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Biofuels for Aviation

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Abstract

Paraffinic Kerosene fuels are the backbone of commercial air travel. Kerosene fuels are primarily derived from petroleum processing and contribute significantly to carbon emissions globally. A variety of processes have been proposed to create renewable or semi-renewable sources of kerosene fuel suitable for aviation. One such process outlined in a 2019 white paper published by Gevo proposes the use of bio-based alcohol feed stocks to produce isobutanol which may be converted to kerosene mixtures through well-established dehydration and oligomerizations processes. The proposed Alcohol to Jet Fuel Pathway (ATJ-SPK) is a potentially net carbon neutral process which can greatly reduce the emissions generated by commercial air travel. The pathway would also allow airlines to integrate green Synthetic Paraffinic Fuel technology without expensive overhaul of existing fleets to accommodate new fuel sources, or research currently infeasible electric air travel (Gevo, 2019).

A plant was designed around the use of a Nickel-FM catalyst to convert feedstocks of ethanol and methanol to isobutanol via the Guerbet chemistry pathway (Olson et al., 2004). Due to the presence of side reactions and excess methanol feed, distillation and liquid-liquid separation were proposed as methods of delivering an isobutanol-water mixture to the downstream dehydration and oligomerization steps. The economics of the downstream processes are estimated and included in the profitability analysis along with a detailed estimation of the isobutanol production step. Selling the fuel product at market price was not found to be profitable; however, if a green premium of 4.55x is applied to the product fuel price the plant is 2 both technically and economically feasible. With the green premium levied on the price of the product fuel the Internal Rate of Return (IRR) is 15%, with a Net Present Value (NPV) of $51.7 MM, and a third year Return on Investment (ROI) of 13.58%. Significant market research is needed to assess the viability of the green premium that must be levied on the fuel price to yield a reasonable return. It may be the case that it is currently inadvisable to invest in the proposed plant but may become advisable in the coming years as consumer and regulatory awareness begins to grow over the environmental impacts of air travel.

Keywords

Guerbet chemistry, biojet fuel, isobutanol, isobutyl alcohol, 2-methyl-1-propanol

Disciplines

Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering

University of Pennsylvania, School of Engineering and Applied Science
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Dear Professor Bruce Vrana and Dr. Sean Holleran,

The enclosed report contains the technical and economic analysis for the conversion of ethanol and methanol to green kerosene fuel for aviation. The proposed process produces 140,000 short tons of isobutanol a year, which is subsequently dehydrated and oligomerized to produce 110,000 short tons of the target kerosene fuel ATJ-SPK (Alcohol-to-Jet Synthetic Paraffinic Kerosene). The plant will be located in Clinton, IA, and will operate on a continuous basis for 24 hours per day, 328.5 days per year. This will allow for over-the-fence acquisition of ethanol feedstock, and access to the Mississippi river for shipping purposes.

The technical focus of this report is the conversion of ethanol and methanol to isobutanol via Guerbet chemistry and a novel Ni-FM catalyst. The dehydration and oligomerization of isobutanol are well established processes, and while they are not analyzed from a technical standpoint, they are included in the economic analysis enclosed. The isobutanol production process consists of a reaction train and subsequent separation via distillation and liquid-liquid separation to yield a product which is 78 wt% isobutanol to be further purified after the dehydration step to nearly pure isobutene.

This process yields a 15% IRR with a 4.55x green premium applied to the selling price of the product jet fuel. While this green premium is currently high, the market for renewable fuel sources may develop quickly in the coming years as biomethanol becomes more readily available and crude oil begins to phase out of energy and fuel production. Before recommending this process, significant market research is needed to determine if the premium levied on the produced fuel is economically feasible.

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Biofuels for Aviation

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1. Abstract

Paraffinic Kerosene fuels are the backbone of commercial air travel. Kerosene fuels are primarily derived from petroleum processing and contribute significantly to carbon emissions globally. A variety of processes have been proposed to create renewable or semi-renewable sources of kerosene fuel suitable for aviation. One such process outlined in a 2019 white paper published by Gevo proposes the use of bio-based alcohol feed stocks to produce isobutanol which may be converted to kerosene mixtures through well-established dehydration and oligomerizations processes. The proposed Alcohol to Jet Fuel Pathway (ATJ-SPK) is a potentially net carbon neutral process which can greatly reduce the emissions generated by commercial air travel. The pathway would also allow airlines to integrate green Synthetic Paraffinic Fuel technology without expensive overhaul of existing fleets to accommodate new fuel sources, or research currently infeasible electric air travel (Gevo, 2019).

A plant was designed around the use of a Nickel-FM catalyst to convert feedstocks of ethanol and methanol to isobutanol via the Guerbet chemistry pathway (Olson et al., 2004). Due to the presence of side reactions and excess methanol feed, distillation and liquid-liquid separation were proposed as methods of delivering an isobutanol-water mixture to the downstream dehydration and oligomerization steps. The economics of the downstream processes are estimated and included in the profitability analysis along with a detailed estimation of the isobutanol production step. Selling the fuel product at market price was not found to be profitable; however, if a green premium of 4.55x is applied to the product fuel price the plant is both technically and economically feasible. With the green premium levied on the price of the product fuel the Internal Rate of Return (IRR) is 15%, with a Net Present Value (NPV) of $51.7 MM, and a third year Return on Investment (ROI) of 13.58%. Significant market research is needed to assess the viability of the green premium that must be levied on the fuel price to yield a reasonable return. It may be the case that it is currently inadvisable to invest in the proposed plant but may become advisable in the coming years as consumer and regulatory awareness begins to grow over the environmental impacts of air travel.

Keywords: Guerbet chemistry, biojet fuel, isobutanol, isobutyl alcohol, 2-methyl-1-propanol

2. *Introduction*

2.1 Background

Kerosene jet fuel is the most commonly used aviation fuel in conventional turboprop/turbofan style engines. The worldwide demand of jet fuel has been steadily climbing in recent decades with 96 billion gallons of fuel being used for commercial purposes in 2019 (Statista). Kerosene fuels have high energy density and allow jet powered aircraft to maintain a large thrust to weight ratio required for flight. Kerosene, also commonly referred to as paraffin, is a mixture of hydrocarbon chains between 10 and 16 carbons in length. The mixture may contain straight and branched alkanes, along with cyclohexanes of varying size. The mixture composition depends on geographic source and methods of processing used on crude oil, or other carbon source, to produce the kerosene (Chevron, 2007)

Kerosene fuels are produced largely via crude oil processing, which is relatively inexpensive and has provided for affordable jet fuel; however, crude oil is not a sustainable resource, and the use of crude oil fuels contributes significantly to pollution and the addition of greenhouse gases to the atmosphere. While other markets, such as the automotive and household energy markets can pivot to fully renewable electric and battery systems, the aviation market will require combustible fuel for the foreseeable future, as modern battery and electric systems cannot compete with conventional jet propulsion in terms of capacity or range.

2.2 Motivation and Goals

A 2019 white paper by the company Gevo discusses the potential importance of the Alcohol to Jet Fuel pathway as means to create a closed carbon loop in the aviation fuel industry. Ethanol derived from carbon consuming corn, and methanol can be transformed into isobutanol, which then may be dehydrated to isobutene and oligomerized to longer carbon chains which make up Synthetic Paraffinic Kerosene (SPK), a substitute for kerosene derived from crude oil. Carbon emission that occurs during fuel combustion is offset by the carbon consumption of corn used in the feedstocks. The process is theoretically carbon neutral and thus a potential alternative to petroleum derived jet fuel.

Gevo has proposed the use of a propriety fermentation method to produce isobutanol from yeast and corn. While Gevo has seen viability in the process another proposed process is the use of Guerbet chemistry to produce a mixture of larger alcohols and other byproducts from ethanol and methanol feeds. The goal of this design project is to investigate the viability of a process based on the research presented in *Higher-Alcohols Biorefinery* which shows a 90% yield of isobutanol in a Guerbet reaction conducted in a Ni-FM catalyst bed reactor (Olson et al. 2004). Originally the economic goal of the process was to create a process with a transformational cost of $0.50/kg of jet fuel. This goal was updated, and instead a sensitivity analysis was conducted on the selling price of the product jet fuel to yield an IRR of 15%. Along with the economic goals, the process was also designed to be a relatively eco-friendly process, with adequate recycle and heat integration in order to minimize waste and utility usage.

3. *Objective Time Chart*

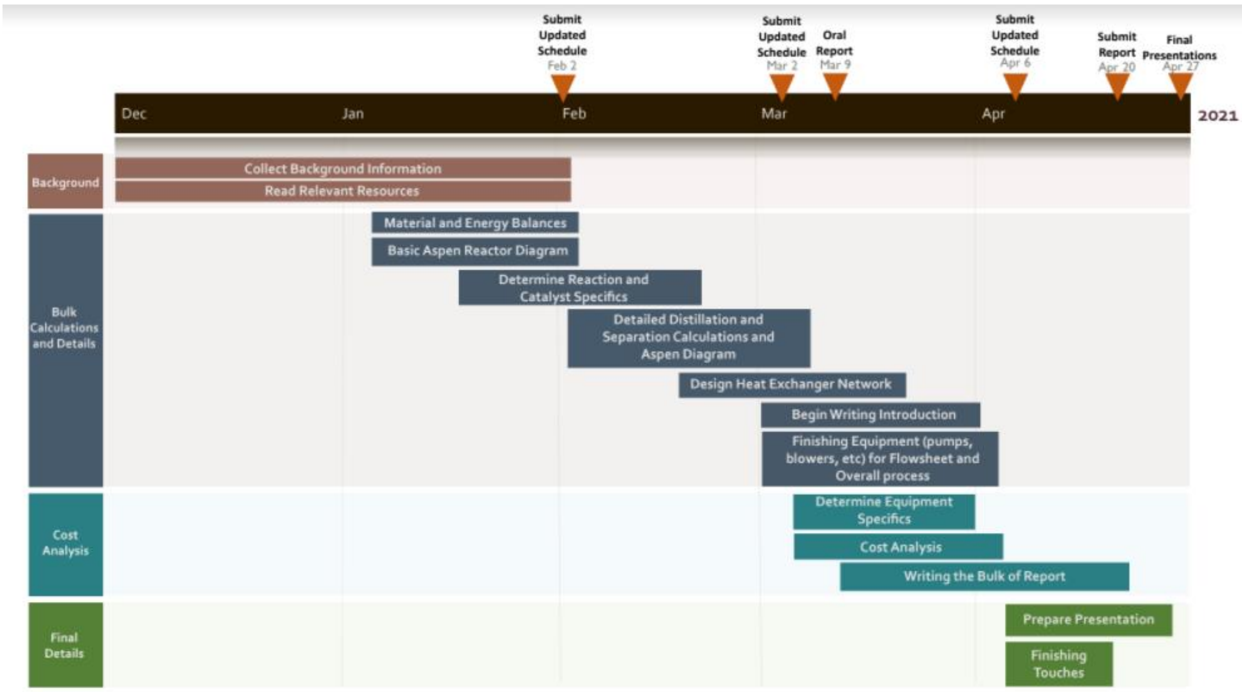

Figure 3.1 Objective Time Chart for project and proposal completion.

4. Innovation Map

N/A

5. Market and Competitive Analysis

5.1 Market Analysis

The market for environmentally friendly energy continues to grow as society faces the increasing effects of climate change. As shown in Figure 5.1.1, over the past six years the market demand for bioenergy has grown and is expected to continue increasing. Aviation is a huge factor in carbon emissions per year, making this mode of transportation desperately in need of a more sustainable energy source (Renewable Power Generation Market Size Report, 2020). While methods of land travel, such as cars, have adapted to using electricity as a more environmental fuel source, batteries are not yet available to be used in aviation due to their lack of duration and heavy weight. This emphasizes the importance and demand of creating a reasonably priced biofuel to replace the conventionally used jet fuel. As more carbon taxes and climate change regulations get implemented, airline companies will be looking to purchase alternative sources of jet fuel.

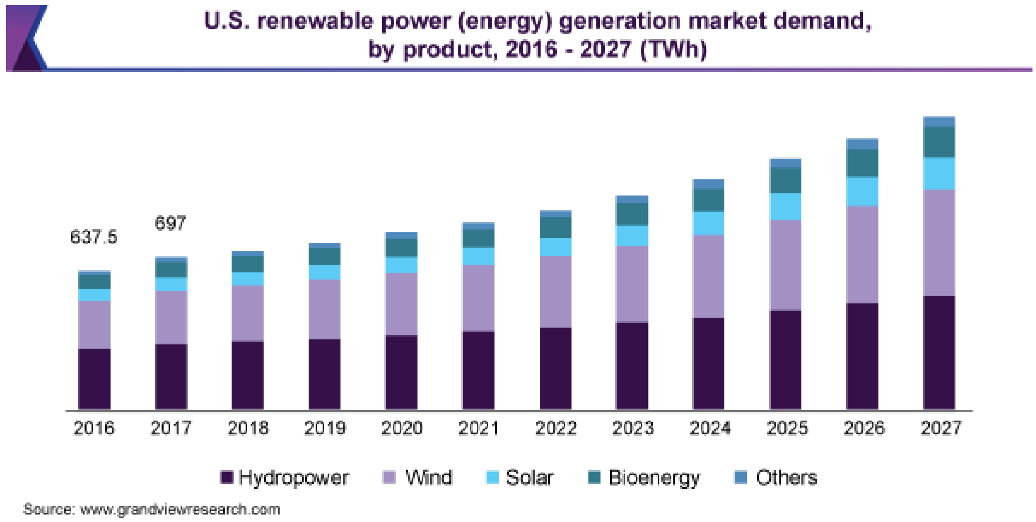

Figure 5.1.1 Market trends and resulting expectations of sustainable energy sources for the years 2016-2027.

5.2 Competitive Analysis

While demand increases due to governmental policies and pollution taxes, it is also increasing because of the consumer's desire to purchase sustainable products. Since 2014, investment in global sustainability and environmentally friendly consumer products has increased by 68%. This means that consumers are driving the market interest towards eco-friendly products and companies are looking to advertise how green they are.

A study about the consumer market in 2020 shows that nearly 57% of consumers are willing to purchase products directly invested in benefitting the environment. Most of these environmentally conscious consumers also state they would be willing to pay a green premium on these products (Haller, 2020). Figure 5.2.1 shows another study outlining the maximum percent premium consumers would be willing to pay for different industries. As shown, they found that about 80% of consumers are willing to pay a 5% premium cost for a green automotive product, but this drops to about 10% of consumers when the premium hits 25% (Miremadi, 2012). While the premium for eco-friendly jet fuel may be too high for consumers to purchase green plane tickets today, these studies show that there is value in an environmentally manufactured product.

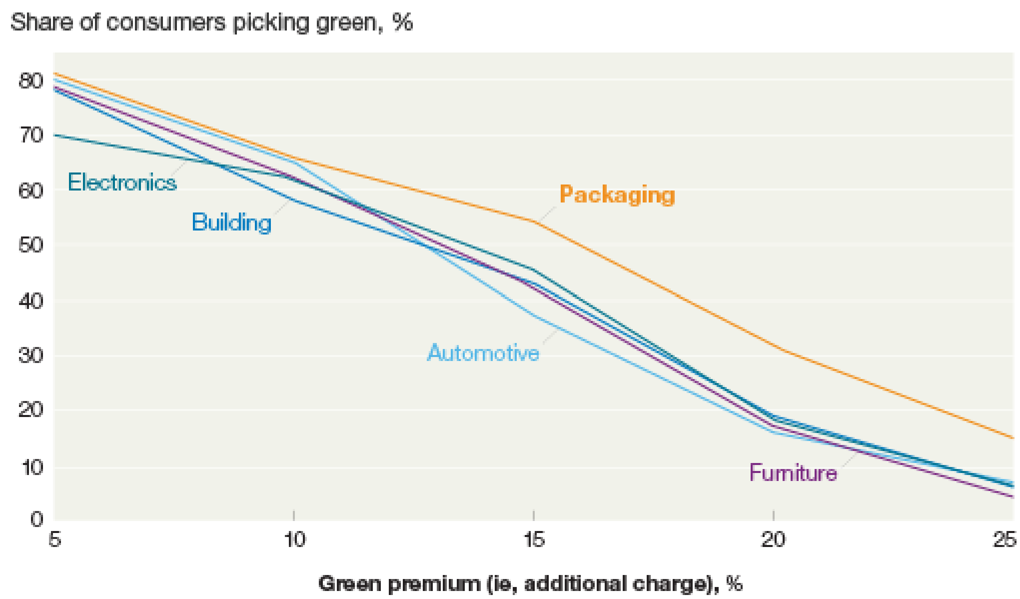

Figure 5.2.1 Trends of percent green premium consumers are willing to pay in different industries.

The environmentally produced jet fuel in this report is not net-zero carbon emission, as it would be difficult to acquire enough renewable energy to meet the needs of the entire process, although it is a step in the eco-friendly direction. As sustainable energy demands raise and consumers continue to drive the market to be more environmentally conscious, biofuel may become a more legitimate source for aviation.

6. *Customer Requirements*

To be charged a green premium on airline ticket price, consumers are expecting a jet fuel product that has been officially deemed sustainable and meets strict environmental certifications. As shown in Figure 6.1, consumers buying products that claim to be sustainable both rely on brand trust and do their own research before purchasing (Haller, 2020). Therefore, this jet fuel must obey eco-friendly regulations to appeal to the targeted audiences.

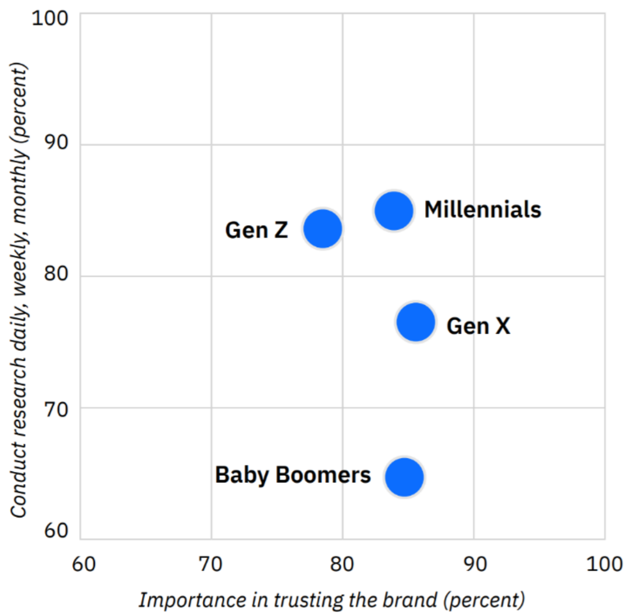

Figure 6.1 Percent of personal research conducted and value of brand trust for consumers in various generations.

The consumers also expect their air flight experience with biofuel to be the exact same as with conventional jet fuel. As the product from this process has the same composition of jet fuel made from other sources, they will perform the same (Gevo, 2019).

7. Product Requirements

N/A

8. Product Concepts

N/A

9. Superior Product Concepts

N/A

10. Competitive (Patent) Analysis

This process was modelled around the ideas presented in the white paper titled *Sustainable Aviation Fuel* released by Gevo in 2019. The paper details six different possible biofuels for aviation: hydro-processed esters and fatty acids (HEFA-SPK), synthetic gas Fischer-Tropsch synthesized paraffinic kerosene (FT-SPK), power-to-liquids Fischer-Tropsch synthesized paraffinic kerosene (PtL FT-SPK), synthesized isoparaffins (SIP), and alcohol-to-jet synthesized paraffinic kerosene (ATJ-SPK). ATJ-SPK was chosen over the other options for a variety of reasons. As aviation biofuels are in their beginning stages of development, viable fuel options need to be supplemented with convention jet fuel and thus must have a very similar composition to allow for mixing. This requirement eliminated SIP and some variations of HEFA-SPK as possible options. The feedstock was also an important consideration, and ATJ-SPK had an advantage over FT-SPK and ptL FT-SPK, as corn is more readily available and beneficial than synthesis gas. Furthermore, the infrastructure to produce bioethanol already exists which reduces the carbon footprint as opposed to starting from scratch (Gevo, 2019).

The final product of the process detailed in this report is isobutanol, which is then sent to separate dehydration and oligomerization procedures before becoming jet fuel. To optimize the production and purification of isobutanol, two different dehydration steps were analyzed. One patent, by Total Petrochemicals Research Feluy, allowed for a mixture of 95 mass% isobutanol and 5 mass% water to be fed to the dehydration step for full conversion to be observed (Simultaneous Dehydration, 2011). However, other literature titled *Dehydration of Fermented Isobutanol for the Production of Renewable Chemicals and Fuels*, stated that a mixture of 85 mass% isobutanol and 15 mass% water was sufficient to achieve conversion over 99% (Taylor et al., 2010). Cost analysis showed that the money saved from a decrease in final purity was more substantial to money lost due to conversion rates and extra equipment. Therefore, the Total Petrochemicals Research patent was not used for this process.

11. Preliminary Process Synthesis

Numerous alternative designs were considered throughout the project. Some of these ideas will be presented here.

11.1 Combined Reactor/Exchangers

Because the exothermic reaction was conducted isothermally in the paper that bases this project, it was of initial priority to design an isothermal reactor sequence around the reaction temperature of 360 °C. To accomplish this, it was proposed to use reactor/heat exchanger combination equipment to perform the Guerbet chemistry reactions similar to the reactors used in butane oxidation to form maleic anhydride. The reactors would have looked like shell and tube heat exchangers with the reactive stream flowing through the tubes and a cooling fluid on the shell side.

However, issues were raised due to the high surface area on the tubes required for the reaction. This surface area was a result of the reaction needs and was not based on heat removal considerations. First, it was proposed to use the latent heat of vaporization of water to cool the reactive streams. However, due to the large temperature difference and surface area for heat transfer, an overall heat transfer coefficient of ~2 $W/m^2 \cdot K$ was required. The heat transfer coefficient for producing 450 psig (~30 bar) steam at 236 °C is estimated to be between 10 and 40 $W/m^2 \cdot K$. Thus, producing 450 psig steam would have resulted in an over-cooling of the reactive stream. Then, it was proposed to use lower pressure, 160 psig (~10 bar) steam and superheat it in the reaction cooling process. The estimated heat transfer coefficient for this process is 3 to 10 $W/m^2 \cdot K$, still too high for the process. Also, an estimated 220,000 lb/hr of the 160 psig steam would be required, likely making the process uneconomical. Using molten salts as the cooling fluid was then considered. The molten salts would not vaporize, and after being heated, would be used to generate steam in a separate exchanger. This would again by similar to the process used in the butane oxidation reaction to form maleic anhydride. Ultimately, a less complex reactor/cooling network was chosen and is discussed in detail in Section 14.2 involving the use of five adiabatic packed bed reactors in series with steam-generating kettle reboilers cooling the effluent after each reactor.

11.2 Pre-distillation Flash Drum

As discussed in the Guerbet chemistry section (Section 12.3), many light gases are formed as byproducts in the reaction from methanol and ethanol to isobutanol and water. It was hypothesized early that a flash drum would be greatly beneficial prior to the effluent stream entering the first distillation column. The flash drum would cause nearly all of the light gases to be separated from the effluent prior to the first column.

However, processes were also considered and analyzed that did not include this preliminary flash drum. Because the condenser in the first column was decided to be a partial condenser, it was theorized that a prior flash drum would not be necessary as the light gases could exit the column in the vapor distillate while the majority of the methanol was recovered in the liquid distillate. Upon realization that the first column needed to be operated under vacuum, this alternative was ultimately discarded as it became important for the vacuum pump to have a small load. By utilizing a pre-distillation flash drum, the load on the vacuum pump is drastically reduced.

11.3 Reusing Hot Condensate in Second Column Reboiler

The chosen reactor/cooler network produces 150 psig steam for use in the separation steps. Initially, it was considered that the steam would supplement the required additional steam for the reboilers of the first distillation column. The steam produced in the process was ~11% of the steam required in these reboilers. Then, the hot condensate leaving the first reboilers was considered to be the heating source for the reboiler of the much smaller, second distillation column. However, this process implementation would confuse the economics for the plant's required steam utility because the quoted price for steam assumes that saturated liquid water is returned to the boiler house, not subcooled condensate.

Ultimately, a more straightforward use of the steam generated was chosen. The steam generated is first sent to the reboiler of the smaller, second column. Only a small amount of the generated steam is required in this reboiler. Then, the remaining generated steam is again used to supplement the steam required for the first column's reboilers now providing ~10% of the required steam. For a deeper discussion of this process, see Section 15.2.

11.4 Plant Location

After design of the first distillation column, a plant location on the Gulf Coast was considered for equipment shipping purposes. It was desired to have the plant near a large body of water to facilitate the delivery of this large diameter column (~20 ft) as transportation by road was likely impossible. Ultimately, it was determined that a plant location closer to major sources of the ethanol feed stock was more preferential. This led to a plant location adjacent to an ethanol plant in Iowa with river access provided via the Mississippi River for column transportation.

