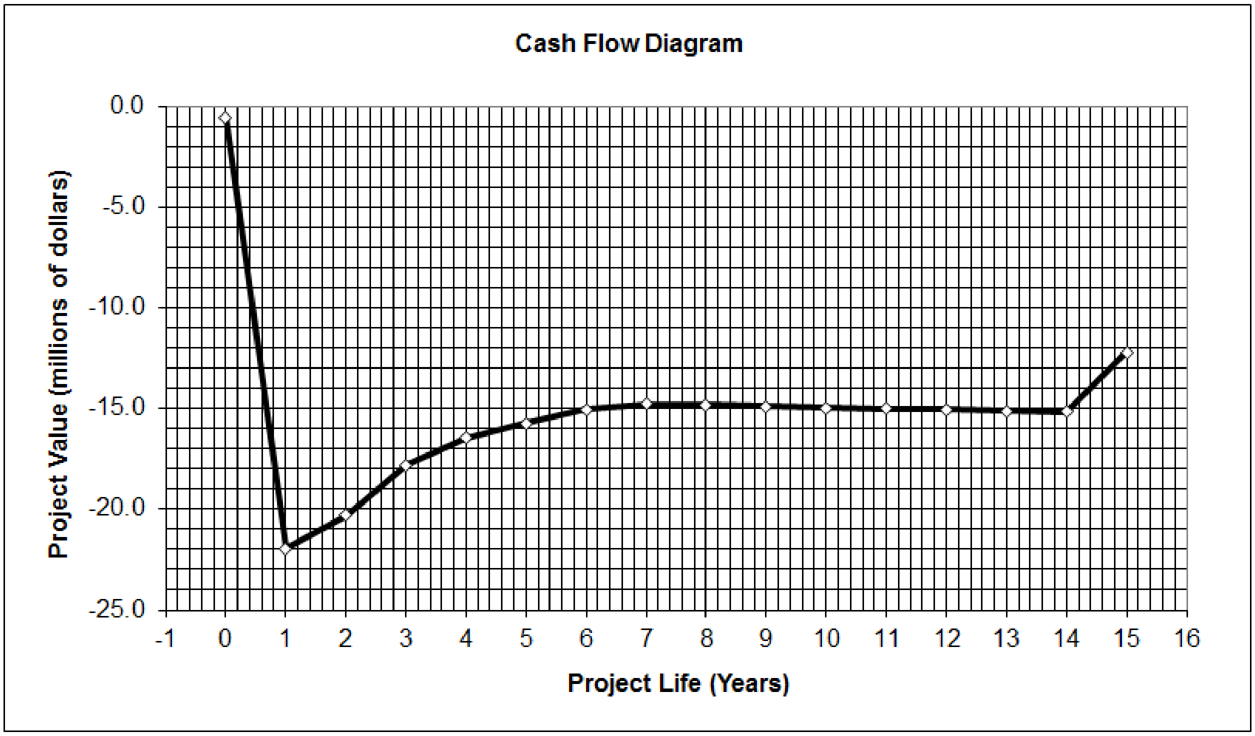

Figure 16: Cash Flow Diagram after HENS optimization

As can be seen in Figure 16, implementing the HENS significantly improves the feasibility of the project. However, the project value does not break even within the lifetime of the project. Table 29 shows the discounted and non-discounted profitability criteria for after HENS optimization. The net present value and rate of return on investment are both negative and the payback period is undefined. These criteria make it clear that this project is not economically feasible without significant adjustments.

Table 29: Discounted and non-discounted profitability criteria after HENS optimization

Discounted Profitibility Criterion		Non-Discounted Profitibility Criteria	
Net Present Value (millions)	(12.20)	Cumulative Cash Position (millions)	(6.88)
Discounted Cash Flow Rate of Return	10.00%	Rate of Return on Investment	-6.13%
Discounted Payback Period (years)	Undefined	Payback Period (years)	Undefined

Within the CAPCOST program, there is the ability to run a Monte Carlo simulation which models various possibilities for variation in key parameters. Table 30 shows the possible variation values for several parameters used in the simulation.

Table 30: Possible variation of key parameters over plant life used in Monte Carlo simulation after HENS

	Lower Limit	Upper Limit	Base Value
FCIL	-30%	30%	$ 28,335,300
Price of Product	-10%	20%	$ 42,980,075
Working Capital	-50%	10%	$ 5,880,000
Income Tax Rate*	-20%	20%	35%
Interest Rate*	-10%	20%	7%
Raw Material Price	-15%	15%	$ 30,296,268
Salvage Value	-50%	30%	$ 2,833,530

Figure 17 shows the results of the Monte Carlo simulation for possible Net Present Value with the aforementioned variations in parameters.

Low NPV	-69.2
High NPV	35.8

Bins	Upper Value	# points/bin	Cumulative
0	-69.2	0	0
1	-58.7	6	6
2	-48.2	27	33
3	-37.7	82	115
4	-27.2	163	278
5	-16.7	217	495
6	-6.2	208	703
7	4.3	163	866
8	14.8	82	948
9	25.3	41	989
10	35.8	11	1000

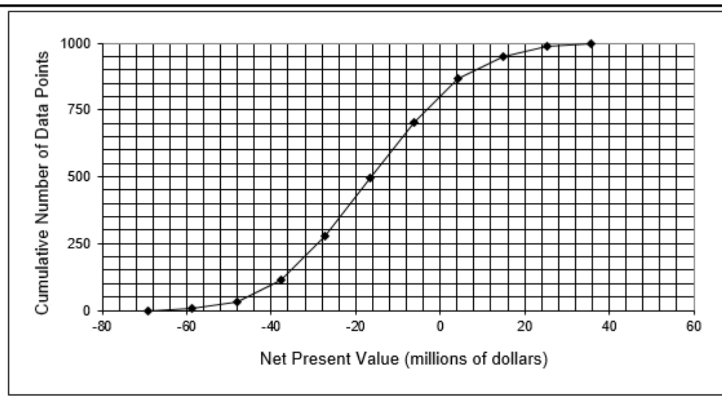

Figure 17: Net Present Value data from Monte Carlo simulation

Figure 17 shows that there is the possibility of a positive Net Present Value at the end of the project's life. This also indicates the possibility of return on investment. Even though this simulation brings hope and the possibility of payback, it is a relatively low possibility and is still likely not economically feasible.

Multi-criteria decision matrix

After discussing the safety, sustainability, and economic factors which indicate feasibility, they must be weighted according to stakeholder values. Table 31 is the multi-criteria decision matrix we completed to compare the base case of selling the C4 mixture feed as low-grade fuel and our process to upgrade to rubber precursors. As a team, we discussed and decided on the weighting factors used in the matrix.

Table 31: Multi-criteria decision matrix for the base case of selling the feed fuel value and upgrade to rubber precursors

Economics and sustainability indicators	Weighting factor: 0-1	Selling feed as low-grade fuel	Upgrade feed to rubber precursors
Economic indicators			
Net present value NPV	1	+	-
Payback period PBP	0.85	+	-
Rate of return ROR	0.7	+	-
Economic constraint EC	0.9	-	+
Impact on employment	0.95	-	+
Impact on customers	0.6	+	+
Impact on economy	0.95	-	+
Impact on utility	0.7	+	-
Sustainability indicators			
Material intensity	0.6	+	-
Energy intensity	0.85	+	-
Environmental impact: GHG in production	0.8	-	-
Environmental impact: GHG in utilization	0.9	-	+
Toxic/waste material emissions-	0.9	+	-
Potential for technological improvements	0.7	-	+
Security/reliability	1	+	+
Political stability and legitimacy	0.85	-	+
Quality of life	0.3	-	+
Total positive score		**9**	**9**
Total minus score		**8**	**8**
Net score (positive-minus)		**1**	**1**
Weighted total score		**0.85**	**0.75**

The results of the multi-criteria decision matrix conclude that the addition of the process to upgrade the feed is not of higher value than simply selling the feed as a low-grade fuel. Although the proposed process has some positive impacts, such as on employment and GHG utilitation, the negative economic indicators outweigh the positive aspects.

Individual Comments, Discussions, and Recommendations

Delaney:

When we selected this design problem statement as our project, I was very intrigued and thought there were many possibilities for innovation and increased sustainability. Instead of selling the low-grade fuel byproduct from ethylene cracking, we had the opportunity to upgrade the stream and produce a high purity product used in rubber production. Upon extensive research and modeling, this proved to be much more difficult than anticipated. Even with the use of extractive rectification, the separation of the C4 hydrocarbon mixture to produce high purity 1,3-Butadiene requires multiple columns and process equipment. The expenses from utilities, equipment, and catalyst ultimately outweigh the revenue from the product streams. Although our design is not feasible, I believe there is potential for further research to be done. If a less expensive catalyst or extragent could be used then the process may be feasible.

Update of Self-Evaluation of Teamwork:

1: Novice (poor); 2: Apprentice; 3: Proficient; 4: Exemplary (excellent)

Teamwork	**1**	**2**	**3**	**4**
Problem identifying and solution: Participated in identifying and defining problems and working toward solutions				**X**
Organization: Approached tasks in systematic manner				**X**
Acceptance of responsibility: Shared responsibility for tasks to be accomplished in process design, safety, and green engineering				**X**
Initiative/motivation: Made suggestions, sought feedback, showed interest in group decision making and planning in process design			**X**	
Task completion: Completing own contributions to group project in process design, engineering economics, safety, and green engineering				**X**
Attendance: Attended planned sessions, was prompt, and participated in decision making				**X**
Collaboration: Worked cooperatively with others in process design, engineering economics, safety, and green engineering			**X**	
Participation: Contributed ‘fair share’ to process design			**X**	
Participation: Contributed ‘fair share’ to safety and green engineering			**X**	
Participation: Contributed ‘fair share’ to engineering economics				**X**
Participation: Contributed ‘fair share’ to preparing reports and presentations				**X**
Attitude: Displayed positive approach and made constructive comments in working toward goal			**X**	
Independence: Carried out tasks without overly depending on the other members			**X**	
Communication: Expressed thoughts clearly			**X**	

Please list specific suggestions to increase the effectiveness of design teamwork:
The nature of this project makes it difficult at times to divide and conquer. There were weeks where only one member was working on things because their work was necessary for the completion of everything else. With COVID-19 and moving to online instruction, this proved extra challenging as communication was more difficult. It would have been nice if the lab lecture time could have been used for teamwork earlier in the semester. As a class, we didn't make as much progress on our projects before moving to remote learning so the quality of resulting projects were significantly impacted.

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1: Novice (poor); 2: Apprentice; 3: Proficient; 4: Exemplary (excellent), NA: Not applicable

ABET Engineering Outcomes
1. an ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics

Performance Criteria	**1**	**2**	**3**	**4**	**NA**
Identify key information and assumptions needed			X		
Selects appropriate principles, equations, and/or approach to formulate the solution			X		
Solution procedure				X	

2. an ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors

Generating and analyzing multiple design solutions			X		
Public health, safety, and welfare design considerations				X	
Global, cultural, social, and environmental factors				X	
Economic factors				X	

3. an ability to communicate effectively with a range of audiences

Organization				X	

Content			X		
Presentation				X	

4. an ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts

Recognition of ethical and professional responsibilities				X	
Consideration of global, economic, environmental, and societal contexts.				X	
Ability to make informed judgements			X		

5. an ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives

Leadership			X		
Collaborative and inclusive environment			X		
Establish goals				X	
Plan tasks			X		
Meet objectives				X	

7. an ability to acquire and apply new knowledge as needed, using appropriate learning strategies

Acquiring new knowledge			X		
Applying new concepts			X		

Lindsey:

Overall I found this project to be unique and promising. While there exists a variety of methods for creating 1,3-Butadiene from other C-4 stream components that would prove useful to this project, it was interesting to see how much a process can really cost to create when a lab-scale catalytic reaction is suddenly an industrial-scale process requiring intensive energy and resource use. My initial thoughts were that we would be saving so much money from the increased value of the waste stream, that it was going to be a clearly obvious choice to invest in the process. I was surprised to see how the costs of materials and equipment add up and continue to contribute to slower payback periods even over the course of a long project. One of the biggest hurdles in the way of making this process a feasible addition to an ethylene cracking process is that the particular catalyst we can use to get more butadiene from the stream is not a catalyst that is currently commercially available. It is also possible that the reaction we are expecting would behave differently in a large industrial-scale reactor, so lots of testing and investigation would be required for the development of the physical reactor and process. This project certainly shows promise for a variety of future research topics, particularly large-scale catalytic reactions with uncommon catalysts for hydrocarbon recovery.

Update of Self-Evaluation of Teamwork:

1: Novice (poor); 2: Apprentice; 3: Proficient; 4: Exemplary (excellent)

Teamwork	1	2	3	4
Problem identifying and solution: Participated in identifying and defining problems and working toward solutions				**x**
Organization: Approached tasks in systematic manner			**x**	
Acceptance of responsibility: Shared responsibility for tasks to be accomplished in process design, safety, and green engineering				**x**
Initiative/motivation: Made suggestions, sought feedback, showed interest in group decision making and planning in process design				**x**
Task completion: Completing own contributions to group project in process design, engineering economics, safety, and green engineering			**x**	
Attendance: Attended planned sessions, was prompt, and participated in decision making				**x**
Collaboration: Worked cooperatively with others in process design, engineering economics, safety, and green engineering				**x**
Participation: Contributed ‘fair share’ to process design		**x**		
Participation: Contributed ‘fair share’ to safety and green engineering				**x**
Participation: Contributed ‘fair share’ to engineering economics		**x**		

Participation: Contributed 'fair share' to preparing reports and presentations				**x**
Attitude: Displayed positive approach and made constructive comments in working toward goal				**x**
Independence: Carried out tasks without overly depending on the other members			**x**	
Communication: Expressed thoughts clearly			**x**	

Please list specific suggestions to increase the effectiveness of design teamwork:
Having the entire year to work on the project would allow us to clear up confusion and specifications for the projects. Our group was able to narrow down our project and select one that stuck throughout the semester but overall having the entire year would allow people to work out the kinks in a project without having to essentially start over midway through the semester.

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ABET Engineering Outcomes
1. an ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics

Performance Criteria	**1**	**2**	**3**	**4**	**NA**
Identify key information and assumptions needed				x	
Selects appropriate principles, equations, and/or approach to formulate the solution			x		
Solution procedure			x		

2. an ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors

Generating and analyzing multiple design solutions			x		
Public health, safety, and welfare design considerations				x	

Global, cultural, social, and environmental factors				x	
Economic factors				x	

3. an ability to communicate effectively with a range of audiences

Organization				x	
Content				x	
Presentation				x	

4. an ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts

Recognition of ethical and professional responsibilities				x	
Consideration of global, economic, environmental, and societal contexts.				x	
Ability to make informed judgements				x	

5. an ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives

Leadership				x	
Collaborative and inclusive environment				x	
Establish goals				x	
Plan tasks				x	
Meet objectives				x	

7. an ability to acquire and apply new knowledge as needed, using appropriate learning strategies

Acquiring new knowledge				x	

Applying new concepts			x		

Andy:

The ability to work on the design and feasibility of this engineering project was a very valuable and enriching experience. From research, I learned a lot about pricing and design specifications for a plant and how this pricing plays into the economic feasibility of the plant. Despite our project not being economically feasible, I still believe it was a worthwhile effort to pursue. Our team really worked well together to accomplish this project. We divided tasks between us and kept each other on track. As a team, we especially did a good job of adapting to meet the needs of our changing project. Ultimately, I believe we found the best design for our project by using separation columns and a reactor to separate the mixture into sellable products. However, this design was not profitable with the cost of equipment and utilities. I found it quite surprising the cost of different utilities as we tested different sources of heating and cooling. Based upon this, it would be best to continue selling the C4 waste stream as low grade fuel oil instead of separating out 1,3-Butadiene for sale as a rubber precursor.

Update of Self-Evaluation of Teamwork:
1: Novice (poor); 2: Apprentice; 3: Proficient; 4: Exemplary (excellent)

Teamwork	**1**	**2**	**3**	**4**
Problem identifying and solution: Participated in identifying and defining problems and working toward solutions			**x**	
Organization: Approached tasks in systematic manner			**x**	
Acceptance of responsibility: Shared responsibility for tasks to be accomplished in process design, safety, and green engineering		**x**		
Initiative/motivation: Made suggestions, sought feedback, showed interest in group decision making and planning in process design		**x**		
Task completion: Completing own contributions to group project in process design, engineering economics, safety, and green engineering				**x**
Attendance: Attended planned sessions, was prompt, and participated in decision making			**x**	
Collaboration: Worked cooperatively with others in process design, engineering economics, safety, and green engineering				**x**

Participation: Contributed 'fair share' to process design				**x**
Participation: Contributed 'fair share' to safety and green engineering			**x**	
Participation: Contributed 'fair share' to engineering economics			**x**	
Participation: Contributed 'fair share' to preparing reports and presentations			**x**	
Attitude: Displayed positive approach and made constructive comments in working toward goal				**x**
Independence: Carried out tasks without overly depending on the other members			**x**	
Communication: Expressed thoughts clearly			**x**	

Please list specific suggestions to increase the effectiveness of design teamwork:
N/A

ABET Student-Self-Assessment for chemical engineering process design and safety CHME 453/853 Spring 2020
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ABET Engineering Outcomes
1. an ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics

Performance Criteria	**1**	**2**	**3**	**4**	**NA**
Identify key information and assumptions needed				x	
Selects appropriate principles, equations, and/or approach to formulate the solution			x		
Solution procedure			x		

2. an ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors

Generating and analyzing multiple design solutions		x			
Public health, safety, and welfare design considerations			x		
Global, cultural, social, and environmental factors		x			
Economic factors		x			

3. an ability to communicate effectively with a range of audiences

Organization			x		
Content			x		
Presentation			x		

4. an ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts

Recognition of ethical and professional responsibilities			x		
Consideration of global, economic, environmental, and societal contexts.				x	
Ability to make informed judgements			x		

5. an ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives

Leadership				x	
Collaborative and inclusive environment			x		
Establish goals				x	
Plan tasks		x			
Meet objectives				xx	

7. an ability to acquire and apply new knowledge as needed, using appropriate learning strategies

Acquiring new knowledge				x	
Applying new concepts			x		

Firdavs:

I found this dive into the feasibility of a plant addition incredibly interesting and fascinating to research. 1,3 butadiene purification and conversion from a mixed low grade fuel stream seemed like a feasible, profitable, and sustainable approach for a plant to branch out its operations, however the potential gain was simply too low to ever support such an endeavour. It was shocking to see how expenses compared to the profits of selling a reaction-grade material. Despite all of its setbacks, however, I can say I am very proud of what my team and I have assembled to present. It is a clear representation of what a thorough market search with careful examination and simulation can achieve, and despite the final result being disappointing, I can safely say it is an excellent and accurate presentation of a possible addition a plant may pursue should the cost be mitigated more. Plants which produce a low grade fuel that is very rich (50-60<) in 1,3 butadiene should strongly consider the leap to selling such a critical rubber precursor.

Update of Self-Evaluation of Teamwork:

1: Novice (poor); 2: Apprentice; 3: Proficient; 4: Exemplary (excellent)

Teamwork	1	2	3	4
Problem identifying and solution: Participated in identifying and defining problems and working toward solutions				**X**
Organization: Approached tasks in systematic manner			**X**	
Acceptance of responsibility: Shared responsibility for tasks to be accomplished in process design, safety, and green engineering			**X**	
Initiative/motivation: Made suggestions, sought feedback, showed interest in group decision making and planning in process design				**X**
Task completion: Completing own contributions to group project in process design, engineering economics, safety, and green engineering			**X**	
Attendance: Attended planned sessions, was prompt, and participated in decision making			**X**	

Collaboration: Worked cooperatively with others in process design, engineering economics, safety, and green engineering			**X**	
Participation: Contributed 'fair share' to process design				**X**
Participation: Contributed 'fair share' to safety and green engineering		**X**		
Participation: Contributed 'fair share' to engineering economics		**X**		
Participation: Contributed 'fair share' to preparing reports and presentations			**X**	
Attitude: Displayed positive approach and made constructive comments in working toward goal			**X**	
Independence: Carried out tasks without overly depending on the other members			**X**	
Communication: Expressed thoughts clearly			**X**	

Please list specific suggestions to increase the effectiveness of design teamwork:
Unfortunately with so much being left out of our control in terms of meeting in person to work together with advancement fo COVID-19, I think we did very well in adapting to online meetings and lectures to successfully complete this project. I think it would be helpful to convert one of the examples in the lab to allotted group work time. This could be done every few weeks to ensure that teams have a guaranteed time to work together with easy accessibility to the professor should they have questions.

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ABET Engineering Outcomes
1. an ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics

Performance Criteria	**1**	**2**	**3**	**4**	**NA**
Identify key information and assumptions needed			X		

Selects appropriate principles, equations, and/or approach to formulate the solution			X		
Solution procedure			X		

2. an ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors

Generating and analyzing multiple design solutions				X	
Public health, safety, and welfare design considerations				X	
Global, cultural, social, and environmental factors			X		
Economic factors			X		

3. an ability to communicate effectively with a range of audiences

Organization			X		
Content			X		
Presentation				X	

4. an ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts

Recognition of ethical and professional responsibilities			X		
Consideration of global, economic, environmental, and societal contexts.			X		
Ability to make informed judgements			X		

5. an ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives

Leadership			X		

Collaborative and inclusive environment				X	
Establish goals				X	
Plan tasks				X	
Meet objectives			X		

7. an ability to acquire and apply new knowledge as needed, using appropriate learning strategies

Acquiring new knowledge				X	
Applying new concepts				X	

Gitau:

Working on a feasible solution for the design problem statement has been mentally engaging, overall. The evolution of the proposed process design has been remarkable, and I can say that I am proud of the final design, despite its infeasibility. I was surprised by how taxing the literature review could be, but thankful for the growth achieved from it. Ultimately, it would be more profitable to sell the original C4 hydrocarbon stream as low-grade fuel instead of processing it to isolate and purify 1,3-butadiene, a highly sought rubber precursor, for commercial sale. Minimization of the utility costs and catalyst purchase cost would be critical in increasing the feasibility of the process. One way to potentially reduce heating utility costs would be to employ geothermal energy to produce the required stream. However, this adds other constraints, such as finding a suitable location with a reliable water supply and easy access to geothermal pockets. The importance of accurate and reliable price data for raw materials was also conveyed by this design project as we ended up approximating some of the values, such as the purchase cost for the catalyst. The uncertainty associated with our cost assumptions might have negatively impacted the feasibility of the overall process if the actual costs were less than our assumed costs.

Update of Self-Evaluation of Teamwork:

1: Novice (poor); 2: Apprentice; 3: Proficient; 4: Exemplary (excellent)

Teamwork	**1**	**2**	**3**	**4**
Problem identifying and solution: Participated in identifying and defining problems and working toward solutions				**X**
Organization: Approached tasks in systematic manner			**X**	

Acceptance of responsibility: Shared responsibility for tasks to be accomplished in process design, safety, and green engineering			**X**	
Initiative/motivation: Made suggestions, sought feedback, showed interest in group decision making and planning in process design				**X**
Task completion: Completing own contributions to group project in process design, engineering economics, safety, and green engineering				**X**
Attendance: Attended planned sessions, was prompt, and participated in decision making				**X**
Collaboration: Worked cooperatively with others in process design, engineering economics, safety, and green engineering				**X**
Participation: Contributed 'fair share' to process design				**X**
Participation: Contributed 'fair share' to safety and green engineering			**X**	
Participation: Contributed 'fair share' to engineering economics		**X**		
Participation: Contributed 'fair share' to preparing reports and presentations				**X**
Attitude: Displayed positive approach and made constructive comments in working toward goal				**X**
Independence: Carried out tasks without overly depending on the other members				**X**
Communication: Expressed thoughts clearly			**X**	

Please list specific suggestions to increase the effectiveness of design teamwork:
The design projects should run for the entire senior year instead of the last semester. This change would enable teams to dedicate more effort to their design solutions over a more extended period, minimizing burnout. The semester was rushed, irrespective of the COVID-19 pandemic and transition to remote learning, as we barely spent any time in class working on our projects. It may be worth omitting some topics from the course syllabus to free up more time for groups to work on their design projects. I am confident that some modules can easily be condensed into a single session, as was evident after the

transition to online classes. The first semester could be dedicated to the literature review and the second semester to the rest of the project.

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ABET Engineering Outcomes
1. an ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics

Performance Criteria	**1**	**2**	**3**	**4**	**NA**
Identify key information and assumptions needed				**X**	
Selects appropriate principles, equations, and/or approach to formulate the solution				**X**	
Solution procedure			**X**		

2. an ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors

Generating and analyzing multiple design solutions				**X**	
Public health, safety, and welfare design considerations			**X**		
Global, cultural, social, and environmental factors			**X**		
Economic factors			**X**		

3. an ability to communicate effectively with a range of audiences

Organization			**X**		
Content			**X**		
Presentation			**X**		

4. an ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts

Recognition of ethical and professional responsibilities			**X**		
Consideration of global, economic, environmental, and societal contexts.			**X**		
Ability to make informed judgements				**X**	

5. an ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives

Leadership			**X**		
Collaborative and inclusive environment				**X**	
Establish goals				**X**	
Plan tasks				**X**	
Meet objectives				**X**	

7. an ability to acquire and apply new knowledge as needed, using appropriate learning strategies

Acquiring new knowledge			**X**		
Applying new concepts			**X**		

Nomenclature

Term	**Meaning**
atm	atmosphere, as in unit of pressure
barg	bars gauge pressure
BFD	Block Flow Diagram
Bi-Mo-O	Bismuth molybdate systems
Butadiene	1,3-Butadiene

BWR-LS	Benedict-Webb-Rubin-Lee-Starling
BWRS	Benedict-Webb-Rubin-Starling
C	Degree celsius, °C
CAPCOST	Title of an excel sheet used to calculate capital cost
CPI	Consumer price index
D	Inner tube diameter
D/dps	Tube diameter to equivalent pellet spherical diameter ratio
di	Pellet inner diameter
di/do	pellet inner diameter to pellet outer diameter ratio
DMF	Dimethylformamide
do	Pellet outer diameter
dps	Equivalent pellet spherical diameter
GJ	Gigajoule
h	Pellet height
h/do	pellet height to pellet outer diameter ratio
HAZOP	Hazard and operability study
hr	Hour
JHA	Job hazard analysis
JIS	Job Instruction Sheet
kW	Kilowatts
kWhr	Kilowatt-hour, as in unit price of electricity
lb	Pound
LEL	Lower explosive limit
LK-PLOCK	Lee-Kesler-Plöcker
MOC	Material of Construction
MT	Metric Ton
N/A	Not Applicable
NFPA	National Fire Protection Association
NPS	Nominal pipe size
NPV	Net Present Value
PBP	Payback period

PFD	Process Flow Diagram
PLC	Programmable logic controller
PR-BM	Peng-Robinson-Boston-Mathias
RAGAGEP	Recognized and Generally Accepted Good Engineering Practices
RKS-BM	Redlich-Kwong-Soave-Boston-Mathias
ROR	Rate of Return
SCADA	Supervisory control and data acquisition (plant operator display)
SOP	Standard Operating Procedure
sqm	Square meter
Tbp	Temperature, boiling point
Term	**Meaning**
Tfp	Temperature, flash point (closed cup)
UA	Unavailable

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Appendix

A-1: List of Chemical Names Used

Many of the chemicals in this system are ubiquitous in industry and have a variety of nicknames. This table contains some of the many common names for these chemicals.

Table A-1: List of Chemical Names Used

Chemical Formula	Name used in Aspen Simulation	Other known nicknames
C4H6-4	1,3-BD	1,3-Butadiene, Butadiene,
C4H8-5	ISOBUTYL	Isobutylene, 2-methylpropene, Isobutene
C4H8-1	1-BUTENE	1-Butene, 1-Butylene
C4H10-1	N-BUTANE	N-butane, Butane*

C4H10-2	ISOBUTAN	Isobutane, Butane*
C4H8-2	CIS-2B	Cis-2-butene
C4H8-3	TRANS-2B	Trans-2-butene
C4H4	BUTENYNE	Butenyne, Vinylacetylene, 1-Buten-3-yne, 1-butenyne
C4H6-1	1-BUTYNE	1-Butyne, Ethylacetylene
C3H8	PROPANE	Propane
C3H4-1	ALLENE	Propadiene, Allene
C3H4-2	PROPYNE	Methylacetylene, Propyne
C5H12-2	ISOPENT	2-methyl-butane, Isopentane
H20	WATER	Water
C3H7NO	DMF	N,N-Dimethylformamide
H2	H2	Hydrogen gas
AIR	AIR	Air

**Butane is colloquially used to refer to either structural isomer. For this reason, the report will specifically refer to 1-butene or n-butane to avoid confusion.*

A-2: Physical Properties of Relevant Chemicals

An SDS sheet is available for each chemical relevant to this process, as cited. We used these SDS documents to create a table of Physical Properties of Relevant Chemicals.

Table A-2: Description of important physical properties and primary hazards associated with chemicals used in the process

Chemical	Primary Hazard	Mitigation	Tbp (°C)	Tfp (°C)	LEL/UEL (% concentration)
1,3-Butadiene	Carcinogen/ Flammable	Keep away from heat & ignition sources. Workers should remove contaminated clothing before entering eating or smoking areas. Store in cool, ventilated area.	-4.41	-85	2/12
Isobutylene	Flammable	Keep away from heat & ignition sources. Store in a	-6.9	-76.1	1.8/9.6

		cool, ventilated area.			
1-Butene	Flammable	Keep away from heat & ignition sources. Store in a cool, ventilated area	-6.47	-80	1.6/10
N-butane	Flammable	Keep away from heat & ignition sources. Store in a cool, ventilated area.	-0.5	-60	1.8/8.4
Isobutane	Flammable	Keep away from heat & ignition sources. Store in a cool, ventilated area.	-12	-83.15	1.8/8.4
Cis-2-butene	Flammable	Keep away from heat & ignition sources. Store in a cool, ventilated area.	3.7	UA	1.5/9
Trans-2-butene	Flammable	Keep away from heat & ignition sources. Store in a cool, ventilated area.	1	UA	1.8/9.7
Vinylacetylene	Flammable	Keep away from heat & ignition sources. Store in a cool, ventilated area.	5	-5	2/100 (decomposes)
Ethylacetylene	Flammable	Keep away from heat & ignition sources. Store in cool, ventilated area.	8	-7	1.3/99.9 (decomposes)
Propane	Flammable	Keep away from heat & ignition sources. Store in a cool, ventilated area.	-42.1	-104.4	UA
Propadiene/ Allene	Flammable	Keep away from heat & ignition sources. Store in a cool, ventilated area.	-34.5	UA	2.1/13
Methyl Acetylene	Flammable	Keep away from heat & ignition sources. Store in a cool, ventilated area.	-23.2	UA	2.4/11.7
Isopentane	Flammable	Keep away from heat & ignition sources. Store in cool, ventilated area.	27.8	-51	1.4/7.6
Water	N/A	N/A	100	N/A	N/A
N-pentane	Flammable	Keep away from heat & ignition sources. Store in cool, ventilated area.	36.06	-40	1.5/7.8

DMF	Flammable, toxic	Store in a well-ventilated area, tightly close container	153	58	2.2/15.2
NMP	Toxic, combustible	Avoid heat, flames, sparks, exposure to air, light, & water	202	91	1.3/9.5

A-3: Equations

Equation term	**Meaning**
A	1-butene
B	Oxygen
C	1,3-butadiene
D	Hydrogen
E	Trans-2-butene
F	Cis-2-butene
r	Reaction rate
k	Rate constant
P	Pressure
F	Flow rate
W	Weight
d_{po}	Outer diameter of pellet
d_{pi}	Inner diameter of pellet
R	Gas constant 1.985×10^{-3} (kcal*K^{-1} *mol^{-1})
H	Height

Material balances:

Main reactions:

$$\textbf{A1: } A + B \rightarrow C + D \quad (1)$$

$$\textbf{E1: } E + B \rightarrow C + D \quad (2)$$

Side reactions:

A2: A + B → F (3)

E2: E + B → F (4)

A3: A + B → E (5)

E3: E + B → A (6)

Rate equations:

$r_{A1} = k_A P_A^{0.8} P_B^{-0.2}$ (Zhai et. al, 2015) (7)

$r_{E1} = k_E P_E^{0.9} P_B^{0.1}$ (Zhai et. al, 2015) (8)

$r_{A2} = (125/800)*(-r_{A1})$ (9)

$r_{A3} = (75/800)*(-r_{A1})$ (10)

$r_{E2} = r_{E3} = (½)*(-r_{E1})$ (11)

Pressure equations:

$P_A = P_0*(F_A//F_T)*(F_{T0}/F_T)$ (12)

$P_B = P_0*(F_B/F_T)*(F_{T0}/F_T)$ (13)

$P_E = P_0*(F_E/F_T)*(F_{T0}/F_T)$ (14)

Differential equations:

$dF_A/dW = r_{E3} - (r_{A1} + r_{A2} + r_{A3}) = (½)*(r_{E1}) - (5/4)*(r_{A1})$ (15)

$dF_B/dW = - (r_{A1} + r_{A2} + r_{A3}+ r_{E1} + r_{E2} + r_{E3}) = - (5/4)*(r_{A1}) - 2*(r_{E1})$ (16)

$dF_C/dW = r_{A1} + r_{E1}$ (17)

$dF_D/dW = r_{A1} + r_{E1}$ (18)

$dF_E/dW = r_{A3} - (r_{E1} + r_{E2} + r_{E3}) = (75/800)*(r_{A1}) - (2)*(-r_{E1})$ (19)

$dF_F/dW = r_{A2} + r_{E2} = (125/800)*(-r_{A1}) + (½)*(-r_{E1})$ (20)

Rate constant equations:

$$k_{MATLAB}(625) = k_{original}(625) \times (\frac{1000\ g}{125\ mg}) \times (\frac{3600\ kmol}{1000\ hr})$$

(21)

$$k_{Aspen\ Plus}(625) = k_{MATLAB}(625) \times 1{,}640\ kg/m^3$$
(22)

$$k_A(523) = k_A(625) * exp[\frac{E_A}{R} * (625^{-1} - 523^{-1})$$
(23)

$$k_E(523) = k_E(625) * exp[\frac{E_E}{R} * (625^{-1} - 523^{-1})$$
(24)

$$k_{cis-2-butene}(523) = k_{1,3-butadiene}(523) \times \left(\frac{selectivity_{cis-2-butene}}{selectivity_{1,3-butadiene}}\right)$$
(25)

$$k_{trans-2-butene}(523) = k_{1,3-butadiene}(523) \times \left(\frac{selectivity_{trans-2-butene}}{selectivity_{1,3-butadiene}}\right)$$
(26)

Pellet geometry:

$$volume_{full\ cylinder} = \pi \times (d_{po}/2)^2 \times H$$
(27)

$$surface\ area_{full\ cylinder} = (2\pi \times (d_{po}/2)^2) + (\pi \times d_{po} \times H)$$
(28)

$$volume_{hole} = \pi \times (d_{pi}/2)^2 \times H$$
(29)

$$surface\ area_{hole} = (2\pi \times (d_{pi}/2)^2) + (\pi \times d_{pi} \times H)$$
(30)

$$volume_{catalyst\ pellet} = volume_{full\ cylinder} - volume_{hole}$$
(31)

$$surface\ area_{pellet} = (2\pi \times ((d_{po}/2)^2 - (d_{pi}/2)^2)) + (\pi \times H \times (d_{po} + d_{pi}))$$
(32)

$$d_{ps} = 2 \times (\frac{3}{4\pi} \times volume_{catalyst\ pellet})^{1/3}$$
(33)

A-4: Example calculations

Catalyst

Table A-4.1: Cost of chemicals to form catalyst, Sigma Aldrich prices

Chemical	Quantity	Unit	Average cost ($/unit)	Cost of Amount Used ($)	Assumptions
$Bi(NO_3)_3 \cdot 5H_2O$	48.5	g	$0.24	$11.43	Reagent grade, 98%
HNO_3	37	mL	$0.04	$1.37	Based on 69%
NH_4VO_3	11.4	g	$1.04	$11.80	ACS reagent, >99%
$(NH_4)_6Mo_7O_{24} \cdot 4H_2O$	17.6	g	$0.47	$8.27	81-83% MoO3 basis
H_2O	600	mL	$0.00	$0.00	No cost

We made an assumption that approximately 80 g of catalyst in total was made during this process described. This assumption is relevant when the cost estimate is upscaled as calculations continue.

Table A-4.2: Cost of energy used to produce catalyst

Equipment	Approx. Wattage	Total run time	Energy Consumed (kWh)	Cost of energy ($/kWh)	Cost of process
Oven	1404	15	21.06	$0.09	$1.90

The oven is the most energy-intensive part of the process. The other equipment (spray dryer, eg.) is used for far less time and is far less wattage. For this reason, the assumption is that the energy cost of the oven dominates the energy cost of the rest of the equipment and is the best representation. We assumed that a cost of energy for Nebraska is a valid input, and used the ubiquitously used $0.09/kWh figure, sourced from Payless Power, updated in February 2020. This cost is shown to be marginal when compared to the chemical costs. The comparison of these contributing costs can be found in Table A-4.3 below.

Table A-4.3: Final cost calculation including chemicals, energy, and labor

Cost	Cost ($/80g of product)	Total Cost ($/kg)	Cost ($/gal)	Note
Chemicals	$32.87	$365.70	$1,386.00	Est, 1 gal approx 3.79 kg
Energy	$1.90	=(((B2+B3)/100)*1000) +18'		
Labor	$18.00			Minimum wage $9/hr * 2 hours

Because an operator does not need to be actively present and working only on the catalyst production during the hours the catalyst is in the oven, we made an assumption that only about 2 hours of the total production process will need to be directly monitored and are thus billable. Assuming minimum wage, $9 in Nebraska, this labor cost is then approximately $18 for a round of catalyst production. This is added onto the calculation because the labor itself is not, within reason, assumed to be dependent on quantity; that is to say that to produce 80 g of catalyst vs 500 g vs 1 kg is not assumed to be significantly different in terms of time required for labor. To further solidify the validity of this estimation, we worked with Everchem, a chemical catalyst company, to get quotes for various quantities of another bismuth catalyst and compare their sale price with our estimated cost.

Table A-4.4: Comparison to a bismuth catalyst available for purchase from Everchem.

Item	Quantity	Unit	Cost	Cost/unit
BiCAT 8840	1	gallon	$200.00	$200.00
BiCAT 8840	5	gallon	$600.00	$120.00
BiCAT 8840	441	lb	$4,096.89	$9.29
BiCAT 8842	1	gallon	$250.00	$250.00
BiCAT 8842	5	gallon	$800.00	$160.00
BiCAT 8842	441	lb	$6,615.00	$15.00

These prices are as quoted from Everchem by Bill Lewis, a sales representative at Everchem (Personal communication, April 14th, 2020). While this catalyst is cheaper in all likelihood based on the differing composition, we used it as a baseline approximation for cost based on the fact that it is an industrially available bismuth-based catalyst.

Rate constant

We scaled the original rate constants for k_A and k_E for the MATLAB model as shown below:

$$k_{A,MATLAB}(625) = 0.0001585 \times (\frac{1000\ g}{125\ mg}) \times (\frac{3600\ kmol}{1000\ hr}) = 4.65\ hr^{-1}$$

$$k_{E,MATLAB}(625) = 0.00001474 \times (\frac{1000\ g}{125\ mg}) \times (\frac{3600\ kmol}{1000\ hr}) = 0.42\ hr^{-1}$$

We scaled the original rate constants for k_A and k_E for the Aspen simulation as shown below:

$$k_{A,Aspen\ Plus}(625) = 4.65\ hr^{-1} \times 1{,}640\ kg/m^3 = 7{,}486.27\ hr^{-1}$$

$$k_{E,Aspen\ Plus}(625) = 0.42\ hr^{-1} \times 1{,}640\ kg/m^3 = 696.20\ hr^{-1}$$

We then scaled the MATLAB model rate constants from their values at 625 K to the reactor temperature equivalents at 523 K using the following rate equations:

$$k_{A,MATLAB}(523) = 4.56\ hr^{-1} \times exp[\frac{9.2}{1.987E-03} \times (625^{-1} - 523^{-1}) = 1.075\ hr^{-1}$$

$$k_{E,MATLAB}(523) = 0.42\ hr^{-1} \times exp[\frac{17.4}{1.987E-03} \times (625^{-1} - 523^{-1}) = 2.732 \times 10^{-2}\ hr^{-1}$$

The Aspen simulation rate constants were scaled automatically according to their temperature, so example calculations for that are not included. Using kA,MATLAB as an example, the rate constants for the isomerization of 1-butene to cis-2-butene and trans-2-butene were determined as follows:

$$k_{A,cis-2-butene}(523) = 1.075\ hr^{-1} \times \left(\frac{0.125}{0.8}\right) = 0.71\ hr^{-1}$$

$$k_{A,trans-2-butene}(523) = 1.075\ hr^{-1} \times \left(\frac{0.075}{0.8}\right) = 0.43\ hr^{-1}$$

Cost Calculations

Table A-4.5: CAPCOST input summary for feasibility analysis before HENS

Economic Options

Cost of Land	$	726,000
Taxation Rate		35%
Annual Interest Rate		7%
Salvage Value	$	3,630,000
Working Capital	$	6,680,000
FCI_L	$	36,300,000
Total Module Factor		1.18
Grass Roots Factor		0.50

Economic Information Calculated From Given Information

Revenue From Sales	$	42,980,075
C_{RM} (Raw Materials Costs)	$	30,296,268
C_{UT} (Cost of Utilities)	$	9,204,300
C_{WT} (Waste Treatment Costs)	$	63
C_{OL} (Cost of Operating Labor)	$	158,700

Factors Used in Calculation of Cost of Manufacturing (COM_d)

Comd = 0.18*FCIL + 2.73*COL + 1.23*(CUT + CWT + CRM)

Multiplying factor for FCIL		0.18
Multiplying factor for C_{OL}		2.73
Facotrs for C_{UT}, C_{WT}, and C_{RM}		1.23
COM_d	$	55,553,027

Factors Used in Calculation of Working Capital

Working Capital = $A*C_{RM} + B*FCI_L + C*C_{OL}$

A	0.10
B	0.10
C	0.10

Project Life (Years after Startup)	15

Construction period	2

Distribution of Fixed Capital Investment (must sum to one)

End of year One	60%
End of year Two	40%
End of year Three	
End of year Four	
End of year Five	

Table A-4.6: CAPCOST input summary for feasibility analysis after HENS

Economic Options

Cost of Land	$	566,706
Taxation Rate		35%
Annual Interest Rate		7%
Salvage Value	$	2,833,530
Working Capital	$	5,880,000
FCI_L	$	28,335,300
Total Module Factor		1.18
Grass Roots Factor		0.50

Economic Information Calculated From Given Information

Revenue From Sales	$	42,980,075
C_{RM} (Raw Materials Costs)	$	30,296,268
C_{UT} (Cost of Utilities)	$	294,229
C_{WT} (Waste Treatment Costs)	$	63
C_{OL} (Cost of Operating Labor)	$	158,700

Factors Used in Calculation of Cost of Manufacturing (COM_d)

Comd = 0.18*FCIL + 2.73*COL + 1.23*(CUT + CWT + CRM)

Multiplying factor for FCIL		0.18
Multiplying factor for C_{OL}		2.73
Facotrs for C_{UT}, C_{WT}, and C_{RM}		1.23
COM_d	$	43,159,994

Factors Used in Calculation of Working Capital

Working Capital = $A*C_{RM} + B*FCI_L + C*C_{OL}$

A	0.10
B	0.10
C	0.10

Project Life (Years after Startup)	15

Construction period	2

Distribution of Fixed Capital Investment (must sum to one)

End of year One	60%
End of year Two	40%
End of year Three	
End of year Four	
End of year Five	

A-5: Input Summary for Aspen Plus Simulation

```
;
;Input Summary created by Aspen Plus Rel. 37.0 at 19:31:38 Mon Apr 20, 2020
;Directory C:\Users\dbachman3\Downloads  Filename
C:\Users\DBACHM~1\AppData\Local\Temp\~apc87.txt
;

DYNAMICS
   DYNAMICS RESULTS=ON

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr'  &
      HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C  &
      VOLUME=cum DELTA-T=C HEAD=meter MASS-DENSITY='kg/cum'  &
      MOLE-ENTHALP='kcal/mol' MASS-ENTHALP='kcal/kg'  &
      MOLE-VOLUME='cum/kmol' HEAT=Gcal MOLE-CONC='mol/l'  &
      PDROP=bar SHORT-LENGTH=mm

DEF-STREAMS CONVEN ALL

MODEL-OPTION

DESCRIPTION "
   Chemical Simulation with Metric Units :
   C, bar, kg/hr, kmol/hr, Gcal/hr, cum/hr.

   Property Method: NRTL

   Flow basis for input: Mole

   Stream report composition: Mole flow
   "

DATABANKS 'APV110 PURE37' / 'APV110 AQUEOUS' / 'APV110 SOLIDS' &
       / 'APV110 INORGANIC' / 'APESV110 AP-EOS' /  &
      'NISTV110 NIST-TRC' / NOASPENPCD
```

```
PROP-SOURCES 'APV110 PURE37' / 'APV110 AQUEOUS' /  &
        'APV110 SOLIDS' / 'APV110 INORGANIC' / 'APESV110 AP-EOS' &
         / 'NISTV110 NIST-TRC'

COMPONENTS
    1,3-BD C4H6-4 /
    ISOBUTYL C4H8-5 /
    1-BUTENE C4H8-1 /
    N-BUTANE C4H10-1 /
    ISOBUTAN C4H10-2 /
    CIS-2B C4H8-2 /
    TRANS-2B C4H8-3 /
    BUTENYNE C4H4 /
    1-BUTYNE C4H6-1 /
    PROPANE C3H8 /
    ALLENE C3H4-1 /
    PROPYNE C3H4-2 /
    ISOPENT C5H12-2 /
    DMF C3H7NO /
    H2 H2 /
    AIR AIR /
    WATER H2O

SOLVE
    RUN-MODE MODE=SIM

FLOWSHEET
    BLOCK HT-01 IN=FEED OUT=S-01
    BLOCK CMP-01 IN=S-01 OUT=S-02
    BLOCK HT-02 IN=S-02 OUT=S-03
    BLOCK COL-01 IN=S-03 OUT=PROPYNE HEAVIES S-04
    BLOCK MX-01 IN=S-04 DMF R-08 OUT=S-05
    BLOCK SEP-01 IN=S-05 D-01 OUT=R-01 S-06
    BLOCK SEP-02 IN=S-06 OUT=1,3-BD D-01
    BLOCK SEP-03 IN=R-01 OUT=R-02 ISOBUTYL
    BLOCK MX-02 IN=R-02 A-02 OUT=R-03
    BLOCK HT-04 IN=R-03 OUT=R-04
    BLOCK RX-01 IN=R-04 OUT=R-05
    BLOCK CMP-02 IN=R-05 OUT=R-06
    BLOCK HT-03 IN=AIR OUT=A-02
    BLOCK HT-05 IN=R-06 OUT=R-07
    BLOCK SEP-04 IN=R-07 OUT=H2+AIR R-08
    BLOCK HT-06 IN=1,3-BD OUT=1,3-BD-C
```

```
  BLOCK HT-07 IN=ISOBUTYL OUT=ISOBUT-C
  BLOCK HT-08 IN=HEAVIES OUT=HEAVY-C
  BLOCK HT-09 IN=PROPYNE OUT=PROPY-C

PROPERTIES PR-BM

PROP-DATA PRKBV-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr'  &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C  &
    VOLUME=cum DELTA-T=C HEAD=meter MASS-DENSITY='kg/cum'  &
    MOLE-ENTHALP='kcal/mol' MASS-ENTHALP='kcal/kg'  &
    MOLE-VOLUME='cum/kmol' HEAT=Gcal MOLE-CONC='mol/l'  &
    PDROP=bar SHORT-LENGTH=mm
  PROP-LIST PRKBV
  BPVAL 1,3-BD 1-BUTENE 2.20000000E-3 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL 1-BUTENE 1,3-BD 2.20000000E-3 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL 1,3-BD N-BUTANE .0141000000 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL N-BUTANE 1,3-BD .0141000000 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL 1-BUTENE N-BUTANE 1.10000000E-3 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL N-BUTANE 1-BUTENE 1.10000000E-3 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL N-BUTANE ISOBUTAN -4.0000000E-4 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL ISOBUTAN N-BUTANE -4.0000000E-4 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL N-BUTANE PROPANE 3.30000000E-3 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL PROPANE N-BUTANE 3.30000000E-3 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL N-BUTANE ISOPENT 2.92000000E-3 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL ISOPENT N-BUTANE 2.92000000E-3 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL N-BUTANE H2 -.3970000000 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL H2 N-BUTANE -.3970000000 0.0 0.0 -273.1500000  &
    726.8500000
  BPVAL ISOBUTAN PROPANE -7.8000000E-3 0.0 0.0 -273.1500000  &
    726.8500000
```

```
    BPVAL PROPANE ISOBUTAN -7.8000000E-3 0.0 0.0 -273.1500000  &
        726.8500000
    BPVAL PROPANE PROPYNE .0758000000 0.0 0.0 -273.1500000  &
        726.8500000
    BPVAL PROPYNE PROPANE .0758000000 0.0 0.0 -273.1500000  &
        726.8500000
    BPVAL PROPANE ISOPENT .0111000000 0.0 0.0 -273.1500000  &
        726.8500000
    BPVAL ISOPENT PROPANE .0111000000 0.0 0.0 -273.1500000  &
        726.8500000
    BPVAL PROPANE H2 -.0833000000 0.0 0.0 -273.1500000  &
        726.8500000
    BPVAL H2 PROPANE -.0833000000 0.0 0.0 -273.1500000  &
        726.8500000

STREAM AIR
    SUBSTREAM MIXED TEMP=25. PRES=1. <atm> MOLE-FLOW=1.
    MOLE-FRAC AIR 1.

STREAM DMF
    SUBSTREAM MIXED TEMP=39. PRES=5.5 <atm> MOLE-FLOW=15.
    MASS-FRAC DMF 1.

STREAM FEED
    SUBSTREAM MIXED TEMP=150. PRES=1. <atm>  &
        MASS-FLOW=15. <tons/hr>
    MASS-FRAC 1,3-BD 0.43 / ISOBUTYL 0.234 / 1-BUTENE 0.124 /  &
        N-BUTANE 0.045 / ISOBUTAN 0.05 / CIS-2B 0.041 /  &
        TRANS-2B 0.053 / BUTENYNE 0.007 / 1-BUTYNE 0.002 /  &
        PROPANE 0. / ALLENE 0.002 / PROPYNE 0.007 / ISOPENT  &
        0.005

BLOCK MX-01 MIXER
    PARAM

BLOCK MX-02 MIXER
    PARAM MAXIT=200 TOL=0.5

BLOCK SEP-01 SEP
    PARAM TOL=1E-06
    FRAC STREAM=R-01 SUBSTREAM=MIXED COMPS=1,3-BD ISOBUTYL  &
        1-BUTENE N-BUTANE ISOBUTAN CIS-2B TRANS-2B FRACS=0.006  &
        0.99 1. 1. 1. 1. 1.
    UTILITY UTILITY-ID=LPS
```

```
BLOCK SEP-02 SEP
    PARAM
    FRAC STREAM=1,3-BD SUBSTREAM=MIXED COMPS=1,3-BD FRACS=1.
    UTILITY UTILITY-ID=LPS

BLOCK SEP-03 SEP
    PARAM
    FRAC STREAM=ISOBUTYL SUBSTREAM=MIXED COMPS=1,3-BD ISOBUTYL  &
        1-BUTENE N-BUTANE ISOBUTAN CIS-2B TRANS-2B BUTENYNE  &
        1-BUTYNE PROPANE ALLENE PROPYNE ISOPENT DMF H2 AIR  &
        FRACS=0. 1. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.  &
        0. 0.
    UTILITY UTILITY-ID=CW

BLOCK SEP-04 SEP
    PARAM
    FRAC STREAM=H2+AIR SUBSTREAM=MIXED COMPS=H2 AIR FRACS=1.  &
        1.
    UTILITY UTILITY-ID=CW

BLOCK HT-01 HEATER
    PARAM TEMP=55. PRES=1. <atm> DPPARMOPT=NO
    UTILITY UTILITY-ID=CW

BLOCK HT-02 HEATER
    PARAM TEMP=48. PRES=5.5 <atm> DPPARMOPT=NO
    UTILITY UTILITY-ID=CW

BLOCK HT-03 HEATER
    PARAM TEMP=200. PRES=1. <atm> TOL=0.01 DPPARMOPT=NO
    UTILITY UTILITY-ID=HPS

BLOCK HT-04 HEATER
    PARAM TEMP=250. PRES=1. <atm> DPPARMOPT=NO
    UTILITY UTILITY-ID=HPS

BLOCK HT-05 HEATER
    PARAM TEMP=48. PRES=5.5 <atm> DPPARMOPT=NO
    UTILITY UTILITY-ID=CW

BLOCK HT-06 HEATER
    PARAM TEMP=25. PRES=5.5 DPPARMOPT=NO
    UTILITY UTILITY-ID=CHILL-W
```

```
BLOCK HT-07 HEATER
   PARAM TEMP=25. PRES=5.5 DPPARMOPT=NO
   UTILITY UTILITY-ID=CHILL-W

BLOCK HT-08 HEATER
   PARAM TEMP=25. PRES=5.5 DPPARMOPT=NO
   UTILITY UTILITY-ID=CHILL-W

BLOCK HT-09 HEATER
   PARAM TEMP=25. PRES=5.5 DPPARMOPT=NO
   UTILITY UTILITY-ID=LPS

BLOCK COL-01 RADFRAC
   SUBOBJECTS INTERNALS = CS-1
   PARAM NSTAGE=75 ALGORITHM=STANDARD HYDRAULIC=NO MAXOL=50  &
      TOLOL=0.001 DAMPING=NONE
   PARAM2 STATIC-DP=YES
   COL-CONFIG CONDENSER=TOTAL KEY-SELECT=SPLIT-FRACTI  &
      CA-CONFIG=INT-1
   FEEDS S-03 26
   PRODUCTS HEAVIES 75 L / PROPYNE 1 L / S-04 42 L  &
      MASS-FLOW=14.5 <tons/hr>
   P-SPEC 1 5.5 <atm>
   COL-SPECS QN=1247.3 <kW> MASS-D=0.45799 <tons/hr>
   SPEC 1 MOLE-RECOV 0.7 COMPS=PROPYNE STREAMS=PROPYNE  &
      SPEC-DESCRIP="Mole recovery, 0.7"
   SPEC 2 MOLE-RECOV 0.7 COMPS=ISOPENT STREAMS=HEAVIES  &
      SPEC-DESCRIP="Mole recovery, 0.7"
   VARY 1 MASS-D 0. 900.
   VARY 2 QN 0.8 20.
   REPORT NOHYDRAULIC TARGET HYDANAL
   INTERNALS CS-1 STAGE1=2 STAGE2=74 P-UPDATE=NO  &
      TRAY-SPACE=0.8096
   TRAY-SIZE 1 2 74 SIEVE
   UTILITIES COND-UTIL=CHILL-W REB-UTIL=HPS

BLOCK RX-01 RPLUG
   PARAM TYPE=T-SPEC NTUBE=135 LENGTH=21. <ft> DIAM=2.067 <in>  &
      INT-TOL=1E-06
   T-SPEC 0.0 250.
   COOLANT TOL=0.001
   REACTIONS RXN-IDS=R-1
```

```
BLOCK CMP-01 COMPR
    PARAM TYPE=ISENTROPIC PRES=5.5 <atm> SEFF=0.72 MEFF=0.9  &
        SB-MAXIT=30 SB-TOL=0.0001
    UTILITY UTILITY-ID=ELECTR

BLOCK CMP-02 COMPR
    PARAM TYPE=ISENTROPIC PRES=5.5 <atm> SEFF=0.72 MEFF=0.9  &
        SB-MAXIT=30 SB-TOL=0.0001
    UTILITY UTILITY-ID=ELECTR

UTILITY CHILL-W GENERAL
    DESCRIPTION "Cooling Water, Inlet Temp=20 C, Outlet Temp=25 C"
    COST ENERGY-PRICE=0.4 <$/GJ>
    PARAM UTILITY-TYPE=WATER PRES=1. <atm> PRES-OUT=1. <atm>  &
        TIN=3. TOUT=8. CALOPT=FLASH MIN-TAPP=10.  &
        HTC=0.0135 <GJ/hr-sqm-C>

UTILITY CW GENERAL
    DESCRIPTION "Cooling Water, Inlet Temp=20 C, Outlet Temp=25 C"
    COST ENERGY-PRICE=0.3609 <$/GJ>
    PARAM UTILITY-TYPE=WATER PRES=1. <atm> PRES-OUT=1. <atm>  &
        TIN=15. TOUT=25. CALOPT=FLASH MIN-TAPP=10.  &
        HTC=0.0135 <GJ/hr-sqm-C>

UTILITY ELECTR GENERAL
    DESCRIPTION "Electrical Utility"
    COST ELEC-PRICE=0.06117 <$/kWhr>
    PARAM UTILITY-TYPE=ELECTRICITY CALCCO2=YES FACTORSOURCE= &
        "US-EPA-Rule-E9-5711" FUELSOURCE="Coal-electric_power"  &
        CO2FACTOR=4.16544732E-7 EFFICIENCY=0.58

UTILITY HPS GENERAL
    DESCRIPTION  &
        "High Pressure Steam, Inlet Temp=250 C, Outlet Temp=249 C, Pres=572 psia"
    COST ENERGY-PRICE=18.05 <$/GJ>
    PARAM UTILITY-TYPE=STEAM PRES=41. TIN=254. TOUT=244.  &
        VFR-OUT=0. CALOPT=FLASH MIN-TAPP=10. CALCCO2=YES  &
        FACTORSOURCE="US-EPA-Rule-E9-5711" FUELSOURCE= &
        "Coal-commercial" CO2FACTOR=4.20438456E-7 EFFICIENCY=0.85  &
        HTC=0.0216 <GJ/hr-sqm-C>

UTILITY LPS GENERAL
    DESCRIPTION  &
        "Low Pressure Steam, Inlet Temp=125 C, Outlet Temp=124 C"
```

```
    COST ENERGY-PRICE=14.32 <$/GJ>
    PARAM UTILITY-TYPE=STEAM PRES=5. <barg> TIN=160. TOUT=150.  &
        VFR-OUT=0. CALOPT=FLASH MIN-TAPP=10. CALCCO2=YES  &
        FACTORSOURCE="US-EPA-Rule-E9-5711" FUELSOURCE= &
        "Coal-commercial" CO2FACTOR=4.20438456E-7 EFFICIENCY=0.85  &
        HTC=0.0216 <GJ/hr-sqm-C>

EO-CONV-OPTI

CALCULATOR AIRFLOW
    DEFINE AIRFLOW STREAM-VAR STREAM=AIR SUBSTREAM=MIXED  &
        VARIABLE=MOLE-FLOW UOM="kmol/hr"
    DEFINE TRN2BF MOLE-FLOW STREAM=R-04 SUBSTREAM=MIXED  &
        COMPONENT=TRANS-2B UOM="kmol/hr"
F     AIRFLOW = (1.5*TRN2BF)/0.21
    READ-VARS TRN2BF
    WRITE-VARS AIRFLOW

SENSITIVITY NTUBES
    DEFINE X1BF MOLE-FLOW STREAM=R-04 SUBSTREAM=MIXED  &
        COMPONENT=1-BUTENE UOM="kmol/hr"
    DEFINE X1BP MOLE-FLOW STREAM=R-05 SUBSTREAM=MIXED  &
        COMPONENT=1-BUTENE UOM="kmol/hr"
F     X1BUTENE = (X1BF - X1BP)/X1BF
    TABULATE 1 "X1BF"
    TABULATE 2 "X1BP"
    TABULATE 3 "X1BUTENE"
    VARY BLOCK-VAR BLOCK=RX-01 VARIABLE=NTUBE SENTENCE=PARAM
    RANGE OPT-LIST=RANGE LOWER="50" UPPER="70" INCR="1"

CONV-OPTIONS
    PARAM TEAR-METHOD=BROYDEN TOL=0.001
    WEGSTEIN MAXIT=30

TEAR
    TEAR D-01 0.035 / A-02 0.01 / R-02 0.2

STREAM-REPOR MOLEFLOW

PROPERTY-REP PCES

REACTIONS R-1 GENERAL
    REAC-DATA 1 NAME=M1 PHASE=V CBASIS=PARTIALPRES RATE-UNITV= &
        "KMOL/CUM-HR" PRES-UNIT="ATM"
```

```
REAC-DATA 2 NAME=M2 PHASE=V CBASIS=PARTIALPRES RATE-UNITV= &
   "KMOL/CUM-HR" PRES-UNIT="ATM"
REAC-DATA 3 NAME=S1 PHASE=V CBASIS=PARTIALPRES RATE-UNITV= &
   "KMOL/CUM-HR" PRES-UNIT="ATM"
REAC-DATA 4 NAME=S2 PHASE=V CBASIS=PARTIALPRES RATE-UNITV= &
   "KMOL/CUM-HR" PRES-UNIT="ATM"
REAC-DATA 5 NAME=S3 PHASE=V CBASIS=PARTIALPRES RATE-UNITV= &
   "KMOL/CUM-HR" PRES-UNIT="ATM"
REAC-DATA 6 NAME=S4 PHASE=V CBASIS=PARTIALPRES RATE-UNITV= &
   "KMOL/CUM-HR" PRES-UNIT="ATM"
RATE-CON 1 PRE-EXP=7486.27 ACT-ENERGY=9.2 T-REF=625. <K>
RATE-CON 2 PRE-EXP=696.2 ACT-ENERGY=17.4 T-REF=625. <K>
RATE-CON 3 PRE-EXP=1169.73 ACT-ENERGY=9.2 T-REF=625. <K>
RATE-CON 4 PRE-EXP=701.84 ACT-ENERGY=9.2 T-REF=625. <K>
RATE-CON 5 PRE-EXP=348.1 ACT-ENERGY=17.4 T-REF=625. <K>
RATE-CON 6 PRE-EXP=348.1 ACT-ENERGY=17.4 T-REF=625. <K>
STOIC 1 MIXED 1-BUTENE -1. / 1,3-BD 1. / H2 1.
STOIC 2 MIXED TRANS-2B -1. / 1,3-BD 1. / H2 1.
STOIC 3 MIXED 1-BUTENE -1. / CIS-2B 1.
STOIC 4 MIXED 1-BUTENE -1. / TRANS-2B 1.
STOIC 5 MIXED TRANS-2B -1. / CIS-2B 1.
STOIC 6 MIXED TRANS-2B -1. / 1-BUTENE 1.
DFORCE-EXP 1 MIXED 1-BUTENE 0.8
DFORCE-EXP 2 MIXED TRANS-2B 0.9
DFORCE-EXP 3 MIXED 1-BUTENE 0.8
DFORCE-EXP 4 MIXED 1-BUTENE 0.8
DFORCE-EXP 5 MIXED TRANS-2B 0.9
DFORCE-EXP 6 MIXED TRANS-2B 0.9

DISABLE
   SENSITIVITY NTUBES
;
```