12. *Assembly of Database*

12.1 Price of Raw Materials, Utilities, Products, and Byproducts

The prices of the raw materials, utilities, products, and byproducts can be seen in Table 12.1.1. For the process, catalyst regeneration is treated as a raw material, the final product is the biojet fuel, and a stream with significant fuel value is sold to a boiler house as byproduct. A breakdown of the annual costs and costs per unit of jet fuel can be found for each entity in Section 20. The utility prices were taken from Chapter 17 of *Product and Process Design Principles* (Seider et al., 2017). The ethanol feed price was taken as the 5-year average ethanol price. A 5-year average was also taken for the methanol feed price with an additional 2x "green premium" factor applied to assume the methanol was sourced from bio-products. The product price was the multiplication of conventional jet fuel and a green premium factor for biojet. The price of the boiler house fuel byproduct was taken to be equal to the price of natural gas. More details on the pricing can be found in Section 22.

Table 12.1.1 Prices of Raw Materials, Utilities and Products

Entity	Economic Designation	Cost (USD) per Unit
Biomethanol	Raw Materials	$0.36/lb
Ethanol		$0.23/lb
Catalyst Regeneration		$5.00/lb
Boiler House Fuel	Byproduct	$5.00/1,000 SCF
Biojet Product	Product	$1.09/lb
Steam (150 psig)	Utilities	$7.00/1,000 lb
Cooling Water		$0.10/1,000 gal
Electricity		$0.070/kW-hr
Natural Gas		$5.00/1,000 SCF
Refrigerant (chilled water/glycol)		$1.75/ton-day
Wastewater Treatment		$0.15/lb organic removed

12.2 Chemical Toxicities of Major Chemicals

The Material Safety Data Sheets (MSDSs) for the major components in the process are provided in the appendix (Section 26.2). For brevity, the MSDSs for methanol, ethanol, isobutanol, and water have been chosen to be included and were found on chemicalsafety.com. As desired, the MSDSs of the minor components can be found on the same site.

12.3 Guerbet Chemistry Reactions

The process is built around the Guerbet Chemistry Reactor Sequence, which was researched by Olson et al. (2004). Guerbet chemistry involves numerous reactions to eventually produce isobutanol from methanol and ethanol feeds. All of the reactions involved can be seen in Figure 12.3.1. The nomenclature 2-methyl-1-propanol is identically isobutanol.

$$CH_3OH \rightarrow CH_2{=}O + H_2 \quad (1)$$

$$CH_3CH_2OH \rightarrow CH_3CH{=}O + H_2 \quad (2)$$

$$CH_2{=}O + CH_3CH{=}O \rightarrow HOCH_2CH_2CH{=}O \rightarrow CH_2{=}CHCH{=}O + H_2 \quad (3)$$

$$CH_2{=}CHCH{=}O + 2H_2 \rightarrow CH_3CH_2CH_2OH \ (1\text{-propanol}) \quad (4)$$

$$CH_3CH_2CH{=}O + CH_2{=}O \rightarrow HOCH_2CH(CH_3)CH{=}O \quad (5)$$

$$HOCH_2CH(CH_3)CH{=}O + 2H_2 \rightarrow CH_3CH(CH_3)CH_2OH \ (2\text{-methyl-1-propanol}) \quad (6)$$

$$2CH_3CH{=}O \rightarrow CH_3CH{=}CHCH{=}O + H_2O \quad (7)$$

$$CH_3CH{=}CHCH{=}O \overset{H_2}{\rightarrow} CH_3CH_2CH_2CHO \overset{H_2}{\rightarrow} CH_3CH_2CH_2CH_2OH \quad (8)$$

$$CH_3CH_2CH_2CH{=}O + CH_2{=}O \rightarrow \rightarrow CH_3CH_2CH(CH_3)CH_2OH \quad (9)$$

Figure 12.3.1 Full Guerbet chemistry reaction sequence.

The full reaction path is complicated, but it can be broken down and generalized to the “net” reaction shown in Figure 12.3.2. The large amount of water formed in the reaction along with the presence of numerous light alcohols are what causes the non-ideality in the downstream separation steps.

2 Methanol + Ethanol → Isobutanol + 2 Water

Figure 12.3.2 “Net” Guerbet chemistry reaction.

No kinetic data was provided by in the research paper by Olson et al. (2004). Instead, yields were given for the reaction. Table 12.3.1 shows the yields to the light gas products. Ice traps were used to analyze the yields to alcohols and heavier products as shown in Table 12.3.2. The Ni-FM case was used as the base for this project in Table 12.3.2. Again, note that 2-Me-1-PrOH is identically isobutanol. Also, please note that the nitrogen was used as the carrier gas in the laboratory experiment, so that is why it appears in Table 12.3.1. Nitrogen was assumed to not be present in the analysis for this process which does not require a carrier gas.

Table 12.3.1 Yields to the Light Gas Byproducts

Gas	Weight (mg)	mmol	Composition (mmol%)
Hydrogen	3.0	1.500	8.40
Carbon dioxide	8.1	0.200	1.12
Propane	0.7	0.015	0.08
Acetylene	3.5	0.140	0.78
i-Butane	1.5	0.026	0.15
t-Butane	3.2	0.055	0.31
trans-2-Butene	1.6	0.028	0.16
cis-2-Butene	7.0	0.123	0.70
Ethene	1.2	0.040	0.22
Oxygen	2.8	0.087	0.49
Methane	4.0	0.230	1.30
Carbon monoxide	8.2	0.293	1.64
Nitrogen	424.6	15.153	84.65
Total	44.7	17.900	100.00

Table 12.3.2 Yields to the Alcohols and Heavier Products

Catalyst	Recovered MeOH (mmol)	Recovered EtOH (mmol)	EtOH conversion (%)	2-Me propanal (mmol [%])	1-PrOH (mmol [%])	2-Me-1-PrOH (mmol [%])	2-Me-1-BuOH (mmol [%])	Others (mmol)
FM	89.03	0	100	1.13 (7)	0.44 (3)	13.19 (76)	0.28 (3)	1.3
Ni-FM	89.25	0	100	0.15 (1)	0.60 (3)	15.69 (90)	0.15 (2)	1.1

[a] Flow rate, 0.1 mL/min; carrier flow, 66 cm^3/min; MeOH, 125 mmol; EtOH, 17.4 mmol; temperature, 360°C; time, 60 min. Percentages given in parenthesis refer to percent yield based on millimoles of product per millimole of ethanol converted.

The yields given were then used to scale up the process to produce the required amount of isobutanol, and in turn, jet fuel per year. Note that the yields above do not include water and also include an arbitrary “Others” category. To account for the water formed in the reaction, an atom balance was performed after scaling the process up to produce the required amount of isobutanol. The results of the atom balance showed that there was slightly more carbon entering the process than leaving and much more hydrogen and oxygen entering the process than leaving as expected due to the lack of accounting for water in the product. To close the atom balance, first the small amount of “extra” carbon was assumed to be sourced from methanol, the dominant species in the process by mass. After the carbon, hydrogen, and oxygen allotment to methanol, the remaining hydrogens were all assumed to be sourced from water. After the allotment of the hydrogen and associated oxygen to water, the small amount of remaining oxygen was assumed to be from oxygen gas. After these corrections, the mass balance error was less than a hundredth of a percent.

12.4 ASPEN PLUS Chemical Alias Mapping

For convenience, a mapping of the ASPEN PLUS chemical IDs and aliases to the full chemical names is provided on the succeeding page in Table 12.4.1.

Table 12.4.1 ASPEN PLUS ID/Alias to Chemical Name

ASPEN PLUS ID	ALIAS	FULL CHEMICAL NAME
METHANOL	CH4O	METHANOL
ETHANOL	C2H6O-2	ETHANOL
IB-ALDEH	C4H8O-2	ISOBUTYRALDEHYDE
PROPANOL	C3H8O-1	1-PROPANOL
ISBUT-OH	C4H10O-3	ISOBUTANOL
2-ME1BOH	C5H12O-2	2-METHYL-1-BUTANOL
H2	H2	HYDROGEN
CO2	CO2	CARBON-DIOXIDE
PROPANE	C3H8	PROPANE
C2H2	C2H2	ACETYLENE
ISOBU-01	C4H10-2	ISOBUTANE
N-BUT-01	C4H10-1	N-BUTANE
TRANS-01	C4H8-3	TRANS-2-BUTENE
CIS-2-01	C4H8-2	CIS-2-BUTENE
C2H4	C2H4	ETHYLENE
O2	O2	OXYGEN
CH4	CH4	METHANE
CO	CO	CARBON-MONOXIDE
WATER	H2O	WATER
IBUTENE	C4H8-5	ISOBUTYLENE
PROPENE	C3H6-2	PROPYLENE
2ME1BENE	C5H10-5	2-METHYL-1-BUTENE
IBUTENE	C4H8-5	ISOBUTYLENE
PROPENE	C3H6-2	PROPYLENE
2ME1BENE	C5H10-5	2-METHYL-1-BUTENE

12.5 ASPEN PLUS Simulation Specifications/Parameters

All of the chemicals in the process are conventional chemicals in the ASPEN PLUS database. To handle the non-ideality of the reactor effluent streams as well as the liquid-liquid phase separation required for a decantation step, the NRTL property method was used as recommended by Professor Len Fabiano. The binary interaction parameters pulled from ASPEN PLUS's database can be seen in Table 12.5.1 for the relevant chemical species.

Table 12.5.1 NRTL Binary Interaction Parameters

Component i	Component j	Source	Temp. Units	A_{ij}	A_{ji}	B_{ij}	B_{ji}	C_{ij}	T_{lower}	T_{upper}
METHANOL	ETHANOL	APV110 VLE-IG	C	4.7119	-2.3127	-1162.2949	483.8436	0.3	20	78.4
METHANOL	PROPANOL	APV110 VLE-IG	C	0	0	19.5547	-8.8867	0.3	60.02	97.12
METHANOL	ISBUT-OH	APV110 VLE-IG	C	-16.0411	14.3289	5443.7725	-4751.3677	0.3	40	70
METHANOL	N-BUT-01	APV110 VLE-LIT	C	0	0	380.4331	551.7243	0.3	50	50
METHANOL	WATER	APV110 VLE-IG	C	-0.693	2.7322	172.9871	-617.2687	0.3	24.99	100
ETHANOL	PROPANOL	APV110 VLE-IG	C	8.2606	-9.721	-2846.6829	3409.6863	0.3	40	97.16
ETHANOL	ISBUT-OH	APV110 VLE-IG	C	-0.3474	-0.8327	167.9138	252.5334	0.3	40	105.9
ETHANOL	WATER	APV110 VLE-IG	C	-0.8009	3.4578	246.18	-586.0809	0.3	24.99	100
IB-ALDEH	ISBUT-OH	APV110 VLE-IG	C	0	0	504.1191	-282.9924	0.3	63.3	107.3
IB-ALDEH	WATER	APV110 LLE-ASPEN	C	-2.3344	8.2408	987.1738	-1408.5771	0.2	26.45	67.95
PROPANOL	ISBUT-OH	APV110 VLE-IG	C	-0.9906	0.7245	110.2754	69.2322	0.3	40	106.8
PROPANOL	N-BUT-01	APV110 VLE-IG	C	0	0	193.2439	314.7243	0.3	10	40
PROPANOL	WATER	APV110 VLE-IG	C	-1.7411	5.4486	576.4458	-861.1792	0.3	25	100
ISBUT-OH	WATER	APV110 VLE-IG	C	0	0	-23.0994	1343.6896	0.3	89.67	106.6
2-ME1BOH	WATER	APV110 LLE-ASPEN	C	-1.8935	9.9206	410.6462	-1319.3188	0.2	20	30
N-BUT-01	TRANS-01	APV110 VLE-IG	C	0	0	-167.7039	227.2447	0.3	5	5
N-BUT-01	CIS-2-01	APV110 VLE-IG	C	0	0	-182.7351	260.7721	0.3	5	5
TRANS-01	CIS-2-01	APV110 VLE-IG	C	0	0	147.144	-126.6744	0.3	5	5
METHANOL	IBUTENE	APV110 VLE-IG	C	0	0	412.2995	840.5508	0.47	50	50
METHANOL	PROPENE	APV110 VLE-IG	C	0	0	207.6027	660.5184	0.3	25	25
METHANOL	2ME1BENE	APV110 VLE-IG	C	0	0	520.3923	755.7555	0.47	27.38	44.7

Also, hydrogen gas, carbon dioxide, oxygen gas, and carbon monoxide were included as Henry Components in the ASPEN PLUS simulations to model their solubilities more accurately in the water and the various alcohols. The Henry parameters used can be seen in Table 12.5.2 on the succeeding page.

Table 12.5.2 Henry Component Parameters

Component i	Component j	Source	Temp. Units	Property Units	A_{ij}	B_{ij}	C_{ij}	D_{ij}	T_{lower}	T_{upper}
H2	METHANOL	APV110 HENRY-AP	C	bar	-61.4347	1867.4000	12.6430	-0.0272	-60	69.85
H2	ETHANOL	APV110 HENRY-AP	C	bar	-39.8852	1472.4000	8.5486	-0.0177	-60	50
H2	PROPANOL	APV110 HENRY-AP	C	bar	-66.3659	2023.3000	13.3810	-0.0277	-60	25
H2	WATER	APV110 BINARY	C	bar	180.0661	-6993.5100	-26.3119	0.0150	0.85	65.85
CO2	METHANOL	APV110 HENRY-AP	C	bar	15.4699	-3426.7000	1.5108	-0.0255	0	20
CO2	ETHANOL	APV110 HENRY-AP	C	bar	89.5831	-5018.7998	-11.8910	0.0000	10	40
CO2	PROPANOL	APV110 HENRY-AP	C	bar	82.5921	-4594.6001	-10.9140	0.0000	10	40
CO2	ISBUT-OH	APV110 HENRY-AP	C	bar	-5.3023	-628.3700	2.1790	-0.0001	0.83	54.85
CO2	WATER	APV110 BINARY	C	bar	159.8651	-8741.5500	-21.6690	0.0011	-0.15	79.85
O2	METHANOL	APV110 HENRY-AP	C	bar	26.6982	-767.5700	-2.9774	0.0022	-25	50
O2	ETHANOL	APV110 HENRY-AP	C	bar	-30.2976	651.8400	7.0212	-0.0149	-25	50
O2	PROPANOL	APV110 HENRY-AP	C	bar	7.0946	59.1580	0.0000	0.0000	0	40
O2	ISBUT-OH	APV110 HENRY-AP	C	bar	-0.7656	667.8300	0.5362	0.0086	0.94	54.81
O2	WATER	APV110 BINARY	C	bar	144.4081	-7775.0600	-18.3974	-0.0094	0.85	74.85
CO	METHANOL	APV110 HENRY-AP	C	bar	4.2119	1144.4000	0.0000	0.0000	20	25
CO	ETHANOL	APV110 HENRY-AP	C	bar	7.6405	10.7080	0.0000	0.0000	20	25
CO	PROPANOL	APV110 HENRY-AP	C	bar	7.5935	0.0000	0.0000	0.0000	25	25
CO	ISBUT-OH	APV110 HENRY-AP	C	bar	59.7622	-783.5200	-10.1630	0.0272	0.9	54.83
CO	WATER	APV110 BINARY	C	bar	171.7751	-8296.7500	-23.3372	0.0000	-0.15	79.85

13. PFD and Material Balances

A generalized, basic process flowsheet of the process is given below in Figure 13.1. Please note that only the main chemicals in the process are included in the simplified flowsheet in Figure 13.1 while many other chemicals are involved in the actual process. This is why the mass balance does not close in the figure.

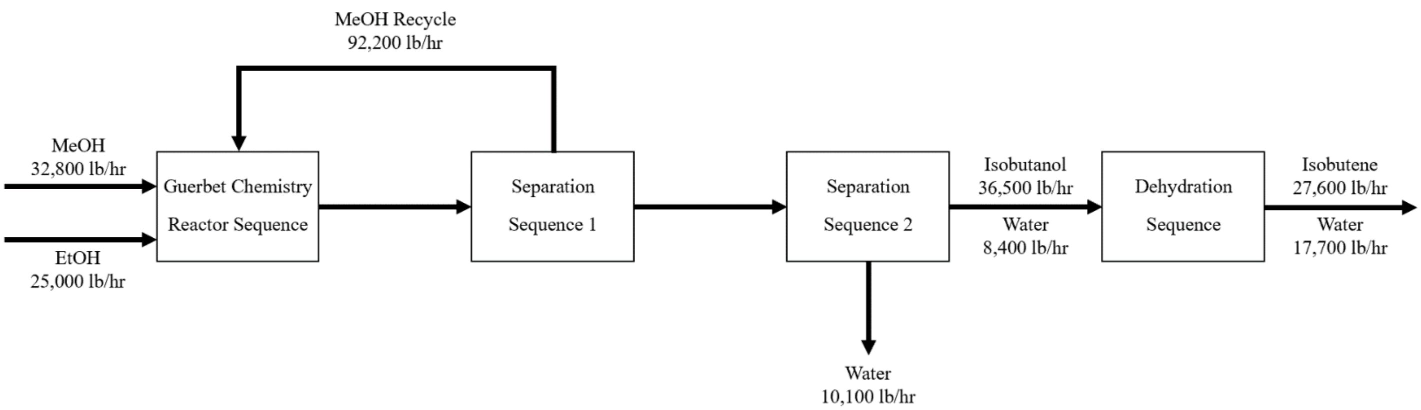

Figure 13.1 Simplified, overall process flowsheet for the production of isobutanol/isobutene from methanol and ethanol via Guerbet chemistry.

Broadly, the process involves the conversion of methanol and ethanol feedstocks into isobutanol via the Guerbet Chemistry Reactor Sequence. This process involves many side reactions including the generation of a large amount of water (see Section 12.3 for the chemical reactions involved). Then, methanol is distilled out of the effluent and recycled back to the reactor feed in Separation Sequence 1. In Separation Sequence 2, most of the water is removed from the isobutanol product stream. Finally, the Dehydration Sequence converts the isobutanol into isobutene which can then be further processed and oligomerized into jet fuel.

The major scope of this project ends with the isobutanol production and purification step i.e., prior to the Dehydration Sequence. The Dehydration Sequence is included in the process flowsheets because the pre-reaction fired heater (FH-2) and effluent cooler (ST-7) needed to be included in the economic analysis. The cost of the dehydration reactor (R-6) is included in a supplied economic factor and needed not be re-costed or sized in the process (see Section 18).

The full process flow diagrams (PFDs) for the process will be shown on the succeeding pages. If needed, the full chemical names for the abbreviations/IDs used in ASPEN PLUS can be found in Section 12.4. The overall process flowsheet will be shown first in Figure 13.2. Then, the flowsheet will be broken down into the four major parts: the Guerbet Chemistry Reactor Sequence (Figure 13.3), Separation Sequence 1 (Figure 13.4), Separation Sequence 2 (Figure 13.5), and the Dehydration Sequence (Figure 13.6). To reduce clutter, the stream results/material balances and short unit descriptions will be shown only after each of the four reduced parts of the overall process.

A total process mass balance will follow the presentation of the flowsheets (Table 13.5) and will also appear in the ASPEN PLUS report in Appendix 26.5 with more significant figures. Note that the amount of isobutanol (ISBUT-OH) leaving the process and being generated in the process is very small in Table 13.5. This is because all of the isobutanol is assumed to be dehydrated to isobutene (IBUTENE) in the Dehydration Sequence. Table 13.6 shows the total mass balances excluding the Dehydration Sequence to provide a better sense of the isobutanol production in the process.

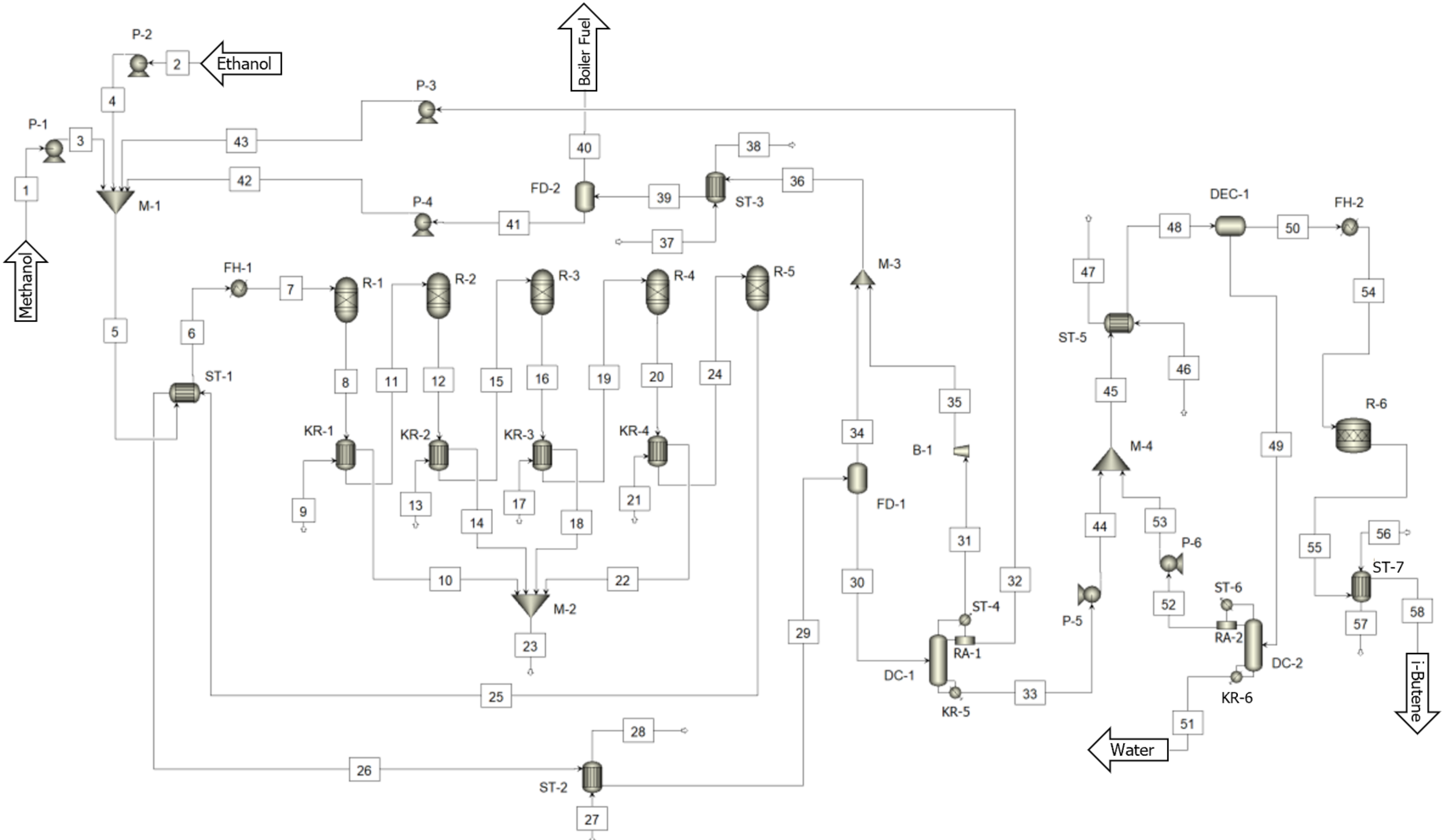

Figure 13.2 Complete process flowsheet.