A-6: Aspen Plus Simulation Report

```
+ + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
+ + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
+ +                                                  + +
+ +              ASPEN PLUS CALCULATION REPORT              + +
+ +                                                  + +
+ + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
+ + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
```

ASPEN PLUS IS A TRADEMARK OF HOTLINE:
ASPEN TECHNOLOGY, INC. U.S.A. 888/996-7100
781/221-6400 EUROPE (44) 1189-226555

PLATFORM: WIN-X64 APRIL 20, 2020
VERSION: 37.0 Build 395 MONDAY
INSTALLATION: 5:22:00 P.M.

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RUN CONTROL SECTION

RUN CONTROL INFORMATION

THIS COPY OF ASPEN PLUS LICENSED TO UNIV OF NEBRASKA

TYPE OF RUN: NEW

INPUT FILE NAME: _4646lgy.inm

OUTPUT PROBLEM DATA FILE NAME: _4646lgy
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:\Program Files\AspenTech\Aspen Plus V11.0\Engine\\xeq

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

DESCRIPTION

Chemical Simulation with Metric Units : C, bar, kg/hr, kmol/hr,
Gcal/hr, cum/hr. Property Method: NRTL Flow basis for input: Mole
Stream report composition: Mole flow

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FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
FEED	----	HT-01	DMF	----	MX-01
AIR	----	HT-03	S-01	HT-01	CMP-01
S-02	CMP-01	HT-02	S-03	HT-02	COL-01
PROPYNE	COL-01	HT-09	HEAVIES	COL-01	HT-08

S-04	COL-01	MX-01	S-05	MX-01	SEP-01
R-01	SEP-01	SEP-03	S-06	SEP-01	SEP-02
1,3-BD	SEP-02	HT-06	D-01	SEP-02	SEP-01
R-02	SEP-03	MX-02	ISOBUTYL	SEP-03	HT-07
R-03	MX-02	HT-04	R-04	HT-04	RX-01
R-05	RX-01	CMP-02	R-06	CMP-02	HT-05
A-02	HT-03	MX-02	R-07	HT-05	SEP-04
H2+AIR	SEP-04	----	R-08	SEP-04	MX-01
1,3-BD-C	HT-06	----	ISOBUT-C	HT-07	----
HEAVY-C	HT-08	----	PROPY-C	HT-09	----

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
HT-01	FEED	S-01
CMP-01	S-01	S-02
HT-02	S-02	S-03
COL-01	S-03	PROPYNE HEAVIES S-04
MX-01	S-04 DMF R-08	S-05
SEP-01	S-05 D-01	R-01 S-06
SEP-02	S-06	1,3-BD D-01
SEP-03	R-01	R-02 ISOBUTYL
MX-02	R-02 A-02	R-03
HT-04	R-03	R-04
RX-01	R-04	R-05
CMP-02	R-05	R-06
HT-03	AIR	A-02
HT-05	R-06	R-07
SEP-04	R-07	H2+AIR R-08
HT-06	1,3-BD	1,3-BD-C
HT-07	ISOBUTYL	ISOBUT-C
HT-08	HEAVIES	HEAVY-C
HT-09	PROPYNE	PROPY-C

CONVERGENCE STATUS SUMMARY

TEAR STREAM SUMMARY
==================

STREAM ID	VARIABLE ID	MAXIMUM ERR/TOL	MAX. ERR. RELATIVE	ABSOLUTE ERROR	CONV STAT	BLOCK

```
  ------   --------       --------    -------     ---------   ----  -----
  D-01     PROPYNE MOLEFLOW  0.95332      0.33366E-01  0.19813E-03  #    $OLVER01
  R-02     MASS ENTHALPY     0.26927      0.53853E-01  0.27300E-03  #    $OLVER01
  A-02     AIR MOLEFLOW      0.72976     -0.72976E-02  0.92646E-03  #    $OLVER01
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                        FLOWSHEET SECTION

 CONVERGENCE STATUS SUMMARY (CONTINUED)

  #  = CONVERGED
  *  = NOT CONVERGED

 CALCULATOR BLOCK:   AIRFLOW
 ---------------------------

  SAMPLED VARIABLES:
   AIRFLOW  : TOTAL MOLEFLOW IN STREAM AIR SUBSTREAM MIXED
   TRN2BF   : TRANS-2BMOLEFLOW IN STREAM R-04 SUBSTREAM MIXED

  FORTRAN STATEMENTS:
      AIRFLOW = (1.5*TRN2BF)/0.21

  READ VARIABLES:  TRN2BF

  WRITE VARIABLES: AIRFLOW

  VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:
   VARIABLE       VALUE READ      VALUE WRITTEN    UNITS
   --------       ----------      -------------    -----
   AIRFLOW         306.446         453.702        KMOL/HR
   TRN2BF          63.5183                        KMOL/HR

 CONVERGENCE BLOCK:  $OLVER01
 ----------------------------
   Tear Stream  :  D-01       R-02       A-02
   Tolerance used:  0.350D-01  0.350D-01  0.350D-01
   Trace molefrac:  0.350D-03  0.200D-02  0.100D-03

   MAXIT =   30 WAIT =   2
   METHOD: BROYDEN       STATUS: CONVERGED
   TOTAL NUMBER OF ITERATIONS:     8

                     *** FINAL VALUES ***
```

VAR# TEAR STREAM VAR STREAM SUBSTREA COMPONEN UNIT VALUE
PREV VALUE ERR/TOL
---- ---------------- ------ -------- -------- ---- ----- ---------- -------
1 TOTAL MOLEFLOW D-01 MIXED KMOL/HR 542.4967 524.9987
0.9523
2 TOTAL MOLEFLOW R-02 MIXED KMOL/HR 520.0881 505.0950
0.1484
3 TOTAL MOLEFLOW A-02 MIXED KMOL/HR 453.7021 457.0373 -
0.7298
4 MOLE-FLOW D-01 MIXED 1,3-BD KMOL/HR 0.0 0.0 0.0
5 MOLE-FLOW D-01 MIXED ISOBUTYL KMOL/HR 0.5731 0.5731 -
6.1587-05
6 MOLE-FLOW D-01 MIXED 1-BUTENE KMOL/HR 0.0 0.0 0.0
7 MOLE-FLOW D-01 MIXED N-BUTANE KMOL/HR 0.0 0.0 0.0
8 MOLE-FLOW D-01 MIXED ISOBUTAN KMOL/HR 0.0 0.0 0.0
9 MOLE-FLOW D-01 MIXED CIS-2B KMOL/HR 0.0 0.0 0.0
10 MOLE-FLOW D-01 MIXED TRANS-2B KMOL/HR 0.0 0.0 0.0
11 MOLE-FLOW D-01 MIXED BUTENYNE KMOL/HR 38.0349 36.8068
0.9533
12 MOLE-FLOW D-01 MIXED 1-BUTYNE KMOL/HR 8.4718 8.1982
0.9533
13 MOLE-FLOW D-01 MIXED PROPANE KMOL/HR 0.0 0.0 0.0
14 MOLE-FLOW D-01 MIXED ALLENE KMOL/HR 6.9852-03 6.7597-03
0.9533
15 MOLE-FLOW D-01 MIXED PROPYNE KMOL/HR 22.0898 21.3766
0.9533
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FLOWSHEET SECTION

CONVERGENCE BLOCK: $OLVER01 (CONTINUED)
16 MOLE-FLOW D-01 MIXED ISOPENT KMOL/HR 8.7614 8.4785
0.9533
17 MOLE-FLOW D-01 MIXED DMF KMOL/HR 464.5587 449.5587
0.9533
18 MOLE-FLOW D-01 MIXED H2 KMOL/HR 0.0 0.0 0.0
19 MOLE-FLOW D-01 MIXED AIR KMOL/HR 0.0 0.0 0.0
20 MOLE-FLOW D-01 MIXED WATER KMOL/HR 0.0 0.0 0.0
21 PRESSURE D-01 MIXED BAR 5.5729 5.5729 0.0
22 MASS ENTHALPY D-01 MIXED KCAL/KG -592.8299 -594.5743 8.3823-
02
23 MOLE-FLOW R-02 MIXED 1,3-BD KMOL/HR 0.8541 0.8594 -3.0827-02

24 MOLE-FLOW R-02 MIXED ISOBUTYL KMOL/HR 0.0 0.0 0.0
25 MOLE-FLOW R-02 MIXED 1-BUTENE KMOL/HR 30.1867 30.1845
3.6160-04
26 MOLE-FLOW R-02 MIXED N-BUTANE KMOL/HR 0.0 0.0 0.0
27 MOLE-FLOW R-02 MIXED ISOBUTAN KMOL/HR 0.0 0.0 0.0
28 MOLE-FLOW R-02 MIXED CIS-2B KMOL/HR 424.7669 410.5328
0.1734
29 MOLE-FLOW R-02 MIXED TRANS-2B KMOL/HR 64.2804 63.5183
5.9989-02
30 MOLE-FLOW R-02 MIXED BUTENYNE KMOL/HR 0.0 0.0 0.0
31 MOLE-FLOW R-02 MIXED 1-BUTYNE KMOL/HR 0.0 0.0 0.0
32 MOLE-FLOW R-02 MIXED PROPANE KMOL/HR 0.0 0.0 0.0
33 MOLE-FLOW R-02 MIXED ALLENE KMOL/HR 0.0 0.0 0.0
34 MOLE-FLOW R-02 MIXED PROPYNE KMOL/HR 0.0 0.0 0.0
35 MOLE-FLOW R-02 MIXED ISOPENT KMOL/HR 0.0 0.0 0.0
36 MOLE-FLOW R-02 MIXED DMF KMOL/HR 0.0 0.0 0.0
37 MOLE-FLOW R-02 MIXED H2 KMOL/HR 0.0 0.0 0.0
38 MOLE-FLOW R-02 MIXED AIR KMOL/HR 0.0 0.0 0.0
39 MOLE-FLOW R-02 MIXED WATER KMOL/HR 0.0 0.0 0.0
40 PRESSURE R-02 MIXED BAR 5.5729 5.5729 0.0
41 MASS ENTHALPY R-02 MIXED KCAL/KG -114.5588 -121.0793
0.2693
42 MOLE-FLOW A-02 MIXED 1,3-BD KMOL/HR 0.0 0.0 0.0
43 MOLE-FLOW A-02 MIXED ISOBUTYL KMOL/HR 0.0 0.0 0.0
44 MOLE-FLOW A-02 MIXED 1-BUTENE KMOL/HR 0.0 0.0 0.0
45 MOLE-FLOW A-02 MIXED N-BUTANE KMOL/HR 0.0 0.0 0.0
46 MOLE-FLOW A-02 MIXED ISOBUTAN KMOL/HR 0.0 0.0 0.0
47 MOLE-FLOW A-02 MIXED CIS-2B KMOL/HR 0.0 0.0 0.0
48 MOLE-FLOW A-02 MIXED TRANS-2B KMOL/HR 0.0 0.0 0.0
49 MOLE-FLOW A-02 MIXED BUTENYNE KMOL/HR 0.0 0.0 0.0
50 MOLE-FLOW A-02 MIXED 1-BUTYNE KMOL/HR 0.0 0.0 0.0
51 MOLE-FLOW A-02 MIXED PROPANE KMOL/HR 0.0 0.0 0.0
52 MOLE-FLOW A-02 MIXED ALLENE KMOL/HR 0.0 0.0 0.0
53 MOLE-FLOW A-02 MIXED PROPYNE KMOL/HR 0.0 0.0 0.0
54 MOLE-FLOW A-02 MIXED ISOPENT KMOL/HR 0.0 0.0 0.0
55 MOLE-FLOW A-02 MIXED DMF KMOL/HR 0.0 0.0 0.0
56 MOLE-FLOW A-02 MIXED H2 KMOL/HR 0.0 0.0 0.0
57 MOLE-FLOW A-02 MIXED AIR KMOL/HR 453.7021 457.0373 -0.7298
58 MOLE-FLOW A-02 MIXED WATER KMOL/HR 0.0 0.0 0.0
59 PRESSURE A-02 MIXED BAR 1.0133 1.0133 0.0
60 MASS ENTHALPY A-02 MIXED KCAL/KG 42.1315 42.1315 0.0

*** ITERATION HISTORY ***
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FLOWSHEET SECTION

CONVERGENCE BLOCK: $OLVER01 (CONTINUED)

TEAR STREAMS AND TEAR VARIABLES:

ITERATION	MAX-ERR/TOL	VAR#	STREAM ID	VAR DESCRIPTION	SUBSTREA	COMPONEN	ATTRIBUT	ELEMENT
1	0.1000E+07	21	D-01	PRESSURE	MIXED			
2	0.6070E+05	60	A-02	MASS ENT	MIXED			
3	14.29	15	D-01	MOLE-FLO	MIXED	PROPYNE		
4	28.25	3	A-02	TOTAL MO	MIXED			
5	4.489	12	D-01	MOLE-FLO	MIXED	1-BUTYNE		
6	2.716	15	D-01	MOLE-FLO	MIXED	PROPYNE		
7	1.608	17	D-01	MOLE-FLO	MIXED	DMF		
8	0.9533	15	D-01	MOLE-FLO	MIXED	PROPYNE		

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:
LPS HPS CHILL-W ELECTR CW HT-01 CMP-01 HT-02 *COL-01 HT-09 HT-08
$OLVER01 MX-02 *HT-04 RX-01 CMP-02 HT-05 SEP-04 MX-01 SEP-01 *SEP-03
| *SEP-02 AIRFLOW *HT-03
(RETURN $OLVER01)
HT-07 HT-06

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
CONVENTIONAL COMPONENTS				
(KMOL/HR)				
1,3-BD	108.175	141.610	33.4304	-0.373664E-04
ISOBUTYL	56.7521	56.7521	0.00000	0.448382E-07
1-BUTENE	30.0738	0.786133E-02	-30.0637	0.726528E-04
N-BUTANE	10.5353	10.5353	0.00000	0.157212E-07
ISOBUTAN	11.7059	11.7059	0.00000	0.671793E-07
CIS-2B	9.94374	3.23611	7.52648	1.43146
TRANS-2B	12.8541	1.19889	-10.8931	0.592867E-01
BUTENYNE	1.82915	0.601055	0.00000	0.671402

1-BUTYNE	0.503138	0.229595	0.00000	0.543673
PROPANE	0.00000	0.00000	0.00000	0.00000
ALLENE	0.679289	0.679063	0.00000	0.332061E-03
PROPYNE	2.37751	1.66426	0.00000	0.300000
ISOPENT	0.943016	0.660123	0.00000	0.299988
DMF	15.0000	0.00000	0.00000	1.00000
H2	0.00000	33.4304	33.4304	0.00000
AIR	453.702	457.037	0.00000	-0.729756E-02
WATER	0.00000	0.00000	0.00000	0.00000
TOTAL BALANCE				
MOLE(KMOL/HR)	715.074	719.348	33.4304	0.405309E-01
MASS(KG/HR)	27839.3	25870.4		0.707218E-01
ENTHALPY(GCAL/HR)	1.97357	1.81546		0.801155E-01

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FLOWSHEET SECTION

OVERALL FLOWSHEET BALANCE (CONTINUED)

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	KG/HR
PRODUCT STREAMS CO2E	0.00000	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	7586.96	KG/HR
TOTAL CO2E PRODUCTION	7586.96	KG/HR

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PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME
1,3-BD	C	C4H6-4	1,3-BUTADIENE
ISOBUTYL	C	C4H8-5	ISOBUTYLENE
1-BUTENE	C	C4H8-1	1-BUTENE
N-BUTANE	C	C4H10-1	N-BUTANE
ISOBUTAN	C	C4H10-2	ISOBUTANE
CIS-2B	C	C4H8-2	CIS-2-BUTENE
TRANS-2B	C	C4H8-3	TRANS-2-BUTENE
BUTENYNE	C	C4H4	VINYLACETYLENE
1-BUTYNE	C	C4H6-1	1-BUTYNE
PROPANE	C	C3H8	PROPANE
ALLENE	C	C3H4-1	PROPADIENE

PROPYNE C C3H4-2 METHYL-ACETYLENE
ISOPENT C C5H12-2 2-METHYL-BUTANE
DMF C C3H7NO N,N-DIMETHYLFORMAMIDE
H2 C H2 HYDROGEN
AIR C AIR AIR
WATER C H2O WATER

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REACTION SECTION

REACTION: R-1 TYPE: GENERAL

Unit operations referencing this reaction model:

Reactor Name: RX-01 Block Type: RPLUG

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U-O-S BLOCK SECTION

BLOCK: CMP-01 MODEL: COMPR

INLET STREAM: S-01
OUTLET STREAM: S-02
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	246.372	246.372	0.00000
MASS(KG/HR)	13607.8	13607.8	0.00000
ENTHALPY(GCAL/HR)	2.24210	2.63690	-0.149721

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	KG/HR
PRODUCT STREAMS CO2E	0.00000	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	315.041	KG/HR
TOTAL CO2E PRODUCTION	315.041	KG/HR

*** INPUT DATA ***

ISENTROPIC CENTRIFUGAL COMPRESSOR
OUTLET PRESSURE BAR 5.57288

ISENTROPIC EFFICIENCY 0.72000
MECHANICAL EFFICIENCY 0.90000

U-O-S BLOCK SECTION

BLOCK: CMP-01 MODEL: COMPR (CONTINUED)