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P-1
MeOH Pump

P-2
EtOH Pump

M-1
Feed/Recy.
Mixer

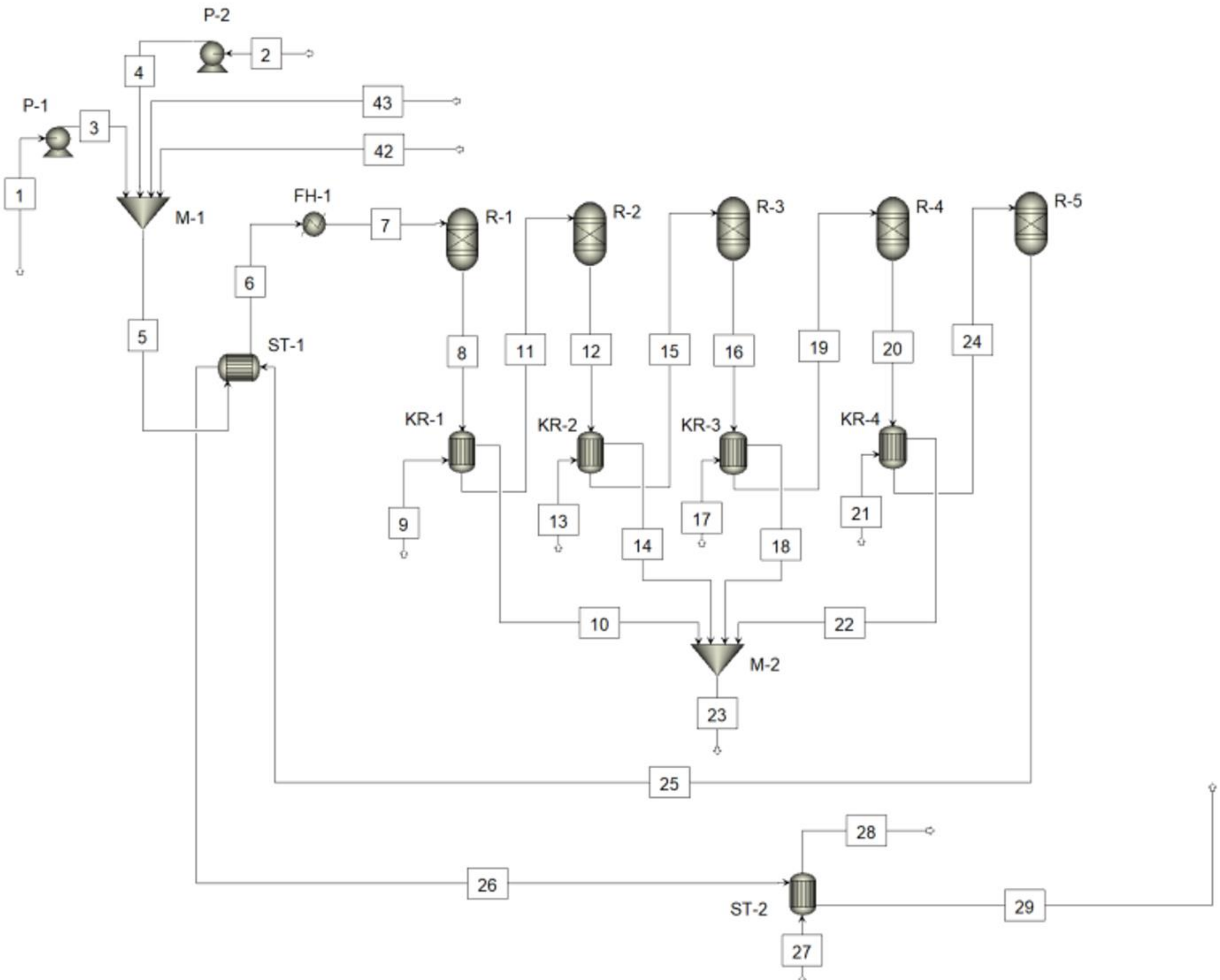
ST-1
Feed/Effl.
HX

FH-1
Reactant
Fired Heater

R-1
Reactor 1

R-2
Reactor 2

R-3
Reactor 3



R-4
Reactor 4

R-5
Reactor 5

KR-1
Ket. Rebr. 1

KR-2
Ket. Rebr. 2

KR-3
Ket. Rebr. 3

KR-4
Ket. Rebr. 4

M-2
Steam Mixer

ST-2
Effl. Cooler

Figure 13.3 Guerbet Chemistry Reactor Sequence.

Table 13.1 Stream Summary Table for the Guerbet Chemistry Reactor Sequence

Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Temperature (°C)	23.0	23.0	23.3	23.4	36.3	109.5	332.0	393.8	185.6	185.8	343.0	386.5	185.6	185.8	347.9	382.5
Pressure (psig)	5	5	63	63	53	52	50	44	151	150	41	35	151	151	33	27
Mass Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.27	1.00	1.00	0.00	1.00	1.00	1.00	0.00	1.00	1.00	1.00
Mass Flows (lb/hr)	32,766	25,005	32,766	25,005	150,857	150,857	150,857	150,858	8,626	8,626	150,858	150,858	6,592	6,592	150,858	150,858
Comp. Mass Flows (lb/hr):																
METHANOL	32,766	0	32,766	0	124,940	124,940	124,940	115,693	0	0	115,693	107,356	0	0	107,356	100,686
ETHANOL	0	25,005	0	25,005	25,005	25,005	25,005	17,611	0	0	17,611	11,321	0	0	11,321	6,289
IB-ALDEH	0	0	0	0	338	338	338	102	0	0	102	187	0	0	187	255
PROPANOL	0	0	0	0	4	4	4	339	0	0	339	622	0	0	622	849
ISBUT-OH	0	0	0	0	32	32	32	10,950	0	0	10,950	20,075	0	0	20,075	27,374
2-ME1BOH	0	0	0	0	0	0	0	124	0	0	124	228	0	0	228	311
H2	0	0	0	0	0	0	0	28	0	0	28	52	0	0	52	71
CO2	0	0	0	0	22	22	22	83	0	0	83	152	0	0	152	207
PROPANE	0	0	0	0	16	16	16	6	0	0	6	11	0	0	11	16
C2H2	0	0	0	0	38	38	38	34	0	0	34	63	0	0	63	86
ISOBU-01	0	0	0	0	43	43	43	14	0	0	14	26	0	0	26	36
N-BUT-01	0	0	0	0	64	64	64	30	0	0	30	55	0	0	55	75
TRANS-01	0	0	0	0	46	46	46	15	0	0	15	27	0	0	27	37
CIS-2-01	0	0	0	0	204	204	204	65	0	0	65	119	0	0	119	162
C2H4	0	0	0	0	9	9	9	11	0	0	11	19	0	0	19	26
O2	0	0	0	0	0	0	0	53	0	0	53	97	0	0	97	132
CH4	0	0	0	0	4	4	4	35	0	0	35	64	0	0	64	87
CO	0	0	0	0	0	0	0	77	0	0	77	142	0	0	142	193
WATER	0	0	0	0	91	91	91	5,586	8,626	8,626	5,586	10,241	6,592	6,592	10,241	13,965

Stream Number	17	18	19	20	21	22	23	24	25	26	27	28	29	42	43	–
Temperature (°C)	185.6	185.8	351.8	377.6	185.6	185.8	185.8	355.7	372.9	110.0	32.2	39.4	40.0	10.4	38.9	–
Pressure (psig)	151	151	24	18	151	151	150	15	9	8	7	2	6	63	53	–
Mass Vapor Fraction	0.00	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	0.00	0.00	0.01	0.00	0.00	–
Mass Flows (lb/hr)	5,263	5,263	150,858	150,858	3,772	3,772	24,254	150,858	150,858	150,858	6,621,966	6,621,966	150,858	718	92,368	–
Comp. Mass Flows (lb/hr):																–
METHANOL	0	0	100,686	95,683	0	0	0	95,683	92,349	92,349	0	0	92,349	643	91,531	–
ETHANOL	0	0	6,289	2,516	0	0	0	2,516	0	0	0	0	0	0	0	–
IB-ALDEH	0	0	255	306	0	0	0	306	339	339	0	0	339	3	335	–
PROPANOL	0	0	849	1,018	0	0	0	1,018	1,132	1,132	0	0	1,132	1	3	–
ISBUT-OH	0	0	27,374	32,849	0	0	0	32,849	36,499	36,499	0	0	36,499	32	1	–
2-ME1BOH	0	0	311	373	0	0	0	373	415	415	0	0	415	0	0	–
H2	0	0	71	85	0	0	0	85	95	95	0	0	95	0	0	–
CO2	0	0	207	249	0	0	0	249	276	276	0	0	276	1	21	–
PROPANE	0	0	16	19	0	0	0	19	21	21	0	0	21	0	16	–
C2H2	0	0	86	103	0	0	0	103	114	114	0	0	114	1	38	–
ISOBU-01	0	0	36	43	0	0	0	43	47	47	0	0	47	1	42	–
N-BUT-01	0	0	75	90	0	0	0	90	100	100	0	0	100	1	63	–
TRANS-01	0	0	37	44	0	0	0	44	49	49	0	0	49	1	46	–
CIS-2-01	0	0	162	195	0	0	0	195	217	217	0	0	217	3	201	–
C2H4	0	0	26	32	0	0	0	32	35	35	0	0	35	0	9	–
O2	0	0	132	158	0	0	0	158	176	176	0	0	176	0	0	–
CH4	0	0	87	104	0	0	0	104	116	116	0	0	116	0	3	–
CO	0	0	193	232	0	0	0	232	258	258	0	0	258	0	0	–
WATER	5,263	5,263	13,965	16,758	3,772	3,772	24,254	16,758	18,620	18,620	6,621,966	6,621,966	18,620	31	60	–

FD-1
Flash
Drum 1

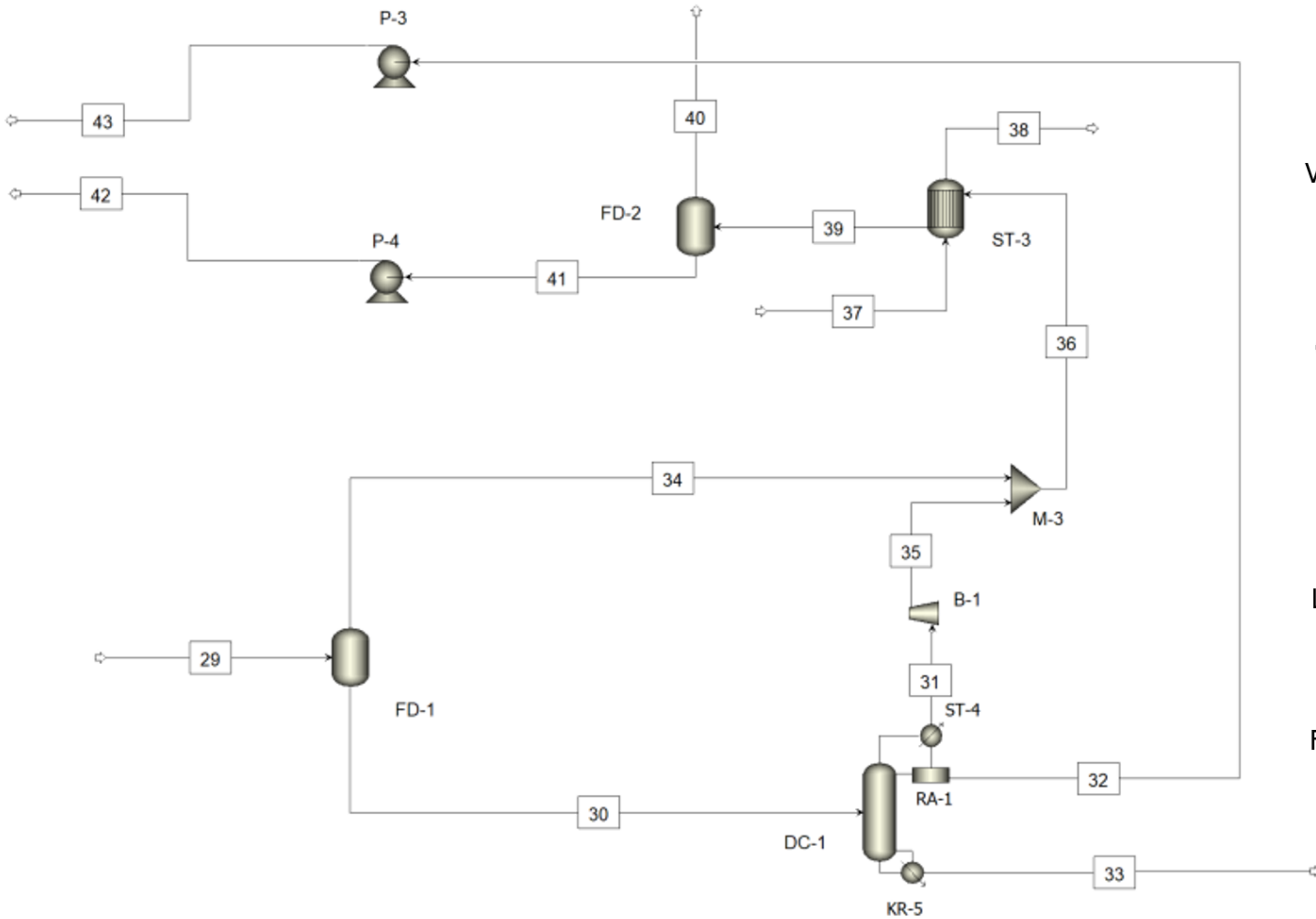
DC-1
MeOH Dist.
Column

KR-5
DC-1 Ket.
Rebrs.

ST-4
DC-1 Partial
Condensers

RA-1
DC-1 Reflux
Accumulator

B-1
Vapor Dist.
Blower



M-3
Vap. Stream
Mixer

ST-3
Vapor
Condenser

FD-2
Flash
Drum 2

P-3
Liquid Dist.
Pump

P-4
FD-2 Liquid
Pump

Figure 13.4 Separation Sequence 1.

Table 13.2 Stream Summary Table for Separation Sequence 1

Stream Number	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
Temperature (°C)	40.0	40.0	38.6	38.6	85.0	40.0	124.3	55.5	2.0	7.3	10.0	10.0	10.0	10.4	38.9
Pressure (psig)	6	5	-8	-8	-3	5	5	5	3	3	4	1	1	63	53
Mass Vapor Fraction	0.01	0.00	1.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.62	1.00	0.00	0.00	0.00
Mass Flows (lb/hr)	150,858	149,373	455	92,368	56,551	1,484	455	1,939	52,189	52,189	1,939	1,221	718	718	92,368
Comp. Mass Flows (lb/hr):															
METHANOL	92,349	91,862	315	91,531	16	487	315	802	0	0	802	160	643	643	91,531
IB-ALDEH	339	336	1	335	0	4	1	5	0	0	5	2	3	3	335
PROPANOL	1,132	1,130	0	3	1,127	1	0	1	0	0	1	0	1	1	3
ISBUT-OH	36,499	36,467	0	1	36,466	32	0	32	0	0	32	0	32	32	1
2-ME1BOH	415	415	0	0	415	0	0	0	0	0	0	0	0	0	0
H2	95	1	1	0	0	94	1	95	0	0	95	95	0	0	0
CO2	276	64	43	21	0	212	43	255	0	0	255	254	1	1	21
PROPANE	21	18	2	16	0	3	2	5	0	0	5	5	0	0	16
C2H2	114	63	26	38	0	51	26	77	0	0	77	76	1	1	38
ISOBU-01	47	45	2	42	0	3	2	5	0	0	5	4	1	1	42
N-BUT-01	100	85	22	63	0	15	22	38	0	0	38	37	1	1	63
TRANS-01	49	47	2	46	0	2	2	4	0	0	4	3	1	1	46
CIS-2-01	217	208	7	201	0	8	7	15	0	0	15	12	3	3	201
C2H4	35	17	8	9	0	18	8	27	0	0	27	26	0	0	9
O2	176	4	4	0	0	171	4	176	0	0	176	176	0	0	0
CH4	116	19	15	3	0	97	15	112	0	0	112	112	0	0	3
CO	258	6	5	0	0	252	5	257	0	0	257	257	0	0	0
WATER	18,620	18,587	0	60	18,527	33	0	33	52,189	52,189	33	2	31	31	60

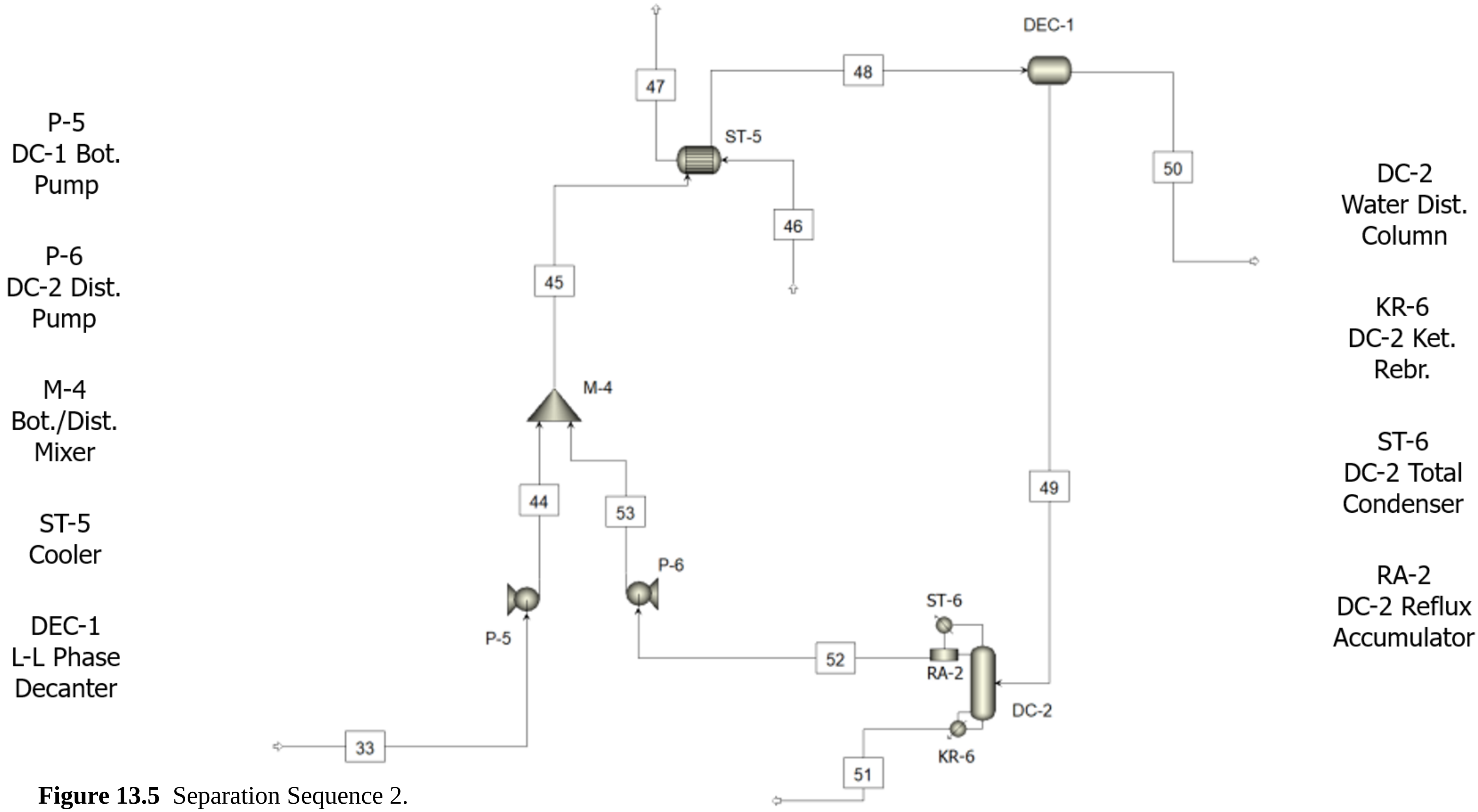


Figure 13.5 Separation Sequence 2.

Table 13.3 Stream Summary Table for Separation Sequence 2

Stream Number	33	44	45	46	47	48	49	50	51	52	53
Temperature (°C)	85.0	83.5	83.6	32.2	37.6	40.0	40.0	40.0	105.3	92.2	90.0
Pressure (psig)	-3	5	5	3	2	4	3	3	3	1	5
Mass Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mass Flows (lb/hr)	56,551	56,551	57,854	424,649	424,649	57,854	11,386	46,468	10,083	1,303	1,303
Comp. Mass Flows (lb/hr):											
METHANOL	16	16	21	0	0	21	5	15	0	5	5
IB-ALDEH	0	0	0	0	0	0	0	0	0	0	0
PROPANOL	1,127	1,127	1,197	0	0	1,197	70	1,127	0	70	70
ISBUT-OH	36,466	36,466	37,067	0	0	37,067	601	36,466	0	601	601
2-ME1BOH	415	415	418	0	0	418	4	415	0	4	4
WATER	18,527	18,527	19,151	424,649	424,649	19,151	10,706	8,445	10,083	624	624

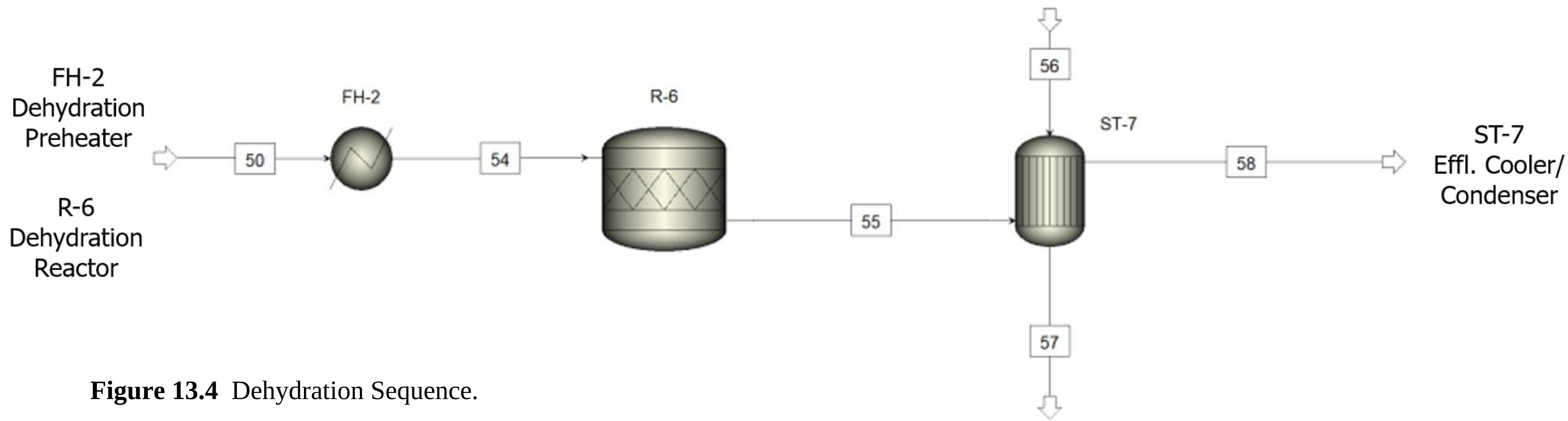


Figure 13.4 Dehydration Sequence.

Table 13.4 Stream Summary Table for the Dehydration Sequence

Stream Number	50	54	55	56	57	58
Temperature (°C)	40.0	325.0	198.0	32.2	48.9	90.0
Pressure (psig)	3	13	8	9	7	7
Mass Vapor Fraction	0.00	1.00	1.00	0.00	0.00	0.73
Mass Flows (lb/hr)	46,468	46,468	46,468	500,774	500,774	46,468
Comp. Mass Flows (lb/hr):						
METHANOL	15	15	15	0	0	15
PROPANOL	1,127	1,127	0	0	0	0
ISBUT-OH	36,466	36,466	0	0	0	0
2-ME1BOH	415	415	0	0	0	0
WATER	8,445	8,445	17,730	500,774	500,774	17,730
IBUTENE	0	0	27,603	0	0	27,603
PROPENE	0	0	789	0	0	789
2ME1BENE	0	0	330	0	0	330

Table 13.5 Complete Process Mass Balances

Components (lb/hr):	In	Out	Generation	Relative Diff.
METHANOL	1.02E+03	5.46E+00	-1.02E+03	-3.95E-05
ETHANOL	5.43E+02	0.00E+00	-5.43E+02	-3.79E-06
IB-ALDEH	0.00E+00	2.16E-02	2.16E-02	-3.79E-04
PROPANOL	0.00E+00	8.55E-04	8.23E-04	-3.81E-02
ISBUT-OH	0.00E+00	1.79E-03	9.41E-04	-4.73E-01
2-ME1BOH	0.00E+00	5.73E-06	-2.34E-06	-1.41E+00
H2	0.00E+00	4.71E+01	4.71E+01	-1.74E-06
CO2	0.00E+00	5.78E+00	5.78E+00	-1.88E-06
PROPANE	0.00E+00	1.09E-01	1.09E-01	-7.46E-06
C2H2	0.00E+00	2.92E+00	2.92E+00	-2.61E-06
ISOBU-01	0.00E+00	7.62E-02	7.62E-02	-1.86E-05
N-BUT-01	0.00E+00	6.30E-01	6.30E-01	-4.75E-06
TRANS-01	0.00E+00	5.42E-02	5.42E-02	-2.81E-05
CIS-2-01	0.00E+00	2.16E-01	2.16E-01	-3.09E-05
C2H4	0.00E+00	9.39E-01	9.39E-01	-2.32E-06
O2	0.00E+00	5.49E+00	5.49E+00	-1.74E-06
CH4	0.00E+00	7.00E+00	7.00E+00	-1.79E-06
CO	0.00E+00	9.19E+00	9.19E+00	-1.74E-06
WATER	0.00E+00	4.25E+05	4.25E+05	-4.24E-09
IBUTENE	0.00E+00	4.92E+02	4.92E+02	0.00E+00
PROPENE	0.00E+00	1.88E+01	1.88E+01	0.00E+00
2ME1BENE	0.00E+00	4.71E+00	4.71E+00	0.00E+00
Total (lb/hr):	7.68E+06	7.68E+06	-	-1.94E-07

Table 13.6 Complete Process Mass Bal. (excl. Dehydration Seq.)

Components (lb/hr):	In	Out	Generation	Relative Diff.
METHANOL	1.02E+03	5.46E+00	-1.02E+03	-3.95E-05
ETHANOL	5.43E+02	0.00E+00	-5.43E+02	-3.79E-06
IB-ALDEH	0.00E+00	2.16E-02	2.16E-02	-3.79E-04
PROPANOL	0.00E+00	1.88E+01	1.88E+01	-1.74E-06
ISBUT-OH	0.00E+00	4.92E+02	4.92E+02	-1.72E-06
2-ME1BOH	0.00E+00	4.71E+00	4.71E+00	-1.72E-06
H2	0.00E+00	4.71E+01	4.71E+01	-1.74E-06
CO2	0.00E+00	5.78E+00	5.78E+00	-1.88E-06
PROPANE	0.00E+00	1.09E-01	1.09E-01	-7.46E-06
C2H2	0.00E+00	2.92E+00	2.92E+00	-2.61E-06
ISOBU-01	0.00E+00	7.62E-02	7.62E-02	-1.86E-05
N-BUT-01	0.00E+00	6.30E-01	6.30E-01	-4.75E-06
TRANS-01	0.00E+00	5.42E-02	5.42E-02	-2.81E-05
CIS-2-01	0.00E+00	2.16E-01	2.16E-01	-3.09E-05
C2H4	0.00E+00	9.39E-01	9.39E-01	-2.32E-06
O2	0.00E+00	5.49E+00	5.49E+00	-1.74E-06
CH4	0.00E+00	7.00E+00	7.00E+00	-1.79E-06
CO	0.00E+00	9.19E+00	9.19E+00	-1.74E-06
WATER	0.00E+00	3.96E+05	3.96E+05	-4.55E-09
IBUTENE	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PROPENE	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2ME1BENE	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Total (lb/hr):	7.18E+06	7.18E+06	-	-2.08E-07

14. Process Descriptions

14.1 Feed and Product Storage

Because the plant will require a large amount of methanol (~786,000 lb/day), 10 days of methanol storage will be held in two storage tanks. Due to the plant's proposed close proximity to a separate ethanol plant, only three days of ethanol storage will be held in one storage tank. The storage tanks will hold the feedstocks at 23 °C and ~5 psig. The feeds are assumed to be pure methanol and ethanol. A small day tank will be used to hold the isobutanol product for quality assurance purposes before it is shipped "over-the-fence" to an adjacent plant to undergo the dehydration and oligomerization steps to produce the jet fuel. The days of raw material/product held were recommended by project author Dr. Bockrath.

14.2 Guerbet Chemistry Reactor Sequence

The feedstocks will first be mixed with one large methanol recycle stream (Stream 43) and another smaller one (Stream 42). The flow through the process will be pressure driven with the streams being pressurized high enough at the feed stage for travel through the reactor sequence. Pressure drops through the reactors were calculated using the Ergun Equation (see appendix Section 26.3.3) and pressure drops through the heat exchangers were calculated using ASPEN Exchanger Design and Rating (EDR) software. The large methanol recycle stream is pressurized to ~53 psig. The fresh methanol, fresh ethanol, and the smaller methanol recycle streams will be mixed with the large methanol recycle stream in series by entering at pressures 10 psig higher than that of the large methanol stream. The choice of these starting pressures was optimized to provide just enough pressure to force the stream through the reactor sequence. Maintaining as low of a pressure as possible was important in this design as the reaction data comes from laboratory experiments conducted at atmospheric pressure (Olson et al., 2004).

The combined feed stream (Stream 5) at 36 °C is then passed through a feed/effluent preheater (ST-1) to efficiently recover some heat energy from the hot reactor effluent. Here the liquid feed is heated to 110 °C and undergoes partial vaporization (~27% mass vapor fraction in Stream 6). The now warm, partially vaporized feed is fully vaporized in the fired heater (FH-1).

The reactor sequence consists of five equally-sized, vertical, packed-bed reactors with the reactor feeds entering from the top. The reaction is performed adiabatically and utilizes a Ni-FM catalyst that is 90% selective to isobutanol (Olson et al., 2004). Of the unreacted methanol, 99.8% is recovered and recycled to the beginning of the reactor train. Full conversion of the ethanol is assumed as evidenced by the same research article. This is supported by project author Dr. Bockrath's assumption that a catalyst 3x more effective than the one used in the referenced paper will be available by the time of project startup. Also, the reactors are proportionally oversized by 100% and the methanol is fed in great excess relative to the ethanol (~7.2 molar ratio) to ensure full conversion of the ethanol. Still, to ensure the process's efficacy does not fully depend on the full conversion of ethanol, sensitivity analyses were run with varying levels of ethanol conversion. Conversions as low as 95% did not affect the process as almost all of the ethanol was recycled with the methanol in the methanol recycle streams. The small amount of ethanol that would escape within the isobutanol/water product stream (Stream 50) would be dehydrated and participate in the oligomerization steps in the downstream processes anyway.

Table 14.2.1 Ethanol Conversion Selectivity

EtOH Conversion [%]	EtOH entering Separation Sequence 1 [kmol/hr]	EtOH that Leaves in IBuOH/Water Product Stream [%]	EtOH that is Recylced [%]	EtOH that Leaves in Flare Stream [%]	EtOH that Leaves in Water Stream [%]	EtOH Conversion [%]
99	2.46	0.02	99.94	0.04	trace	99
95	12.31	11.2	88.7	0.04	trace	95

The laboratory experiment for the reaction performed the reaction isothermally at 360 °C. Therefore, the adiabatic temperature rises in the reactors in the sequence were optimized to closely straddle the reaction temperature of 360 °C. It is assumed that the first reactor will convert 30% of the feed ethanol, followed by 25% in the second reactor, 20% in the third, 15% in the fourth, and 10% in the final reactor. With this assumption, the fired heater heats the first reactor's feed to 332 °C which then exits the first reactor at 394 °C. The succeeding reactors' feeds and effluents also straddle the 360 °C reaction temperature but involve smaller adiabatic temperature rises due to the assumed decreasing conversion through the process.

After the stream leaves each of the first four reactors, it must be cooled appropriately before entering the next reactor. To do this efficiently, each of the first four reactors has an associated kettle reboiler to remove heat from the hot effluents. The kettle reboilers produce saturated steam at 150 psig (~186 °C) for use in the reboilers of the two later distillation columns.

It is recognized that the exact proportions of conversion for each reactor are unknown. The 30/25/20/15/10 assumption was supported by numerous industrial consultants. It is logical that fresh, reactors earlier in the sequence will provide more of the conversion than older, more-coked reactors. The amount of excess air in the fired heater and the water levels in the kettle reboilers can be adjusted as necessary to appropriately straddle the reaction temperature in each of the five reactors. Also, there is a sixth reactor in turn-around which will enter the process as necessary as reactors become coked. The Guerbet chemistry results in the formation of many light gas products as well as other compounds. Refer to Section 12.3 for information on the chemical reactions involved.

The hot effluent from the final reactor in the train is not used to produce steam. Instead, this hot, vapor effluent is used in the feed/effluent preheater discussed earlier (ST-1). Here, the hot effluent is cooled from 373 °C to 110 °C but remains a vapor. The final process unit in this section is the effluent condenser (ST-2). Here, cooling water is used to reduce the temperature from 110 °C to 40 °C, and the vapor quality is decreased from 1 to ~0.01 (Stream 29).

As mentioned above and in the process assumptions in Section 20.1, the packed bed reactors will need to be decoked periodically. Each reactor will be decoked every two months with an assumed 10% fresh catalyst regeneration required after each decoking. The decoking process is a standard operating procedure that involves the use of a dilute air stream of 1% oxygen to burn off the coke from the catalyst. The dilute stream will be manufactured by mixing 5 parts air with 95 parts nitrogen. The process will not need to be shut down during the decoking process. Instead, a valve will turn off flow into the reactor that needs to be decoked, and the process stream will be redirected into the previously decoked/unused swing reactor.

14.3 Separation Sequence 1

The cooled, condensed reactor effluent is then sent to a flash drum (FD-1) operating at 40 °C and ~5 psig. The purpose of this flash drum is to remove most of the light gas byproducts from the Guerbet Chemistry Reaction Sequence. Only 1,484 lb/hr leave in the vapor stream (Stream 34) while 149,373 lb/hr leave in the liquid stream (Stream 30). The operating conditions of the flash drum were chosen to optimize a large amount of light gas byproduct removal in the vapor phase while not sacrificing too much methanol to the vapor stream as well. Only 0.5% of the incoming methanol is lost to the vapor stream, but even the majority of this methanol is recovered in a later process that will be described shortly.

The liquid from the flash drum (FD-1) is then sent to the methanol distillation column (DC-1). The feed to the column is primarily methanol, water, and isobutanol, and the purpose of the column is to remove the methanol from the top of the column. This column is operated below atmospheric pressure with the top stage/condenser pressure being about -8 psig. This was a necessary operating condition to achieve a satisfactory methanol separation. Operating the column above atmospheric caused too much methanol to be lost to the bottoms of the column. At the top of the column, two partial, cooling water condensers are used in parallel to handle the large cooling requirement. Partial condensers were used instead of total condensers as there are still small amounts of light gas byproducts that were not removed in the prior flash drum. Of the total distillate, only 0.5% is vapor distillate with the remaining light gases (Stream 31) while the remaining liquid distillate (Stream 32) is 99% methanol by mass. The small amount of vapor distillate required is beneficial as this means the vacuum pressure-changer load is small. The liquid distillate is then pumped up to the appropriate feed pressure and returned to the reactor sequence to be mixed with the fresh feeds and the smaller methanol recycle stream which will be discussed shortly. Similar to the condensers, two kettle reboilers are used in parallel to achieve the large, required heat duty for the boil-up of this column. The heating fluid for the reboilers is 150 psig steam with ~90% of the required steam coming from a third-party steam plant and the other 10% coming from the reactor effluent kettle reboilers from the Guerbet Chemistry Reactor Sequence. The bottoms stream (Stream 33) is primarily water, isobutanol, and a small amount of methanol and other light alcohols and is sent to Separation Sequence 2.

The small vapor distillate stream is blown and mixed with the vapor from the earlier flash drum. This combined stream (Stream 36) is still 41% methanol by mass, so another flash event was designed to recover the majority of this methanol. Stream 36, which now contains methanol and the light gas products, is cooled from 55°C to 10 °C using a chilled water/glycol coolant in the shell-and-tube heat exchanger ST-3. The coolant enters at 2 °C and exits at ~7 °C. Then, the process stream (now, Stream 39) enters the second flash drum (FD-2) which operates at 10 °C and ~1.5 psig. From this flash drum, the vapor stream (Stream 40), which contains the light gas byproducts, exits the process and is sold as boiler house fuel. 80% of the methanol that enters this flash drum is recovered in the liquid stream (Stream 41). The liquid stream is 90% methanol by mass with the balance being nearly split equally between water and isobutanol. This stream is then pressurized to the reactor sequence feed stream pressure and becomes the small methanol recycle stream (Stream 42).

14.4 Separation Sequence 2

Simple distillation is not an option to purify the bottoms stream from the first distillation column (Stream 33) to obtain a purer isobutanol product. This is because Stream 33 lies almost directly on a binary azeotrope between isobutanol and water. Instead, the immiscibility of isobutanol and water is taken advantage of and used in a liquid-liquid phase separation event in a decanter (DEC-1).

But first, Stream 33 is pressurized and mixed with the distillate from the water distillation column (DC-2). The combined stream (Stream 45) is again mostly isobutanol, water, and some light alcohols. Importantly, the concentration of methanol in this stream is very small (~0.04% by mass) as methanol concentrations as low as 2% by mass can begin to severely impact the liquid-liquid phase split in the decantation step mentioned previously. This small amount of methanol is enabled by the high methanol recovery and recycle in the previous distillation column. The combined stream is then cooled from 84 °C to the decantation temperature of 40 °C using cooling water in ST-5.

The cooled stream then enters the decanter (DEC-1) which operates at 40 °C and ~3.3 psig. The liquid-liquid phase separation on which the decanter depends is discussed in Section 16.3.

Leaving the decanter is an isobutanol-rich liquid (78% isobutanol, 18% water by mass) and a water-rich liquid (5% isobutanol, 94% water by mass). The balance of the two phases are the remaining light alcohols i.e., methanol, propanol, 2-methyl-1-butanol. The decanter is able to knock out more than half of the water in the isobutanol product stream with 56% of the water entering the decanter leaving in the water-rich stream (Stream 49). The alcohol-rich stream (Stream 50) is the primary product stream for the scope of this project but is sent to the Dehydration Sequence for conversion of isobutanol to isobutene.

The water-rich stream is then sent to the water distillation column (DC-2) to recover the remaining isobutanol. This column is much smaller than the first column and utilizes a total, cooling water condenser at the top. Of the material entering the column, 99.995% of the isobutanol and 99.8% of the remaining light alcohols are recovered in the distillate, while 94.2% of the water is recovered in the bottoms. The top stage/condenser pressure in this column is ~1.3

psig, as sub-atmospheric operation is not required. The bottoms water stream is nearly pure at 99.998% water by mass and is sent to a wastewater treatment plant for further processing. The distillate containing the alcohols (importantly, the isobutanol) is recycled with the bottoms of the methanol distillation column (DC-1) and is returned to the decantation process.

14.5 Dehydration Sequence

The primary isobutanol/water product stream (Stream 50) is then sent to the Dehydration Sequence with the purpose of dehydrating the isobutanol to isobutene as well as the small amount of other light alcohols to their corresponding alkenes. This sequence is included in the process as the economics of the fired heater (FH-2) and effluent cooler/condenser (ST-7) within the sequence are needed to provide a more accurate economic evaluation.

First, Stream 50 is vaporized and heated from 40 °C to the dehydration reaction temperature of 325 °C in FH-2 (Taylor et al., 2010). The hot, vapor stream (Stream 54) then enters the dehydration reactor, which is modeled as a simple stoichiometric, adiabatic reactor (R-6). Full conversion of the alcohols is assumed as evidenced by the previous paper. The dehydration reaction is endothermic and results in an effluent temperature of 198 °C. The effluent (Stream 55) is then cooled further to 90 °C with cooling water to knock out the majority of the water in the effluent in ST-7. The final product stream (Stream 58) for the process is mostly isobutene and yields 27,603 lb/hr of isobutene. This stream would then be shipped over-the-fence to the adjacent plant to perform the oligomerization process.

15. Energy Balance/Utility Requirements

15.1 Feed Vaporization

To begin the process, the ethanol and methanol feed streams, initially in liquid phase for storage purposes, are heated from around 23°C to the reaction temperature. These substances are fully vaporized before being fed to the reactor sequence. This is done via the heat exchanger ST-1 and fired heater FH-1. This heat exchanger operates using the effluent from the end of the reaction sequence, utilizing the energy produced from the exothermic reaction. The effluent temperature drops by 257°C, vaporizing 25% of the mixed feed. This liquid vapor mixture is then fed to the fired heater to complete the phase change and increase the temperature, which is operated by natural gas producing 72.8 MM BTU/hr. The reactor effluent stream is then further cooled down to 40°C – the temperature required for the first flash drum – using typical cooling water in the heat exchanger ST-2. The energy and utility requirements for the heat exchangers and fired heater can be found in Table 15.1.

15.2 Steam Generation

In total, the exothermic reaction produces 24.9 MM BTU/hr, split up among the five reactors in sequence. To maintain the correct reaction temperature of 360°C, kettle reboilers are placed after each reactor, excluding the last one where the effluent is fed to ST-1 as previously noted. As described in Section 16.1, the conversion in the reactors will vary depending on the amount of coking, also altering the energy produced. Each kettle reboiler is sized for maximum conversion; however, the hot water inlet flow will fluctuate based on the expected heat production. Most of the produced steam from these reboilers is recycled and used in the second distillation columns reboiler (KR-6), where the water is condensed and sent back to the reactor sequence creating an integrated steam loop. Since the amount of steam produced exceeds the energy requirements of KR-6, the remaining steam is sent to the first distillation columns reboiler (KR-5) to reduce the amount of purchased steam utility by 10%, and then recycled in the same manner. Table 15.1 shows the flow rates and energy requirements within this loop.

15.3 Chilled Water

Heat exchanger ST-3 is used to cool down one of the methanol recycle streams to the desired temperature for the second flash drum. As this unit requires the cooling water to be at a starting temperature of 2°C, an ethylene glycol water mixture is used to lower the freezing point of the chilled water. The energy and utility requirements for this unit can be found in Table 15.1.

15.4 Flare Byproduct

The second flash drum FD-2 is used to remove undesired hydrocarbons from one of the methanol recycle streams. The effluent from this unit has a flow rate of 1220 lb/hr can be burned to provide 13.6 MM BTU/hr, which is sold as a natural gas byproduct. The composition of this stream and energy calculations can be found in Section 26.3.1.

15.5 Other Equipment Utilities

Both distillation columns use typical cooling water for their condensers, as well as the heat exchanger (ST-5) which is used to cool down the decanter inlet stream. Due to a simplifying assumption used for the dehydration step, an extra heat exchanger (ST-7) and fired heater (FH-2) were designed and are detailed in Section 16. The flow rates and energy requirements for all these units can be seen in Table 15.1. To provide a reasonable pressure drop throughout the whole process, six pumps and one blower are required. The electricity utility for these units is presented in Table 15.2.

Table 15.1 Utility Energy Requirements and Quantities

Utility	Equipment	Energy Requirement [BTU/hr]	Quantity [lb/hr]
Cooling Water	ST-2	85.5 MM	6.62 MM
	ST-4	175 MM	19.7 MM
	ST-5	4.20 MM	424000
	ST-6	1.57 MM	52200
	ST-7	16.0 MM	534000
Hot Water	KR-1/KR-2/KR-3/KR-4	7.39 MM	8630
150 psig Steam	KR-5	182 MM	209000
	KR-6	2.89 MM	3330
Chilled Water	ST-3	0.475 MM	52200
		[BTU/hr]	**[SCF/hr]**
Natural gas	FH-1	72.8 MM	70200
	FH-2	30.2 MM	29100

Table 15.2 Electricity Requirements

Equipment	kW Required
P-1	4.02
P-2	3.30
P-3	9.76
P-4	0.158
P-5	0.852
P-6	0.0186
B-1	7.56

16. Equipment List and Unit Descriptions

Apart from the reactors, all equipment specifications were designed and optimized using ASPEN. Costing is detailed in Section 18 and was performed using Seider et al. (2017) design specifications. Due to the location of Iowa, it was assumed that wind and earthquakes would pose no problem and therefore were not accounted for in design costing specifications. Stainless steel was used for pieces of equipment where corrosion due to carbonic acid was a possibility or temperatures were too high for carbon steel. More detailed specification sheets for these equipment designs can be found in Section 17.

16.1 Reactors

The reaction converting methanol and ethanol to isobutanol will take place in five packed-bed vertical reactors in series (R-1, R-2, R-3, R-4, and R-5). The flow rate of feedstock into this reactor sequence is 151000 lb/hr of a gaseous methanol/ethanol mixture with a ratio of 5:1 weight% respectively. There will be an extra reactor unit so that process flow can continue while the decoking process, see Section 14.2, occurs on one reactor at a time. This multiple reactor design was chosen for sizing considerations, plausible heat removal strategy and viable decoking time periods. While these reactors are identical in design and sizing, due to the coking, it is expected that the cleanest reactor will account for 30% of the reaction conversion and the successive reactors will account for 25%, 20%, 15% and 10% based on coking amounts. A Ni-FM catalyst, with 90% isobutanol selectivity, packed via activated carbon will be used to ensure 100% conversion of the ethanol (Olson et al., 2004). The total volume of catalyst used in the reactors is 7060 ft^3, with each reactor being decoked and replenished every two months. This volume was calculated by upscaling the amount used in the reaction reference paper, but accounting for the project description assumption of a 3x stronger catalyst. Based on the volume of catalyst needed in each reactor, the diameter and depth of the units was determined to be 13.4 ft. The reactor sizing design was also upscaled by 100% to ensure conversion and account for coking factors. These calculations can be seen in Section 26.3.2. The initial price of the catalyst is $4.00 MM, with an associated utility regeneration cost.

An estimated pressure drop across each reactor was calculated using Ergun's Equation, as seen in Section 26.3.3 from the catalyst properties, flow rate and size of each reactor. This was determined to be 29.2 psig across all five vessels and is accounted for by pumping the feedstock material to an inlet pressure of 62.6 psig. The reference laboratory reaction was performed at 360°C. Due to the adiabatic temperature rise caused by the exothermic reaction, heat exchangers are located after the first four reactors to keep the temperature in the range 330°C to 400°C. The reactors are made from stainless steel to account for the high temperatures and the total vessel cost is $4.7 MM.

16.2 Distillation Columns

16.2.1 DC-1

The first distillation column occurs after the reaction sequence and first flash drum (FD-1) and is used to separate 99.6% of the total methanol from the isobutanol. The feed stream has a flow rate of 149000 lb/hr with 99.998% of the isobutanol leaving in the bottoms product. This column was chosen to operate at a vacuum pressure of -7.70 psig due to the difficulty of separation caused by fluid properties and water/alcohol interactions. The methanol percentage leaving in the bottom's product was required to be less than ~10 weight% because of decanter specifications to be discussed in Section 16.3. Sensitivity analysis and efficiency calculations were performed, shown in Section 26.3.4, to determine a reflux ratio of 2.8 with 50 required trays in the column and a tray efficiency of 0.505. The feed will be located on tray 23. The length of the column was calculated to be 114 ft, while the diameter is 20.0 ft. The distillation vessel is made from stainless steel and the cost was determined to be $11.2 MM.

This column contains two, stainless steel partial condensers (ST-4) used in parallel due to the large cooling requirement. Partial condensers were chosen to remove trace amounts of light gas byproducts in the vapor distillate that were not removed via the first flash drum (FD-1). From these, the methanol is recovered as the liquid distillate and is further purified and recycled back to the initial feedstock. These condensers operate at a temperature of 38.6°C and require a total heat duty of 175 MM BTU/hr, satisfied by cooling water with a temperature change of ~5°C. Modelled as shell and tube heat exchanges, these condensers have a tube length of 19.7 ft, heat transfer area of 31000 ft^2, and total of 8262 tubes each. The cost for both was determined to be $6.99 MM.

The reflux drum accumulator (RA-1) was determined to be 18.3 ft in length, with a 9.17 ft diameter. Priced as a horizontal, stainless steel pressure vessel, the cost was determined to be $0.295 MM.

The column also contains two carbon steel reboilers (KR-5) operating in parallel and will be maintained at a temperature of 84.6°C. The required heat duty is 182 MM BTU/hr and is satisfied by high pressure steam, modelled as a kettle reboiler. This steam is purchased as a utility but supplemented from steam generated in the reaction sequence as described in Section 15.2. The tube length was calculated to be 18.5 ft, with a total heat transfer area of 2050 ft^2 and a total of 211 tubes each. The cost was determined to be $0.553 MM.

16.2.2 DC-2

The second distillation column occurs at the end of the process and is used to purify and recycle isobutanol from water, lost from the decanter separation unit. The feed stream has a flow rate of 11400 lb/hr and recovers 99.995% of the isobutanol as distillate product. This column successfully removes 94.2% of the incoming water in the bottoms, which is sent for wastewater treatment and discarded. The operating pressure is set to 1.30 psig. Sensitivity analysis and efficiency calculations were performed, shown in Section 26.3.5, to determine a reflux ratio of 1.0 with 29 required trays in the column and an efficiency of 0.313. The feed will be located on tray 13. The length of the column was calculated to be 70.0 ft, while the diameter is 1.70 ft. This distillation vessel is made from carbon steel and the cost was determined to be $0.321 MM.

This column contains a single carbon steel condenser (ST-6) maintained at an operating temperature of 92.2°C. The required heat duty is 1.57 MM BTU/hr and is satisfied by cooling water with a temperature change of ~17°C. Modelled as a shell and tube heat exchanger, this condenser has a tube length of 24.0 ft, total heat transfer area of 87.4 ft^2, and total of 44 tubes. The cost was determined to be $51100 total.

The reflux drum accumulator (RA-1) was determined to be 3.50 ft in length, with a 1.75 ft diameter. Priced as a horizontal, carbon steel pressure vessel, the cost was determined to be $31000.

The reboiler for this column (KR-6) is designed as a carbon steel kettle reboiler and will be maintained at a temperature of 105°C. The required heat duty is 2.89 MM BTU/hr and is satisfied by the steam generated throughout the reactor sequence as described in Section 15.2. The tube length was calculated to be 6.89 ft, with a total heat transfer area of 52.4 ft^2 and a total of 19 tubes. The cost was determined to be $0.136 MM.

16.3 Decanter

After the main separation section, where the light gases and methanol is removed from the isobutanol stream, a decanter (DEC-1) is used to remove the water via liquid-liquid separation. Due to the azeotrope of isobutanol and water shown in Figure 16.3.1, and immiscibility of the two liquids, it was determined that a decanter would be more cost effective and efficient than a distillation column. The decanter is maintained at a pressure of 3.30 psig and a temperature of 40°C. The feed rate is 57900 lb/hr and contains approximately a 70:30 weight% isobutanol to water split. The length was calculated as 12.2 ft, with a diameter of 6.11 ft.

Figure 16.3.1 shows the ternary diagram for a methanol, isobutanol, water mixture. Represented by the red diamond and yellow circle, the feed concentration is extremely close to the azeotrope making a distillation separation difficult. The blue section signifies the concentration mixtures of these three substances where there is a liquid-liquid phase split. Therefore, for separation to be possible in the decanter the feed must be in this blue zone, meaning methanol concentration must be below ~10 weight%. This was a driving factor for the design of the first distillation column described in Section 16.2.1. The ternary diagrams for the other trace amounts of substances such as propanol and 2-methyl-1-butanol had larger two-phase regions and were not considered an issue.