*** RESULTS ***

INDICATED HORSEPOWER REQUIREMENT KW 459.152
BRAKE HORSEPOWER REQUIREMENT KW 510.169
NET WORK REQUIRED KW 510.169
POWER LOSSES KW 51.0169
ISENTROPIC HORSEPOWER REQUIREMENT KW 330.589
CALCULATED OUTLET TEMP C 127.274
ISENTROPIC TEMPERATURE C 109.924
EFFICIENCY (POLYTR/ISENTR) USED 0.72000
OUTLET VAPOR FRACTION 1.00000
HEAD DEVELOPED, METER 8,918.33
MECHANICAL EFFICIENCY USED 0.90000
INLET HEAT CAPACITY RATIO 1.10759
INLET VOLUMETRIC FLOW RATE , CUM/HR 6,505.48
OUTLET VOLUMETRIC FLOW RATE, CUM/HR 1,380.76
INLET COMPRESSIBILITY FACTOR 0.98063
OUTLET COMPRESSIBILITY FACTOR 0.93812
AV. ISENT. VOL. EXPONENT 1.06275
AV. ISENT. TEMP EXPONENT 1.09984
AV. ACTUAL VOL. EXPONENT 1.09983
AV. ACTUAL TEMP EXPONENT 1.13220

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY ELECTR
RATE OF CONSUMPTION 510.1686 KW
COST 31.2070 $/HR
CO2 EQUIVALENT EMISSIONS 315.0414 KG/HR

BLOCK: CMP-02 MODEL: COMPR

INLET STREAM: R-05
OUTLET STREAM: R-06
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

```
               ***  MASS AND ENERGY BALANCE  ***
                        IN            OUT       RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(KMOL/HR )          995.563        995.563        0.00000
     MASS(KG/HR   )          41569.5        41569.5        0.350062E-15
     ENTHALPY(GCAL/HR )       3.63682        6.30364       -0.423060

               ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             0.00000      KG/HR
   PRODUCT STREAMS CO2E          0.00000      KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
   UTILITIES CO2E PRODUCTION     2128.07      KG/HR
   TOTAL CO2E PRODUCTION         2128.07      KG/HR
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                    U-O-S BLOCK SECTION

 BLOCK:  CMP-02   MODEL: COMPR (CONTINUED)

                  ***  INPUT DATA  ***

  ISENTROPIC CENTRIFUGAL COMPRESSOR
   OUTLET PRESSURE  BAR                           5.57288
   ISENTROPIC EFFICIENCY                          0.72000
   MECHANICAL EFFICIENCY                          0.90000

                  ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  KW             3,101.51
   BRAKE      HORSEPOWER REQUIREMENT  KW             3,446.12
   NET WORK REQUIRED                  KW             3,446.12
   POWER LOSSES                       KW             344.612
   ISENTROPIC HORSEPOWER REQUIREMENT  KW             2,233.09
   CALCULATED OUTLET TEMP  C                         381.209
   ISENTROPIC TEMPERATURE  C                         346.509
   EFFICIENCY (POLYTR/ISENTR) USED                   0.72000
   OUTLET VAPOR FRACTION                             1.00000
   HEAD DEVELOPED,       METER                       19,720.3
   MECHANICAL EFFICIENCY USED                        0.90000
   INLET HEAT CAPACITY RATIO                         1.11730
   INLET VOLUMETRIC FLOW RATE , CUM/HR               42,682.8
   OUTLET VOLUMETRIC FLOW RATE, CUM/HR               9,703.53
   INLET  COMPRESSIBILITY FACTOR                     0.99873
   OUTLET COMPRESSIBILITY FACTOR                     0.99838
```

AV. ISENT. VOL. EXPONENT 1.10931
AV. ISENT. TEMP EXPONENT 1.11026
AV. ACTUAL VOL. EXPONENT 1.15084
AV. ACTUAL TEMP EXPONENT 1.15111

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY ELECTR
RATE OF CONSUMPTION 3446.1246 KW
COST 210.7994 $/HR
CO2 EQUIVALENT EMISSIONS 2128.0651 KG/HR

BLOCK: COL-01 MODEL: RADFRAC

INLETS - S-03 STAGE 26
OUTLETS - PROPYNE STAGE 1
HEAVIES STAGE 75
S-04 STAGE 42
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE
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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

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

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	246.372	246.372	-0.230722E-15
MASS(KG/HR)	13607.8	13607.8	-0.248551E-08
ENTHALPY(GCAL/HR)	1.02510	1.02865	-0.345385E-02

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E 0.00000 KG/HR
PRODUCT STREAMS CO2E 0.00000 KG/HR
NET STREAMS CO2E PRODUCTION 0.00000 KG/HR

UTILITIES CO2E PRODUCTION 2093.43 KG/HR
TOTAL CO2E PRODUCTION 2093.43 KG/HR

****
**** INPUT DATA ****
****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	75
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	BROYDEN
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	50
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.00100000

U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST		0.0
REBOILER DUTY	GCAL/HR	1.07248
MASS DISTILLATE RATE	KG/HR	415.482

**** PROFILES ****

P-SPEC STAGE 1 PRES, BAR 5.57288

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

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS		

	PROPYNE	HEAVIES	S-04
COMPONENT:			
1,3-BD	.19656E-08	.10877E-02	.99891
ISOBUTYL	.34154E-07	.22205E-03	.99978
1-BUTENE	.28522E-07	.26137E-03	.99974
N-BUTANE	.32468E-09	.19597E-01	.98040
ISOBUTAN	.11280E-04	.38370E-05	.99998
CIS-2B	.28525E-11	.32544	.67456
TRANS-2B	.30630E-10	.93269E-01	.90673
BUTENYNE	.22952E-11	.32860	.67140
1-BUTYNE	.74839E-13	.45633	.54367
ALLENE	.99967	0.0000	.33203E-03
PROPYNE	.70000	.11272E-11	.30000
ISOPENT	0.0000	.70001	.29999

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	C	20.3663
BOTTOM STAGE TEMPERATURE	C	59.9706
TOP STAGE LIQUID FLOW	KMOL/HR	943.416
BOTTOM STAGE LIQUID FLOW	KMOL/HR	6.27040
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOILUP VAPOR FLOW	KMOL/HR	878.518
MOLAR REFLUX RATIO		402.575
MOLAR BOILUP RATIO		140.106
CONDENSER DUTY (W/O SUBCOOL)	GCAL/HR	-4.22873
REBOILER DUTY	GCAL/HR	4.23229

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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

**** MANIPULATED VARIABLES ****

		BOUNDS		CALCULATED
		LOWER	UPPER	VALUE
MASS DISTILLATE RATE	KG/HR	0.0000	900.00	93.892

REBOILER DUTY GCAL/HR 0.80000 20.000 4.2323

**** DESIGN SPECIFICATIONS ****

NO	SPEC-TYPE	QUALIFIERS	UNIT	SPECIFIED VALUE	CALCULATED VALUE
1	MOLE-RECOV	STREAMS: PROPYNE COMPS: PROPYNE		0.70000	0.70000
2	MOLE-RECOV	STREAMS: HEAVIES COMPS: ISOPENT		0.70000	0.70001

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

DEW POINT 0.42397E-04 STAGE= 19
BUBBLE POINT 0.69047E-04 STAGE= 21
COMPONENT MASS BALANCE 0.72498E-05 STAGE= 26 COMP=ISOPENT
ENERGY BALANCE 0.11344E-03 STAGE= 75

**** PROFILES ****

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

STAGE	TEMPERATURE C	PRESSURE BAR	ENTHALPY KCAL/MOL LIQUID	ENTHALPY KCAL/MOL VAPOR	HEAT DUTY GCAL/HR
1	20.366	5.5729	39.862	44.408	-4.2287
2	20.994	5.5729	39.764	44.333	
3	21.539	5.5729	39.679	44.266	
25	32.543	5.5729	21.395	31.035	
26	36.231	5.5729	16.297	26.102	
27	37.292	5.5729	14.695	24.349	
37	47.178	5.5729	3.4247	8.1602	
38	47.495	5.5729	3.3665	7.9152	
39	47.750	5.5729	3.4137	7.8404	
41	48.167	5.5729	3.7372	8.0659	
42	48.368	5.5729	3.9771	8.3137	
43	48.588	5.5729	4.2445	8.6215	
74	58.738	5.5729	0.97418E-01	5.7217	
75	59.971	5.5729	-1.6511	4.9265	4.2322

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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

STAGE	FLOW RATE KMOL/HR		FEED RATE KMOL/HR			PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	945.8	0.000		2.3434			
2	937.0	945.8					
3	931.6	939.4					
25	905.2	910.0					
26	1147.	907.5	246.3716				
27	1148.	903.4					
37	1164.	919.7					
38	1165.	920.3					
39	1165.	920.6					
41	1164.	920.3					
42	1163.	919.7		237.7577			
43	924.2	918.9					
74	884.8	882.4					
75	6.270	878.5		6.2704			

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE KG/HR		FEED RATE KG/HR			PRODUCT RATE KG/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.3789E+05	0.000			93.8924		
2	0.3754E+05	0.3789E+05					
3	0.3733E+05	0.3764E+05					
25	0.4282E+05	0.4110E+05					
26	0.5686E+05	0.4291E+05	.13608+05				
27	0.5764E+05	0.4335E+05					
37	0.6414E+05	0.5042E+05					
38	0.6427E+05	0.5063E+05					
39	0.6435E+05	0.5076E+05					
41	0.6437E+05	0.5087E+05					
42	0.6434E+05	0.5086E+05			.13154+05		
43	0.5113E+05	0.5082E+05					
74	0.5007E+05	0.4955E+05					
75	359.7	0.4971E+05			359.6999		

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

STAGE	1,3-BD	ISOBUTYL	1-BUTENE	N-BUTANE	ISOBUTAN

1	0.90732E-07	0.82712E-06	0.36602E-06	0.14596E-08	0.56345E-04
2	0.18346E-06	0.14952E-05	0.66643E-06	0.31703E-08	0.81936E-04
3	0.36396E-06	0.26496E-05	0.11897E-05	0.67421E-08	0.11671E-03
25	0.19000	0.12222	0.64304E-01	0.14945E-01	0.48523E-01
26	0.25736	0.15484	0.81666E-01	0.21834E-01	0.52790E-01
27	0.27382	0.16590	0.87501E-01	0.22922E-01	0.57788E-01
37	0.42043	0.25019	0.13227	0.34202E-01	0.74185E-01
38	0.42765	0.25071	0.13260	0.35362E-01	0.70601E-01
39	0.43453	0.24996	0.13226	0.36753E-01	0.66299E-01
41	0.44796	0.24418	0.12933	0.40660E-01	0.55620E-01
42	0.45448	0.23864	0.12646	0.43443E-01	0.49234E-01
43	0.46054	0.23078	0.12235	0.47002E-01	0.42126E-01

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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

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

STAGE	1,3-BD	ISOBUTYL	1-BUTENE	N-BUTANE	ISOBUTAN
74	0.23743E-01	0.26797E-02	0.16546E-02	0.37468E-01	0.10762E-04
75	0.18765E-01	0.20097E-02	0.12536E-02	0.32926E-01	0.71631E-05

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

STAGE	CIS-2B	TRANS-2B	BUTENYNE	1-BUTYNE	ALLENE
1	0.12104E-10	0.16801E-09	0.17915E-11	0.16068E-13	0.28977
2	0.31491E-10	0.39861E-09	0.46771E-11	0.48528E-13	0.23529
3	0.80317E-10	0.92682E-09	0.12001E-10	0.14378E-12	0.18849
25	0.98752E-02	0.15043E-01	0.18555E-02	0.42589E-03	0.19651E-02
26	0.16922E-01	0.23843E-01	0.31482E-02	0.79516E-03	0.16025E-02
27	0.17513E-01	0.24822E-01	0.32621E-02	0.82136E-03	0.11791E-02
37	0.22880E-01	0.34943E-01	0.42690E-02	0.10446E-02	0.15643E-04
38	0.23354E-01	0.36259E-01	0.43514E-02	0.10564E-02	0.93400E-05
39	0.23986E-01	0.38030E-01	0.44594E-02	0.10700E-02	0.55043E-05
41	0.26211E-01	0.44005E-01	0.48331E-02	0.11130E-02	0.17867E-05
42	0.28212E-01	0.49021E-01	0.51653E-02	0.11505E-02	0.94863E-06
43	0.31255E-01	0.56207E-01	0.56668E-02	0.12079E-02	0.44785E-06
74	0.53200	0.21170	0.97628E-01	0.35862E-01	0.23732E-17
75	0.51609	0.19120	0.95856E-01	0.36616E-01	0.91540E-18

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

STAGE	PROPYNE	ISOPENT
1	0.71017	0.22158E-19
2	0.76463	0.11685E-18

3	0.81139	0.60103E-18
25	0.53054	0.30729E-03
26	0.38412	0.10729E-02
27	0.34338	0.10840E-02
37	0.24396E-01	0.11718E-02
38	0.16868E-01	0.11751E-02
39	0.11471E-01	0.11783E-02
41	0.49130E-02	0.11853E-02
42	0.29999E-02	0.11898E-02
43	0.16587E-02	0.11956E-02
74	0.96405E-12	0.57257E-01
75	0.42740E-12	0.10528

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

STAGE	1,3-BD	ISOBUTYL	1-BUTENE	N-BUTANE	ISOBUTAN
1	0.43968E-07	0.44780E-06	0.19677E-06	0.65692E-09	0.37867E-04
2	0.90732E-07	0.82712E-06	0.36602E-06	0.14596E-08	0.56345E-04
3	0.18322E-06	0.14935E-05	0.66568E-06	0.31661E-08	0.81872E-04
25	0.12725	0.88316E-01	0.46311E-01	0.92811E-02	0.41384E-01
26	0.18951	0.12190	0.64138E-01	0.14906E-01	0.48398E-01
27	0.20714	0.13385	0.70436E-01	0.16070E-01	0.54092E-01
37	0.40442	0.25258	0.13338	0.30537E-01	0.84702E-01
38	0.41437	0.25487	0.13466	0.31823E-01	0.81136E-01
39	0.42351	0.25552	0.13508	0.33291E-01	0.76600E-01
41	0.44074	0.25189	0.13332	0.37234E-01	0.64840E-01
42	0.44919	0.24726	0.13094	0.39993E-01	0.57650E-01
43	0.45746	0.24026	0.12731	0.43515E-01	0.49570E-01
74	0.29345E-01	0.34944E-02	0.21362E-02	0.41600E-01	0.15861E-04

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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

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

STAGE	1,3-BD	ISOBUTYL	1-BUTENE	N-BUTANE	ISOBUTAN
75	0.23779E-01	0.26845E-02	0.16575E-02	0.37500E-01	0.10787E-04

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

STAGE	CIS-2B	TRANS-2B	BUTENYNE	1-BUTYNE	ALLENE
1	0.45552E-11	0.69302E-10	0.67385E-12	0.52143E-14	0.35113
2	0.12104E-10	0.16801E-09	0.17915E-11	0.16068E-13	0.28977
3	0.31442E-10	0.39804E-09	0.46699E-11	0.48447E-13	0.23543
25	0.52051E-02	0.85982E-02	0.98576E-03	0.20341E-03	0.30831E-02

26	0.98497E-02	0.15004E-01	0.18507E-02	0.42480E-03	0.27083E-02
27	0.10486E-01	0.16055E-01	0.19739E-02	0.45301E-03	0.20351E-02
37	0.17639E-01	0.28927E-01	0.33246E-02	0.76019E-03	0.32555E-04
38	0.18142E-01	0.30241E-01	0.34135E-02	0.77490E-03	0.19546E-04
39	0.18744E-01	0.31907E-01	0.35180E-02	0.78984E-03	0.11571E-04
41	0.20677E-01	0.37271E-01	0.38462E-02	0.82955E-03	0.37831E-05
42	0.22354E-01	0.41705E-01	0.41267E-02	0.86127E-03	0.20155E-05
43	0.24883E-01	0.48051E-01	0.45465E-02	0.90850E-03	0.95510E-06
74	0.53395	0.22847	0.96814E-01	0.34106E-01	0.60565E-17
75	0.53211	0.21185	0.97640E-01	0.35857E-01	0.23836E-17

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

STAGE	PROPYNE	ISOPENT
1	0.64883	0.40923E-20
2	0.71017	0.22158E-19
3	0.76449	0.11661E-18
25	0.66930	0.79270E-04
26	0.53100	0.30650E-03
27	0.48710	0.31891E-03
37	0.43238E-01	0.45273E-03
38	0.30089E-01	0.45789E-03
39	0.20565E-01	0.46227E-03
41	0.88781E-02	0.47022E-03
42	0.54410E-02	0.47451E-03
43	0.30204E-02	0.47956E-03
74	0.21322E-11	0.30069E-01
75	0.96788E-12	0.56914E-01

**** K-VALUES ****

STAGE	1,3-BD	ISOBUTYL	1-BUTENE	N-BUTANE	ISOBUTAN
1	0.48460	0.54140	0.53759	0.45006	0.67205
2	0.49458	0.55320	0.54922	0.46041	0.68765
3	0.50343	0.56366	0.55953	0.46960	0.70148
25	0.66960	0.72266	0.72018	0.62063	0.85324
26	0.73623	0.78728	0.78536	0.68241	0.91716
27	0.75632	0.80680	0.80497	0.70076	0.93638
37	0.96192	1.0095	1.0084	0.89286	1.1418
38	0.96895	1.0166	1.0156	0.89993	1.1492
39	0.97462	1.0223	1.0213	0.90581	1.1554
41	0.98389	1.0316	1.0309	0.91575	1.1658
42	0.98835	1.0361	1.0355	0.92059	1.1710
43	0.99328	1.0411	1.0405	0.92582	1.1767
74	1.2367	1.3039	1.2910	1.1102	1.4736
75	1.2679	1.3357	1.3222	1.1389	1.5058

U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

**** K-VALUES ****

STAGE	CIS-2B	TRANS-2B	BUTENYNE	1-BUTYNE	ALLENE
1	0.37636	0.41250	0.37615	0.32454	1.2117
2	0.38438	0.42150	0.38304	0.33113	1.2315
3	0.39149	0.42948	0.38914	0.33698	1.2490
25	0.52691	0.57143	0.53111	0.47726	1.5699
26	0.58183	0.62908	0.58769	0.53384	1.6912
27	0.59856	0.64660	0.60493	0.55115	1.7272
37	0.77096	0.82784	0.77878	0.72772	2.0811
38	0.77679	0.83403	0.78444	0.73355	2.0928
39	0.78145	0.83899	0.78890	0.73816	2.1022
41	0.78887	0.84698	0.79579	0.74532	2.1174
42	0.79234	0.85076	0.79893	0.74860	2.1247
43	0.79614	0.85490	0.80230	0.75214	2.1326
74	1.0036	1.0792	0.99176	0.95103	2.5524
75	1.0310	1.1079	1.0187	0.97928	2.6042

**** K-VALUES ****

STAGE	PROPYNE	ISOPENT
1	0.91364	0.18470
2	0.92880	0.18964
3	0.94221	0.19403
25	1.2616	0.25780
26	1.3825	0.28545
27	1.4187	0.29397
37	1.7724	0.38634
38	1.7838	0.38965
39	1.7928	0.39232
41	1.8071	0.39670
42	1.8137	0.39880
43	1.8209	0.40112
74	2.2120	0.52513
75	2.2648	0.54060

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

STAGE	1,3-BD	ISOBUTYL	1-BUTENE	N-BUTANE	ISOBUTAN
1	0.12249E-06	0.11583E-05	0.51257E-06	0.21175E-08	0.81739E-04
2	0.24768E-06	0.20938E-05	0.93325E-06	0.45991E-08	0.11886E-03

3	0.49136E-06	0.37104E-05	0.16660E-05	0.97805E-08	0.16931E-03
25	0.21726	0.14495	0.76268E-01	0.18362E-01	0.59619E-01
26	0.28093	0.17532	0.92467E-01	0.25610E-01	0.61919E-01
27	0.29509	0.18545	0.97811E-01	0.26544E-01	0.66919E-01
37	0.41284	0.25483	0.13472	0.36087E-01	0.78275E-01
38	0.41916	0.25489	0.13481	0.37243E-01	0.74357E-01
39	0.42539	0.25382	0.13430	0.38662E-01	0.69742E-01
41	0.43803	0.24767	0.13117	0.42722E-01	0.58442E-01
42	0.44434	0.24202	0.12824	0.45639E-01	0.51723E-01
43	0.45027	0.23404	0.12408	0.49378E-01	0.44256E-01
74	0.22696E-01	0.26570E-02	0.16406E-02	0.38485E-01	0.11054E-04
75	0.17694E-01	0.19657E-02	0.12261E-02	0.33361E-01	0.72579E-05

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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

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

STAGE	CIS-2B	TRANS-2B	BUTENYNE	1-BUTYNE	ALLENE
1	0.16950E-10	0.23528E-09	0.23285E-11	0.21693E-13	0.28976
2	0.44098E-10	0.55821E-09	0.60790E-11	0.65515E-13	0.23528
3	0.11247E-09	0.12979E-08	0.15598E-10	0.19410E-12	0.18848
25	0.11712E-01	0.17841E-01	0.20426E-02	0.48698E-03	0.16643E-02
26	0.19160E-01	0.26996E-01	0.33085E-02	0.86798E-03	0.12956E-02
27	0.19577E-01	0.27747E-01	0.33845E-02	0.88516E-03	0.94115E-03
37	0.23304E-01	0.35590E-01	0.40357E-02	0.10257E-02	0.11378E-04
38	0.23744E-01	0.36863E-01	0.41061E-02	0.10354E-02	0.67806E-05
39	0.24356E-01	0.38618E-01	0.42029E-02	0.10475E-02	0.39912E-05
41	0.26585E-01	0.44634E-01	0.45499E-02	0.10884E-02	0.12940E-05
42	0.28611E-01	0.49714E-01	0.48619E-02	0.11248E-02	0.68696E-06
43	0.31696E-01	0.57001E-01	0.53339E-02	0.11809E-02	0.32431E-06
74	0.52748	0.20990	0.89843E-01	0.34280E-01	0.16802E-17
75	0.50478	0.18701	0.87018E-01	0.34527E-01	0.63933E-18

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

STAGE	PROPYNE	ISOPENT
1	0.71015	0.39901E-19
2	0.76460	0.21042E-18
3	0.81135	0.10823E-17
25	0.44932	0.46867E-03
26	0.31057	0.15622E-02
27	0.27409	0.15582E-02
37	0.17743E-01	0.15348E-02

38	0.12246E-01	0.15363E-02
39	0.83174E-02	0.15386E-02
41	0.35583E-02	0.15460E-02
42	0.21724E-02	0.15517E-02
43	0.12012E-02	0.15591E-02
74	0.68255E-12	0.73003E-01
75	0.29850E-12	0.13241

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

STAGE	1,3-BD	ISOBUTYL	1-BUTENE	N-BUTANE	ISOBUTAN
1	0.59360E-07	0.62710E-06	0.27555E-06	0.95300E-09	0.54934E-04
2	0.12249E-06	0.11583E-05	0.51257E-06	0.21175E-08	0.81739E-04
3	0.24736E-06	0.20914E-05	0.93220E-06	0.45929E-08	0.11877E-03
25	0.15241	0.10972	0.57534E-01	0.11944E-01	0.53260E-01
26	0.21678	0.14464	0.76101E-01	0.18322E-01	0.59488E-01
27	0.23352	0.15652	0.82367E-01	0.19467E-01	0.65526E-01
37	0.39903	0.25850	0.13651	0.32376E-01	0.89802E-01
38	0.40746	0.25996	0.13735	0.33625E-01	0.85730E-01
39	0.41548	0.26002	0.13746	0.35094E-01	0.80749E-01
41	0.43132	0.25570	0.13533	0.39154E-01	0.68185E-01
42	0.43937	0.25087	0.13285	0.42034E-01	0.60593E-01
43	0.44736	0.24371	0.12914	0.45726E-01	0.52089E-01
74	0.28267E-01	0.34914E-02	0.21343E-02	0.43058E-01	0.16417E-04
75	0.22732E-01	0.26620E-02	0.16436E-02	0.38522E-01	0.11081E-04

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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

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

STAGE	CIS-2B	TRANS-2B	BUTENYNE	1-BUTYNE	ALLENE
1	0.63791E-11	0.97050E-10	0.87585E-12	0.70397E-14	0.35112
2	0.16950E-10	0.23528E-09	0.23285E-11	0.21693E-13	0.28976
3	0.44031E-10	0.55740E-09	0.60697E-11	0.65406E-13	0.23542
25	0.64665E-02	0.10682E-01	0.11366E-02	0.24363E-03	0.27351E-02
26	0.11687E-01	0.17802E-01	0.20381E-02	0.48592E-03	0.22946E-02
27	0.12263E-01	0.18774E-01	0.21424E-02	0.51071E-03	0.16993E-02
37	0.18053E-01	0.29605E-01	0.31580E-02	0.75005E-03	0.23791E-04
38	0.18504E-01	0.30845E-01	0.32314E-02	0.76198E-03	0.14236E-04
39	0.19074E-01	0.32469E-01	0.33227E-02	0.77487E-03	0.84079E-05
41	0.20989E-01	0.37834E-01	0.36237E-02	0.81182E-03	0.27422E-05
42	0.22680E-01	0.42314E-01	0.38860E-02	0.84244E-03	0.14602E-05
43	0.25241E-01	0.48742E-01	0.42804E-02	0.88845E-03	0.69182E-06

74	0.53349	0.22828	0.89780E-01	0.32852E-01	0.43211E-17
75	0.52764	0.21007	0.89864E-01	0.34278E-01	0.16878E-17

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

STAGE	PROPYNE	ISOPENT
1	0.64882	0.73695E-20
2	0.71015	0.39901E-19
3	0.76446	0.20999E-18
25	0.59375	0.12664E-03
26	0.44990	0.46765E-03
27	0.40673	0.47955E-03
37	0.31598E-01	0.59582E-03
38	0.21915E-01	0.60057E-03
39	0.14943E-01	0.60492E-03
41	0.64354E-02	0.61380E-03
42	0.39419E-02	0.61909E-03
43	0.21878E-02	0.62555E-03
74	0.15213E-11	0.38634E-01
75	0.68533E-12	0.72573E-01

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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

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

*** THERMAL ANALYSIS ***

STAGE	TEMPERATURE	PRESSURE	ENTHALPY DEFICIT	EXERGY LOSS	CARNOT FACTOR
	C	BAR	GCAL/HR	GCAL/HR	
1	20.366	5.5729	4.2287	0.47809E-02	-.15787E-01
2	20.994	5.5729	4.2182	0.85382E-02	-.13620E-01
3	21.539	5.5729	4.2090	0.72653E-02	-.11743E-01
25	32.543	5.5729	0.28130	0.46014E-01	0.24676E-01
26	36.231	5.5729	4.9165	0.94853E-01	0.36301E-01
27	37.292	5.5729	4.9687	0.55886E-02	0.39596E-01
37	47.178	5.5729	3.7158	0.28502E-02	0.69236E-01