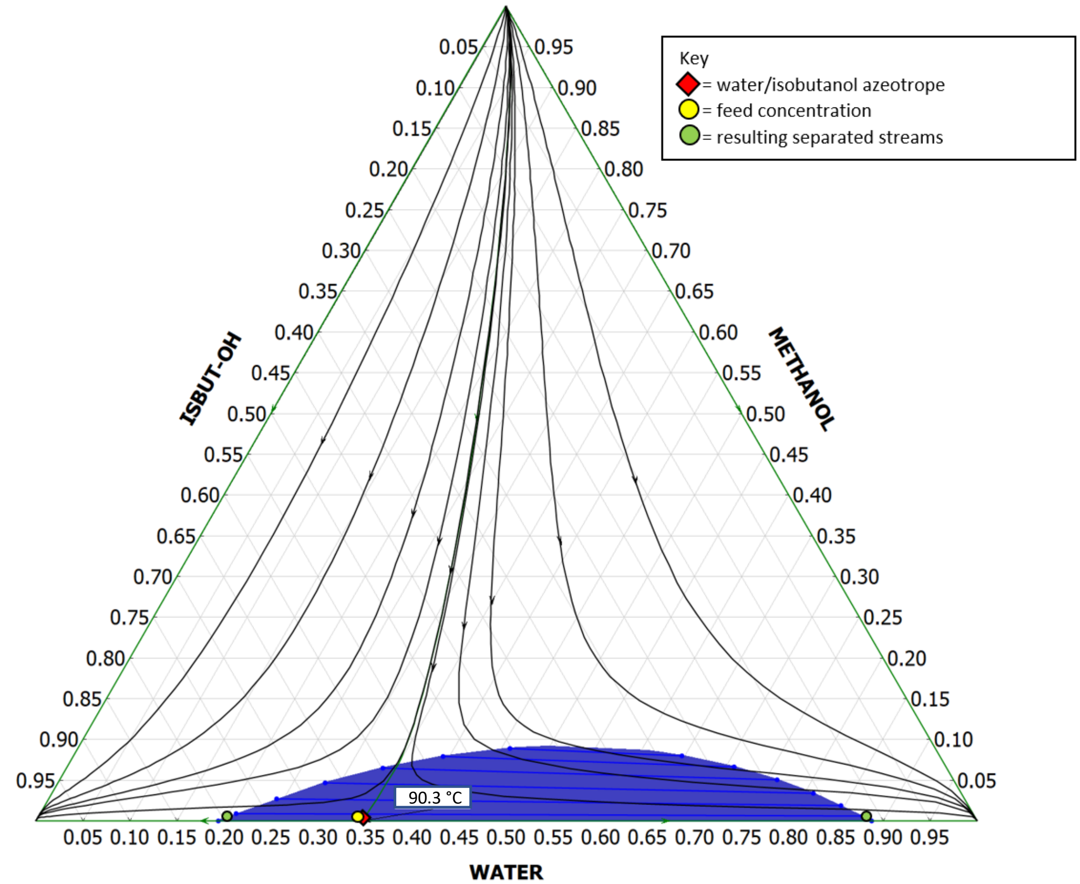


Figure 16.3.1 Ternary diagram for isobutanol, methanol and water showing the liquid-liquid phase split.

The green circles represent the two resulting streams after the liquid-liquid phase split, which follow the tie lines shown within the blue region. The right-side concentration is about 10% isobutanol and 90% water. This is fed to the second distillation column described in Section

16.2.2 so the lost isobutanol can be recycled back to the decanter. The left-side concentration is about 80% isobutanol and 20% water and is the final product for this outlined process. This stream has a flow rate of 46500 lb/hr and is fed to a pre-outlined and priced dehydration step. Research showed that the extra amounts of water in this product stream will not affect the conversion and efficiency of the dehydration step and therefore an assumption, detailed in Section 20.1, was made that no further separation was needed (Taylor et al., 2010). To account for an increase in overall flow to the dehydration step, an extra heat exchanger and fired heater, detailed in Section 16.5.5 and Section 16.7.2 were designed and priced. The cost of this decanter was determined to be \$0.110 MM – much less than an expected distillation column that would produce the same results.

16.4 Flash Drums

16.4.1 FD-1

The first flash drum (FD-1) is utilized immediately after the reaction sequence to separate out the majority of the light gas byproducts formed in the reaction. The feed has flow rate of 151000 lb/hr and the drum is maintained at a pressure of 5.30 psig and a temperature of 40°C. These conditions eliminated unwanted gas byproducts through vaporization, leaving a liquid mix of methanol, isobutanol and water in the bottom product stream. The vapor stream is further separated so that the lost methanol can be recycled back into the feedstock. The size of this flash drum, calculated as a vertical pressure vessel is 36.9 ft in length and 18.4 ft in diameter. The cost was determined to be \$1.35 MM.

16.4.2 FD-2

The second flash drum (FD-2) is located immediately after FD-1, to further purify the methanol in the vapor stream for recycling purposes by removing even more of the light gases. The feed, which has been cooled down by a heat exchanger (ST-3), has a flow rate of 1940 lb/hr. The drum is maintained at a pressure of 1.30 psig and a temperature of 10°C. These conditions allow for a resulting methanol stream of 89.6 weight% purity to be mixed with the feedstock. The vaporized light gases are burned to provide a natural gas utility requirement and described in Section 15.4. The size of this flash drum, calculated as a vertical pressure vessel is 34.5 ft in length and 17.3 ft in diameter. The cost was determined to be $1.23 MM.

16.5 Heat Exchangers

16.5.1 ST-1

The first heat exchanger (ST-1) is used to heat up the mixed feed of ethanol and methanol to the desired reaction temperature. The cold stream is the feedstock with a flow rate of 151000 lb/hr, and an initial temperature of 36.3°C. The hot stream is the effluent from the reactor sequence, utilizing the exothermic nature of the reaction, with an initial temperature of 373°C. This heat exchanger is a typical stainless-steel shell and tube model with a tube length of 17.7 ft, a total heat transfer area of 5630 ft^2, and 1652 tubes. The cost was determined to be $0.681 MM.

16.5.2 KR-1, KR-2, KR-3, KR-4

The discussed reaction is exothermic and therefore, kettle reboilers are located after the first four reactors to remove heat before entering the next reactor. As previously discussed, each reactor will perform a varying percentage of the overall reaction process due to levels of coking. Each kettle reboiler was designed to handle the maximum amount of heat removal but will be adjusted based on the expected conversion rate of each reactor. For the maximum design, the hot stream entering the kettle reboiler, which is reactor effluent will have a flow rate of 151000 lb/hr and a temperature of 394°C. The cold stream will be high pressure water at a flow rate of 8630 lb/hr and a temperature of 186°C, that will be fully vaporized in the reboiler. This generated steam will be used for the second distillation columns reboiler as described in Section 15.2. The tube length in each reboiler will be 4.43 ft, with a total heat transfer area of 277 ft^2 and 51 tubes. The shell cover will be made from carbon steel, with the tube sheets stainless steel due to the heat. The total cost of all four kettle reboilers was determined to be $1.57 MM.

16.5.3 ST-2

While the reaction effluent is cooled down from ST-1, more cooling is necessary so that the flow can reach the appropriate temperature of 40°C for FD-1. Heat exchanger ST-2 utilizes a cold stream of cooling water at 32.2°C with a flow rate of 6.62 MM lb/hr. The hot reactor effluent has a flow rate of 151000 lb/hr and an inlet temperature of 110°C. This heat exchanger is a typical shell and tube model with a tube length of 18.2 ft, a total heat transfer area of 16500 ft^2, and 4743 tubes. The shell cover will be made from carbon steel, with the tube sheets stainless steel due to the heat. The cost was determined to be $1.81 MM.

16.5.4 ST-3

Heat exchanger ST-3 is used to cool a methanol recycle stream to the appropriate temperature of 10°C for FD-2. The cold stream is a glycol-water mixture used as a refrigerant with an inlet flow rate of 52200 lb/hr, and temperature of 2.00°C. The hot steam is mostly methanol with small amounts of light gases, has flow rate of 1940 lb/hr and an inlet temperature of 55.5°C. This heat exchanger is a typical stainless-steel shell and tube model with a tube length of 5.45 ft, a total heat transfer area of 125 ft^2, and 47 tubes. The cost was determined to be $0.176 MM.

16.5.5 ST-5

Heat exchanger ST-5 is used to cool the decanter inlet stream to the appropriate temperature of 40°C. The cold stream is typical cooling water with a flow rate of 425000 lb/hr and a temperature of 32.2°C. The hot stream contains mostly water and isobutanol with a flow rate of 57900 lb/hr and an inlet temperature of 83.6°C. This heat exchanger is a typical carbon steel shell and tube model with a tube length of 1.05 ft, a total heat transfer area of 921 ft^2, and 268 tubes. The cost was determined to be $83800.

16.5.5 ST-7

Due to the assumption outlined in Section 20.1, where an isobutanol/water mixture of 80:20 weight% can be fed to the dehydration step, an extra heat exchanger was designed to account for increased flow. The cold stream is typical cooling water with a flow rate of 534000lb/hr and a temperature of 32.2°C. The hot stream of isobutanol and water has a flow rate of 46400 lb/hr and an inlet temperature of 198°C. This heat exchanger is a typical carbon steel shell and tube model with a tube length of 4.95 ft, a total heat transfer area of 629 ft^2, and 245 tubes. The cost was determined to be $54600.

16.7 Fired Heater

16.7.1 FH-1

A fired heater (FH-1) is used to fully vaporize and heat the ethanol and methanol feed streams to the reaction temperature. ST-1 begins this process, but more utility is needed for the feedstock to reach a temperature of 330°C. While the desired temperature for the reaction is 360°C, there is an adiabatic temperature rise, hence why the feed stream is slightly lower. The feed to the fired heater has a flow rate of 151000 lb/hr and a temperature of 109°C. Natural gas provides 72.8 MM BTU/hr for this process unit. The operating pressure is 66.3 psig and the material is Cr-Mo ally steel. The cost was determined to be $4.14 MM.

16.7.1 FH-2

Another fired heater (FH-2) is used to prepare the product stream from this process for dehydration. Due to the assumption that a higher concentration of water can be present in the dehydration inlet, detailed in Section 20.1, an extra fired heater was designed and costed to raise the isobutanol/water stream to a higher temperature. The feed to the fired heater has a flow rate of 46500 lb/hr and a temperature of 40°C. Natural gas provides 30.2 MM BTU/hr for this process unit. The operating pressure is 3.30 psig and the material is Cr-Mo ally steel. The cost was determined to be $2.07 MM.

16.8 Pumps and Blowers

There are five pumps and one blower that account for the pressure drops throughout the process and allow the material to continuously flow. These are standardized units, operated with electricity, that have a total cost of $0.181 MM.

16.9 Storage Tanks

There will be a total of four storage tanks, three of which are used for the feed, and the remaining one to be used for product. Two methanol storage tanks, containing 10 days' worth of storage, each with a volume of 987000 gallons were determined to cost $4.40 MM. Only one ethanol storage tank, containing three days' worth of storage, is needed due to the plant's proximity to an ethanol plant. This tank has a volume of 449000 gallons and a cost of $1.48 MM. The feedstock is contained at a temperature of 23 °C and a pressure around 5 psig. The last storage tank is used to hold a days' worth of isobutanol, with a volume of 267000 gallons and a price of $1.13 MM.

17. *Specification Sheets*

R *Packed-Bed Reactors*		
Identification:	**Item** R-1, R-2, R-3, R-4, R-5, R-6 No. Req. 6	
Function: React methanol and ethanol to form isobutanol and byproducts		
Operation: Continuous		
Materials Handled:	Feed	Effluent
Stream #	7/11/15/19/24	38/12/16/20/25
Temperature (°C)	332-355	394-372
Pressure (psig)	49.8-15.3	44.0-9.44
Vapor Mass Fraction	1	1
Mass Flow (lb/hr)	151000	151000
Design Data:		
	Adiabatic Temp. Rise:	~40°C
	Catalyst Volume:	7060 ft^3
	Material:	Stainless Steel
	Diameter:	13 ft
	Height:	13 ft
	Orientation:	Vertical
	Heat Release:	24.9 MM BTU/hr
	Pressure Drop:	~ 5.84 psig
Utilities:		
Comments: Five reactors in use at a time. One extra for when a reactor must be decoked. Reaction conversion in reactors vary based on coking.		

D-1 *Distillation Column 1*

Identification:	**Item**	D-1		
	No. Req.	1		

Function: Separate methanol from isobutanol

Operation: Continuous

Materials Handled:	Feed	Vapor Dist.	Liquid Dist.	Bottoms
Stream #	30	31	32	33
Temperature (°C)	40.0	38.6	38.6	84.9
Pressure (psig)	5.30	-7.70	-7.70	-2.80
Vapor Mass Fraction	0	1	0	0
Mass Flow (lb/hr)	149000	455	92400	56600

Design Data:

Number of Trays:	50
Feed Stage:	23
Height:	114 ft
Diameter:	20.0 ft
Tray Efficiency:	0.505
Tray Spacing:	2.00 ft
Reflux Ratio:	2.80
Column Material:	Stainless Steel
Condensor Material:	Stainless Steel
Reboiler Material:	Carbon Steel
Condensor Duty:	175 MM BTU/hr
Reboiler Duty:	182 MM BTU/hr

Utilities: 188000 lb/hr of steam. 19.7 MM lb/hr of cooling water

Comments: There are two condensors and two reboilers in parallel. The condensors are designed as partial condensors to remove extra light gases from the feed. The reboilers are kettle reboilers.

D-2 ***Distillation Column 2***

Identification:	**Item**	D-2
	No. Req.	1

Function: Recover lost isobutanol and separate from water

Operation: Continuous

Materials Handled:	Feed	Liquid Dist.	Bottoms
Stream #	49	52	51
Temperature (°C)	40.0	92.2	105.0
Pressure (psig)	3.30	1.30	3.01
Vapor Mass Fraction	0	0	0
Mass Flow (lb/hr)	11400	1300	10000

Design Data:

Number of Trays:	29
Feed Stage:	13
Height:	70.0 ft
Diameter:	1.70 ft
Tray Efficiency:	0.313
Tray Spacing:	2.00 ft
Reflux Ratio:	1.00
Column Material:	Carbon Steel
Condensor Material:	Carbon Steel
Reboiler Material:	Carbon Steel
Condensor Duty:	1.57 MM BTU/hr
Reboiler Duty:	2.89 MM BTU/hr

Utilities: Steam utility is satisfied by generated steam from reactor sequence. 52200 lb/hr of cooling water

Comments: The reboiler is a kettle reboiler.

DEC-1 *Decanter*

Identification:	**Item**	DEC-1	
	No. Req.	1	
Function: Separate water from isobutanol			
Operation: Continuous			
Materials Handled:	Feed	Effluent 1	Effluent 2
Stream #	48	49	50
Temperature (°C)	40.0	40.0	40.0
Pressure (psig)	3.68	3.30	3.30
Vapor Mass Fraction	0	0	0
Mass Flow (lb/hr)	57800	11400	46500
Isobutanol Weight%	0.641	0.0528	0.00892
Water Weight%	0.331	0.94	0.182
Design Data:			
	Length:	12.2 ft	
	Diameter:	6.11 ft	
	Material:	Carbon Steel	
Utilities:			
Comments: A ternary diagram showing the liquid-liquid separation can be found in Section 16.3			

FD-1 *Flash Drum 1*

Identification:	**Item**	FD-1
	No. Req.	1

Function: Remove light gases from reactor effluent

Operation: Continuous

Materials Handled:	Feed	Effluent 1	Effluent 2
Stream #	29	30	34
Temperature (°C)	40.0	40.0	40.0
Pressure (psig)	6.10	5.30	5.30
Vapor Mass Fraction	0	0	1
Mass Flow (lb/hr)	151000	149000	1480
Isobutanol Weight%	0.242	0.244	0.0215
Byproduct Weight%	0.758	0.756	0.978

Design Data:

Length:	36.9 ft
Diameter:	18.4 ft
Material:	Stainless Steel

Utilities:

Comments:

FD-2 *Flash Drum 2*

Identification: **Item** FD-2
No. Req. 1

Function: Remove light gases from methanol recycle stream

Operation: Continuous

Materials Handled:	Feed	Effluent 1	Effluent 2
Stream #	39	40	41
Temperature (°C)	10.0	10.0	10.0
Pressure (psig)	4.18	1.3	1.3
Vapor Mass Fraction	0.616	1	0
Mass Flow (lb/hr)	1940	1220	717
Methanol Weight%	0.414	0.131	0.896
Byproduct Weight%	0.586	0.869	0.104

Design Data:

Length:	34.5 ft
Diameter:	17.3 ft
Material:	Stainless Steel

Utilities:

Comments:

ST-1 *Preheater*

Identification:	**Item**	ST-1		
	No. Req.	1		
Function: Heat methanol and ethanol feed streams				
Operation: Continuous				
Materials Handled:	Cold In	Cold Out	Hot In	Hot Out
Stream #	5	6	25	26
Temperature (°C)	36.3	110	373	110
Pressure (psig)	52.6	51.9	9.44	7.51
Vapor Mass Fraction	0	0.731	1	1
Mass Flow (lb/hr)	151000	151000	151000	151000

Design Data:

Type:	Shell and Tube
Eff. Surface Area:	5640 ft^2
Heat Exchanged:	33.4 MM BTU/hr
Tube Side Material:	Stainless Steel
Shell Side Material:	Stainless Steel
No.Tubes:	1652
Tube Passes:	1
Length of Tubes	17.7 ft
Baffle Spacing:	1.14 ft
Shell Diameter:	3.77 ft

Utilities:

Comments: The reactor effluent is on the tube side, and the feed is on the shell side

KR ***Reactor Cooler***

Identification:	**Item**	KR-1, KR-2, KR-3, KR-4			
	No. Req.	4			
Function: Cool reactor effluent					
Operation: Continuous					
Materials Handled:		Cold In	Cold Out	Hot In	Hot Out
Stream #		9/13/17/21	10/14/18/22	8/12/16/20	11/15/19/24
Temperature (°C)		185	185	394	343
Pressure (psig)		151	150	44.0	41.2
Vapor Mass Fraction		1	0	0	0
Mass Flow (lb/hr)		8630	8630	151000	151000
Design Data:					
	Type:	Kettle Reboiler			
	Eff. Surface Area:	277 ft^2			
	Heat Exchanged:	7.40 MM BTU/hr			
	Tube Side Material:	Stainless Steel			
	Shell Side Material:	Carbon Steel			
	No.Tubes:	51			
	Tube Passes:	2			
	Length of Tubes	4.43 ft			
	Shell Diameter:	2.61 ft			

Utilities: 8630 lb/hr of heated water

Comments: The hot water is on the shell side, and reactor effluent is on the tube side.

ST-2 *Effluent Cooler*

Identification:	**Item**	ST-2			
	No. Req.	1			
Function: Cool reactor effluent					
Operation: Continuous					
Materials Handled:		Cold In	Cold Out	Hot In	Hot Out
Stream #		27	28	26	29
Temperature (°C)		32.2	39.4	110	40
Pressure (psig)		7.30	2.25	7.51	6.10
Vapor Mass Fraction		0	0	1	0
Mass Flow (lb/hr)		6620000	6620000	151000	151000
Design Data:					
	Type:	Shell and Tube			
	Eff. Surface Area:	16500 ft^2			
	Heat Exchanged:	85.5 MM BTU/hr			
	Tube Side Material:	Stainless Steel			
	Shell Side Material:	Carbon Steel			
	No.Tubes:	4743			
	Tube Passes:	2			
	Length of Tubes	18.2 ft			
	Baffle Spacing:	1.59 ft			
	Shell Diameter:	6.05 ft			
Utilities: 6620000 lb/hr of cooling water					
Comments: The reactor effluent is on the tube side, and the feed is on the shell side					

ST-3 *Recycle Cooler*

Identification:	**Item**	ST-3
	No. Req.	1

Function: Cool reactor effluent

Operation: Continuous

Materials Handled:	Cold In	Cold Out	Hot In	Hot Out
Stream #	37	38	36	39
Temperature (°C)	2.00	7.26	55.5	10.0
Pressure (psig)	3.30	2.72	5.3	4.18
Vapor Mass Fraction	0	0	1	0.616
Mass Flow (lb/hr)	2890	2890	107	107

Design Data:

Type:	Shell and Tube
Eff. Surface Area:	125 ft^2
Heat Exchanged:	0.475 MM BTU/hr
Tube Side Material:	Stainless Steel
Shell Side Material:	Stainless Steel
No.Tubes:	47
Tube Passes:	1
Length of Tubes	5.45 ft
Baffle Spacing:	0.361 ft
Shell Diameter:	0.720 ft

Utilities: 2890 lb/hr of chilled water-glycol mixture

Comments: The cooling water is on the tube side, and methanol recycle stream is on the shell side

ST-4 *Distillation Column 1 Condenser*

Identification:	**Item**	ST-4
	No. Req.	2

Function: Distillation column condenser

Operation: Continuous

Materials Handled:	Cold In	Cold Out	Hot In	Hot Out
Stream #	-	-	30	31/32
Temperature (°C)	32.2	37.2	52.6	37.6
Pressure (psig)	7.30	0.430	-6.70	-8.10
Vapor Mass Fraction	0	0	1	0.00512
Mass Flow (lb/hr)	19700000	19700000	353000	353000

Design Data:

Type:	Shell and Tube
Eff. Surface Area:	31000 ft^2
Heat Exchanged:	176 MM BTU/hr
Tube Side Material:	Stainless Steel
Shell Side Material:	Stainless Steel
No.Tubes:	8268
Tube Passes:	2
Length of Tubes	19.7 ft
Baffle Spacing:	1.49 ft
Shell Diameter:	0.662 ft

Utilities: 19.7 MM lb/hr of cooling water

Comments: The distillation column requires two condensers in parallel. They are partial condensers. The cooling water is on the tube side and the distillation feed is on the shell side.

ST-5 *Decanter Cooler*

Identification:	**Item**	ST-5			
	No. Req.	1			
Function: Cool reactor effluent					
Operation: Continuous					
Materials Handled:		Cold In	Cold Out	Hot In	Hot Out
Stream #		46	47	45	48
Temperature (°C)		32.20	37.6	83.6	40.0
Pressure (psig)		3.30	1.96	5.30	3.68
Vapor Mass Fraction		0	0	0	0
Mass Flow (lb/hr)		424000	424000	57900	57900

Design Data:

Type:	Shell and Tube
Eff. Surface Area:	921 ft^2
Heat Exchanged:	4.20 MM BTU/hr
Tube Side Material:	Carbon Steel
Shell Side Material:	Carbon Steel
No.Tubes:	268
Tube Passes:	1
Length of Tubes	1.05 ft
Baffle Spacing:	0.443 ft
Shell Diameter:	1.50 ft

Utilities: 424000 lb/hr of cooling water

Comments: The cooling water is on the tube side, and decanter inlet stream is on the shell side

ST-6 *Distillation Column 2 Condenser*

Identification:	**Item**	ST-6			
	No. Req.	1			
Function: Distillation column condenser					
Operation: Continuous					
Materials Handled:		Cold In	Cold Out	Hot In	Hot Out
Stream #		-	-	49	52
Temperature (°C)		32.2	48.9	97.3	90.2
Pressure (psig)		7.30	4.42	2.10	1.51
Vapor Mass Fraction		0	0	1	0
Mass Flow (lb/hr)		52200	52200	2610	2610
Design Data:					
	Type:	Shell and Tube			
	Eff. Surface Area:	87.4 ft^2			
	Heat Exchanged:	1.56 MM BTU/hr			
	Tube Side Material:	Carbon Steel			
	Shell Side Material:	Carbon Steel			
	No.Tubes:	44			
	Tube Passes:	2			
	Length of Tubes	2.00 ft			
	Baffle Spacing:	1.35 ft			
	Shell Diameter:	0.718 ft			

Utilities: 52200 lb/hr of cooling water

Comments: The cooling water is on the tube side and the distillation feed is on the shell side.

ST-7 *Dehydration Cooler*

Identification:	**Item**	ST-7			
	No. Req.	1			
Function: Cool reactor effluent					
Operation: Continuous					
Materials Handled:		Cold In	Cold Out	Hot In	Hot Out
Stream #		56	57	55	58
Temperature (°C)		32.2	48.9	198	87.8
Pressure (psig)		3.30	1.96	5.30	3.68
Vapor Mass Fraction		0	0	0	0.7
Mass Flow (lb/hr)		534000	534000	46400	46400
Design Data:					
	Type:	Shell and Tube			
	Eff. Surface Area:	629 ft^2			
	Heat Exchanged:	16.0 MM BTU/hr			
	Tube Side Material:	Carbon Steel			
	Shell Side Material:	Carbon Steel			
	No.Tubes:	245			
	Tube Passes:	1			
	Length of Tubes	4.95 ft			
	Baffle Spacing:	1.79 ft			
	Shell Diameter:	1.67 ft			

Utilities: 534000 lb/hr of cooling water

Comments: The cooling water is on the tube side, and decanter outlet stream is on the shell side

KR-5 *Distillation Column 1 Reboiler*

Identification: **Item** KR-5
No. Req. 2

Function: Distillation column reboiler

Operation: Continuous

Materials Handled:	Cold In	Cold Out	Hot In	Hot Out
Stream #	30	33	-	-
Temperature (°C)	85.0	83.1	186	184
Pressure (psig)	-2.48	-3.68	150	147
Vapor Mass Fraction	0	0.831	1	0
Mass Flow (lb/hr)	425000	425000	210000	210000

Design Data:

Type:	Kettle Reboiler
Eff. Surface Area:	2090 ft^2
Heat Exchanged:	180 MM BTU/hr
Tube Side Material:	Carbon Steel
Shell Side Material:	Carbon Steel
No.Tubes:	211
Tube Passes:	2
Length of Tubes	1.54 ft
Baffle Spacing:	-
Shell Diameter:	2.53 ft

Utilities: 210000 lb/hr of high pressure steam

Comments: The distillation column requires two reboilers in parallel.
10% of the required steam is taken from the steam integration loop.
The steam is on the tube side and the distillation feed is on the shell side.

KR-6 *Distillation Column 2 Reboiler*

Identification:	**Item**	KR-6
	No. Req.	1

Function: Distillation column reboiler

Operation: Continuous

Materials Handled:	Cold In	Cold Out	Hot In	Hot Out
Stream #	49	51	-	-
Temperature (°C)	105	104	186	184
Pressure (psig)	3.01	2.25	160	149
Vapor Mass Fraction	0	0.297	1	0
Mass Flow (lb/hr)	13100	13100	3330	3330

Design Data:

Type:	Kettle Reboiler
Eff. Surface Area:	52.4 ft^2
Heat Exchanged:	2.86 MM BTU/hr
Tube Side Material:	Carbon Steel
Shell Side Material:	Carbon Steel
No.Tubes:	19
Tube Passes:	2
Length of Tubes	6.89 ft
Baffle Spacing:	-
Shell Diameter:	0.719 ft

Utilities: 3330 lb/hr of high pressure steam

Comments: The required steam is taken from the steam integration loop. The steam is on the tube side and the distillation feed is on the shell side.

FH-1 *Fired Heater 1*

Identification:	**Item**	FH-1
	No. Req.	1

Function: Vaporize and heat up feed streams

Operation: Continuous

Materials Handled:	Feed	Effluent
Stream #	6	7
Temperature (°C)	109	332
Pressure (psig)	51.9	49.9
Vapor Mass Fraction	0.269	1
Mass Flow (lb/hr)	151000	151000

Design Data:

Material:	Cr-Mo Ally Steel
Heat Duty:	72.8 MM BTU/hr

Utilities: Natural gas is used for the heat duty

Comments:

FH-2 *Fired Heater 2*

Identification:	**Item**	FH-2
	No. Req.	1

Function: Heat up dehydration feed

Operation: Continuous

Materials Handled:	Feed	Effluent
Stream #	50	54
Temperature (°C)	40	325
Pressure (psig)	3.30	13.0
Vapor Mass Fraction	0	1
Mass Flow (lb/hr)	46500	46500

Design Data:

Material:	Cr-Mo Ally Steel
Heat Duty:	30.2 MM BTU/hr

Utilities: Natural gas is used for the heat duty

Comments:

18. Equipment Cost Summary

Tables 18.1-18.4 shows the equipment cost for this process. The design specifications for equipment in the ethanol and methanol to isobutanol step were determined in ASPEN. Additional considerations were given to the reactors and heat exchangers in the reactor train. Since the reactors rotate in and out of operation, and the catalyst cokes up the reactors and heat exchangers variable heat and pressure loads, and thus they are all standardized to the largest size necessary. The distillation columns are also given an additional tray efficiency consideration outside of ASPEN using the O'Connell method. The summary table, 18.4, includes entries for downstream dehydration and oligomerization steps. The prices were determined to incorporate the known CAPEX for the downstream steps. The total cost of equipment without consideration of the downstream steps is $47.4MM. The first table, table 18.1 shows the individual and total costs of fabricated equipment.

Table 18.1 Fabricated Equipment Costs Table

Equipment Description	Purchase Cost	Bare Module Factor	Bare Module Cost
DC-1	$2,686,541	4.16	$11,176,011
FH-1	$1,889,372	2.19	$4,137,725
ST-4 (DC-1 Condenser 1)	$1,102,623	3.17	$3,495,315
ST-4 (DC-1 Condenser 2)	$1,102,623	3.17	$3,495,315
FH-2	$946,865	2.19	$2,073,634
ST-2	$572,436	3.17	$1,814,622
FD-1	$325,016	4.16	$1,352,067
FD-2	$296,743	4.16	$1,234,451
R-1	$186,921	4.16	$777,591
R-2	$186,921	4.16	$777,591
R-3	$186,921	4.16	$777,591
R-4	$186,921	4.16	$777,591
R-5	$186,921	4.16	$777,591
R-6	$186,921	4.16	$777,591
ST-1	$214,960	3.17	$681,423
KR-1	$123,666	3.17	$392,021
KR-2	$123,666	3.17	$392,021
KR-3	$123,666	3.17	$392,021
KR-4	$123,666	3.17	$392,021
DC-2	$77,227	4.16	$321,264
RA-1	$70,918	4.16	$295,019
KR-5 (DC-1 Reboiler 1)	$87,242	3.17	$276,557
KR-5 (DC-1 Reboiler 2)	$87,242	3.17	$276,557
ST-3	$55,475	3.17	$175,856
KR-6	$42,870	3.17	$127,444
DEC-1	$26,349	4.16	$109,612
ST-5	$26,439	3.17	$83,812
ST-7	$17,229	3.17	$54,616
ST-6	$16,132	3.17	$51,138
RA-2	$7,452	4.16	$31,000
Total			**$37,497,068**

Table 18.2 shows the prices for the process machinery in the process. The process machinery is mostly pumping and motors.

Table 18.2 Process Machinery Equipment Costs

Equipment Description	**Purchase Cost**	**Bare Module Factor**	**Bare Module Cost**
P-3 (pump)	$9,176	3.3	$30,281
P-4 (pump)	$7,920	3.3	$26,136
P-6 (pump)	$7,816	3.3	$25,793
P-1 (pump)	$7,791	3.3	$25,710
P-5 (pump)	$7,733	3.3	$25,519
P-2 (pump)	$7,724	3.3	$25,489
B-1 (blower)	$8,030	2.15	$17,265
P-3 (motor)	$1,485	3.3	$4,901
P-4 (motor)	$1,059	3.3	$3,495
P-1 (motor)	$980	3.3	$3,234
P-2 (motor)	$925	3.3	$3,053
B-1 (motor)	$841	3.3	$2,775
P-5 (motor)	$755	3.3	$2,492
P-6 (motor)	$750	3.3	$2,475
Total			**$198,618**

Table 18.3 shows the equipment costs for the storage units needed for feedstocks and product storage. Ethanol is acquired over-the-fence so 3 days of critical storage is used to size the storage tanks. Since methanol is not acquired over-the-fence, ten days of storage are allocated to size the storage tanks. Isobutanol and water storage is sized as a day tank.

Table 18.3 Storage Equipment Costs

Equipment Description	**Purchase Cost**	**Bare Module Factor**	**Bare Module Cost**
Methanol Storage 1	$550,079	4	$1,698,276
Methanol Storage 2	$550,079	4	$1,698,276
Ethanol Storage 1	$368,928	4	$1,139,000
Isobutanol/water storage	$283,350	4	$1,133,400
Total			**$5,668,952**

Table 18.4 summarizes the equipment costs and adds in costs for initial purchase of catalyst as well as a bare module cost for the downstream steps to account for the CAPEX of the downstream processes.

Table 18.4 Equipment Cost Summaries

Description	**Bare Module Cost**
Total Fabricated Equipment Costs	$37,497,068
Total Process Machinery Costs	$198,618
Total Storage Costs	$5,668,952
Initial Catalyst Purchase	$4,035,642
Downstream Equipment Costs	$14,953,727
Total Bare Module Costs	**$62,354,007**

19. Fixed Capital Investment Summary

The Total Capital Investment (TCI) for this process is $115.9 MM, using the estimation methods in Chapter 16 of Seider et al. (2017), and the corresponding excel spreadsheet. As discussed in Section 17 the CAPEX of the downstream dehydration and oligomerization steps as well as the initial purchase of the catalyst are incorporated in the bare module costs for the process and thus accounted for in the TCI. The TCI is calculated using the equation below where C_{TDC} is Total Depreciable Capital (TDC), C_{wc} is Working Capital, C_{land} is the cost of land, and C_{start} is the cost of plant startup

$$C_{TCI} = C_{TDC} + C_{WC} + C_{land} + C_{start}$$

TDC, cost of land, and cost of startup are all included in the calculation of Total Permanent Investment (TPI). Table 19.1 details the assumptions and factors used to calculate TPI.

Table 19.1 Total Permanent Investment Assumptions and Factors

Cost of Site Preparations:	5.00%	of Total Bare Module Costs
Cost of Service Facilities:	5.00%	of Total Bare Module Costs
Cost of Contingencies and Contractor Fees:	18.00%	of Direct Permanent Investment
Cost of Land:	2.00%	of Total Depreciable Capital
Cost of Plant Start-Up:	10.00%	of Total Depreciable Capital

Total Depreciable Capital is calculated with the bare module costs given in the equipment costing table in Section 18 as well as the cost of site preparation, service facilities, and contingency/contractor fees. Table 19.2 details the Total Depreciable Capital summary and calculations.

Table 19.2 Total Depreciable Capital Summary

Total Bare Module Costs:			
Fabricated Equipment	$	37,497,070	
Process Machinery	$	198,616	
Spares	$	-	
Storage	$	5,668,952	
Other Equipment	$	14,953,727	
Catalysts	$	4,035,642	
Computers, Software, Etc.	$	-	
Total Bare Module Costs:			**$ 62,354,007**
Direct Permanent Investment			
Cost of Site Preparations:	$	3,117,700	
Cost of Service Facilities:	$	3,117,700	
Allocated Costs for utility plants and related facilities:	$	-	
Direct Permanent Investment			**$ 68,589,407**
Total Depreciable Capital			
Cost of Contingencies & Contractor Fees	$	12,346,093	
Total Depreciable Capital			**$ 80,935,501**

The TPI is then found by factoring in land and plant startup costs. These costs are set percentages of the TDC. The location factor is also accounted for in TPI, with a factor of 1.15. This factor corresponds to the site factor for plants in the Midwest. Table 19.3 details the Total Permanent Investment summary and calculation.

Table 19.3 Total Permanent Investment Summary

Total Permanent Investment				
Cost of Land:	$	1,618,710		
Cost of Royalties:	$	-		
Cost of Plant Start-Up:	$	8,093,550		
Total Permanent Investment - Unadjusted			$	90,647,761
Site Factor				1.15
Total Permanent Investment			**$**	**104,244,925**

The Working Capital Costs are calculated with an assumption of 30 days of Accounts Receivable, Accounts Payable, and Cash Reserves, as well as 4 days of fuel product inventory and 7 days of raw material storage. 7 days of raw material storage was chosen a functional midpoint between the ethanol and methanol storage capacities, as ethanol will be purchased as an over-the-fence input and has a 3-day critical storage capacity while the methanol has a full 10-day storage capacity. Table 19.4 details the working capital needed for plant operation as well as the final TCI from TPI and working capital

Table 19.4 Working Capital and Total Capital Investment

Working Capital		**2023**		**2024**		**2025**
Accounts Receivable	$	8,900,425	$	4,450,213	$	4,450,213
Cash Reserves	$	1,462,434	$	731,217	$	731,217
Accounts Payable	$	(6,039,382)	$	(3,019,691)	$	(3,019,691)
Jet Fuel Inventory	$	1,186,723	$	593,362	$	593,362
Raw Materials	$	1,197,370	$	598,685	$	598,685
Total	**$**	**6,707,570**	**$**	**3,353,785**	**$**	**3,353,785**
Total Capital Investment					**$**	**115,993,311**

20. *Operating Cost/Cost of Manufacture*

20.1 Major Process Assumptions

The design of this process was facilitated by a few major assumptions. First, it is assumed that the isobutanol in the 78 wt% isobutanol, 18 wt% water product in Stream 50 is able to be completely dehydrated to isobutene. Coming into the project, it was to be assumed that the dehydration and oligomerization steps experience 100% yields since they are well-established technologies (see appendix Section 26.1). However, this assumption was based on a purer isobutanol product stream. It was feared that the larger-than-expected amount of water in the product stream would hurt the yield of the dehydration process since water is a product in isobutanol dehydration (Figure 20.1.1).

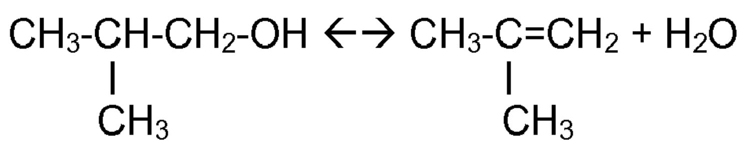


Figure 20.1.1 Dehydration of isobutanol to isobutene.

However, research has showed that isobutanol feed streams of similar water content still have highly selective conversions of 99+% of isobutanol to isobutene in dehydration reactions (Taylor et al., 2010). This assumption enables the designation of Stream 50 as an adequate product stream and prevents the need for an additional, capital-intensive isobutanol-water distillation column.

Other assumptions provided by project author Dr. Bockrath (see appendix Section 26.1) in the problem statement include:

- Ni-FM catalyst performance reported in Olson et al. (2004) can be markedly improved by a factor of three resulting in less catalyst required,
- Although the catalyst is assumed to be 3x more effective, the reactors will be twice as large as calculated using the more effective catalyst to ensure that 100% ethanol conversion is achieved as demonstrated in Olson et al. (2004),
- Each packed bed reactor is assumed to require decoking every two months with 10% catalyst regeneration after each decoking (see Section 14.2 for details on the decoking process),
- The Ni-FM catalyst cost is $5/lb which is approximately 25% higher than that of Fluid Catalytic Cracker catalyst, and
- The cost of biomethanol is assumed to be 2x the price of conventional methanol in the base, main profitability analysis of this report.

20.2 Raw Materials

Table 20.2.1 shows the annual costs of the raw materials required for the process. Catalyst regeneration is included as a raw material along with the methanol and ethanol feedstocks.

Table 20.2.1 Raw Material Costs

Raw Material	Annual Cost (USD)	Cost (USD)/lb Jet Fuel
Methanol	$63,028,439	$0.286
Ethanol	$75,286,271	$0.341
Catalyst Regeneration	$428,108	$0.002
Total	$138,742,819	$0.629

20.3 Boiler House Fuel Byproduct

The flare stream (Stream 40) is sold as boiler house fuel as there is a significant amount of fuel value associated with it at 1.36E+07 BTU/hr. The price assumed for the sale is the same as the price for the natural gas utility at $4.82E-06/BTU. This results in a credit for the process of $516,720 per year, or equivalently, about $0.002/lb of jet fuel.

20.4 Utilities

Table 20.4.1 summarizes the utility costs for the process. The utilities required include 150 psig steam for the first column's reboiler, cooling water, electricity, natural gas for the fired heaters, refrigerant for the second flash drum (FD-2), wastewater treatment, and a value for the Operating Expenditure supplied for the downstream dehydration and oligomerization steps. The refrigerant used is a water/glycol mixture, and was used to cool a process stream down to 10 °C. The utility prices were taken from Chapter 17 of *Product and Process Design Principles* (Seider et al., 2017).

Table 20.4.1 Utility Costs

Utility	Typical Factor in American Engineering Units	Annual Cost (USD)	Cost (USD)/lb Jet Fuel
Steam (150 psig)	$7.00/1,000 lb	$10,399,450	$0.047
Cooling Water	$0.10/1,000 gal	$2,594,997	$0.012
Electricity	$0.070/kW-hr	$14,167	$0.000064
Natural Gas	$5.00/1,000 SCF	$3,958,877	$0.018
Refrigerant (chilled water/glycol)	$1.75/ton-day	$20,902	$0.000095
Wastewater Treatment	$0.15/lb organic removed	$234	$0.000001
Downstream OPEX	-	$7,555,555	$0.034
Total	-	$24,544,184	$0.111

20.5 Labor

It is assumed that the plant will operate using a 5-shift schedule with 5 operators per shift earning $40 per hour. Also, it is assumed that 2 engineers will be required at the plant with each earning

$200,000/yr including benefits. $500M will be spent each year on laboratory and quality assurance services. The plant maintenance required was calculated as percentages of the Total Depreciable Capital and the Maintenance Wages and Benefits as shown in Figure 20.5.1.

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

Figure 20.5.1 Calculation parameters for the plant's maintenance.

The total yearly fixed costs for labor are shown in Figure 20.5.2.

Operations			
	Direct Wages and Benefits	$	2,080,000
	Direct Salaries and Benefits	$	312,000
	Operating Supplies and Services	$	124,800
	Technical Assistance to Manufacturing	$	500,000
	Control Laboratory	$	400,000
	Total Operations	**$**	**3,416,800**
Maintenance			
	Wages and Benefits	$	3,642,098
	Salaries and Benefits	$	910,524
	Materials and Services	$	3,642,098
	Maintenance Overhead	$	182,105
	Total Maintenance	**$**	**8,376,824**

Figure 20.5.2 Annual fixed costs for the Operations and Maintenance**.**

20.6 Remaining Fixed Costs

The calculation parameters of the remaining fixed costs are given in Figure 20.6.1 with the results following in Figure 20.6.2.

Operating Overhead	
General Plant Overhead:	7.10% of Maintenance and Operations Wages and Benefits
Mechanical Department Services:	2.40% of Maintenance and Operations Wages and Benefits
Employee Relations Department	5.90% of Maintenance and Operations Wages and Benefits
Business Services	7.40% of Maintenance and Operations Wages and Benefits
Property Taxes and Insurance	
Property Taxes and Insurance:	2.00% of Total Depreciable Capital
Straight Line Depreciation	
Direct Plant:	8.00% of Total Depreciable Capital, less 1.18 times the Allocated Costs for Utility Plants and Related Facilities
Allocated Plant:	6.00% of 1.18 times the Allocated Costs for Utility Plants and Related Facilities
Other Annual Expenses	
Rental Fees (Office and Laboratory Space):	$0
Licensing Fees:	$0
Miscellaneous:	$0
Depletion Allowance	
Annual Depletion Allowance:	$0

Figure 20.6.1 Calculation parameters for the remaining fixed costs.

Operating Overhead		
General Plant Overhead:	$	493,068
Mechanical Department Services:	$	166,671
Employee Relations Department:	$	409,733
Business Services:	$	513,902
Total Operating Overhead	**$**	**1,583,374**
Property Taxes and Insurance		
Property Taxes and Insurance:	$	1,618,710

Figure 20.6.2 Annual costs for the remaining fixed costs.

The total annual fixed costs for the plant are just shy of $15MM.

20.7 Other Variable Costs and Working Capital

Other factors contributing to the plant's variable costs and the working capital are calculated using the parameters given in Figure 20.7.1.

Other Variable Costs			
General Expenses			
Selling / Transfer Expenses:	3.00% of Sales		
Direct Research:	4.80% of Sales		
Allocated Research:	0.50% of Sales		
Administrative Expense:	2.00% of Sales		
Management Incentive Compensation:	1.25% of Sales		
Working Capital			
Accounts Receivable		⇨	**30 Days**
Cash Reserves (excluding Raw Materials)		⇨	**30 Days**
Accounts Payable		⇨	**30 Days**
Jet Fuel Inventory		⇨	**4 Days**
Raw Materials		⇨	**7 Days**

Figure 20.7.1 Calculation parameters for other variable cost factors and working capital.

The total variable costs are summarized in Figure 20.7.2, while the working capital calculation is shown in Figure 20.7.3.

General Expenses			
Selling / Transfer Expenses:		$	7,219,234
Direct Research:		$	11,550,774
Allocated Research:		$	1,203,206
Administrative Expense:		$	4,812,823
Management Incentive Compensation:		$	3,008,014
Total General Expenses		$	27,794,050
Raw Materials	$0.629328 per lb of Jet Fuel		$138,742,819
Byproducts	$0.002344 per lb of Jet Fuel		($516,720)
Utilities	$0.111331 per lb of Jet Fuel		$24,544,184
Total Variable Costs		**$**	**190,564,333**

Figure 20.7.2 Summary and total of the variable costs for the plant.

		2023		2024		2025
Accounts Receivable	$	8,900,425	$	4,450,213	$	4,450,213
Cash Reserves	$	1,462,434	$	731,217	$	731,217
Accounts Payable	$	(6,039,382)	$	(3,019,691)	$	(3,019,691)
Jet Fuel Inventory	$	1,186,723	$	593,362	$	593,362
Raw Materials	$	1,197,370	$	598,685	$	598,685
Total	**$**	**6,707,570**	**$**	**3,353,785**	**$**	**3,353,785**
Present Value at 8%	*$*	*6,210,713*	*$*	*2,875,330*	*$*	*2,662,343*

Figure 20.7.3 Working capital for the plant.

The Total Permanent Investment discussed in Section 18 and the working capital sum to provide the Total Capital Investment of the plant which comes in at about $116MM.

21. Considerations

21.1 Health and Safety

The proposed process is conducted at high temperatures, with flammable, as well as toxic materials present. The reactor section is specifically designed to minimize the chance of a runaway temperature event, with oversized reactor beds and oversized heat exchangers. The controls in the reactor section must be closely monitored in the event of any temperature anomalies. Additionally, the feedstocks, as well as many of the products of this reaction are flammable. Due to flammability concerns the plant must be constructed with explosion proof equipment, and each part of the process must be monitored for leaks and potential formation of flammable vapor clouds. The process also produces a variety of hazardous chemicals, which can lead to significant health and environmental hazards with prolonged exposure. Due to these hazards, operators will be required to wear protective equipment, and the process must be regularly checked for material leakage and potential points of exposure. The storage tanks are constructed with floating heads to prevent both explosions and exposure to feedstocks and products.

21.2 Environmental Considerations

The process is designed to be an eco-friendly alternative to petroleum derived jet fuel. It is imperative that the energy demands of this process do not have a significant effect of the carbon neutral nature of the corn to fuel cycle. A majority of the equipment in the process uses steam and water to provide heating and cooling. The water and steam may require fuel sources to be heated and pumped. Additionally, the fired heater in the process uses natural gas as fuel. While natural gas burns cleaner than many other fuels, it still releases carbon into the atmosphere. Depending on the exact methods of farming and processing used, this process may still have a net carbon emission; however, it will be much lower than the processing and use of petroleum-based fuel.

There is also significant consideration due for the waste produced by this process. The water that leaves the process must be processed to remove organics and other pollutants before release into any body of water. Additionally, the light gases produced are used as fuel elsewhere, to offset use of shale gas and other fuels. Effective waste management is critical for both safety and the integrity of this process as a green process.

21.3 Location and Market Timing

The location of Clinton, IA was specifically chosen for access to ethanol manufacture in Iowa, which is the largest producer of ethanol in the United States. Iowa also supports a variety of programs that can give tax advantages to land purchases used for industry. Analysis of these programs was not included in this report because it is unclear whether or not the proposed plant would get approval for these tax advantages; nevertheless, it is important to acknowledge their existence as this may yield a more profitable venture. Clinton specifically offers a location advantage due to its proximity to the Mississippi River. The river may be used as a source of water and transportation of especially large equipment such as the first distillation tower.

There should also be consideration given to the timing of bringing this process to market. Currently, the product fuel of this process would need to sell for 4.55 times the price of conventional jet fuel. Fuel prices contribute significantly to ticket costs, so this increase in price may be unacceptable for today's consumers. Additionally, green sources of methanol are beginning to emerge, but the market is still in the early stages of formation. Another report, *CO_2 Capture and Conversion with Binding Organic Liquid*, proposes a process by which sequestered CO_2 can be converted into methanol, which would meet the green criteria sought by this process. However, the proposed sequestration process produces about 26,000 short tons of methanol per year which is too little for the scale of this process. The economics of this process are designed around construction beginning in 2023; however, it may be advisable to wait for the green methanol/biomethanol market to develop further, the emergence of more environmentally conscious generations, and additional regulations on non-renewable fuel and energy. This can potentially result in favorable market conditions for the product fuel, and a higher return.

22. *Profitability Analysis*

The profitability analysis of the plant was greatly facilitated by the use of the Profitability Analysis 4.0 Excel spreadsheet created by Mr. Brian Downey and maintained by Professor Bruce Vrana that was provided to the senior design class.

It assumed that design of the plant will commence in 2022 with construction beginning in 2023. Production and sales will begin the following year in 2024 initially starting at 45% capacity. In 2025, the production capacity will be upped to 67.5% with the remaining 13 years operating at 90% capacity. An income tax rate of 23% and a cost of capital/discount rate of 8% is used as recommended by Professor Vrana. A general inflation rate of 2% is used for all aspects of the plant's economics except for the product's inflation rate of 1.5% which was again recommended by Professor Vrana.

Instead of assuming a product price from the start, the green jet fuel price was calculated as to provide an internal rate of return (IRR) of 15%. The initial product price is the multiplication of the price of conventional jet fuel from crude oil ($0.24/lb) and a "green premium" factor. The necessary green premium was calculated to be 4.55. This is on point with renewable chemical company Gevo's estimation that the cost of producing biojet is "two to seven times greater than conventional jet fuel" (Gevo, 2019). The price required to achieve an IRR of 15% is then $1.09/lb of jet fuel, accordingly. The cash flow sheet for the life of the plant is shown on the following page in Table 22.1.