38	47.495	5.5729	3.6896	0.22644E-02	0.70155E-01
39	47.750	5.5729	3.6963	0.18938E-02	0.70896E-01
41	48.167	5.5729	3.9077	0.18308E-02	0.72102E-01
42	48.368	5.5729	4.2427	0.22486E-02	0.72680E-01
43	48.588	5.5729	4.2427	0.22181E-02	0.73313E-01
74	58.738	5.5729	4.2408	0.10640E-01	0.10166
75	59.971	5.5729	4.2323	0.82728E-02	0.10498

U-O-S BLOCK SECTION

BLOCK: COL-01 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 C	
STAGE	LIQUID FROM	VAPOR TO
1	20.366	20.994
2	20.994	21.539
3	21.539	22.001
25	32.543	36.231
26	36.231	37.292
27	37.292	38.518

37	47.178	47.495
38	47.495	47.750
39	47.750	47.968
41	48.167	48.368
42	48.368	48.588
43	48.588	48.795
74	58.738	59.971
75	59.971	59.971

	MASS FLOW KG/HR		VOLUME FLOW CUM/HR		MOLECULAR WEIGHT	
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	37893.	37893.	61.387	3742.4	40.066	40.066
2	37543.	37637.	60.634	3725.4	40.066	40.066
3	37327.	37421.	60.129	3711.0	40.067	40.067
25	42820.	42914.	70.533	3737.9	47.306	47.288
26	56860.	43346.	94.475	3728.8	49.554	47.981
27	57637.	44123.	96.039	3741.2	50.193	48.794
37	64140.	50626.	109.32	3867.5	55.086	55.009
38	64273.	50759.	109.58	3870.8	55.187	55.137
39	64349.	50835.	109.72	3872.8	55.254	55.221
41	64375.	50861.	109.74	3874.0	55.317	55.301

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U-O-S BLOCK SECTION

BLOCK: COL-01   MODEL: RADFRAC (CONTINUED)

	MASS FLOW KG/HR		VOLUME FLOW CUM/HR		MOLECULAR WEIGHT	
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
42	64338.	50824.	109.65	3873.4	55.326	55.312
43	51133.	50773.	87.110	3872.3	55.326	55.312
74	50068.	49709.	85.067	3842.0	56.588	56.582
75	359.70	0.0000	0.61196	0.0000	57.365	

	DENSITY KG/CUM		VISCOSITY CP		SURFACE TENSION DYNE/CM
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM
1	617.27	10.125	0.13834	0.84218E-02	12.913
2	619.17	10.103	0.13983	0.84290E-02	13.049

3	620.79	10.084	0.14113	0.84350E-02	13.165
25	607.10	11.481	0.14030	0.85133E-02	11.842
26	601.85	11.625	0.13716	0.85104E-02	11.260
27	600.14	11.794	0.13606	0.85057E-02	11.083
37	586.72	13.090	0.12599	0.84333E-02	9.6547
38	586.53	13.113	0.12578	0.84324E-02	9.6267
39	586.47	13.126	0.12566	0.84325E-02	9.6102
41	586.61	13.129	0.12562	0.84351E-02	9.6021
42	586.78	13.122	0.12569	0.84374E-02	9.6073
43	586.99	13.112	0.12579	0.84398E-02	9.6173
74	588.58	12.938	0.12887	0.85552E-02	9.9532
75	587.79		0.12917		9.8898

STAGE	MARANGONI INDEX DYNE/CM	FLOW PARAM	QR CUM/HR	REDUCED F-FACTOR (GM-L)**.5/MIN
1		0.12808	483.29	0.19847E+06
2	0.13674	0.12742	479.80	0.19735E+06
3	0.11550	0.12713	476.86	0.19640E+06
25	-.53255	0.13722	518.95	0.21109E+06
26	-.65103E-01	0.18231	523.30	0.21189E+06
27	-.17686	0.18312	529.69	0.21414E+06
37	-.42733E-01	0.18924	584.23	0.23321E+06
38	-.27960E-01	0.18933	585.35	0.23362E+06
39	-.16495E-01	0.18937	585.99	0.23385E+06
41	-.55234E-03	0.18935	586.15	0.23395E+06
42	0.51765E-02	0.18930	585.81	0.23385E+06
43	0.10043E-01	0.15052	585.32	0.23370E+06
74	-.24298E-01	0.14934	576.00	0.23033E+06
75	-.63402E-01		0.0000	0.0000

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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

****
***** TRAY SIZING CALCULATIONS *****
****

****
*** SECTION 1 ***

****

STARTING STAGE NUMBER		2
ENDING STAGE NUMBER		74
FLOODING CALCULATION METHOD		GLITSCH6

DESIGN PARAMETERS

PEAK CAPACITY FACTOR		1.00000
SYSTEM FOAMING FACTOR		1.00000
FLOODING FACTOR		0.80000
MINIMUM COLUMN DIAMETER	METER	0.30480
MINIMUM DC AREA/COLUMN AREA		0.100000
HOLE AREA/ACTIVE AREA		0.100000
DOWNCOMER DESIGN BASIS		EQUAL FLOW PATH LENGTH

TRAY SPECIFICATIONS

TRAY TYPE		SIEVE
NUMBER OF PASSES		1
TRAY SPACING	METER	0.80960

***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER		40
COLUMN DIAMETER	METER	1.69433
DC AREA/COLUMN AREA		0.10148
DOWNCOMER VELOCITY	M/SEC	0.13327
FLOW PATH LENGTH PER PANEL	METER	1.15868
SIDE DOWNCOMER WIDTH	METER	0.26782
SIDE WEIR LENGTH	METER	1.23621
CENTER DOWNCOMER WIDTH	METER	0.0
CENTER WEIR LENGTH	METER	MISSING
OFF-CENTER DOWNCOMER WIDTH	METER	0.0
OFF-CENTER SHORT WEIR LENGTH	METER	MISSING
OFF-CENTER LONG WEIR LENGTH	METER	MISSING
TRAY CENTER TO OCDC CENTER	METER	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA	SIDE DC AREA
	METER	SQM	SQM	SQM

2	1.6943	2.2547	1.7971	0.22880
3	1.6943	2.2547	1.7971	0.22880
4	1.6943	2.2547	1.7971	0.22880
5	1.6943	2.2547	1.7971	0.22880
6	1.6943	2.2547	1.7971	0.22880
7	1.6943	2.2547	1.7971	0.22880
8	1.6943	2.2547	1.7971	0.22880
9	1.6943	2.2547	1.7971	0.22880
10	1.6943	2.2547	1.7971	0.22880
11	1.6943	2.2547	1.7971	0.22880

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U-O-S BLOCK SECTION

BLOCK: COL-01   MODEL: RADFRAC (CONTINUED)

STAGE	DIAMETER METER	TOTAL AREA SQM	ACTIVE AREA SQM	SIDE DC AREA SQM
12	1.6943	2.2547	1.7971	0.22880
13	1.6943	2.2547	1.7971	0.22880
14	1.6943	2.2547	1.7971	0.22880
15	1.6943	2.2547	1.7971	0.22880
16	1.6943	2.2547	1.7971	0.22880
17	1.6943	2.2547	1.7971	0.22880
18	1.6943	2.2547	1.7971	0.22880
19	1.6943	2.2547	1.7971	0.22880
20	1.6943	2.2547	1.7971	0.22880
21	1.6943	2.2547	1.7971	0.22880
22	1.6943	2.2547	1.7971	0.22880
23	1.6943	2.2547	1.7971	0.22880
24	1.6943	2.2547	1.7971	0.22880
25	1.6943	2.2547	1.7971	0.22880
26	1.6943	2.2547	1.7971	0.22880
27	1.6943	2.2547	1.7971	0.22880
28	1.6943	2.2547	1.7971	0.22880
29	1.6943	2.2547	1.7971	0.22880
30	1.6943	2.2547	1.7971	0.22880
31	1.6943	2.2547	1.7971	0.22880
32	1.6943	2.2547	1.7971	0.22880
33	1.6943	2.2547	1.7971	0.22880
34	1.6943	2.2547	1.7971	0.22880
35	1.6943	2.2547	1.7971	0.22880
36	1.6943	2.2547	1.7971	0.22880
37	1.6943	2.2547	1.7971	0.22880

38	1.6943	2.2547	1.7971	0.22880
39	1.6943	2.2547	1.7971	0.22880
40	1.6943	2.2547	1.7971	0.22880
41	1.6943	2.2547	1.7971	0.22880
42	1.6943	2.2547	1.7971	0.22880
43	1.6943	2.2547	1.7971	0.22880
44	1.6943	2.2547	1.7971	0.22880
45	1.6943	2.2547	1.7971	0.22880
46	1.6943	2.2547	1.7971	0.22880
47	1.6943	2.2547	1.7971	0.22880
48	1.6943	2.2547	1.7971	0.22880
49	1.6943	2.2547	1.7971	0.22880
50	1.6943	2.2547	1.7971	0.22880
51	1.6943	2.2547	1.7971	0.22880
52	1.6943	2.2547	1.7971	0.22880
53	1.6943	2.2547	1.7971	0.22880
54	1.6943	2.2547	1.7971	0.22880
55	1.6943	2.2547	1.7971	0.22880
56	1.6943	2.2547	1.7971	0.22880
57	1.6943	2.2547	1.7971	0.22880
58	1.6943	2.2547	1.7971	0.22880
59	1.6943	2.2547	1.7971	0.22880
60	1.6943	2.2547	1.7971	0.22880
61	1.6943	2.2547	1.7971	0.22880
62	1.6943	2.2547	1.7971	0.22880

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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

STAGE	DIAMETER METER	TOTAL AREA SQM	ACTIVE AREA SQM	SIDE DC AREA SQM
63	1.6943	2.2547	1.7971	0.22880
64	1.6943	2.2547	1.7971	0.22880
65	1.6943	2.2547	1.7971	0.22880
66	1.6943	2.2547	1.7971	0.22880
67	1.6943	2.2547	1.7971	0.22880
68	1.6943	2.2547	1.7971	0.22880
69	1.6943	2.2547	1.7971	0.22880
70	1.6943	2.2547	1.7971	0.22880
71	1.6943	2.2547	1.7971	0.22880
72	1.6943	2.2547	1.7971	0.22880
73	1.6943	2.2547	1.7971	0.22880

74	1.6943	2.2547	1.7971	0.22880

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP BAR	DC BACKUP METER	DC BACKUP/ (TSPC+WHT)
2	60.22	0.6531E-02	0.2417	27.56
3	59.82	0.6512E-02	0.2406	27.43
4	59.50	0.6497E-02	0.2396	27.32
5	59.24	0.6485E-02	0.2389	27.24
6	59.03	0.6475E-02	0.2383	27.17
7	58.87	0.6467E-02	0.2379	27.12
8	58.75	0.6462E-02	0.2375	27.08
9	58.65	0.6458E-02	0.2373	27.05
10	58.59	0.6455E-02	0.2371	27.03
11	58.54	0.6453E-02	0.2370	27.02
12	58.51	0.6452E-02	0.2369	27.01
13	58.50	0.6451E-02	0.2368	27.00
14	58.50	0.6452E-02	0.2369	27.01
15	58.53	0.6454E-02	0.2369	27.02
16	58.58	0.6458E-02	0.2371	27.03
17	58.66	0.6463E-02	0.2374	27.06
18	58.82	0.6473E-02	0.2378	27.11
19	59.03	0.6487E-02	0.2385	27.19
20	59.40	0.6512E-02	0.2396	27.31
21	59.96	0.6551E-02	0.2413	27.51
22	60.85	0.6614E-02	0.2440	27.82
23	62.15	0.6707E-02	0.2481	28.29
24	63.95	0.6840E-02	0.2540	28.96
25	66.15	0.7006E-02	0.2615	29.81
26	70.59	0.7265E-02	0.2959	33.73
27	71.55	0.7338E-02	0.2994	34.14
28	72.63	0.7422E-02	0.3036	34.61
29	73.79	0.7513E-02	0.3081	35.13
30	74.96	0.7605E-02	0.3127	35.66
31	76.07	0.7694E-02	0.3172	36.17
32	77.06	0.7773E-02	0.3213	36.63

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U-O-S BLOCK SECTION

BLOCK: COL-01   MODEL: RADFRAC (CONTINUED)

STAGE	FLOODING FACTOR	PRES. DROP BAR	DC BACKUP METER	DC BACKUP/ (TSPC+WHT)
33	77.90	0.7841E-02	0.3247	37.02
34	78.57	0.7896E-02	0.3275	37.34
35	79.08	0.7938E-02	0.3297	37.59
36	79.45	0.7969E-02	0.3313	37.77
37	79.71	0.7991E-02	0.3324	37.89
38	79.87	0.8006E-02	0.3331	37.97
39	79.97	0.8014E-02	0.3334	38.02
40	80.00	0.8018E-02	0.3336	38.03
41	79.99	0.8018E-02	0.3335	38.02
42	79.93	0.8015E-02	0.3332	37.99
43	76.14	0.7794E-02	0.2996	34.16
44	76.06	0.7788E-02	0.2992	34.12
45	75.98	0.7781E-02	0.2989	34.08
46	75.90	0.7775E-02	0.2986	34.04
47	75.82	0.7768E-02	0.2983	34.01
48	75.75	0.7761E-02	0.2980	33.98
49	75.68	0.7754E-02	0.2977	33.95
50	75.61	0.7747E-02	0.2975	33.92
51	75.55	0.7740E-02	0.2973	33.89
52	75.49	0.7732E-02	0.2970	33.87
53	75.43	0.7725E-02	0.2968	33.84
54	75.37	0.7718E-02	0.2966	33.82
55	75.32	0.7712E-02	0.2964	33.80
56	75.27	0.7705E-02	0.2962	33.78
57	75.22	0.7699E-02	0.2961	33.76
58	75.17	0.7693E-02	0.2959	33.74
59	75.12	0.7688E-02	0.2957	33.72
60	75.08	0.7683E-02	0.2956	33.70
61	75.03	0.7679E-02	0.2954	33.68
62	74.99	0.7675E-02	0.2952	33.66
63	74.95	0.7671E-02	0.2950	33.64
64	74.90	0.7668E-02	0.2949	33.62
65	74.86	0.7665E-02	0.2947	33.60
66	74.81	0.7662E-02	0.2944	33.57
67	74.76	0.7660E-02	0.2942	33.55
68	74.71	0.7657E-02	0.2940	33.53
69	74.67	0.7656E-02	0.2938	33.50
70	74.63	0.7654E-02	0.2937	33.48
71	74.60	0.7654E-02	0.2935	33.47
72	74.60	0.7656E-02	0.2935	33.47

73	74.65	0.7661E-02	0.2937	33.49
74	74.79	0.7674E-02	0.2944	33.56

U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

STAGE	HEIGHT OVER WEIR METER	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.1258	0.5987	0.2235	42.51
3	0.1244	0.5989	0.2243	42.18
4	0.1233	0.5991	0.2249	41.90
5	0.1224	0.5992	0.2254	41.68
6	0.1217	0.5993	0.2258	41.51
7	0.1211	0.5994	0.2261	41.37
8	0.1207	0.5994	0.2263	41.27
9	0.1204	0.5995	0.2265	41.19
10	0.1202	0.5995	0.2266	41.13
11	0.1200	0.5995	0.2267	41.09
12	0.1199	0.5996	0.2268	41.06
13	0.1199	0.5996	0.2268	41.05
14	0.1199	0.5996	0.2268	41.05
15	0.1200	0.5996	0.2268	41.07
16	0.1202	0.5995	0.2267	41.11
17	0.1205	0.5995	0.2265	41.17
18	0.1211	0.5995	0.2262	41.28
19	0.1220	0.5994	0.2258	41.45
20	0.1234	0.5992	0.2251	41.73
21	0.1256	0.5990	0.2241	42.16
22	0.1293	0.5987	0.2225	42.85
23	0.1350	0.5983	0.2202	43.89
24	0.1435	0.5976	0.2172	45.36
25	0.1559	0.5968	0.2137	47.23
26	0.2191	0.5960	0.2132	48.32
27	0.2226	0.5956	0.2117	49.11
28	0.2264	0.5953	0.2101	50.03
29	0.2306	0.5949	0.2085	51.01
30	0.2347	0.5945	0.2068	52.02
31	0.2386	0.5942	0.2054	52.98
32	0.2421	0.5938	0.2041	53.84
33	0.2451	0.5935	0.2030	54.57
34	0.2474	0.5933	0.2022	55.16

35	0.2492	0.5932	0.2015	55.62
36	0.2505	0.5930	0.2011	55.95
37	0.2514	0.5930	0.2008	56.19
38	0.2520	0.5929	0.2006	56.34
39	0.2523	0.5929	0.2004	56.43
40	0.2524	0.5929	0.2004	56.46
41	0.2523	0.5929	0.2004	56.46
42	0.2522	0.5930	0.2004	56.42
43	0.2162	0.5930	0.2005	56.19
44	0.2160	0.5931	0.2006	56.12
45	0.2157	0.5931	0.2007	56.05
46	0.2154	0.5931	0.2008	55.98
47	0.2151	0.5931	0.2009	55.91
48	0.2149	0.5932	0.2010	55.85
49	0.2147	0.5932	0.2011	55.79
50	0.2144	0.5932	0.2012	55.73

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U-O-S BLOCK SECTION

BLOCK: COL-01 MODEL: RADFRAC (CONTINUED)

STAGE	HEIGHT OVER WEIR METER	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
51	0.2142	0.5932	0.2013	55.67
52	0.2140	0.5932	0.2014	55.61
53	0.2138	0.5931	0.2015	55.55
54	0.2136	0.5931	0.2016	55.50
55	0.2134	0.5931	0.2016	55.45
56	0.2132	0.5931	0.2017	55.40
57	0.2130	0.5931	0.2018	55.35
58	0.2129	0.5931	0.2019	55.30
59	0.2127	0.5931	0.2019	55.25
60	0.2125	0.5931	0.2020	55.20
61	0.2124	0.5931	0.2021	55.15
62	0.2122	0.5931	0.2021	55.10
63	0.2120	0.5931	0.2022	55.05
64	0.2119	0.5931	0.2022	55.00
65	0.2117	0.5932	0.2023	54.95
66	0.2115	0.5932	0.2023	54.90
67	0.2114	0.5932	0.2023	54.85
68	0.2112	0.5933	0.2024	54.79
69	0.2110	0.5933	0.2024	54.74

70	0.2109	0.5934	0.2024	54.70
71	0.2108	0.5934	0.2025	54.66
72	0.2108	0.5934	0.2025	54.65
73	0.2110	0.5934	0.2024	54.68
74	0.2116	0.5934	0.2023	54.80

*** ASSOCIATED UTILITIES ***

UTILITY USAGE: CHILL-W (WATER)

CONDENSER 8.4368+05 7.0819
------------- -------------
TOTAL: 8.4368+05 KG/HR 7.0819 $/HR
=============
UTILITY USAGE: HPS (STEAM)

REBOILER 1.0119+04 319.8412 2093.4299
------------- ------------- -------------
TOTAL: 1.0119+04 KG/HR 319.8412 $/HR 2093.4299 CO2 KG/HR
=============

BLOCK: HT-01 MODEL: HEATER

INLET STREAM: FEED
OUTLET STREAM: S-01
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	246.372	246.372	0.00000
MASS(KG/HR)	13607.8	13607.8	0.00000
ENTHALPY(GCAL/HR)	2.81403	2.24210	0.203241

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U-O-S BLOCK SECTION

BLOCK: HT-01 MODEL: HEATER (CONTINUED)

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

TOTAL CO2E PRODUCTION 0.00000 KG/HR

*** INPUT DATA ***

TWO PHASE TP FLASH
SPECIFIED TEMPERATURE C 55.0000
SPECIFIED PRESSURE BAR 1.01325
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

*** RESULTS ***

OUTLET TEMPERATURE C 55.000
OUTLET PRESSURE BAR 1.0132
HEAT DUTY GCAL/HR -0.57193
OUTLET VAPOR FRACTION 1.0000

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
1,3-BD	0.43907	0.43680	0.43907	5.6760
ISOBUTYL	0.23035	0.22040	0.23035	5.9015
1-BUTENE	0.12207	0.11701	0.12207	5.8907
N-BUTANE	0.42762E-01	0.46484E-01	0.42762E-01	5.1945
ISOBUTAN	0.47513E-01	0.40716E-01	0.47513E-01	6.5893
CIS-2B	0.40361E-01	0.50213E-01	0.40361E-01	4.5387
TRANS-2B	0.52174E-01	0.60500E-01	0.52174E-01	4.8695
BUTENYNE	0.74244E-02	0.91322E-02	0.74244E-02	4.5906
1-BUTYNE	0.20422E-02	0.26507E-02	0.20422E-02	4.3504
ALLENE	0.27572E-02	0.12638E-02	0.27572E-02	12.319
PROPYNE	0.96501E-02	0.51022E-02	0.96501E-02	10.680
ISOPENT	0.38276E-02	0.97289E-02	0.38276E-02	2.2215

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR WATER CW
RATE OF CONSUMPTION 5.7328+04 KG/HR
COST 0.8642 $/HR

BLOCK: HT-02 MODEL: HEATER

INLET STREAM: S-02

OUTLET STREAM: S-03
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

U-O-S BLOCK SECTION

BLOCK: HT-02 MODEL: HEATER (CONTINUED)

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	246.372	246.372	0.00000
MASS(KG/HR)	13607.8	13607.8	0.00000
ENTHALPY(GCAL/HR)	2.63690	1.02510	0.611249

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

TWO PHASE TP FLASH
SPECIFIED TEMPERATURE C 48.0000
SPECIFIED PRESSURE BAR 5.57288
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

*** RESULTS ***

OUTLET TEMPERATURE C 48.000
OUTLET PRESSURE BAR 5.5729
HEAT DUTY GCAL/HR -1.6118
OUTLET VAPOR FRACTION 0.0000

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
1,3-BD	0.43907	0.43907	0.43264	0.97997
ISOBUTYL	0.23035	0.23035	0.23812	1.0281

1-BUTENE	0.12207	0.12207	0.12608	1.0272
N-BUTANE	0.42762E-01	0.42762E-01	0.39207E-01	0.91185
ISOBUTAN	0.47513E-01	0.47513E-01	0.55568E-01	1.1631
CIS-2B	0.40361E-01	0.40361E-01	0.31869E-01	0.78529
TRANS-2B	0.52174E-01	0.52174E-01	0.44246E-01	0.84342
BUTENYNE	0.74244E-02	0.74244E-02	0.59103E-02	0.79172
1-BUTYNE	0.20422E-02	0.20422E-02	0.15220E-02	0.74121
ALLENE	0.27572E-02	0.27572E-02	0.58524E-02	2.1110
PROPYNE	0.96501E-02	0.96501E-02	0.17462E-01	1.7996
ISOPENT	0.38276E-02	0.38276E-02	0.15202E-02	0.39499

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR WATER CW
RATE OF CONSUMPTION 1.6156+05 KG/HR
COST 2.4355 $/HR

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U-O-S BLOCK SECTION

BLOCK: HT-03 MODEL: HEATER

INLET STREAM: AIR
OUTLET STREAM: A-02
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

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**********************************************************************
*                                                                    *
*    BLOCK IS IN MASS IMBALANCE                                      *
*                                                                    *
**********************************************************************
```

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	453.702	457.037	-0.729756E-02
MASS(KG/HR)	13135.1	13231.6	-0.729756E-02
ENTHALPY(GCAL/HR)	-0.913253E-03	0.557470	-1.00164

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 0.00000 KG/HR
PRODUCT STREAMS CO2E 0.00000 KG/HR

NET STREAMS CO2E PRODUCTION 0.00000 KG/HR
UTILITIES CO2E PRODUCTION 274.183 KG/HR
TOTAL CO2E PRODUCTION 274.183 KG/HR

*** INPUT DATA ***

TWO PHASE TP FLASH
SPECIFIED TEMPERATURE C 200.000
SPECIFIED PRESSURE BAR 1.01325
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.0100000

*** RESULTS ***

OUTLET TEMPERATURE C 200.00
OUTLET PRESSURE BAR 1.0132
HEAT DUTY GCAL/HR 0.55431
OUTLET VAPOR FRACTION 1.0000

BLOCK: HT-03 MODEL: HEATER (CONTINUED)

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
AIR	1.0000	1.0000	1.0000	MISSING

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR STEAM HPS
RATE OF CONSUMPTION 1325.3200 KG/HR
COST 41.8905 $/HR
CO2 EQUIVALENT EMISSIONS 274.1826 KG/HR

BLOCK: HT-04 MODEL: HEATER

INLET STREAM: R-03
OUTLET STREAM: R-04
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

```
**********************************************************************
*                                         *
*   MINIMUM APPROACH TEMPERATURE VIOLATED WITH UTILITY          *
*                                         *
**********************************************************************

             ***  MASS AND ENERGY BALANCE  ***
                      IN          OUT       RELATIVE DIFF.
  TOTAL BALANCE
    MOLE(KMOL/HR )         962.132       962.132       0.00000
    MASS(KG/HR   )         41569.5       41569.5       0.00000
    ENTHALPY(GCAL/HR )     -2.87366      2.70625      -1.94174

             ***  CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E           0.00000      KG/HR
  PRODUCT STREAMS CO2E        0.00000      KG/HR
  NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
  UTILITIES CO2E PRODUCTION    2760.01      KG/HR
  TOTAL CO2E PRODUCTION        2760.01      KG/HR

               ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE             C                250.000
  SPECIFIED PRESSURE              BAR                1.01325
  MAXIMUM NO. ITERATIONS                              30
  CONVERGENCE TOLERANCE                               0.000100000


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                      U-O-S BLOCK SECTION

 BLOCK:  HT-04    MODEL: HEATER (CONTINUED)

                ***  RESULTS  ***
  OUTLET TEMPERATURE    C                        250.00
  OUTLET PRESSURE       BAR                     1.0132
  HEAT DUTY             GCAL/HR                 5.5799
  OUTLET VAPOR FRACTION                          1.0000
```

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
1,3-BD	0.89320E-03	0.89320E-03	0.89320E-03	MISSING
1-BUTENE	0.31372E-01	0.31372E-01	0.31372E-01	MISSING
CIS-2B	0.42669	0.42669	0.42669	MISSING
TRANS-2B	0.66018E-01	0.66018E-01	0.66018E-01	MISSING
AIR	0.47503	0.47503	0.47503	MISSING

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR STEAM HPS
RATE OF CONSUMPTION 1.3341+04 KG/HR
COST 421.6839 $/HR
CO2 EQUIVALENT EMISSIONS 2760.0129 KG/HR

BLOCK: HT-05 MODEL: HEATER

INLET STREAM: R-06
OUTLET STREAM: R-07
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	995.563	995.563	0.00000
MASS(KG/HR)	41569.5	41569.5	0.00000
ENTHALPY(GCAL/HR)	6.30364	0.248015	0.960655

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

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U-O-S BLOCK SECTION

BLOCK: HT-05 MODEL: HEATER (CONTINUED)

*** INPUT DATA ***
TWO PHASE TP FLASH
SPECIFIED TEMPERATURE C 48.0000

SPECIFIED PRESSURE BAR 5.57288
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

*** RESULTS ***

OUTLET TEMPERATURE C 48.000
OUTLET PRESSURE BAR 5.5729
HEAT DUTY GCAL/HR -6.0556
OUTLET VAPOR FRACTION 1.0000

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
1,3-BD	0.34443E-01	0.55092E-01	0.34443E-01	0.95580
1-BUTENE	0.12133E-03	0.18399E-03	0.12133E-03	1.0082
CIS-2B	0.41992	0.83804	0.41992	0.76606
TRANS-2B	0.52860E-01	0.97808E-01	0.52860E-01	0.82625
H2	0.33579E-01	0.32880E-03	0.33579E-01	156.14
AIR	0.45907	0.85460E-02	0.45907	82.126

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR WATER CW
RATE OF CONSUMPTION 6.0700+05 KG/HR
COST 9.1501 $/HR

BLOCK: HT-06 MODEL: HEATER

INLET STREAM: 1,3-BD
OUTLET STREAM: 1,3-BD-C
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	141.493	141.493	0.00000
MASS(KG/HR)	7653.57	7653.57	0.00000
ENTHALPY(GCAL/HR)	3.05656	2.96609	0.295974E-01

U-O-S BLOCK SECTION

BLOCK: HT-06 MODEL: HEATER (CONTINUED)

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

TWO PHASE TP FLASH

SPECIFIED TEMPERATURE	C	25.0000
SPECIFIED PRESSURE	BAR	5.50000
MAXIMUM NO. ITERATIONS		30
CONVERGENCE TOLERANCE		0.000100000

*** RESULTS ***

OUTLET TEMPERATURE	C	25.000
OUTLET PRESSURE	BAR	5.5000
HEAT DUTY	GCAL/HR	-0.90466E-01
OUTLET VAPOR FRACTION		0.0000

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
1,3-BD	1.0000	1.0000	1.0000	0.55188

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR WATER	CHILL-W
RATE OF CONSUMPTION	1.8049+04 KG/HR
COST	0.1515 $/HR

BLOCK: HT-07 MODEL: HEATER

INLET STREAM: ISOBUTYL
OUTLET STREAM: ISOBUT-C
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	78.7741	78.7741	0.00000
MASS(KG/HR)	4464.24	4464.24	0.00000
ENTHALPY(GCAL/HR)	-1.25609	-1.31128	0.420898E-01

U-O-S BLOCK SECTION

BLOCK: HT-07 MODEL: HEATER (CONTINUED)

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

TWO PHASE TP FLASH

SPECIFIED TEMPERATURE	C	25.0000
SPECIFIED PRESSURE	BAR	5.50000
MAXIMUM NO. ITERATIONS		30
CONVERGENCE TOLERANCE		0.000100000

*** RESULTS ***

OUTLET TEMPERATURE	C	25.000
OUTLET PRESSURE	BAR	5.5000
HEAT DUTY	GCAL/HR	-0.55192E-01
OUTLET VAPOR FRACTION		0.0000

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
ISOBUTYL	0.72028	0.72028	0.72055	0.59434
N-BUTANE	0.13112	0.13112	0.10804	0.48956
ISOBUTAN	0.14860	0.14860	0.17141	0.68533

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR WATER CHILL-W
RATE OF CONSUMPTION 1.1011+04 KG/HR
COST 9.2431-02 $/HR

BLOCK: HT-08 MODEL: HEATER

INLET STREAM: HEAVIES
OUTLET STREAM: HEAVY-C
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	6.27040	6.27040	0.00000
MASS(KG/HR)	359.700	359.700	-0.158030E-15
ENTHALPY(GCAL/HR)	-0.103528E-01	-0.173381E-01	0.402889

BLOCK: HT-08 MODEL: HEATER (CONTINUED)

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

*** INPUT DATA ***
TWO PHASE TP FLASH
SPECIFIED TEMPERATURE C 25.0000
SPECIFIED PRESSURE BAR 5.50000
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

*** RESULTS ***
OUTLET TEMPERATURE C 25.000
OUTLET PRESSURE BAR 5.5000
HEAT DUTY GCAL/HR -0.69853E-02

OUTLET VAPOR FRACTION 0.0000

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
1,3-BD	0.18765E-01	0.18765E-01	0.24715E-01	0.55408
ISOBUTYL	0.20097E-02	0.20097E-02	0.28606E-02	0.59878
1-BUTENE	0.12536E-02	0.12536E-02	0.17734E-02	0.59511
N-BUTANE	0.32926E-01	0.32926E-01	0.39102E-01	0.49959
ISOBUTAN	0.71631E-05	0.71631E-05	0.12105E-04	0.71091
CIS-2B	0.51609	0.51609	0.53138	0.43314
TRANS-2B	0.19120	0.19120	0.21342	0.46957
BUTENYNE	0.95856E-01	0.95856E-01	0.10074	0.44212
1-BUTYNE	0.36616E-01	0.36616E-01	0.33865E-01	0.38908
PROPYNE	0.42740E-12	0.42740E-12	0.10726E-11	1.0557
ISOPENT	0.10528	0.10528	0.52124E-01	0.20828

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR WATER CHILL-W
RATE OF CONSUMPTION 1393.6568 KG/HR
COST 1.1698-02 $/HR

BLOCK: HT-09 MODEL: HEATER

INLET STREAM: PROPYNE
OUTLET STREAM: PROPY-C
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE
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U-O-S BLOCK SECTION

BLOCK: HT-09 MODEL: HEATER (CONTINUED)

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	2.34346	2.34346	0.00000
MASS(KG/HR)	93.8924	93.8924	0.00000
ENTHALPY(GCAL/HR)	0.934141E-01	0.104040	-0.102135

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 0.00000 KG/HR
PRODUCT STREAMS CO2E 0.00000 KG/HR
NET STREAMS CO2E PRODUCTION 0.00000 KG/HR
UTILITIES CO2E PRODUCTION 5.25603 KG/HR
TOTAL CO2E PRODUCTION 5.25603 KG/HR

*** INPUT DATA ***

TWO PHASE TP FLASH		
SPECIFIED TEMPERATURE	C	25.0000
SPECIFIED PRESSURE	BAR	5.50000
MAXIMUM NO. ITERATIONS		30
CONVERGENCE TOLERANCE		0.000100000

*** RESULTS ***

OUTLET TEMPERATURE	C	25.000
OUTLET PRESSURE	BAR	5.5000
HEAT DUTY	GCAL/HR	0.10626E-01
OUTLET VAPOR FRACTION		1.0000

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
1,3-BD	0.90732E-07	0.18204E-06	0.90732E-07	0.55896
ISOBUTYL	0.82712E-06	0.14917E-05	0.82712E-06	0.62181
1-BUTENE	0.36602E-06	0.66531E-06	0.36602E-06	0.61697
N-BUTANE	0.14596E-08	0.31571E-08	0.14596E-08	0.51849
ISOBUTAN	0.56345E-04	0.82549E-04	0.56345E-04	0.76546
CIS-2B	0.12104E-10	0.31097E-10	0.12104E-10	0.43650
TRANS-2B	0.16801E-09	0.39424E-09	0.16801E-09	0.47792
BUTENYNE	0.17915E-11	0.46330E-11	0.17915E-11	0.43364
1-BUTYNE	0.16068E-13	0.47419E-13	0.16068E-13	0.38000
ALLENE	0.28977	0.23819	0.28977	1.3643
PROPYNE	0.71017	0.76173	0.71017	1.0456

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR STEAM LPS
RATE OF CONSUMPTION 20.9309 KG/HR
COST 0.6371 $/HR
CO2 EQUIVALENT EMISSIONS 5.2560 KG/HR

U-O-S BLOCK SECTION

BLOCK: MX-01 MODEL: MIXER

INLET STREAMS: S-04 DMF R-08
OUTLET STREAM: S-05
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	757.853	757.853	0.00000
MASS(KG/HR)	42521.1	42521.1	0.171114E-15
ENTHALPY(GCAL/HR)	-2.22564	-2.22564	-0.199533E-15

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

TWO PHASE FLASH
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000
OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES

BLOCK: MX-02 MODEL: MIXER

INLET STREAMS: R-02 A-02
OUTLET STREAM: R-03
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	962.132	962.132	0.00000
MASS(KG/HR)	41569.5	41569.5	0.175031E-15
ENTHALPY(GCAL/HR)	-2.87366	-2.87366	-0.154538E-15

U-O-S BLOCK SECTION

BLOCK: MX-02 MODEL: MIXER (CONTINUED)

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

*** INPUT DATA ***
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS 200
CONVERGENCE TOLERANCE 0.50000
OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES

BLOCK: RX-01 MODEL: RPLUG

INLET STREAM: R-04
OUTLET STREAM: R-05
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
TOTAL BALANCE				
MOLE(KMOL/HR)	962.132	995.563	33.4304	-0.114194E-15
MASS(KG/HR)	41569.5	41569.5		-0.175031E-15
ENTHALPY(GCAL/HR)	2.70625	3.63682		-0.255874

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

*** INPUT DATA ***

REACTOR TYPE:
SPECIFIED TEMPERATURE
VAPOR FLUID PHASE
REACTOR TUBE LENGTH METER 6.4008
REACTOR DIAMETER METER 0.52502E-01

```
  REACTOR RISE                    METER           0.0000
  NUMBER OF REACTOR TUBES                            135
  REACTOR VOLUME                  CUM             1.8707
  PRESSURE DROP OPTION:                           SPECIFIED
  HOLDUP OPTION:                                  NO-SLIP
  ERROR TOLERANCE                                 0.10000E-05
  INTEGRATION METHOD                              GEAR
  CORRECTOR METHOD                                NEWTON
  INITIAL STEP SIZE FACTOR                        0.10000E-01
  CORRECTOR TOLERANCE FACTOR                      0.10000
  MAXIMUM NUMBER OF STEPS                         1000

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                    U-O-S BLOCK SECTION

 BLOCK:  RX-01    MODEL: RPLUG (CONTINUED)
  TEMPERATURE PROFILES:

   RELATIVE LOCATION        TEMPERATURE
        0.0000              250.00     C


   REACTION PARAGRAPH          ID:  R-1          TYPE:  GENERAL
   GLOBAL BASES:
   KBASIS                              MOLE-GAMMA
   CBASIS                              MOLARITY
   SBASIS                              GLOBAL

   STOICHIOMETRY:

   REACTION NUMBER:          1
     SUBSTREAM:  MIXED
       1,3-BD      1.0000      1-BUTENE   -1.0000      H2          1.0000

   REACTION NUMBER:          2
     SUBSTREAM:  MIXED
       1,3-BD      1.0000      TRANS-2B   -1.0000      H2          1.0000

   REACTION NUMBER:          3
     SUBSTREAM:  MIXED
       1-BUTENE   -1.0000      CIS-2B      1.0000

   REACTION NUMBER:          4
```

SUBSTREAM: MIXED
1-BUTENE -1.0000 TRANS-2B 1.0000

REACTION NUMBER: 5
SUBSTREAM: MIXED
CIS-2B 1.0000 TRANS-2B -1.0000

REACTION NUMBER: 6
SUBSTREAM: MIXED
1-BUTENE 1.0000 TRANS-2B -1.0000

REAC-DATA ENTRIES:

REACTION NO	TYPE	PHASE	DELT C	BASIS
1	KINETIC	V	0.0000	PARTIALPRES
2	KINETIC	V	0.0000	PARTIALPRES
3	KINETIC	V	0.0000	PARTIALPRES
4	KINETIC	V	0.0000	PARTIALPRES
5	KINETIC	V	0.0000	PARTIALPRES
6	KINETIC	V	0.0000	PARTIALPRES

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U-O-S BLOCK SECTION

BLOCK: RX-01 MODEL: RPLUG (CONTINUED)

*** RESULTS ***

REACTOR DUTY	GCAL/HR	0.93057
RESIDENCE TIME	HR	0.44140E-04
REACTOR MINIMUM TEMPERATURE	C	250.00
REACTOR MAXIMUM TEMPERATURE	C	250.00

*** RESULTS PROFILE (PROCESS STREAM) ***

LENGTH METER	PRESSURE BAR	TEMPERATURE C	VAPOR FRAC	RES-TIME HR
0.0000	1.0132	250.00	1.0000	0.0000
0.64008	1.0132	250.00	1.0000	0.44952E-05

1.2802	1.0132	250.00	1.0000	0.89397E-05
1.9202	1.0132	250.00	1.0000	0.13361E-04
2.5603	1.0132	250.00	1.0000	0.17772E-04
3.2004	1.0132	250.00	1.0000	0.22177E-04
3.8405	1.0132	250.00	1.0000	0.26578E-04
4.4806	1.0132	250.00	1.0000	0.30974E-04
5.1206	1.0132	250.00	1.0000	0.35367E-04
5.7607	1.0132	250.00	1.0000	0.39755E-04
6.4008	1.0132	250.00	1.0000	0.44140E-04

LENGTH METER	DUTY GCAL/HR	LIQUID HOLDUP
0.0000	0.0000	0.0000
0.64008	0.42011	0.0000
1.2802	0.62223	0.0000
1.9202	0.71550	0.0000
2.5603	0.76277	0.0000
3.2004	0.79512	0.0000
3.8405	0.82379	0.0000
4.4806	0.85139	0.0000
5.1206	0.87834	0.0000
5.7607	0.90473	0.0000
6.4008	0.93057	0.0000

*** TOTAL MOLE FRACTION PROFILE (PROCESS STREAM) ***

LENGTH METER	1,3-BD	1-BUTENE	CIS-2B	TRANS-2B
0.0000	0.89320E-03	0.31372E-01	0.42669	0.66018E-01
0.64008	0.16720E-01	0.12382E-01	0.42266	0.64892E-01
1.2802	0.24095E-01	0.41905E-02	0.42092	0.63581E-01
1.9202	0.27398E-01	0.11942E-02	0.42027	0.62190E-01
2.5603	0.29007E-01	0.34514E-03	0.42007	0.60781E-01
3.2004	0.30071E-01	0.16953E-03	0.42001	0.59388E-01
3.8405	0.31001E-01	0.13939E-03	0.41999	0.58023E-01
4.4806	0.31893E-01	0.13196E-03	0.41997	0.56688E-01
5.1206	0.32763E-01	0.12805E-03	0.41996	0.55383E-01
5.7607	0.33612E-01	0.12452E-03	0.41994	0.54107E-01
6.4008	0.34443E-01	0.12133E-03	0.41992	0.52860E-01

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U-O-S BLOCK SECTION

BLOCK: RX-01 MODEL: RPLUG (CONTINUED)

*** TOTAL MOLE FRACTION PROFILE (PROCESS STREAM) ***

LENGTH METER	H2	AIR
0.0000	0.0000	0.47503
0.64008	0.15841E-01	0.46750
1.2802	0.23223E-01	0.46399
1.9202	0.26529E-01	0.46242
2.5603	0.28139E-01	0.46166
3.2004	0.29204E-01	0.46115
3.8405	0.30135E-01	0.46071
4.4806	0.31028E-01	0.46029
5.1206	0.31898E-01	0.45987
5.7607	0.32748E-01	0.45947
6.4008	0.33579E-01	0.45907

*** TOTAL MASS FRACTION PROFILE (PROCESS STREAM) ***

LENGTH METER	1,3-BD	1-BUTENE	CIS-2B	TRANS-2B
0.0000	0.11183E-02	0.40741E-01	0.55411	0.85732E-01
0.64008	0.21270E-01	0.16339E-01	0.55771	0.85626E-01
1.2802	0.30884E-01	0.55712E-02	0.55960	0.84531E-01
1.9202	0.35236E-01	0.15930E-02	0.56064	0.82962E-01
2.5603	0.37367E-01	0.46119E-03	0.56130	0.81217E-01
3.2004	0.38780E-01	0.22678E-03	0.56185	0.79443E-01
3.8405	0.40018E-01	0.18664E-03	0.56235	0.77691E-01
4.4806	0.41208E-01	0.17685E-03	0.56285	0.75973E-01
5.1206	0.42369E-01	0.17176E-03	0.56333	0.74291E-01
5.7607	0.43506E-01	0.16718E-03	0.56380	0.72643E-01
6.4008	0.44619E-01	0.16303E-03	0.56427	0.71030E-01

LENGTH METER	H2	AIR
0.0000	0.0000	0.31830
0.64008	0.75102E-03	0.31830

1.2802	0.11093E-02	0.31830
1.9202	0.12715E-02	0.31830
2.5603	0.13509E-02	0.31830
3.2004	0.14036E-02	0.31830
3.8405	0.14497E-02	0.31830
4.4806	0.14940E-02	0.31830
5.1206	0.15373E-02	0.31830
5.7607	0.15797E-02	0.31830
6.4008	0.16212E-02	0.31830

U-O-S BLOCK SECTION

BLOCK: SEP-01 MODEL: SEP

INLET STREAMS: S-05 D-01
OUTLET STREAMS: R-01 S-06
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	1282.85	1282.85	0.177241E-15
MASS(KG/HR)	79242.3	79242.3	0.00000
ENTHALPY(GCAL/HR)	-24.0591	-24.0453	-0.575125E-03

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 0.00000 KG/HR
PRODUCT STREAMS CO2E 0.00000 KG/HR
NET STREAMS CO2E PRODUCTION 0.00000 KG/HR
UTILITIES CO2E PRODUCTION 6.84424 KG/HR
TOTAL CO2E PRODUCTION 6.84424 KG/HR

*** INPUT DATA ***

INLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES

FLASH SPECS FOR STREAM R-01
TWO PHASE TP FLASH
PRESSURE DROP BAR 0.0
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

FLASH SPECS FOR STREAM S-06
TWO PHASE TP FLASH
PRESSURE DROP BAR 0.0
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

U-O-S BLOCK SECTION

BLOCK: SEP-01 MODEL: SEP (CONTINUED)

FRACTION OF FEED
SUBSTREAM= MIXED
STREAM= R-01 CPT= 1,3-BD FRACTION= 0.0060000
ISOBUTYL 0.99000
1-BUTENE 1.00000
N-BUTANE 1.00000
ISOBUTAN 1.00000
CIS-2B 1.00000
TRANS-2B 1.00000

*** RESULTS ***

HEAT DUTY GCAL/HR 0.13837E-01

COMPONENT = 1,3-BD

STREAM	SUBSTREAM	SPLIT FRACTION
R-01	MIXED	0.0060000
S-06	MIXED	0.99400

COMPONENT = ISOBUTYL

STREAM	SUBSTREAM	SPLIT FRACTION
R-01	MIXED	0.99000
S-06	MIXED	0.0100000

COMPONENT = 1-BUTENE

STREAM	SUBSTREAM	SPLIT FRACTION
R-01	MIXED	1.00000

COMPONENT = N-BUTANE

STREAM	SUBSTREAM	SPLIT FRACTION
R-01	MIXED	1.00000

COMPONENT = ISOBUTAN

STREAM	SUBSTREAM	SPLIT FRACTION
R-01	MIXED	1.00000

COMPONENT = CIS-2B

STREAM	SUBSTREAM	SPLIT FRACTION
R-01	MIXED	1.00000

COMPONENT = TRANS-2B

STREAM	SUBSTREAM	SPLIT FRACTION
R-01	MIXED	1.00000

COMPONENT = BUTENYNE

STREAM	SUBSTREAM	SPLIT FRACTION
S-06	MIXED	1.00000

COMPONENT = 1-BUTYNE

STREAM	SUBSTREAM	SPLIT FRACTION
S-06	MIXED	1.00000

BLOCK: SEP-01 MODEL: SEP (CONTINUED)

COMPONENT = ALLENE

STREAM	SUBSTREAM	SPLIT FRACTION
S-06	MIXED	1.00000

COMPONENT = PROPYNE

STREAM	SUBSTREAM	SPLIT FRACTION
S-06	MIXED	1.00000

COMPONENT = ISOPENT

STREAM	SUBSTREAM	SPLIT FRACTION
S-06	MIXED	1.00000

COMPONENT = DMF

STREAM	SUBSTREAM	SPLIT FRACTION
S-06	MIXED	1.00000

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR STEAM LPS

RATE OF CONSUMPTION 27.2556 KG/HR
COST 0.8296 $/HR
CO2 EQUIVALENT EMISSIONS 6.8442 KG/HR

BLOCK: SEP-02 MODEL: SEP

INLET STREAM: S-06
OUTLET STREAMS: 1,3-BD D-01
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

```
***********************************************************************
*                                              *
*    BLOCK IS IN MASS IMBALANCE                                *
*                                              *
***********************************************************************
```

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	683.989	666.491	0.255823E-01
MASS(KG/HR)	45598.9	44374.7	0.268464E-01
ENTHALPY(GCAL/HR)	-19.4469	-18.7769	-0.344537E-01

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 0.00000 KG/HR
PRODUCT STREAMS CO2E 0.00000 KG/HR
NET STREAMS CO2E PRODUCTION 0.00000 KG/HR
UTILITIES CO2E PRODUCTION 4.12995 KG/HR
TOTAL CO2E PRODUCTION 4.12995 KG/HR

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U-O-S BLOCK SECTION

BLOCK: SEP-02 MODEL: SEP (CONTINUED)

*** INPUT DATA ***

FLASH SPECS FOR STREAM 1,3-BD
TWO PHASE TP FLASH
PRESSURE DROP BAR 0.0
MAXIMUM NO. ITERATIONS 30

CONVERGENCE TOLERANCE 0.000100000

FLASH SPECS FOR STREAM D-01
TWO PHASE TP FLASH
PRESSURE DROP BAR 0.0
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

FRACTION OF FEED
SUBSTREAM= MIXED
STREAM= 1,3-BD CPT= 1,3-BD FRACTION= 1.00000

*** RESULTS ***

HEAT DUTY GCAL/HR 0.83495E-02

COMPONENT = 1,3-BD
STREAM SUBSTREAM SPLIT FRACTION
1,3-BD MIXED 1.00000

COMPONENT = ISOBUTYL
STREAM SUBSTREAM SPLIT FRACTION
D-01 MIXED 1.00000

COMPONENT = BUTENYNE
STREAM SUBSTREAM SPLIT FRACTION
D-01 MIXED 1.00000

COMPONENT = 1-BUTYNE
STREAM SUBSTREAM SPLIT FRACTION
D-01 MIXED 1.00000

COMPONENT = ALLENE
STREAM SUBSTREAM SPLIT FRACTION
D-01 MIXED 1.00000

COMPONENT = PROPYNE
STREAM SUBSTREAM SPLIT FRACTION
D-01 MIXED 1.00000

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U-O-S BLOCK SECTION

BLOCK: SEP-02 MODEL: SEP (CONTINUED)

COMPONENT = ISOPENT

STREAM	SUBSTREAM	SPLIT FRACTION
D-01	MIXED	1.00000

COMPONENT = DMF

STREAM	SUBSTREAM	SPLIT FRACTION
D-01	MIXED	1.00000

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR STEAM LPS
RATE OF CONSUMPTION 16.4466 KG/HR
COST 0.5006 $/HR
CO2 EQUIVALENT EMISSIONS 4.1300 KG/HR

BLOCK: SEP-03 MODEL: SEP

INLET STREAM: R-01
OUTLET STREAMS: R-02 ISOBUTYL
PROPERTY OPTION SET: PR-BM PENG-ROBINSON EQUATION OF STATE