Table 22.1 Cash Flow Summary

Year	Percentage of Design Capacity	Product Unit Price	Sales	Capital Costs	Working Capital	Var Costs	Fixed Costs	Depreciation	Depletion Allowance	Taxible Income	Taxes	Net Earnings	Cash Flow	Cumulative Net Present Value at 8%
2022	0%		-	-	-	-	-	-	-	-	-	-	-	-
2023	0%		-	(104,244,900)	(6,707,600)	-	-	-	-	-	-	-	(110,952,500)	(102,733,800)
2024	45%	$1.09	108,288,500	-	(3,353,800)	(85,753,900)	(14,995,700)	(16,187,100)	-	(8,648,300)	1,989,100	(6,659,200)	6,174,200	(97,440,400)
2025	68%	$1.11	164,869,300	-	(3,353,800)	(131,203,500)	(15,295,600)	(25,899,400)	-	(7,529,300)	1,731,700	(5,797,500)	16,748,000	(84,145,300)
2026	90%	$1.12	223,123,100	-	-	(178,436,800)	(15,601,500)	(15,539,600)	-	13,545,100	(3,115,400)	10,429,700	25,969,300	(65,057,100)
2027	90%	$1.14	226,469,900	-	-	(182,005,600)	(15,913,600)	(9,323,800)	-	19,227,000	(4,422,200)	14,804,800	24,128,600	(48,635,600)
2028	90%	$1.16	229,867,000	-	-	(185,645,700)	(16,231,800)	(9,323,800)	-	18,665,700	(4,293,100)	14,372,600	23,696,300	(33,702,900)
2029	90%	$1.18	233,315,000	-	-	(189,358,600)	(16,556,500)	(4,661,900)	-	22,738,000	(5,229,700)	17,508,300	22,170,200	(20,766,800)
2030	90%	$1.19	236,814,700	-	-	(193,145,800)	(16,887,600)	-	-	26,781,300	(6,159,700)	20,621,600	20,621,600	(9,625,600)
2031	90%	$1.21	240,366,900	-	-	(197,008,700)	(17,225,400)	-	-	26,132,900	(6,010,600)	20,122,300	20,122,300	440,600
2032	90%	$1.23	243,972,400	-	-	(200,948,800)	(17,569,900)	-	-	25,453,700	(5,854,400)	19,599,400	19,599,400	9,518,900
2033	90%	$1.25	247,632,000	-	-	(204,967,800)	(17,921,300)	-	-	24,742,900	(5,690,900)	19,052,000	19,052,000	17,690,000
2034	90%	$1.27	251,346,500	-	-	(209,067,200)	(18,279,700)	-	-	23,999,600	(5,519,900)	18,479,700	18,479,700	25,028,500
2035	90%	$1.29	255,116,700	-	-	(213,248,500)	(18,645,300)	-	-	23,222,900	(5,341,300)	17,881,600	17,881,600	31,603,600
2036	90%	$1.31	258,943,400	-	-	(217,513,500)	(19,018,200)	-	-	22,411,700	(5,154,700)	17,257,000	17,257,000	37,478,900
2037	90%	$1.32	262,827,600	-	-	(221,863,800)	(19,398,500)	-	-	21,565,300	(4,960,000)	16,605,300	16,605,300	42,713,600
2038	90%	$1.34	266,770,000	-	13,415,100	(226,301,000)	(19,786,500)	-	-	20,682,400	(4,757,000)	15,925,500	29,340,600	51,277,800

The capital investment for the plant is recovered in 2031, the 8th year of production. At the end of the plant's life, the net present value (NPV) is a little more than $51MM. The return on investment (ROI) in the third production year is 13.58% as shown in Figure 22.1.

Annual Sales	**223,123,057**
Annual Costs	**(194,038,354)**
Depreciation	**(8,339,594)**
Income Tax	**(4,771,375)**
Net Earnings	**15,973,734**
Total Capital Investment	**117,660,066**
ROI	**13.58%**

Figure 22.1 Return on investment (ROI) calculation in the 3rd year of production.

As the economics of the process are greatly impacted by the product price as well as the variable costs, a two-dimensional sensitivity analysis was conducted by varying the product price and variables costs ±50% as shown in Figure 22.2. The cells highlighted in green indicate analyses yielding IRRs greater than or equal to 50% while those highlighted in yellow indicate analyses yielding IRRs between 15% and 50%.

Product Price \ Variable Costs	$95,282,167	$114,338,600	$133,395,033	$152,451,466	$171,507,900	***$190,564,333***	$209,620,766	$228,677,200	$247,733,633	$266,790,066	$285,846,500
$0.55	-8.01%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.65	17.01%	-0.25%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.76	30.37%	19.61%	4.77%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.87	41.44%	32.32%	22.03%	8.70%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.98	51.40%	43.09%	34.20%	24.30%	12.04%	-18.46%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.09	60.67%	52.85%	44.69%	36.01%	26.45%	15.00%	-4.42%	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.20	69.43%	61.97%	54.27%	46.25%	37.76%	28.50%	17.68%	1.78%	Negative IRR	Negative IRR	Negative IRR
$1.31	77.79%	70.60%	63.23%	55.65%	47.76%	39.45%	30.45%	20.15%	6.23%	Negative IRR	Negative IRR
$1.42	85.82%	78.85%	71.74%	64.47%	57.00%	49.24%	41.09%	32.33%	22.46%	9.85%	Negative IRR
$1.53	93.57%	86.78%	79.89%	72.87%	65.69%	58.31%	50.68%	42.68%	34.14%	24.63%	12.97%
$1.64	101.08%	94.45%	87.73%	80.91%	73.97%	66.87%	59.60%	52.08%	44.23%	35.88%	26.69%

Figure 22.2 Sensitivity analysis on the IRR with varying product price and variable costs.

The biomethanol price had to be estimated, due to lack of availability, as 2x the expected price for petrochemical methanol. However, since the variable costs effect the necessary product price, a sensitivity analysis was conducted, shown in Figure 22.3, by varying the biomethanol "green" multiplication factor to analyze the effect it would have on product price and IRR. The cells highlighted in green indicate an IRR above 15%. If biomethanol production only requires a 1.5x raise in price, then the jet fuel price will only be 4x as expensive as traditional jet fuel. The impact of biomethanol costing on the jet fuel price is not very dramatic, however for this process to succeed, available sources of biomethanol will need to become financially viable.

Biomethanol "Green" Factor	Product Price										
	$ 0.55	$ 0.65	$ 0.76	$ 0.87	$ 0.98	***$ 1.09***	$ 1.20	$ 1.31	$ 1.42	$ 1.53	$ 1.64
0.75	Negative IRR	Negative IRR	5.52%	22.02%	33.93%	44.23%	53.66%	62.49%	70.88%	78.91%	86.65%
1.00	Negative IRR	Negative IRR	-15.05%	14.86%	28.31%	39.27%	49.07%	58.17%	66.76%	74.96%	82.83%
1.25	Negative IRR	Negative IRR	Negative IRR	5.52%	22.11%	34.03%	44.32%	53.73%	62.55%	70.93%	78.95%
1.50	Negative IRR	Negative IRR	Negative IRR	-16.50%	14.93%	28.40%	39.36%	49.16%	58.24%	66.82%	75.00%
1.75	Negative IRR	Negative IRR	Negative IRR	Negative IRR	5.52%	22.20%	34.12%	44.41%	53.81%	62.62%	70.98%
2.00	Negative IRR	Negative IRR	Negative IRR	Negative IRR	-18.46%	15.00%	28.50%	39.45%	49.24%	58.31%	66.87%
2.25	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	5.52%	22.29%	34.22%	44.50%	53.89%	62.68%
2.50	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	-21.39%	15.07%	28.59%	39.54%	49.32%	58.38%
2.75	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	5.52%	22.38%	34.31%	44.59%	53.96%
3.00	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	-26.44%	15.14%	28.69%	39.64%	49.40%
3.25	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	5.52%	22.47%	34.41%	44.67%

Figure 22.3 Sensitivity analysis on the IRR with varying product price and biomethanol "green" factor.

23. Recommendations

The 4.55x green premium factor on the biojet fuel produced in this process is likely too large for the process to be economical today. This factor is on par with that predicted by Gevo for biojet fuel production (Gevo, 2019). Before recommending this process, significant market research will be needed to ensure the green premium levied on the biojet fuel is economically feasible. Currently, the 4.55x green premium factor results in a profitable venture with an IRR of 15%, an NPV of $51.7MM, and a third year ROI of 13.8%. As consumer and regulatory awareness of the environmental impacts of air travel continue to grow in the coming years, the process will become more and more economically viable. In the near future, an increased social swing to renewable products could lead to consumers spending more money on products that positively impact the environment. Furthermore, tax exemptions for renewable processes could reduce the costs of producing biojet fuel.

Also, to achieve true net carbon neutrality in the biojet fuel production process, higher production levels of the bio-sourced and renewable methanol and ethanol will be required. The production of renewable methanol and ethanol will continue to increase as more companies invest in anaerobic digestion of industrial and municipal waste as well as carbon capture from carbon dioxide in flue gas. As biomethanol becomes more readily available, the green premium factor associated with it will likely decrease thus lowering the raw material cost for this process.

It is also recommended to further research the effect of high water content in isobutanol feeds in dehydration reactions to form isobutene. As discussed in this report, current research has shown

99% conversions of isobutanol to isobutene in feeds with up to 15% water content by mass. If more efficient dehydration processes are discovered to allow even larger water contents in isobutanol feeds while still achieving high conversions, the economic costs of the biojet process could be reduced even further.

24. Acknowledgements

Our team would like to acknowledge the multitude of people who made this project possible. Firstly, we would like to acknowledge Professor Bruce Vrana and Dr. Sean Holleran, both of whom dedicated significant time and effort to our team's project and were instrumental in the process and economic analysis enclosed in this report. Additionally, we would like to acknowledge Dr. Richard Bockrath, who authored the unique and challenging problem statement addressed in this report and was also willing to share his expertise and years of experience with us, which was supremely necessary in designing a robust and effective process. We would also like to extend our deepest thanks to Professor Len Fabiano, who's effort and knowledge were indispensable in our mission to complete this project to the best of our abilities. His knowledge of ASPEN and years of process engineering experience played an enormous role in the work presented here. We would like to thank the department of Chemical and Biomolecular Engineering at Penn, from the faculty, to the administration, to our TA's and everyone else who educated, challenged, and guided us over the past four years, and ultimately enabled us to take this project head on. We would also like to extend a special acknowledgment to our families and friends who have supported us throughout our time here and especially during the COVID-19 pandemic, which has presented a variety of both physical and intangible obstacles that needed to be overcome to deliver this report.

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26. Appendix

26.1 Project Description/Problem Statement

The project description/problem statement written by project author Dr. Richard Bockrath is provided on the following pages. Note that the initial recommendation of oversizing the packed bed reactors by 50% was later increased to 100%. Also, the targeted IRR for the project was reduced from 20% to a more reasonable 15%.

Suggested CBE 459 Design Projects – 2020-2021

1. Biofuels for Aviation (Recommended by Rick Bockrath, Consultant – retired from DuPont)

Background

You are the Senior Vice-President for Sustainability at one of the largest Airline carriers. The current core sustainability goals for your company are heavily focused on the improvement of the fuel efficiency of the jet engines and increasingly sophisticated AI-based management of the routes taken by the planes to minimize fuel consumption. There has been a consistent desire to have a third focus by moving into sustainable, bio-based fuels. Yet so far, this has not been a viable commercial option. Aside from some clearly press release-oriented activities, there has been no clear-cut movement toward such sustainable fuels because of their apparently high cost structure.

Gevo is the company that seems to be the furthest along in developing such a biofuel. In December 2019 they released a "White Paper" document entitled "SUSTAINABLE AVIATION FUEL: Alcohol-to-Jet Synthetic Paraffinic Kerosene Is a Proven Pathway to Deliver a Bio-Based, Low-Carbon Option to Travelers". The following statement in the document summarizes the current dilemma:

"… the cost of producing biojet is estimated to be two to seven times greater than conventional jet fuel for the foreseeable future".

Your fear is that "seven times greater" is more likely than "two times greater".

Gevo's overall transformation technology is based on fermentation of corn mash directly to isobutanol followed by dehydration of isobutanol to isobutene which is then oligomerized to an isoparaffinic mix that is about twelve carbons in length, which is a good jet fuel. Gevo has extensively tested their material, which is called ATJ-SPK against Jet Fuel standards (ASTM D1655/7566) and has shown that it meets the required specifications.

The key to any biofuel will be a highly scalable series of unit operations from initial feedstock through final product. This is especially critical for the large volume production of jet fuels. Your company hired an outside technology assessment firm to look at the Gevo process and their key conclusions are given below:

a) The concept of retrofitting US ethanol plants to make isobutanol instead of ethanol is of interest since US ethanol plants are world scale and consistent with bio-fuel volume needs.
b) The dehydration of isobutanol to isobutene is well established technology that is commercially practiced, and the technology is available for licensing from a number of technology providers. Yield is virtually 100%.
c) The oligomerization of isobutene (C4) to an average chain length of twelve is a quite reasonable extension of well-known isooctane (C8) technology which is widely practiced commercially and is available from a number of technology providers. Yield is virtually 100%.
d) The key bottleneck in the overall process is that the retrofit of an ethanol plant to make isobutanol appears to result in a dramatic decrease in overall plant capacity. The plant capacity is no longer world scale. This has the result of making the isobutanol generation step very expensive.
e) To make the corn to isobutanol to biofuel process sequence viable, an alternative way to make isobutanol is needed.

f) Since ethanol plants are highly efficient in making ethanol, a potential route to isobutanol via ethanol and methanol could be quite advantageous and might make the overall corn to bio-fuel story successful. The chemistry involved is called Guerbet chemistry. The overall sequence would then be:

Corn mash to ethanol.
Ethanol and biomethanol to isobutanol.
Well established technologies for the dehydration and oligomerization steps.

Since your company's expertise is neither in chemistry nor catalysis, you contracted with a group of academic/industrial consultants in this field to fully explore the Guerbet chemistry technology landscape for cost efficient transformations. They found the following article to be the most promising; although, it must be realized that the work is at the early stages of R&D development.

"Higher-Alcohols Biorefinery: Improvement of Catalyst for Ethanol Conversion", E. S. Olson, R. K. Sharma and T. R. Aulich, Applied Biochemistry and Biotechnology Vol. 113–116, p 913- 933, 2004

In the article, isobutanol is the dominant product at 90+% yields. Biomethanol can be made from biomethane which can be obtained from a number of different sources. Bioethanol is readily available from current ethanol plants.

The improvements detailed in the article are significant enough to justify further analysis. If the analysis is positive; then, upper management will likely want to approach the owner of the technology to discuss a joint development R&D partnership.

Since the technology is in its early R&D stage, the consultants suggest that the following assumptions be used in the analysis.

a) It is likely that the catalyst activity can be markedly improved and so a rate that is three times higher than the results in Table 4 (Ni-FM case) is reasonable.
b) The product distribution will be more difficult to improve on and so assume the product mix from Table 4 (Ni-FM) for the liquid compounds and Table 3 for the gases for the analysis.
c) The authors demonstrated the successful recycle of the lighter alcohols to the desired product and this should be assumed in the analysis.
d) Catalyst decay rates are not provided. They suggested that you oversize the reactor bed by 50% over the (kg of product/hr)/(kg of catalyst) demonstrated in Table 4. It should be noted that the conversion of the ethanol was 100% and so the flow rate through the reactor could have been higher while still getting very high conversions. Therefore using 100% conversion rate data plus a further 50% increase allows for significant activity decay before the bed must be renewed.
e) Assume the bed has a 2-month life before it must be decoked.
f) Since the support is activated carbon there will be some loss of catalyst in the decoking step. Assume that there is a 10% catalyst loss that must be made up by the addition of fresh catalyst to the top of the bed.
g) The catalyst uses inexpensive metals and salts and is not expected to be expensive. They suggest assuming \$5/lb for the Ni-FM catalyst. This is approximately 25% higher pricing than Fluid Cat Cracker catalyst.

You need a technoeconomic analysis of the overall cost of transformation. You do not want the cost of purchasing bioethanol or biomethanol to confuse the initial analysis, so your focus is on the transformation cost. You have started discussions with your Logistics/Supply organization to answer those feedstock cost questions. This analysis is to focus on the CAPEX and OPEX to take ethanol and methanol through to biofuel. You have had preliminary discussions with the current technology providers for the dehydration and oligomerization steps at the scale of interest to you and so the analysis is to assume the following:

Dehydration step: CAPEX of \$ 0.10/kg/yr of jet fuel, OPEX of \$0.03/kg of jet fuel. 100% yield

Oligomerization step: CAPEX of \$ 0.15/kg/yr. OPEX of \$0.034/kg of jet fuel. 100% yield

Once you have an analysis of the ethanol/methanol to isobutanol step's CAPEX and OPEX, you can then bring all of the transformation steps together and have an overall picture of the process cost structure.

For this analysis assume the plant capacity is 100 kt/yr jet-fuel (129 kiloton isobutanol).

As a framework for comparison, your company pays close attention to the cost difference between crude oil and jet fuel. Over the 2010 to 2019 time period, the spread has averaged \$0.05/kg of jet fuel. Clearly the existing cost of transformation is quite efficient. This spread covers OPEX and a return on the CAPEX. You realize that bio-jet will be more expensive than regular jet fuel, but it is unlikely that you can "afford" more than a \$0.50/kg cost of transformation OPEX and return on CAPEX. Your goal is to find out if this can be achieved.

You will need to make many assumptions in the course of completing the analysis and so management will expect a strongly positive result before proceeding further due to the uncertainties inherent in your analysis. An IRR of greater 20% should be sufficient. You expect that you will exceed 20% but if your analysis falls short then upper management wants to know the required price to reach 20%.

General Considerations

The plant design should be as environmentally friendly as possible. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate. You will need to make many assumptions and these need to be fully documented in your analysis.

References

"Higher-Alcohols Biorefinery: Improvement of Catalyst for Ethanol Conversion", E. S. Olson, R. K. Sharma and T. R. Aulich, Applied Biochemistry and Biotechnology Vol. 113–116, p 913- 933, 2004

" SUSTAINABLE AVIATION FUEL: Alcohol-to-Jet Synthetic Paraffinic Kerosene Is a Proven Pathway to Deliver a Bio-Based, Low-Carbon Option to Travelers", GEVO White Paper, December 2019.

26.2 Material Safety Data Sheets (MSDSs)

The MSDSs of the selected chemicals (methanol, ethanol, isobutanol, and water) can be found in the following pages. Each chemical's MSDS will begin on a new page for convenience.

26.2.1 Methanol

ThermoFisher SCIENTIFIC

SAFETY DATA SHEET

Creation Date 27-Apr-2009 **Revision Date** 11-Apr-2018 **Revision Number** 7

1. Identification

Product Name	**Methanol**
Cat No. :	**A413-4; A413-20; A413-200; A413-500**
CAS-No	67-56-1
Synonyms	Methyl alcohol
Recommended Use	Laboratory chemicals.
Uses advised against	Food, drug, pesticide or biocidal product use

Details of the supplier of the safety data sheet

Company
Fisher Scientific
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Emergency Telephone Number
CHEMTREC®, Inside the USA: 800-424-9300
CHEMTREC®, Outside the USA: 001-703-527-3887

2. Hazard(s) identification

Classification
This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 2
Acute oral toxicity	Category 3
Acute dermal toxicity	Category 3
Acute Inhalation Toxicity - Vapors	Category 3
Specific target organ toxicity (single exposure)	Category 1
Target Organs - Optic nerve.	
Specific target organ toxicity - (repeated exposure)	Category 1
Target Organs - Kidney, Liver, spleen, Blood.	

Label Elements

Signal Word
Danger

Hazard Statements
Highly flammable liquid and vapor
Toxic if swallowed
Toxic in contact with skin
Toxic if inhaled
Causes damage to organs
Causes damage to organs through prolonged or repeated exposure

Precautionary Statements
Prevention
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear protective gloves/protective clothing/eye protection/face protection
Use only outdoors or in a well-ventilated area
Do not breathe dust/fume/gas/mist/vapors/spray
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting/equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Keep cool
Response
IF exposed: Call a POISON CENTER or doctor/physician
Inhalation
IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Call a POISON CENTER or doctor/physician
Skin
Call a POISON CENTER or doctor/physician if you feel unwell
Wash contaminated clothing before reuse
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower
Ingestion
IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
Rinse mouth
Fire
In case of fire: Use CO2, dry chemical, or foam for extinction
Storage
Store locked up
Store in a well-ventilated place. Keep container tightly closed
Disposal
Dispose of contents/container to an approved waste disposal plant
Hazards not otherwise classified (HNOC)

Other hazards
Poison, may be fatal or cause blindness if swallowed. Vapor harmful. Cannot be made non-poisonous.
WARNING. Reproductive Harm - https://www.p65warnings.ca.gov/.

3. Composition/Information on Ingredients

Component	CAS-No	Weight %
Methyl alcohol	67-56-1	>95

4. First-aid measures

General Advice Immediate medical attention is required. Show this safety data sheet to the doctor in attendance.

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

Inhalation Move to fresh air. If breathing is difficult, give oxygen. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.

Ingestion Do not induce vomiting. Call a physician or Poison Control Center immediately.

Most important symptoms and effects Breathing difficulties. May cause blindness: Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Cool closed containers exposed to fire with water spray.

Unsuitable Extinguishing Media Water may be ineffective

Flash Point 12 °C / 53.6 °F

Method - No information available

Autoignition Temperature 455 °C / 851 °F

Explosion Limits

Upper 31.00 vol %

Lower 6.0 vol %

Sensitivity to Mechanical Impact No information available

Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Flammable. Risk of ignition. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Vapors may form explosive mixtures with air.

Hazardous Combustion Products

Carbon monoxide (CO) Formaldehyde

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

NFPA

Health	Flammability	Instability	Physical hazards
1	3	0	N/A

6. Accidental release measures

Personal Precautions Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Use personal protective equipment. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions Should not be released into the environment. See Section 12 for additional ecological information.

Methods for Containment and Clean Up Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

7. Handling and storage

Handling Wear personal protective equipment. Do not breathe vapors or spray mist. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not ingest. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

Storage Keep container tightly closed in a dry and well-ventilated place. Keep away from open flames, hot surfaces and sources of ignition. Flammables area.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	Mexico OEL (TWA)
Methyl alcohol	TWA: 200 ppm STEL: 250 ppm Skin	(Vacated) TWA: 200 ppm (Vacated) TWA: 260 mg/m³ (Vacated) STEL: 250 ppm (Vacated) STEL: 325 mg/m³ Skin TWA: 200 ppm TWA: 260 mg/m³	IDLH: 6000 ppm TWA: 200 ppm TWA: 260 mg/m³ STEL: 250 ppm STEL: 325 mg/m³	TWA: 200 ppm TWA: 260 mg/m³ STEL: 250 ppm STEL: 310 mg/m³

Legend

ACGIH *- American Conference of Governmental Industrial Hygienists*
OSHA *- Occupational Safety and Health Administration*
NIOSH IDLH: *The National Institute for Occupational Safety and Health Immediately Dangerous to Life or Health*

Engineering Measures Use only under a chemical fume hood. Use explosion-proof electrical/ventilating/lighting/equipment. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

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

Hygiene Measures When using, do not eat, drink or smoke. Provide regular cleaning of equipment, work area and clothing.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Colorless
Odor	Alcohol-like
Odor Threshold	No information available
pH	Not applicable
Melting Point/Range	-98 °C / -144.4 °F
Boiling Point/Range	64.7 °C / 148.5 °F @ 760 mmHg
Flash Point	12 °C / 53.6 °F
Evaporation Rate	5.2 (ether = 1)
Flammability (solid,gas)	Not applicable

Flammability or explosive limits	
Upper	31.00 vol %
Lower	6.0 vol %
Vapor Pressure	128 hPa @ 20 °C
Vapor Density	1.11
Specific Gravity	0.791
Solubility	Miscible with water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	455 °C / 851 °F
Decomposition Temperature	No information available
Viscosity	0.55 cP at 20 °C
Molecular Formula	C H4 O
Molecular Weight	32.04
VOC Content(%)	100
Surface tension	0.02255 N/m @ 20°C

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable under normal conditions.

Conditions to Avoid Incompatible products. Heat, flames and sparks. Keep away from open flames, hot surfaces and sources of ignition.

Incompatible Materials Strong oxidizing agents, Strong acids, Acid anhydrides, Acid chlorides, Strong bases, Metals, Peroxides

Hazardous Decomposition Products Carbon monoxide (CO), Formaldehyde

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information
Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Methyl alcohol	**Calc. ATE 60 mg/kg** LD50 > 1187 – 2769 mg/kg (Rat)	**Calc. ATE 60 mg/kg** LD50 = 17100 mg/kg (Rabbit)	**Calc. ATE 0.6 mg/L (vapours) or 0.5 mg/L (mists)** LC50 = 128.2 mg/L (Rat) 4 h

Toxicologically Synergistic Products Carbon tetrachloride

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation May cause skin and eye irritation

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
Methyl alcohol	67-56-1	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects Component substance is listed on California Proposition 65 as a developmental hazard.