```
*********************************************************************
*                                                                   *
*    BLOCK IS IN MASS IMBALANCE                                     *
*                                                                   *
*********************************************************************
```

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	598.862	583.869	0.250359E-01
MASS(KG/HR)	33643.4	32802.1	0.250045E-01
ENTHALPY(GCAL/HR)	-4.59835	-4.68722	0.189613E-01

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

FLASH SPECS FOR STREAM R-02
TWO PHASE TP FLASH
PRESSURE DROP BAR 0.0
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

BLOCK: SEP-03 MODEL: SEP (CONTINUED)

FLASH SPECS FOR STREAM ISOBUTYL
TWO PHASE TP FLASH
PRESSURE DROP BAR 0.0
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

FRACTION OF FEED
SUBSTREAM= MIXED
STREAM= ISOBUTYL CPT= 1,3-BD FRACTION= 0.0

ISOBUTYL	1.00000
1-BUTENE	0.0
N-BUTANE	1.00000
ISOBUTAN	1.00000
CIS-2B	0.0
TRANS-2B	0.0
BUTENYNE	0.0
1-BUTYNE	0.0
PROPANE	0.0
ALLENE	0.0
PROPYNE	0.0
ISOPENT	0.0
DMF	0.0
H2	0.0
AIR	0.0

*** RESULTS ***

HEAT DUTY GCAL/HR -0.46896E-03

COMPONENT = 1,3-BD
STREAM SUBSTREAM SPLIT FRACTION
R-02 MIXED 1.00000

COMPONENT = ISOBUTYL
STREAM SUBSTREAM SPLIT FRACTION
ISOBUTYL MIXED 1.00000

COMPONENT = 1-BUTENE
STREAM SUBSTREAM SPLIT FRACTION
R-02 MIXED 1.00000

COMPONENT = N-BUTANE
STREAM SUBSTREAM SPLIT FRACTION
ISOBUTYL MIXED 1.00000

COMPONENT = ISOBUTAN
STREAM SUBSTREAM SPLIT FRACTION
ISOBUTYL MIXED 1.00000

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U-O-S BLOCK SECTION

BLOCK: SEP-03 MODEL: SEP (CONTINUED)

COMPONENT = CIS-2B
STREAM SUBSTREAM SPLIT FRACTION
R-02 MIXED 1.00000

COMPONENT = TRANS-2B
STREAM SUBSTREAM SPLIT FRACTION
R-02 MIXED 1.00000

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR WATER CW
RATE OF CONSUMPTION 47.0072 KG/HR
COST 7.0860-04 $/HR

BLOCK: SEP-04 MODEL: SEP

INLET STREAM: R-07
OUTLET STREAMS: H2+AIR R-08

PROPERTY OPTION SET: PR-BM   PENG-ROBINSON EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	995.563	995.563	0.00000
MASS(KG/HR)	41569.5	41569.5	-0.175031E-15
ENTHALPY(GCAL/HR)	0.248015	-2.25774	1.10985

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

FLASH SPECS FOR STREAM H2+AIR
TWO   PHASE TP FLASH
PRESSURE DROP   BAR   0.0
MAXIMUM NO. ITERATIONS   30
CONVERGENCE TOLERANCE   0.000100000

U-O-S BLOCK SECTION

BLOCK: SEP-04   MODEL: SEP (CONTINUED)

FLASH SPECS FOR STREAM R-08
TWO   PHASE TP FLASH
PRESSURE DROP   BAR   0.0
MAXIMUM NO. ITERATIONS   30
CONVERGENCE TOLERANCE   0.000100000

FRACTION OF FEED
SUBSTREAM= MIXED
STREAM= H2+AIR   CPT= H2   FRACTION=   1.00000
AIR   1.00000

*** RESULTS ***

HEAT DUTY GCAL/HR -2.5058

COMPONENT = 1,3-BD

STREAM	SUBSTREAM	SPLIT FRACTION
R-08	MIXED	1.00000

COMPONENT = 1-BUTENE

STREAM	SUBSTREAM	SPLIT FRACTION
R-08	MIXED	1.00000

COMPONENT = CIS-2B

STREAM	SUBSTREAM	SPLIT FRACTION
R-08	MIXED	1.00000

COMPONENT = TRANS-2B

STREAM	SUBSTREAM	SPLIT FRACTION
R-08	MIXED	1.00000

COMPONENT = H2

STREAM	SUBSTREAM	SPLIT FRACTION
H2+AIR	MIXED	1.00000

COMPONENT = AIR

STREAM	SUBSTREAM	SPLIT FRACTION
H2+AIR	MIXED	1.00000

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR WATER CW
RATE OF CONSUMPTION 2.5117+05 KG/HR
COST 3.7862 $/HR

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STREAM SECTION

1,3-BD 1,3-BD-C A-02 AIR D-01

STREAM ID	1,3-BD	1,3-BD-C	A-02	AIR	D-01
FROM :	SEP-02	HT-06	HT-03	----	SEP-02
TO :	HT-06	----	MX-02	HT-03	SEP-01
CONV. MAX. REL. ERR:	0.0	0.0	-7.2976-03	0.0	3.3366-02

SUBSTREAM: MIXED

PHASE:	LIQUID	LIQUID	VAPOR	VAPOR	LIQUID
COMPONENTS: KMOL/HR					
1,3-BD	141.4926	141.4926	0.0	0.0	0.0
ISOBUTYL	0.0	0.0	0.0	0.0	0.5731
1-BUTENE	0.0	0.0	0.0	0.0	0.0
N-BUTANE	0.0	0.0	0.0	0.0	0.0
ISOBUTAN	0.0	0.0	0.0	0.0	0.0
CIS-2B	0.0	0.0	0.0	0.0	0.0
TRANS-2B	0.0	0.0	0.0	0.0	0.0
BUTENYNE	0.0	0.0	0.0	0.0	36.8068
1-BUTYNE	0.0	0.0	0.0	0.0	8.1982
PROPANE	0.0	0.0	0.0	0.0	0.0
ALLENE	0.0	0.0	0.0	0.0	6.7597-03
PROPYNE	0.0	0.0	0.0	0.0	21.3766
ISOPENT	0.0	0.0	0.0	0.0	8.4785
DMF	0.0	0.0	0.0	0.0	449.5587
H2	0.0	0.0	0.0	0.0	0.0
AIR	0.0	0.0	457.0373	453.7021	0.0
WATER	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
KMOL/HR	141.4926	141.4926	457.0373	453.7021	524.9987
KG/HR	7653.5665	7653.5665	1.3232+04	1.3135+04	3.6721+04
CUM/HR	12.6719	12.0051	1.7749+04	1.1094+04	54.3732
STATE VARIABLES:					
TEMP C	46.2387	25.0000	200.0000	25.0000	46.2387
PRES BAR	5.5729	5.5000	1.0133	1.0133	5.5729
VFRAC	0.0	0.0	1.0000	1.0000	0.0
LFRAC	1.0000	1.0000	0.0	0.0	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
KCAL/MOL	21.6023	20.9629	1.2197	-2.0129-03	-41.5876
KCAL/KG	399.3642	387.5440	42.1315	-6.9528-02	-594.5743
GCAL/HR	3.0566	2.9661	0.5575	-9.1325-04	-21.8335
ENTROPY:					
CAL/MOL-K	-49.4628	-51.5329	3.2164	-5.7121-03	-94.9443
CAL/GM-K	-0.9144	-0.9527	0.1111	-1.9730-04	-1.3574
DENSITY:					
MOL/CC	1.1166-02	1.1786-02	2.5750-05	4.0896-05	9.6555-03
KG/CUM	603.9775	637.5240	0.7455	1.1840	675.3548
AVG MW	54.0916	54.0916	28.9509	28.9509	69.9453

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STREAM SECTION

DMF FEED H2+AIR HEAVIES HEAVY-C

STREAM ID	DMF	FEED	H2+AIR	HEAVIES	HEAVY-C
FROM :	----	----	SEP-04	COL-01	HT-08
TO :	MX-01	HT-01	----	HT-08	----
SUBSTREAM: MIXED					
PHASE:	LIQUID	VAPOR	VAPOR	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
1,3-BD	0.0	108.1746	0.0	0.1177	0.1177
ISOBUTYL	0.0	56.7521	0.0	1.2602-02	1.2602-02
1-BUTENE	0.0	30.0738	0.0	7.8605-03	7.8605-03
N-BUTANE	0.0	10.5353	0.0	0.2065	0.2065
ISOBUTAN	0.0	11.7059	0.0	4.4916-05	4.4916-05
CIS-2B	0.0	9.9437	0.0	3.2361	3.2361
TRANS-2B	0.0	12.8541	0.0	1.1989	1.1989
BUTENYNE	0.0	1.8292	0.0	0.6011	0.6011
1-BUTYNE	0.0	0.5031	0.0	0.2296	0.2296
PROPANE	0.0	0.0	0.0	0.0	0.0
ALLENE	0.0	0.6793	0.0	5.7399-18	5.7399-18
PROPYNE	0.0	2.3775	0.0	2.6799-12	2.6799-12
ISOPENT	0.0	0.9430	0.0	0.6601	0.6601
DMF	15.0000	0.0	0.0	0.0	0.0
H2	0.0	0.0	33.4304	0.0	0.0
AIR	0.0	0.0	457.0373	0.0	0.0
WATER	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
KMOL/HR	15.0000	246.3716	490.4677	6.2704	6.2704
KG/HR	1096.4208	1.3608+04	1.3299+04	359.6999	359.6999
CUM/HR	1.6131	8475.2467	2347.0958	0.6120	0.5622
STATE VARIABLES:					
TEMP C	39.0000	150.0000	48.0000	59.9706	25.0000
PRES BAR	5.5729	1.0133	5.5729	5.5729	5.5000
VFRAC	0.0	1.0000	1.0000	0.0	0.0
LFRAC	1.0000	0.0	0.0	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
KCAL/MOL	-55.9695	11.4219	0.1508	-1.6511	-2.7651
KCAL/KG	-765.7123	206.7955	5.5600	-28.7817	-48.2015
GCAL/HR	-0.8395	2.8140	7.3943-02	-1.0353-02	-1.7338-02
ENTROPY:					
CAL/MOL-K	-106.8742	-37.7455	-2.4006	-71.0667	-74.5956

CAL/GM-K	-1.4621	-0.6834	-8.8533-02	-1.2389	-1.3004
DENSITY:					
MOL/CC	9.2988-03	2.9070-05	2.0897-04	1.0246-02	1.1153-02
KG/CUM	679.6925	1.6056	5.6662	587.7874	639.7883
AVG MW	73.0947	55.2327	27.1150	57.3647	57.3647

STREAM SECTION

ISOBUT-C ISOBUTYL PROPY-C PROPYNE R-01

STREAM ID	ISOBUT-C	ISOBUTYL	PROPY-C	PROPYNE	R-01
FROM :	HT-07	SEP-03	HT-09	COL-01	SEP-01
TO :	----	HT-07	----	HT-09	SEP-03
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
1,3-BD	0.0	0.0	2.1263-07	2.1263-07	0.8541
ISOBUTYL	56.7395	56.7395	1.9383-06	1.9383-06	56.7395
1-BUTENE	0.0	0.0	8.5775-07	8.5775-07	30.1867
N-BUTANE	10.3289	10.3289	3.4206-09	3.4206-09	10.3289
ISOBUTAN	11.7058	11.7058	1.3204-04	1.3204-04	11.7058
CIS-2B	0.0	0.0	2.8365-11	2.8365-11	424.7669
TRANS-2B	0.0	0.0	3.9372-10	3.9372-10	64.2804
BUTENYNE	0.0	0.0	4.1982-12	4.1982-12	0.0
1-BUTYNE	0.0	0.0	3.7654-14	3.7654-14	0.0
PROPANE	0.0	0.0	0.0	0.0	0.0
ALLENE	0.0	0.0	0.6791	0.6791	0.0
PROPYNE	0.0	0.0	1.6643	1.6643	0.0
ISOPENT	0.0	0.0	5.1926-20	5.1926-20	0.0
DMF	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0
AIR	0.0	0.0	0.0	0.0	0.0
WATER	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
KMOL/HR	78.7741	78.7741	2.3435	2.3435	598.8622
KG/HR	4464.2391	4464.2391	93.8924	93.8924	3.3643+04
CUM/HR	7.3354	7.7767	9.5790	0.1521	55.8735
STATE VARIABLES:					
TEMP C	25.0000	46.2387	25.0000	20.3663	46.2387
PRES BAR	5.5000	5.5729	5.5000	5.5729	5.5729
VFRAC	0.0	0.0	1.0000	0.0	0.0

LFRAC	1.0000	1.0000	0.0	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
KCAL/MOL	-16.6461	-15.9455	44.3960	39.8617	-7.6785
KCAL/KG	-293.7305	-281.3675	1108.0784	994.9053	-136.6792
GCAL/HR	-1.3113	-1.2561	0.1040	9.3414-02	-4.5983
ENTROPY:					
CAL/MOL-K	-85.5041	-83.2356	-9.9691	-25.4223	-74.7758
CAL/GM-K	-1.5088	-1.4687	-0.2488	-0.6345	-1.3310
DENSITY:					
MOL/CC	1.0739-02	1.0130-02	2.4464-04	1.5406-02	1.0718-02
KG/CUM	608.5868	574.0548	9.8019	617.2694	602.1341
AVG MW	56.6714	56.6714	40.0658	40.0658	56.1788

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STREAM SECTION

R-02 R-03 R-04 R-05 R-06

STREAM ID	R-02	R-03	R-04	R-05	R-06
FROM :	SEP-03	MX-02	HT-04	RX-01	CMP-02
TO :	MX-02	HT-04	RX-01	CMP-02	HT-05

CONV. MAX. REL. ERR:	5.3853-02	0.0	0.0	0.0	0.0
SUBSTREAM: MIXED					
PHASE:	LIQUID	MIXED	VAPOR	VAPOR	VAPOR
COMPONENTS: KMOL/HR					
1,3-BD	0.8594	0.8594	0.8594	34.2897	34.2897
ISOBUTYL	0.0	0.0	0.0	0.0	0.0
1-BUTENE	30.1845	30.1845	30.1845	0.1208	0.1208
N-BUTANE	0.0	0.0	0.0	0.0	0.0
ISOBUTAN	0.0	0.0	0.0	0.0	0.0
CIS-2B	410.5328	410.5328	410.5328	418.0593	418.0593
TRANS-2B	63.5183	63.5183	63.5183	52.6252	52.6252
BUTENYNE	0.0	0.0	0.0	0.0	0.0
1-BUTYNE	0.0	0.0	0.0	0.0	0.0
PROPANE	0.0	0.0	0.0	0.0	0.0
ALLENE	0.0	0.0	0.0	0.0	0.0
PROPYNE	0.0	0.0	0.0	0.0	0.0
ISOPENT	0.0	0.0	0.0	0.0	0.0
DMF	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	33.4304	33.4304

AIR	0.0	457.0373	457.0373	457.0373	457.0373
WATER	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
KMOL/HR	505.0950	962.1323	962.1323	995.5627	995.5627
KG/HR	2.8338+04	4.1570+04	4.1570+04	4.1570+04	4.1570+04
CUM/HR	46.7395	1.4698+04	4.1245+04	4.2683+04	9703.5286
STATE VARIABLES:					
TEMP C	46.2387	-21.8045	250.0000	250.0000	381.2093
PRES BAR	5.5729	1.0133	1.0133	1.0133	5.5729
VFRAC	0.0	0.7470	1.0000	1.0000	1.0000
LFRAC	1.0000	0.2530	0.0	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
KCAL/MOL	-6.7930	-2.9868	2.8128	3.6530	6.3317
KCAL/KG	-121.0793	-69.1290	65.1018	87.4877	151.6409
GCAL/HR	-3.4311	-2.8737	2.7063	3.6368	6.3036
ENTROPY:					
CAL/MOL-K	-74.3840	-36.5281	-19.4551	-17.6069	-16.4293
CAL/GM-K	-1.3258	-0.8454	-0.4503	-0.4217	-0.3935
DENSITY:					
MOL/CC	1.0807-02	6.5461-05	2.3327-05	2.3325-05	1.0260-04
KG/CUM	606.2941	2.8283	1.0079	0.9739	4.2840
AVG MW	56.1041	43.2056	43.2056	41.7548	41.7548

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STREAM SECTION

R-07 R-08 S-01 S-02 S-03

STREAM ID	R-07	R-08	S-01	S-02	S-03
FROM :	HT-05	SEP-04	HT-01	CMP-01	HT-02
TO :	SEP-04	MX-01	CMP-01	HT-02	COL-01
SUBSTREAM: MIXED					
PHASE:	VAPOR	LIQUID	VAPOR	VAPOR	LIQUID
COMPONENTS: KMOL/HR					
1,3-BD	34.2897	34.2897	108.1746	108.1746	108.1746
ISOBUTYL	0.0	0.0	56.7521	56.7521	56.7521
1-BUTENE	0.1208	0.1208	30.0738	30.0738	30.0738
N-BUTANE	0.0	0.0	10.5353	10.5353	10.5353
ISOBUTAN	0.0	0.0	11.7059	11.7059	11.7059
CIS-2B	418.0593	418.0593	9.9437	9.9437	9.9437
TRANS-2B	52.6252	52.6252	12.8541	12.8541	12.8541

BUTENYNE	0.0	0.0	1.8292	1.8292	1.8292
1-BUTYNE	0.0	0.0	0.5031	0.5031	0.5031
PROPANE	0.0	0.0	0.0	0.0	0.0
ALLENE	0.0	0.0	0.6793	0.6793	0.6793
PROPYNE	0.0	0.0	2.3775	2.3775	2.3775
ISOPENT	0.0	0.0	0.9430	0.9430	0.9430
DMF	0.0	0.0	0.0	0.0	0.0
H2	33.4304	0.0	0.0	0.0	0.0
AIR	457.0373	0.0	0.0	0.0	0.0
WATER	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
KMOL/HR	995.5627	505.0950	246.3716	246.3716	246.3716
KG/HR	4.1570+04	2.8271+04	1.3608+04	1.3608+04	1.3608+04
CUM/HR	4574.9363	46.7346	6505.4760	1380.7622	23.1531
STATE VARIABLES:					
TEMP C	48.0000	48.0000	55.0000	127.2738	48.0000
PRES BAR	5.5729	5.5729	1.0133	5.5729	5.5729
VFRAC	1.0000	0.0	1.0000	1.0000	0.0
LFRAC	0.0	1.0000	0.0	0.0	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
KCAL/MOL	0.2491	-4.6163	9.1005	10.7029	4.1608
KCAL/KG	5.9663	-82.4777	164.7661	193.7789	75.3317
GCAL/HR	0.2480	-2.3317	2.2421	2.6369	1.0251
ENTROPY:					
CAL/MOL-K	-29.0889	-72.6375	-43.9314	-42.7860	-62.4767
CAL/GM-K	-0.6967	-1.2978	-0.7954	-0.7747	-1.1312
DENSITY:					
MOL/CC	2.1761-04	1.0808-02	3.7871-05	1.7843-04	1.0641-02
KG/CUM	9.0864	604.9156	2.0917	9.8553	587.7290
AVG MW	41.7548	55.9707	55.2327	55.2327	55.2327

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STREAM SECTION

S-04 S-05 S-06

STREAM ID	S-04	S-05	S-06
FROM :	COL-01	MX-01	SEP-01
TO :	MX-01	SEP-01	SEP-02

SUBSTREAM: MIXED

PHASE:	LIQUID	LIQUID	LIQUID

COMPONENTS: KMOL/HR

1,3-BD	108.0569	142.3467	141.4926
ISOBUTYL	56.7395	56.7395	0.5731
1-BUTENE	30.0659	30.1867	0.0
N-BUTANE	10.3289	10.3289	0.0
ISOBUTAN	11.7058	11.7058	0.0
CIS-2B	6.7076	424.7669	0.0
TRANS-2B	11.6552	64.2804	0.0
BUTENYNE	1.2281	1.2281	38.0349
1-BUTYNE	0.2735	0.2735	8.4718
PROPANE	0.0	0.0	0.0
ALLENE	2.2554-04	2.2554-04	6.9852-03
PROPYNE	0.7133	0.7133	22.0898
ISOPENT	0.2829	0.2829	8.7614
DMF	0.0	15.0000	464.5587
H2	0.0	0.0	0.0
AIR	0.0	0.0	0.0
WATER	0.0	0.0	0.0
TOTAL FLOW:			
KMOL/HR	237.7578	757.8528	683.9893
KG/HR	1.3154+04	4.2521+04	4.5599+04
CUM/HR	22.4175	70.3748	67.8621
STATE VARIABLES:			
TEMP C	48.3678	48.1040	46.2387
PRES BAR	5.5729	5.5729	5.5729
VFRAC	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0
ENTHALPY:			
KCAL/MOL	3.9771	-2.9368	-28.4316
KCAL/KG	71.8849	-52.3420	-426.4778
GCAL/HR	0.9456	-2.2256	-19.4469
ENTROPY:			
CAL/MOL-K	-62.7912	-69.2142	-84.6689
CAL/GM-K	-1.1349	-1.2336	-1.2700
DENSITY:			
MOL/CC	1.0606-02	1.0769-02	1.0079-02
KG/CUM	586.7808	604.2093	671.9347
AVG MW	55.3260	56.1073	66.6661

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UTILITY SECTION

UTILITY USAGE: CHILL-W (WATER)

COOLING WATER, INLET TEMP=20 C, OUTLET TEMP=25 C
INPUT DATA:

INLET TEMPERATURE 3.0000 C
OUTLET TEMPERATURE 8.0000 C
INLET PRESSURE 1.0133 BAR
OUTLET PRESSURE 1.0133 BAR
HEAT TRANSFER COEFFICIENT 3224.4196 KCAL/HR-SQM-K
PRICE 1.6747-09 $/CAL
INDEX TYPE FUEL

RESULT:

COOLING VALUE 5.0122 KCAL/KG
INDEXED PRICE 1.6747-09 $/CAL

THIS UTILITY IS PURCHASED

USAGE:

BLOCK ID	MODEL	DUTY GCAL/HR	USAGE RATE KG/HR	COST $/HR
HT-06	HEATER	9.0466-02	1.8049+04	0.1515
HT-07	HEATER	5.5192-02	1.1011+04	9.2431-02
HT-08	HEATER	6.9853-03	1393.6568	1.1698-02
COL-01	RADFRAC	4.2287	8.4368+05	7.0819
	TOTAL:	4.3814	8.7414+05	7.3376

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UTILITY SECTION

UTILITY USAGE: CW (WATER)

COOLING WATER, INLET TEMP=20 C, OUTLET TEMP=25 C
INPUT DATA:

INLET TEMPERATURE 15.0000 C

OUTLET TEMPERATURE 25.0000 C
INLET PRESSURE 1.0133 BAR
OUTLET PRESSURE 1.0133 BAR
HEAT TRANSFER COEFFICIENT 3224.4196 KCAL/HR-SQM-K
PRICE 1.5110-09 $/CAL
INDEX TYPE FUEL

RESULT:

COOLING VALUE 9.9763 KCAL/KG
INDEXED PRICE 1.5110-09 $/CAL

THIS UTILITY IS PURCHASED

USAGE:

BLOCK ID	MODEL	DUTY GCAL/HR	USAGE RATE KG/HR	COST $/HR
SEP-03	SEP	4.6896-04	47.0072	7.0860-04
SEP-04	SEP	2.5058	2.5117+05	3.7862
HT-01	HEATER	0.5719	5.7328+04	0.8642
HT-02	HEATER	1.6118	1.6156+05	2.4355
HT-05	HEATER	6.0556	6.0700+05	9.1501
	TOTAL:	10.7456	1.0771+06	16.2367

UTILITY SECTION

UTILITY USAGE: ELECTR (ELECTRICITY)

ELECTRICAL UTILITY
INPUT DATA:

CO2 DATA SOURCE US-EPA-RULE-E9-5711
CO2 FUEL SOURCE COAL-ELECTRIC_POWER
CO2 EMISSION FACTOR 4.1654-07 KG/CAL
THERMAL EFFICIENCY 0.5800
PRICE 6.1170-02 $/KWHR
INDEX TYPE FUEL

RESULT:

INDEXED PRICE	6.1170-02	$/KWHR
CO2 EMISSION FACTOR	4.1654-07	KG/CAL
TOTAL CO2 EMISSIONS	2443.1066	KG/HR

THIS UTILITY IS PURCHASED

USAGE:

BLOCK ID	MODEL	DUTY GCAL/HR	USAGE RATE KW	COST $/HR	CO2E EMISSIONS KG/HR
CMP-01	COMPR	0.4387	510.1686	31.2070	315.0414
CMP-02	COMPR	2.9631	3446.1246	210.7994	2128.0651
	TOTAL:	3.4018	3956.2932	242.0065	2443.1066

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UTILITY SECTION

UTILITY USAGE: HPS (STEAM)

HIGH PRESSURE STEAM, INLET TEMP=250 C, OUTLET TEMP=249 C, PRES=572 PSIA
INPUT DATA:

INLET TEMPERATURE	254.0000	C
OUTLET TEMPERATURE	244.0000	C
INLET PRESSURE	41.0000	BAR
OUTLET VAPOR FRACTION	0.0	
HEAT TRANSFER COEFFICIENT	5159.0714	KCAL/HR-SQM-K
CO2 DATA SOURCE	US-EPA-RULE-E9-5711	
CO2 FUEL SOURCE	COAL-COMMERCIAL	
CO2 EMISSION FACTOR	4.2044-07	KG/CAL
THERMAL EFFICIENCY	0.8500	
PRICE	7.5572-08	$/CAL
INDEX TYPE	FUEL	

RESULT:

HEATING VALUE 418.2497 KCAL/KG
INDEXED PRICE 7.5572-08 $/CAL
CO2 EMISSION FACTOR 4.2044-07 KG/CAL
TOTAL CO2 EMISSIONS 5127.6255 KG/HR

THIS UTILITY IS PURCHASED

USAGE:

BLOCK ID	MODEL	DUTY GCAL/HR	USAGE RATE KG/HR	COST $/HR	CO2E EMISSIONS KG/HR
HT-03	HEATER	0.5543	1325.3200	41.8905	274.1826
HT-04	HEATER	5.5799	1.3341+04	421.6839	2760.0129
COL-01	RADFRAC	4.2323	1.0119+04	319.8412	2093.4299
	TOTAL:	10.3665	2.4785+04	783.4156	5127.6255

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UTILITY SECTION

UTILITY USAGE: LPS (STEAM)

LOW PRESSURE STEAM, INLET TEMP=125 C, OUTLET TEMP=124 C
INPUT DATA:

INLET TEMPERATURE 160.0000 C
OUTLET TEMPERATURE 150.0000 C
INLET PRESSURE 6.0133 BAR
OUTLET VAPOR FRACTION 0.0
HEAT TRANSFER COEFFICIENT 5159.0714 KCAL/HR-SQM-K
CO2 DATA SOURCE US-EPA-RULE-E9-5711
CO2 FUEL SOURCE COAL-COMMERCIAL
CO2 EMISSION FACTOR 4.2044-07 KG/CAL
THERMAL EFFICIENCY 0.8500
PRICE 5.9955-08 $/CAL
INDEX TYPE FUEL

RESULT:

HEATING VALUE 507.6747 KCAL/KG
INDEXED PRICE 5.9955-08 $/CAL
CO2 EMISSION FACTOR 4.2044-07 KG/CAL
TOTAL CO2 EMISSIONS 16.2302 KG/HR

THIS UTILITY IS PURCHASED

USAGE:

BLOCK ID	MODEL	DUTY GCAL/HR	USAGE RATE KG/HR	COST $/HR	CO2E EMISSIONS KG/HR
SEP-01	SEP	1.3837-02	27.2556	0.8296	6.8442
SEP-02	SEP	8.3495-03	16.4466	0.5006	4.1300
HT-09	HEATER	1.0626-02	20.9309	0.6371	5.2560
	TOTAL:	3.2813-02	64.6332	1.9673	16.2302

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PROBLEM STATUS SECTION

BLOCK STATUS

```
*****************************************************************************
*                                                                           *
* Calculations were completed with warnings                                 *
*                                                                           *
* The following Unit Operation blocks were                                  *
* completed with warnings:                                                  *
*   SEP-02    SEP-03    HT-03     HT-04                                     *
*                                                                           *
* All streams were flashed normally                                         *
*                                                                           *
* All Utility blocks were completed normally                                *
*                                                                           *
* All Convergence blocks were completed normally                            *
*                                                                           *
* All Sensitivity blocks were completed normally                            *
*                                                                           *
```

```
* All Calculator blocks were completed normally                    *
*                                                       *
*******************************************************************************
```

A-7: Input Summary for MATLAB Modeling

A-7a: 'pellet_geometric_properties' script

```
clear; clc
%constants
dpo = 4e-03;%outer pellet diameter (m)
dpi = 0.6*dpo;%hole diameter
H = 1.25*dpo;%pellet height
dt = 0.0525018;%tube diameter (m)

%supplementary calculations
Vfs = pi*( ( dpo/2 )^2 )*H;%full cylinder volume
Sfs = 2*pi*( ( dpo/2 )^2 ) + pi*dpo*H;%full cylinder surface area
Vi = pi*( ( dpi/2 )^2 )*H;%hole volume
Si = 2*pi*( ( dpi/2 )^2 ) + pi*dpi*H;%hole surface area
Vp = Vfs - Vi;%pellet volume
Ap = 2*pi*( ( dpo/2 )^2 - ( dpi/2 )^2 ) + pi*H*( dpo + dpi );%pellet surface area
dps = 2*( ( ( 3 / ( 4*pi ) )*Vp )^( 1/3 ) );%equivalent spherical diameter
a = dt/dps;%tube diameter to equivalent spherical diameter
```

A-7b: 'isothermal' function

```
function dFdW = isothermal(W,F)
dFdW = zeros(6,1);

%given
P0 = 1;%atm
Ntubes = 135;
FT0 = 962.132316219403/Ntubes;%kmol/hr
ka = 1.075;%hr^(-1) @523K
ke = 0.02732;%hr^(-1) @523K

%explicit equations
FT = F(1) + F(2) + F(3) + F(4) + F(5) + F(6);%kmol/hr
Pa = P0*( F(1)/FT )*( FT0/FT );%atm
Pb = P0*( F(2)/FT )*( FT0/FT );%atm
Pe = P0*( F(5)/FT )*( FT0/FT );%atm

%rate equations
ra1 = ka*Pa^(0.8)*Pb^(-0.2);
```

```
re1 = ke*Pe^(0.9)*Pb^(0.1);

%differential equations
dFdW(1) = (1/2)*(re1) - (5/4)*(ra1);
dFdW(2) = -(5/4)*(ra1) - (2)*(re1);
dFdW(3) = ra1 + re1;
dFdW(4) = dFdW(3);
dFdW(5) = (75/800)*ra1 - 2*re1;
dFdW(6) = (125/800)*ra1 + (1/2)*re1;
```

A-7c: ‘conversion’ script

```
clear;clc
%a = 1-butene
%b = oxygen
%c = 1,3-butadiene
%d = hydrogen
%e = trans-2-butene
%f = cis-2-butene

%number of tubes in Aspen reactor
Ntubes = 135;

%reactor feed flowrate
FT0 = 962.132316219403/Ntubes;%kmol/hr

%reactor feed compositions
xa0 = 0.0313724996172619;
xb0 = 0.475025439900785*(0.21);
xc0 = 0.000893201964958037;
xd0 = 0;
xe0 = 0.0660182481039897;
xf0 = 1 - ( xa0 + ( xb0/0.21 ) + xc0 + xd0 + xe0 );

%ode45 input parameters
F0 = [ xa0*FT0 , xb0*FT0 , xc0*FT0 , xd0*FT0 , xe0*FT0 , xf0*FT0 ];
Wspan = [ 0 4 ];

%ode solver for reaction differential equations
[W,F] = ode45('isothermal',Wspan,F0);

%conversion of 1-butene
W = real(W);
x_a = real((F0(1) - F(:,1))/F0(1));
%Aspen conversion is 99.6% - equivalent weight in MATLAB is 3.547
```

```
%kg/reactor tube

%weight to reactor tube length
L = ( W(1:52)/3.54710218061055 )*21;%ft

%Hydrogen to oxygen ratio in reactor
[r,c] = size(F);
H_O2 = zeros(r,1);
for i = 1:r
   H_O2(i) = real(F(i,4)/(F(i,2)*0.21));
end

%Conversion profile in a reactor tube
figure(1)
plot(L,x_a(1:52),'ko')
axis([ 0 21 0 1 ])
xlabel('Reactor tube length [ft])')
ylabel('X')
legend('Conversion of 1-butene','Location','northwest')

%Molar flowrates along a reactor tube
figure(2)
plot(L,real(F(1:52,1)),'ks',L,real(F(1:52,2)*0.21),'kv',L,real(F(1:52,3)),...
   'ko',L,real(F(1:52,4)),'kx')
axis([ 0 21 0 0.25 ])
xlabel('Reactor tube length [ft])')
ylabel('Molar flow rates [kmol/hr]')
legend('1-butene','oxygen','1,3-butadiene','hydrogen','Orientation','horizontal')

%Hydrogen to oxygen ratio inside a reactor tube
figure(3)
semilogy(L,H_O2(1:52),'kx')
axis([ 0 21 0.0001 10 ])
xlabel('Reactor tube length [ft])')
ylabel('Hydrogen:Oxygen')
legend('Hydrogen:Oxygen')
```

A-8: HAZOP Analysis

A comprehensive copy of the HAZOPtimizer tool in excel used for the HAZOP analysis in this project is included for the convenience and reference of the reader.

Company:	Team 2	**Drawing Numbers:**	NA
Facility:	Olefin Refinery- 1,3-Butadiene Production	**Unit/Process:**	Catalytic Reactor (reactor unit)
Date:	25-Apr-20	**Equipment and Lines:**	RX-01, R-04, R-05 (Reactor, inlet stream, outlet stream)
Design Intention:	Identify and mitigate risks for reactor unit and immediately surrounding lines		

Study HAZOP

Level A: 0
Level B: 0
Level C: 7
Level D: 9
Operating Issue: 0

Entry for Likelihood (L#) or Consequence (C#) out of range

Item No.	Deviation	Cause	Consequences	Engineering and Administrative Controls	L	C	R	Recommendations	Comments/ Questions
1.01	High flow	Valve failure, operator error	Catalyst damage, low conversion rate, over pressurizing	Alarms & interlocks for flowrates out of typical operating range	3	2	D	Display flowrates on operator PLC/SCADA to be visible at all times	Interlock closes valve to set %, causing excess incoming flow to bypass reactor to recycle back to mixer MX-01
1.02	No/low flow	Valve failure, operator error, leak in system, reboiler of separator too low, pressure drop inside reactor	Reactor can overheat	Steam alarm & interlock set for reactor temperature	3	3	C	Display temperature data on operator PLC/SCADA	
1.03	Back Flow	Check valve failure	Reactor can overheat	Steam alarm & interlock set for reactor temperature	3	3	C	Display flowrates temperature data on operator PLC/SCADA	
1.04	Loss of containment	Equipment failure- leak	Release of flammable vapors	Pressure relief devices to route flow to safety recycle line	2	4	C	Equipment inspection regularly per manufacturer's instruction and NFPA guidelines	
1.05	High pressure	Valve failure, operator error	Equipment damage causing loss of containment	Alarms, Interlocks, and Pressure relief devices	2	4	C	Display flowrates, temperature, and pressure data on operator PLC/SCADA	
1.06	Low Pressure	Valve failure, operator error, leak in system, inadequate flow causing low pressure	Reactor can overheat	Alarms, Interlocks, and Pressure relief devices	3	2	D	Display flowrates, temperature, and pressure data on operator PLC/SCADA	
1.07	Vacuum	Low pressure, compresser after reactor failing, closed valves causing double block	Implosion of any part of reactor, equipment damage, equipment failure, loss of containment	Alarms, Interlocks, and Pressure relief devices	1	3	D	Display flowrates, temperature, and pressure data on operator PLC/SCADA	
1.08	High temperature	Low flow to reactor	Reactor can overheat, equipment failure	Alarms, Interlocks	3	3	C	Display flowrates, temperature, and pressure data on operator PLC/SCADA	
1.09	Low temperature	High flow to reactor, blockage in steam line	Low conversion	Alarms, Interlocks	3	1	D	Display flowrates, temperature, and pressure data on operator PLC/SCADA	
1.10	Startup	Electrical or pneumatic failure, operator error	Overheating reactor, flash fire, friction in pipes from improper valve use	Interting reactor before startup, LEL interlock in reactor, SOP for startup process	2	4	C	Require operators to review SOP before startup, fill out JHA before startup	
1.11	Shutdown	Electrical or pneumatic failure, operator error	Overheating reactor, flash fire, friction in pipes from improper valve use	Interting reactor before shut down, LEL interlock in reactor, SOP for shut down process	2	4	C	Require operators to review SOP before shut down, fill out JHA before startup	
1.12	Emergency	Severe weather event (i.e. tornado), fire, global pandemic	Equipment damage, loss of containment, BLEVE	Evacuation procedures, emergency shutdown procedures, emergency preparedness procedures, isolation valves	1	4	D	NFPA guidelines for isolation valves in the event of an emergency to isolate flow and reduce the loss of containment and consequences thereof, training and procedures for employees reviewed	
1.13	Contaminants or Impurities	Air stream contamination, catalyst contamination or quality compromise	Affect conversion rate, change reaction, side reactions	Filter in air stream, quality check of catalyst in lab for replacement batches	2	3	D	Training for operators on hazards of operation, monitoring flowrates and conversion on PLC, LEL monitor in Hydrogen line, pressure relief valves on reactor	Severity varies drastically depending on nature of contamination
1.14	Corrosion/ erosion	Steam corrosion of pipes causing rust/ other damage	Reactor tubes breaking down, loss of containment	Inspectoins of piping thickness, SOP for additional inspection when removing coking from reactor tubes, monitor pressure readings in reactor tubes/annulus	3	1	D	Pressure sensors at different parts of reactor can indicate to operators where pressure losses or increases are occuring in the system. Designed intervals for inspection frequency. Inspection of piping thickness at high risk sections (joints, turns, and random intervals otherwise) is critical.	
1.15	Service Failure	Electrical or pneumatic failure, power outage, upstream supply disturbance for any relevant utility, unexpected shutdown of plant	Unexpected shutdown, which increases risk of any aforementioned parameter deviation	Operator procedure for unexpected shutdown, design of fail open/closed valves, pressure relief valve on reactor	2	3	D	Fail open valves: recirculation piping to absorb flow changes Fail closed valves: Incoming air stream, isolation valves Operator training on procedures and expectations in the event of an unexpected shut down or emergency	
1.16	Maintenance	Physical contact with catalyst	Adverse health affects	PPE, Permitting process, SOP for specific maintence tasks, JHA, review SDS	3	2	D	Respirators and gloves to prevent direct contact with catalyst, decontamination after, disposable paint suit	

Company:	Team 2	**Drawing Numbers:**	NA
Facility:	Olefin Refinery- 1,3-Butadiene Production	**Unit/Process:**	Catalytic Reactor (heat exchange before reactor)
Date:	25-Apr-20	**Equipment and Lines:**	HT-04, R-03, R-04
Design Intention:	Identify and mitigate risks for reactor unit and immediately surrounding lines		

		Level C:	4
	Level A: 0	Level D:	11	# Entry for Likelihood (L#) or Consequence (C#) out of range
Study: HAZOP	Level B: 0	Operating Issue:	0

Item No.	Deviation	Cause	Consequences	Engineering and Administrative Controls	L	C	R	Recommendations	Comments/ Questions
1.01	High flow	Valve failure, operator error	Heater cannot keep up with flowrate, stream does not get heated to 250 C, lower conversion	Alarms & interlocks for flowrates out of typical operating range	3	1	D	Display flowrates on operator PLC/SCADA to be visible at all times	
1.02	No/low flow	Valve failure, operator error, leak in system, reboiler of separator too low, pressure drop inside reactor	Heater could heat stream in excess of 250 C, changing reactor conversion, wasting energy, heater could overheat	Temperature, flow alarm & interlock set for inlet and outlet of heater	2	4	C	Display temperature data on operator PLC/SCADA	
1.03	Back Flow	Check valve failure	Stream not getting to heater, heater can overheat	Temperature, flow alarm & interlock set for inlet and outlet of heater	3	3	C	Display flowrates temperature data on operator PLC/SCADA	
1.04	Loss of containment	Equipment failure- leak	Release of flammable vapors	Pressure relief devices to route flow to safety recycle line	2	4	C	Equipment inspection regularly per manufacturer's instruction and NFPA guidelines	
1.05	High pressure	Valve failure, operator error	Equipment damage causing loss of containment	Alarms, Interlocks, and Pressure relief devices on heater	2	4	C	Display flowrates, temperature, and pressure data on operator PLC/SCADA	
1.06	Low Pressure	Valve failure, operator error, leak in system, inadequate flow causing low pressure	Reactor can overheat	Alarms, Interlocks	3	2	D	Display flowrates, temperature, and pressure data on operator PLC/SCADA	
1.07	Vacuum	Low pressure, closed valves causing double block in line before heater	Implosion of any part of heator, equipment damage, equipment failure, loss of containment	Alarms, Interlocks, and vacuum break device	1	3	D	Display flowrates, temperature, and pressure data on operator PLC/SCADA	
1.08	High temperature	Low flow to heater	Reactor can overheat, equipment failure	Alarms, Interlocks	2	3	D	Display flowrates, temperature, and pressure data on operator PLC/SCADA	
1.09	Low temperature	High flow to reactor, blockage in steam line	Damage to heater unlikely, would affect downstream processes	Alarms, Interlocks	3	1	D	Display flowrates, temperature, and pressure data on operator PLC/SCADA	
1.10	Startup	Electrical or pneumatic failure, operator error	Failure to start heater, stream not reaching adequate temperature	SOP for startup process of surrounding units	2	2	D	Require operators to review SOP before startup, fill out JHA before startup	
1.11	Shutdown	Electrical or pneumatic failure, operator error	Failure to shut down heater, heater running with no stream, overheating	SOP for shut down process of surrounding units	2	3	D	Require operators to review SOP before shut down, fill out JHA before startup	
1.12	Emergency	Severe weather event (i.e. tornado), fire, global pandemic	Equipment damage, loss of containment, BLEVE	Evacuation procedures, emergency shutdown procedures, emergency preparedness procedures, isolation valves	1	4	D	NFPA guidelines for isolation valves in the event of an emergency to isolate flow and reduce the loss of containment and consequences thereof, training and procedures for employees reviewed	Severity varies drastically depending on nature of disaster
1.14	Corrosion/ erosion	Steam corrosion of pipes causing rust/ other damage	Heater tubes breaking down, loss of containment	Inspectoins of piping thickness, SOP for additional inspection when removing coking from reactor tubes, monitor pressure readings in reactor tubes/annulus	3	1	D	Pressure sensors at different parts of reactor can indicate to operators where pressure losses or increases are occuring in the system. Designed intervals for inspection frequency. Inspection of piping thickness at high risk sections (joints, turns, and random intervals otherwise) is critical.	
1.15	Service Failure	Electrical or pneumatic failure, power outage, upstream supply disturbance for any relevant utility, unexpected shutdown of plant	Unexpected shutdown, which increases risk of any aforementioned parameter deviation	Operator procedure for unexpected shutdown, design of fail open/closed valves, pressure relief valve on reactor	2	3	D	Heater automatic shutdown in event of emergency or power loss, valves to isolate flow and prevent from continuing through process, possibly recycled	
1.16	Maintenance	Physical injury during maintenance, contacting hot surfaces	Burns, or other contact injuries	PPE, Permitting process, SOP for specific maintence tasks, JHA, review SDS	3	2	D	Mandatory cooldown time and temperature readings of heater before maintenance is performed	

A-9: Meeting Minutes

01/20/2020 Meeting Minutes

Project selection discussion:

Prior to the meeting, each team member investigated one of the suggested project topics. During this meeting, each member shared information about their investigated project.

- Gitau shared the articles and a summary of a few biochar-related projects.
- Delaney shared the Waste Fuel Upgrading to Acetone and Isopropanol project
- Lindsey shared the mixed C4 byproduct stream upgrade project
- Andy presented a whiskey distillery project, using ethanol separation membranes (novel preparation of familiar product)

After lots of consideration, we decided to pursue the mixed C4 byproduct stream upgrade as our senior design project.

Things to research this week:
- Reactions to upgrade major components of C4 waste stream
    - 1-Butene to 1,3-Butadiene
        - Catalytic oxidative dehydrogenation of 1-butene to 1,3-butadiene using CO2
- 14-page sample paper - skim through it and check references
- Refrigerants - figure out separation methods
- Possible BFD

01/25/2020 Meeting Minutes

Preliminary Project Presentation:
- Worked on Presentation
- Found Additional Literature to Research
- Made Gantt Chart
- Made BFD
- Made schedule for next couple months

1/27/2020 Meeting Minutes

Brief informal meeting after the first round of presentations to set priorities in the coming weeks. General takeaways listed below:
- Need more literature (30-40 sources)
    - Finding more literature will be the focus of this week, each person is expected to find roughly 10 papers that we can add to our collection, and begin reading them for useful information and processes

2/16/2020 Meeting Minutes

Need to do before next presentation:
- Finalize our design problem statement
- Finalize BFD
- Make preliminary PFD

- More literature search
- Compile literature survey
    - APA citations for each source
- Overall mass and energy balances
- Safety considerations
- Sustainability considerations
- Thermodynamic model???

Research possible reactions with the following as feed:

1,3-Butadiene: Lindsey
N-Butane: Andy
1-Butene: Delaney
Iso-Butene: Firdavs

Gitau will finish finding chemical prices

2/22/2020 Minutes

- Created presentation
- Refined process and problem statement
- Finalized BFD

2/23/2020 Minutes

- Finalize presentation for tomorrow's presentation
- Items needed in near future but not ASAP
    - Background information on extractive distillation
        - Why are there three preheaters before column 3 (is this normal for extractive distillation? It's a part of the older process *and* the newer process)
    - What exactly is going on in column ⅘ (high and low-pressure desorption)
        - Using a column for the PFD but we will need to figure out and finalize this to model it for real

03/01/2020 Meeting Minutes

Going over plan to complete needed items for next progress presentation
Individual work this meeting:
Lindsey:

- Added dehydrogenation process to PFD
    - Building on Firdavs' most updated PFD
- Added specs to get simulation to run
    - Will add more specific specs and increase accuracy throughout the week

Firdavs:

- Column 1 and 2 scale up to the Fabiano and Nedwick input (3-4 x bigger)

03/04/2020 Minutes

All of Team 2 present, meeting with Dr. Demiral

Discussed primarily the title of the project

- Reflect the innovation to the process in the title
    - Intermediant desorber and catalytic oxidative dehydrogenation
- Liked the concept of the phrasing"towards efficient rubber production"
    - Rather than increasing the scope of our project, we *will* add rubber to the title to bring humanity to the 1,3-Butadiene so that it is more relatable to the public
- Dr. D said he wanted us to include the "challenge, or problem or shortcoming and how we're addressing it"
- Also said our title was good but too long
    - Current title is in Delaney's notes so this is paraphrased:
    - Adding value to waste stream by way of oxidative dehydrogenation for more efficient production of rubber precursors

Questioned what we can do with the Hydrogen

- We could pipe it somewhere else
    - Lots of safety considerations and assumptions for where it's going
        - Local plant in the gulf coast, ex.
- We could burn it to create our own steam in house
    - This idea we all liked much better
    - Dr. D gave us the greenlight for starting work on this idea

3/8/2020 Meeting Minutes

- Progress check-up
- Took inventory of work left to complete before next progress presentation
    - Combine process units on Aspen (Gitau, Firdavs, Lindsey)
    - Perform sensitivity analysis/optimization
    - Update BFD and PFD
    - Pinch analysis (Delaney- after Aspen done)
    - Safety considerations (Andy)
    - Environmental considerations (Andy, broadly)

04/10/2020 Meeting Minutes

Zoom meeting, all present

- Most recent PFD is the PFD wtih Single Reactor document
- For CAPCOST, when distillation columns are too high, we will just choose the "calculate with columns in series" method
- Adjust scale to ⅓ the original, 15 tons/hr total

Hydrogen separation

- Separating hydrogen from cis/trans-2-butene and 1,3-butadiene
- Could condense x 1 to get rid of hydrogen

Utilities anticipated

- Cooling water
- Low or medium pressure steam
- Electricity

Catalyst

- Cost of chemicals to form catalyst
- Properties of catalyst
  - Toxicity etc.
- Figure out a way to price it
  - This could be raw materials and energy and labor
- Design an excel spreadsheet and keep track of assumptions along the way
  - Likely valid since this is new anyway

Lindsey to do:

- Design Excel spreadsheet for the catalyst cost estimation
  - Bismuth molybdate scheelite phase
- Do the memo per Dr. Demirel's guidelines
- Update our new feed flow rate assumption in the report

Gitau to do:

- Scale down reactor
- Start moving equations and work into report

Andy to do:

- Research safety of catalyst and work on the report

Delaney to do:

- Continue cost calculations as equipment is finished in simulation

Firdavs to do:

- Make the simulation work

Meeting Minutes 04/17/2020

Morning meeting on zoom (~9:30 CST)

- Delaney
- Andy
- Gitau
- Lindsey

Current simulation: Gitau Summary & Content

Started a new Aspen file to better understand the processes and units, guess and check won't cut it any longer.

PFD: Getting poor stream results, current PFD has no input of extragent (DMF) should be separating everything else out from the isobutene 1-butene, cis/trans still needs to be separated

Column 1: Pretty much functions as it should, refining this column more is likely more cost and trouble than worth
Worked on internals

Column 2:
- Gitau added/introduced DMF-- lowers energy requirements at the bottom of the column and increases separation. 1:10 or 1:12 ratio. Can likely be reduced significantly when we add the recycle stream.
- May want to sequence another column from the distillate to purify/increase separation and be able to sell out the isobutylene
- Worked on internals

Column 3:Trying to recover the DMF

Desorp-1: Trying to recover the DMF
Firdavs note: Desorp-2 is to purify extragent and intermediate desorbent from each other, can potentially be eliminated

Reactor: Works well, very confident in this unit

Other: Got rid of a few heat exchangers, will let HENS do its job for those calculations, no sense trying to work it all out ahead of time

Questions for Firdavs:
- The N-pentane in DESORP-1 makeup stream is for what?
    - Lowers total boiling point of the mixture, reduces cost in reboiler, does not help with separation
    - In literature somewhere
- How did you get the purity so high in your simulation (Col3_1.2.bkp) DesorbB1D, is this a simulated/calculated number or just an input of what we want? (It's >98%, and in PFD Single Reactor it is ~69%)
-

Big priorities:
1. We need to get the PFD to run so we can summarize results
    a. Even if it still needs to be optimized, we just need it to run
    b. Even if we can't get it for real, we still need a running basic PFD
2. How to separate the butenes from the 1,3-Butadiene (we can separate the isobutylene pretty good)

a. Is there another extragent? Is this what N-pentane is?
b. Delaney to proceed: Maybe take what comes off S-08 and use that as your starting point
c. Everything before Desorp-1 is good, work after that point in the PFD
3. Column optimization - later
    a. will take forever if we do what we did in class with the graphs etc.
    b. May be better to wing it but with GCC and CC (which look jank af rn)
    c. “We’re using the design specs and focusing on purity”
        i. Most columns we cannot use NQ curves
            1. Do we have too many species? Who knows

Tasks:

- Achieve a running PFD
    - Delaney, Andy, Lindsey, Firdavs
- Safety
    - Update list of chemicals, get missing SDS
        - Lindsey
    - Safety limits for equipment
    - Insulation
    - Isolation valves
        - Lindsey
    - Sizing
        - 10% safety limit etc.
    - Leave space for Gitau to talk about reactor safety
        - Temperature probes
        - Pressure sensors
    - Catalyst
        - Andy

Meeting Minutes 04/22/2020

Day of progress report turn-in: Zoom meeting start circa 2pm CST
Present: Lindsey, Andy, Delaney, Gitau -- Firdavs working on presentation unable to load zoom meeting

Working through finalizing details of the report and the presentation before submission:

- Lindsey, Andy, and Delaney pulling information from Aspen
    - NQ curves, stream tables, etc.
- Gitau adding descriptions to figures and tables in the catalyst section
- Lindsey and Delaney- proofreading through Gitau’s catalyst section
- All- revising and adding to the presentation slides
- Firdavs pulling report information to complete the presentation

Meeting Minutes 04/25/2020

Zoom meeting, 12:30 pm CST

Present: Lindsey and Delaney

Began working on HAZOP Analysis

- HAZOP Scope includes reactor, RX-01, and its inlet and outlet streams, R-04 and R-05

Meeting Minutes 04/26/2020

Zoom meeting, 1:30 pm CST
Present: Delaney, Gitau, Lindsey, Andy, Firdavs

- Finished HAZOP Analysis
- Did Multi-Criteria Decision matrix
- Discussed remaining sections of the report and distributed tasks
  - Delaney: feasibility analysis, fixing BFD, finish multi criteria decision matrix, email Demirel
  - Lindsey: adding HAZOP analysis to the report
  - Lindsey: add HAZOP acronyms to the table
  - Lindsey: Improve HAZOP analysis with additional deviation suggestions
  - Lindsey: Add BFD table (Stream names and compositions for inputs/outputs of the system)
  - Andy: Add temperature and pressure to stream table
  - Gitau: costs and disposal of catalyst research
  - Firdavs: fixing Demirel's edits on report and presentation, starting the executive summary
  - Group: Zoom Dr. D
    - Labeling of PFD?
      - Inputs and outputs, for main streams, add table for description
    - NQ curve
      - Creation of/ results of

Meeting Minutes 04/27/2020

Notes from Dr. Demirel when we asked about the generation of NQ curve/ how to improve ours

- Need 2 design specs to activate NQ curve
- System will give you a table for total number of stages
- Can select any by looking at last column, objective function value
- At minimum value, what is corresponding heat and total number of stages
- They are not in "vary" they are default manipulated variables by the NQ curve itself
- Setup: number of stages start from (ex.) 10-35 manipulated variable is number of stages, do not need a vary block, they're just boxes in the setup
  - Built-in optimization block
- Graph should be objective function (vertical) number of stages (horizontal)
  - Looking for sharp change in curve, more or less this is the minimum point to select
  - Looking for region in which you can work with a minimized reflux ratio or reboiler duty
  - Can pick out any value for the number of stages once you find this range

- In the graph you only see the total number of stages, so to find optimum feed location, look at the table (before you open the plot)
    - First column is feed stage location, second column is total number of stages
    - Select the minimum possible objective function value
- Worthwhile to work out minimum reflux ratio or reboiler/condenser duty because the project life is 15+ years so it all adds up
    - Maybe assume 17 years to increase value of catalyst, to get the full 15 years
- Fixed investment for number of stages will be the fixed original cost, and the duty/operating cost will continue to cost over time, so weigh this tradeoff
- Column targeting tools will show you loss over number of stages (different than NQ curve)
    - Both are for RADFRAC columns but this is a thermodynamic approach, whereas NQ curve is optimization method
    - Gives us GCC etc.
    - Shortcoming of Aspen is inability to show us if there is flooding somewhere during these optimization constraints etc. without us looking into it specifically.

Question about report feedback on PFD/BDF labeling for stream clarification

- When we say "feed" elaborate major composition and flowrate to display on BFD/PFD
- Example in Lecture 5 with labeled PFD, at least show flow rates
- BFD should include name of inputs and outputs but some values for flow rates/composition
- Ex. We can say "C-4 mixture" instead of just "Feed"
- Stream tables should also have Flow rate, Temperature, enthalpy, and Pressure
    - Idea is showing some mass/energy balance in a visual table
    - Gives insight for individual streams mass flow rates/ enthalpies/ etc. can be more useful than we are letting
- Fix figures vs tables (it's not about if it's a screenshot, think of the content and organization)
    - Fix if labels are on top or bottom
    - Label as table or figure
- HAZOP
    - In main text you can only show the risk matrix and all the rest can go into the appendix
    - HAZOP analysis will be in the appendix but the risk metrics can be in the main text. Will show how many A,B,C, and D you have
    - C's will need to be mitigated to D's etc.
        - See lecture 5 for risk metrics example
    - Risk metrics will come from HAZOPtimizer
    - "Detail of HAZOP analysis can be seen in Appendix XX"
- MATLAB model mention
    - Basically stick to one source, if you want to talk about MATLAB or Aspen pick one
    -
- Executive summary
    - Show results for
        - Economic
        - Sustainability
        - Safety

    - Show using charts, visuals,
    - “Management” is not interested in how the process works, they’re interested in the RESULTS/metrics
        - Pull numbers, make metrics visible, again, tables, charts, graphics

Meeting Minutes 04/27/2020

Finalizing report and final touches before turning in.
All members present

- Introduction for Table 18 - Lindsey
- Self-evaluation- Firdavs
- Minutes for today added to appendix - Lindsey
- NQ curve explanation- Delaney
- Happy belated birthday, Gitau!
- Team photo

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