Teratogenicity No information available.

STOT - single exposure Optic nerve
STOT - repeated exposure Kidney Liver spleen Blood

Aspiration hazard No information available

Symptoms / effects,both acute and delayed May cause blindness: Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity
.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Methyl alcohol	Not listed	Pimephales promelas: LC50 > 10000 mg/L 96h	EC50 = 39000 mg/L 25 min EC50 = 40000 mg/L 15 min EC50 = 43000 mg/L 5 min	EC50 > 10000 mg/L 24h

Persistence and Degradability Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its volatility.

Component	log Pow
Methyl alcohol	-0.74

13. Disposal considerations

Waste Disposal Methods Should not be released into the environment.

Component	RCRA - U Series Wastes	RCRA - P Series Wastes
Methyl alcohol - 67-56-1	U154	-

14. Transport information

DOT
- **UN-No** UN1230
- **Proper Shipping Name** METHANOL
- **Hazard Class** 3
- **Packing Group** II

TDG
- **UN-No** UN1230
- **Proper Shipping Name** METHANOL
- **Hazard Class** 3
- **Subsidiary Hazard Class** 6.1
- **Packing Group** II

IATA
- **UN-No** UN1230
- **Proper Shipping Name** METHANOL
- **Hazard Class** 3
- **Subsidiary Hazard Class** 6.1
- **Packing Group** II

IMDG/IMO
- **UN-No** UN1230
- **Proper Shipping Name** METHANOL

Hazard Class	3
Subsidiary Hazard Class	6.1
Packing Group	II

15. Regulatory information

International Inventories

Component	TSCA	DSL	NDSL	EINECS	ELINCS	NLP	PICCS	ENCS	AICS	IECSC	KECL
Methyl alcohol	X	X	-	200-659-6	-		X	X	X	X	X

Legend:
X - Listed
E - Indicates a substance that is the subject of a Section 5(e) Consent order under TSCA.
F - Indicates a substance that is the subject of a Section 5(f) Rule under TSCA.
N - Indicates a polymeric substance containing no free-radical initiator in its inventory name but is considered to cover the designated polymer made with any free-radical initiator regardless of the amount used.
P - Indicates a commenced PMN substance
R - Indicates a substance that is the subject of a Section 6 risk management rule under TSCA.
S - Indicates a substance that is identified in a proposed or final Significant New Use Rule
T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.
XU - Indicates a substance exempt from reporting under the Inventory Update Rule, i.e. Partial Updating of the TSCA Inventory Data Base Production and Site Reports (40 CFR 710(B).
Y1 - Indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.
Y2 - Indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule.

U.S. Federal Regulations

TSCA 12(b) Not applicable

SARA 313

Component	CAS-No	Weight %	SARA 313 - Threshold Values %
Methyl alcohol	67-56-1	>95	1.0

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act

Component	HAPS Data	Class 1 Ozone Depletors	Class 2 Ozone Depletors
Methyl alcohol	X		-

OSHA Occupational Safety and Health Administration
Not applicable

CERCLA This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302)

Component	Hazardous Substances RQs	CERCLA EHS RQs
Methyl alcohol	5000 lb	-

California Proposition 65 This product contains the following proposition 65 chemicals

Component	CAS-No	California Prop. 65	Prop 65 NSRL	Category
Methyl alcohol	67-56-1	Developmental	-	Developmental

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Methyl alcohol	X	X	X	X	X

U.S. Department of Transportation

Reportable Quantity (RQ):	Y
DOT Marine Pollutant	N
DOT Severe Marine Pollutant	N

U.S. Department of Homeland Security
This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade	Serious risk, Grade 3

16. Other information

Prepared By	Regulatory Affairs Thermo Fisher Scientific Email: EMSDS.RA@thermofisher.com
Creation Date	27-Apr-2009
Revision Date	11-Apr-2018
Print Date	11-Apr-2018
Revision Summary	This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

Disclaimer
The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS

26.2.2 Ethanol

SAFETY DATA SHEET

Airgas

Ethanol

Section 1. Identification

GHS product identifier : Ethanol

Chemical name : ethanol

Other means of identification : ethyl alcohol; Denatured Alcohol; ALCOHOL; Ethyl alcohol (Ethanol)

Product use : Synthetic/Analytical chemistry.

Synonym : ethyl alcohol; Denatured Alcohol; ALCOHOL; Ethyl alcohol (Ethanol)

SDS # : 001114

Supplier's details : Airgas USA, LLC and its affiliates
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Emergency telephone number (with hours of operation) : 1-866-734-3438

Section 2. Hazards identification

OSHA/HCS status : This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Classification of the substance or mixture : FLAMMABLE LIQUIDS - Category 2

GHS label elements

Hazard pictograms :

Signal word : Danger

Hazard statements : Highly flammable liquid and vapor.
May form explosive mixtures with air.

Precautionary statements

General : Read label before use. Keep out of reach of children. If medical advice is needed, have product container or label at hand.

Prevention : Wear protective gloves. Wear eye or face protection. Keep away from heat, sparks, open flames and hot surfaces. - No smoking. Use explosion-proof electrical, ventilating, lighting and all material-handling equipment. Use only non-sparking tools. Take precautionary measures against static discharge. Keep container tightly closed. Use and store only outdoors or in a well ventilated place.

Response : IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.

Storage : Store in a well-ventilated place. Keep cool.

Disposal : Dispose of contents and container in accordance with all local, regional, national and international regulations.

Hazards not otherwise classified : None known.

Section 3. Composition/information on ingredients

Substance/mixture : Substance

Chemical name : ethanol

Other means of identification : ethyl alcohol; Denatured Alcohol; ALCOHOL; Ethyl alcohol (Ethanol)

CAS number/other identifiers

CAS number : 64-17-5

Product code : 001114

Ingredient name	%	CAS number
ethanol	100	64-17-5

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified as hazardous to health or the environment and hence require reporting in this section.

Occupational exposure limits, if available, are listed in Section 8.

Section 4. First aid measures

Description of necessary first aid measures

Eye contact : Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention if irritation occurs.

Inhalation : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention if adverse health effects persist or are severe. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.

Skin contact : Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Get medical attention if symptoms occur. Wash clothing before reuse. Clean shoes thoroughly before reuse.

Ingestion : Wash out mouth with water. Remove dentures if any. Remove victim to fresh air and keep at rest in a position comfortable for breathing. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Stop if the exposed person feels sick as vomiting may be dangerous. Do not induce vomiting unless directed to do so by medical personnel. If vomiting occurs, the head should be kept low so that vomit does not enter the lungs. Get medical attention if adverse health effects persist or are severe. Never give anything by mouth to an unconscious person. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.

Most important symptoms/effects, acute and delayed

Potential acute health effects

Eye contact : No known significant effects or critical hazards.

Inhalation : No known significant effects or critical hazards.

Skin contact : No known significant effects or critical hazards.

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

Ingestion : No known significant effects or critical hazards.

Over-exposure signs/symptoms

Eye contact : No specific data.

Section 4. First aid measures

Inhalation : No specific data.

Skin contact : No specific data.

Ingestion : No specific data.

Indication of immediate medical attention and special treatment needed, if necessary

Notes to physician : Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.

Specific treatments : No specific treatment.

Protection of first-aiders : No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

See toxicological information (Section 11)

Section 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media : Use dry chemical, CO_2, water spray (fog) or foam.

Unsuitable extinguishing media : Do not use water jet.

Specific hazards arising from the chemical : Highly flammable liquid and vapor. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapor/gas is heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazard.

Hazardous thermal decomposition products : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Special protective actions for fire-fighters : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.

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

Section 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

For non-emergency personnel : No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.

For emergency responders : If specialised clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

Section 6. Accidental release measures

Methods and materials for containment and cleaning up

Small spill : Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Dilute with water and mop up if water-soluble. Alternatively, or if water-insoluble, absorb with an inert dry material and place in an appropriate waste disposal container. Dispose of via a licensed waste disposal contractor.

Large spill : Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see Section 13). Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see Section 1 for emergency contact information and Section 13 for waste disposal.

Section 7. Handling and storage

Precautions for safe handling

Protective measures : Put on appropriate personal protective equipment (see Section 8). Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use only non-sparking tools. Take precautionary measures against electrostatic discharges. Empty containers retain product residue and can be hazardous. Do not reuse container.

Advice on general occupational hygiene : Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.

Conditions for safe storage, including any incompatibilities : Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

Section 8. Exposure controls/personal protection

Control parameters

Occupational exposure limits

Ingredient name	Exposure limits
ethanol	**ACGIH TLV (United States, 3/2012).** STEL: 1000 ppm 15 minutes. **OSHA PEL 1989 (United States, 3/1989).** TWA: 1000 ppm 8 hours. TWA: 1900 mg/m³ 8 hours. **NIOSH REL (United States, 1/2013).** TWA: 1000 ppm 10 hours. TWA: 1900 mg/m³ 10 hours.

Section 8. Exposure controls/personal protection

	OSHA PEL (United States, 6/2010). TWA: 1000 ppm 8 hours. TWA: 1900 mg/m³ 8 hours.

Appropriate engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Environmental exposure controls : Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

Individual protection measures

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Eye/face protection : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: safety glasses with side-shields.

Skin protection

Hand protection : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.

Body protection : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product. When there is a risk of ignition from static electricity, wear anti-static protective clothing. For the greatest protection from static discharges, clothing should include anti-static overalls, boots and gloves.

Other skin protection : Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

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

Section 9. Physical and chemical properties

Appearance

Physical state : Liquid. [CLEAR, COLORLESS LIQUID WITH A WEAK, ETHEREAL, VINOUS ODOR]

Color : Colorless. Clear.

Molecular weight : 46.08 g/mole

Molecular formula : C2-H6-O

Boiling/condensation point : 78.29°C (172.9°F)

Section 9. Physical and chemical properties

Melting/freezing point	:	-114°C (-173.2°F)
Critical temperature	:	Not available.
Odor	:	Characteristic.
Odor threshold	:	Not available.
pH	:	Not available.
Flash point	:	Closed cup: 9.7°C (49.5°F)
Burning time	:	Not applicable.
Burning rate	:	Not applicable.
Evaporation rate	:	1.7 (butyl acetate = 1)
Flammability (solid, gas)	:	Not available.
Lower and upper explosive (flammable) limits	:	Lower: 3.3% Upper: 19%
Vapor pressure	:	5.7 kPa (42.948650611 mm Hg) [room temperature]
Vapor density	:	1.6 (Air = 1)
Specific Volume (ft^3/lb)	:	1.2716
Gas Density (lb/ft^3)	:	0.7864 (25°C / 77 to °F)
Relative density	:	0.8
Solubility	:	Not available.
Solubility in water	:	1000 g/l
Partition coefficient: n-octanol/water	:	-0.35
Auto-ignition temperature	:	455°C (851°F)
Decomposition temperature	:	Not available.
SADT	:	Not available.
Viscosity	:	Dynamic (room temperature): 0.544 to 0.59 mPa·s (0.544 to 0.59 cP)

Section 10. Stability and reactivity

Reactivity	:	No specific test data related to reactivity available for this product or its ingredients.
Chemical stability	:	The product is stable.
Possibility of hazardous reactions	:	Under normal conditions of storage and use, hazardous reactions will not occur.
Conditions to avoid	:	Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition. Do not allow vapor to accumulate in low or confined areas.
Incompatibility with various substances	:	Highly reactive or incompatible with the following materials: oxidizing materials and alkalis.
Hazardous decomposition products	:	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization	:	Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Information on toxicological effects

Acute toxicity

Not available.

Irritation/Corrosion

Not available.

Sensitization

Not available.

Mutagenicity

Not available.

Carcinogenicity

Not available.

Reproductive toxicity

Not available.

Teratogenicity

Not available.

Specific target organ toxicity (single exposure)

Not available.

Specific target organ toxicity (repeated exposure)

Not available.

Aspiration hazard

Not available.

Information on the likely routes of exposure : Not available.

Potential acute health effects

Eye contact : No known significant effects or critical hazards.
Inhalation : No known significant effects or critical hazards.
Skin contact : No known significant effects or critical hazards.
Ingestion : No known significant effects or critical hazards.

Symptoms related to the physical, chemical and toxicological characteristics

Eye contact : No specific data.
Inhalation : No specific data.
Skin contact : No specific data.
Ingestion : No specific data.

Delayed and immediate effects and also chronic effects from short and long term exposure

Short term exposure

Potential immediate effects : Not available.
Potential delayed effects : Not available.

Long term exposure

Section 11. Toxicological information

Potential immediate effects : Not available.

Potential delayed effects : Not available.

Potential chronic health effects

Not available.

General : No known significant effects or critical hazards.

Carcinogenicity : No known significant effects or critical hazards.

Mutagenicity : No known significant effects or critical hazards.

Teratogenicity : No known significant effects or critical hazards.

Developmental effects : No known significant effects or critical hazards.

Fertility effects : No known significant effects or critical hazards.

Numerical measures of toxicity

Acute toxicity estimates

Not available.

Section 12. Ecological information

Toxicity

Not available.

Persistence and degradability

Not available.

Bioaccumulative potential

Product/ingredient name	$LogP_{ow}$	BCF	Potential
ethanol	-0.35	-	low

Mobility in soil

Soil/water partition coefficient (K_{OC}) : Not available.

Other adverse effects : No known significant effects or critical hazards.

Section 13. Disposal considerations

Disposal methods : The generation of waste should be avoided or minimized wherever possible. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible. This material and its container must be disposed of in a safe way. Care should be taken when handling emptied containers that have not been cleaned or rinsed out. Empty containers or liners may retain some product residues. Vapor from product residues may create a highly flammable or explosive atmosphere

Section 13. Disposal considerations

inside the container. Do not cut, weld or grind used containers unless they have been cleaned thoroughly internally. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Section 14. Transport information

	DOT	TDG	Mexico	IMDG	IATA
UN number	UN1170	UN1170	UN1170	UN1170	UN1170
UN proper shipping name	ETHANOL OR ETHYL ALCOHOL OR ETHANOL SOLUTIONS OR ETHYL ALCOHOL SOLUTIONS	ETHANOL MORE THAN 24 PER CENT ETHANOL, BY VOLUME; ETHANOL SOLUTION MORE THAN 24 PER CENT ETHANOL, BY VOLUME; ETHYL ALCOHOL MORE THAN 24 PER CENT ETHANOL, BY VOLUME; OR ETHYL ALCOHOL SOLUTION MORE THAN 24 PER CENT ETHANOL, BY VOLUME	ETHANOL OR ETHYL ALCOHOL OR ETHANOL SOLUTIONS OR ETHYL ALCOHOL SOLUTIONS	ETHANOL (ETHYL ALCOHOL) OR ETHANOL SOLUTION (ETHYL ALCOHOL SOLUTION)	ETHANOL
Transport hazard class(es)	3 	3 	3 	3 	3 
Packing group	II	II	II	II	II
Environment	No.	No.	No.	No.	No.
Additional information	**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: 5 L **Cargo aircraft** Quantity limitation: 60 L **Special provisions** 24, IB2, T4, TP1	**Explosive Limit and Limited Quantity Index** 5 **Passenger Carrying Road or Rail Index** 60	-	-	**Passenger and Cargo Aircraft** Quantity limitation: 5 L **Cargo Aircraft Only** Quantity limitation: 60 L **Limited Quantities - Passenger Aircraft** Quantity limitation: 1 L

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

Special precautions for user : **Transport within user's premises:** always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code : Not available.

Section 15. Regulatory information

U.S. Federal regulations : **TSCA 8(a) CDR Exempt/Partial exemption**: Not determined
United States inventory (TSCA 8b): This material is listed or exempted.

Clean Air Act Section 112 (b) Hazardous Air Pollutants (HAPs) : Not listed

Clean Air Act Section 602 Class I Substances : Not listed

Clean Air Act Section 602 Class II Substances : Not listed

DEA List I Chemicals (Precursor Chemicals) : Not listed

DEA List II Chemicals (Essential Chemicals) : Not listed

SARA 302/304

Composition/information on ingredients

No products were found.

SARA 304 RQ : Not applicable.

SARA 311/312

Classification : Fire hazard

Composition/information on ingredients

Name	%	Fire hazard	Sudden release of pressure	Reactive	Immediate (acute) health hazard	Delayed (chronic) health hazard
ethanol	100	Yes.	No.	No.	No.	No.

State regulations

Massachusetts : This material is listed.

New York : This material is not listed.

New Jersey : This material is listed.

Pennsylvania : This material is listed.

Canada inventory : This material is listed or exempted.

International regulations

International lists : **Australia inventory (AICS)**: This material is listed or exempted.
China inventory (IECSC): This material is listed or exempted.
Japan inventory: This material is listed or exempted.
Korea inventory: This material is listed or exempted.
Malaysia Inventory (EHS Register): Not determined.
New Zealand Inventory of Chemicals (NZIoC): This material is listed or exempted.
Philippines inventory (PICCS): This material is listed or exempted.
Taiwan inventory (CSNN): Not determined.

Chemical Weapons Convention List Schedule I Chemicals : Not listed

Chemical Weapons Convention List Schedule II Chemicals : Not listed

Section 15. Regulatory information

Chemical Weapons Convention List Schedule III Chemicals : Not listed

Canada

WHMIS (Canada) : Class B-2: Flammable liquid
Class D-2B: Material causing other toxic effects (Toxic).

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

Canada Label requirements : Class B-2: Flammable liquid
Class D-2B: Material causing other toxic effects (Toxic).

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

Health	2
Flammability	3
Physical hazards	0

Caution: HMIS® ratings are based on a 0-4 rating scale, with 0 representing minimal hazards or risks, and 4 representing significant hazards or risks Although HMIS® ratings are not required on SDSs under 29 CFR 1910. 1200, the preparer may choose to provide them. HMIS® ratings are to be used with a fully implemented HMIS® program. HMIS® is a registered mark of the National Paint & Coatings Association (NPCA). HMIS® materials may be purchased exclusively from J. J. Keller (800) 327-6868.

The customer is responsible for determining the PPE code for this material.

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

Reprinted with permission from NFPA 704-2001, Identification of the Hazards of Materials for Emergency Response Copyright ©1997, National Fire Protection Association, Quincy, MA 02269. This reprinted material is not the complete and official position of the National Fire Protection Association, on the referenced subject which is represented only by the standard in its entirety.

Copyright ©2001, National Fire Protection Association, Quincy, MA 02269. This warning system is intended to be interpreted and applied only by properly trained individuals to identify fire, health and reactivity hazards of chemicals. The user is referred to certain limited number of chemicals with recommended classifications in NFPA 49 and NFPA 325, which would be used as a guideline only. Whether the chemicals are classified by NFPA or not, anyone using the 704 systems to classify chemicals does so at their own risk.

History

Date of printing : 5/18/2015.
Date of issue/Date of revision : 5/18/2015.
Date of previous issue : 10/28/2014.
Version : 0.02

Section 16. Other information

Key to abbreviations : ATE = Acute Toxicity Estimate
BCF = Bioconcentration Factor
GHS = Globally Harmonized System of Classification and Labelling of Chemicals
IATA = International Air Transport Association
IBC = Intermediate Bulk Container
IMDG = International Maritime Dangerous Goods
LogPow = logarithm of the octanol/water partition coefficient
MARPOL 73/78 = International Convention for the Prevention of Pollution From Ships, 1973 as modified by the Protocol of 1978. ("Marpol" = marine pollution)
UN = United NationsACGIH – American Conference of Governmental Industrial Hygienists
AIHA – American Industrial Hygiene Association
CAS – Chemical Abstract Services
CEPA – Canadian Environmental Protection Act
CERCLA – Comprehensive Environmental Response, Compensation, and Liability Act (EPA)
CFR – United States Code of Federal Regulations
CPR – Controlled Products Regulations
DSL – Domestic Substances List
GWP – Global Warming Potential
IARC – International Agency for Research on Cancer
ICAO – International Civil Aviation Organisation
Inh – Inhalation
LC – Lethal concentration
LD – Lethal dosage
NDSL – Non-Domestic Substances List
NIOSH – National Institute for Occupational Safety and Health
TDG – Canadian Transportation of Dangerous Goods Act and Regulations
TLV – Threshold Limit Value
TSCA – Toxic Substances Control Act
WEEL – Workplace Environmental Exposure Level
WHMIS – Canadian Workplace Hazardous Material Information System

References : Not available.

Indicates information that has changed from previously issued version.

Notice to reader

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

26.2.3 Isobutanol

SAFETY DATA SHEET

Creation Date 22-Jan-2009 **Revision Date** 14-Feb-2020 **Revision Number** 2

1. Identification

Product Name	**Isobutanol**
Cat No. :	**B23091**
CAS-No	78-83-1
Synonyms	Isobutanol; Isobutyl alcohol
Recommended Use	Laboratory chemicals.
Uses advised against	Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company
Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Emergency Telephone Number
During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660.
After normal business hours, call Carechem 24 at (866) 928-0789.

2. Hazard(s) identification

Classification
This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 3
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 1
Specific target organ toxicity (single exposure)	Category 3

Target Organs - Respiratory system, Central nervous system (CNS).

Label Elements

Signal Word
Danger

Hazard Statements
Flammable liquid and vapor
Causes skin irritation
Causes serious eye damage
May cause respiratory irritation

May cause drowsiness or dizziness

Precautionary Statements
Prevention
Wash face, hands and any exposed skin thoroughly after handling
Wear protective gloves/protective clothing/eye protection/face protection
Do not breathe dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting/equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Keep cool
Response
Get medical attention/advice if you feel unwell
Inhalation
IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Call a POISON CENTER or doctor/physician if you feel unwell
Skin
If skin irritation occurs: Get medical advice/attention
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower
Wash contaminated clothing before reuse
Eyes
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
Immediately call a POISON CENTER or doctor/physician
Fire
In case of fire: Use CO2, dry chemical, or foam for extinction
Storage
Store in a well-ventilated place. Keep container tightly closed
Store locked up
Disposal
Dispose of contents/container to an approved waste disposal plant
Hazards not otherwise classified (HNOC)
None identified

3. Composition/Information on Ingredients

Component	CAS-No	Weight %
Isobutyl alcohol	78-83-1	99

4. First-aid measures

General Advice If symptoms persist, call a physician.

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.

Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Most important symptoms and effects	None reasonably foreseeable. Causes severe eye damage. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	Water may be ineffective
Flash Point	28 °C / 82.4 °F
Method -	No information available
Autoignition Temperature	430 °C / 806 °F
Explosion Limits	
Upper	10.9 vol %
Lower	1.6 vol %
Oxidizing Properties	Not oxidising
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical
Flammable. Risk of ignition. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Containers may explode when heated.

Hazardous Combustion Products
Carbon monoxide (CO). Carbon dioxide (CO_2).
Protective Equipment and Precautions for Firefighters
As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
2	3	0	N/A

6. Accidental release measures

Personal Precautions	Use personal protective equipment as required. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.
Environmental Precautions	Should not be released into the environment.
Methods for Containment and Clean Up	Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

7. Handling and storage

Handling	Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not

get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

Storage Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame. Flammables area.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	Mexico OEL (TWA)
Isobutyl alcohol	TWA: 50 ppm	(Vacated) TWA: 50 ppm (Vacated) TWA: 150 mg/m³ TWA: 100 ppm TWA: 300 mg/m³	IDLH: 1600 ppm TWA: 50 ppm TWA: 150 mg/m³	TWA: 50 ppm

Legend

ACGIH *- American Conference of Governmental Industrial Hygienists*
OSHA *- Occupational Safety and Health Administration*
NIOSH IDLH: *NIOSH - National Institute for Occupational Safety and Health*

Engineering Measures Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting/equipment. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

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

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Colorless
Odor	aromatic
Odor Threshold	No information available
pH	No information available
Melting Point/Range	-108 °C / -162.4 °F
Boiling Point/Range	108 °C / 226.4 °F
Flash Point	28 °C / 82.4 °F
Evaporation Rate	0.6
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	10.9 vol %
Lower	1.6 vol %
Vapor Pressure	11.7 mbar @ 20°C
Vapor Density	2.6
Specific Gravity	0.800
Solubility	Soluble
Partition coefficient; n-octanol/water	No data available

Autoignition Temperature	430 °C / 806 °F
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C4 H10 O
Molecular Weight	74.12
VOC Content(%)	100 %

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable under normal conditions.

Conditions to Avoid Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.

Incompatible Materials Strong oxidizing agents, Acid anhydrides, Acid chlorides

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO_2)

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information See actual entry in RTECS for complete information.

Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isobutyl alcohol	LD50 = 2460 mg/kg (Rat)	LD50 = 3400 mg/kg (Rabbit)	LC50 > 6.5 mg/L (Rat) 4 h

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation Severe eye irritant. Irritating to respiratory system and skin.

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
Isobutyl alcohol	78-83-1	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system Central nervous system (CNS)
STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects,both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity
Do not empty into drains. .

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Isobutyl alcohol	1799 mg/l EC50 = 72 h 230 mg/L EC50 = 48 h	LC50: 1120 - 1520 mg/L, 96h flow-through (Oncorhynchus mykiss) LC50: 1480 - 1730 mg/L, 96h flow-through (Lepomis macrochirus) LC50: 1370 - 1670 mg/L, 96h flow-through (Pimephales promelas) LC50: = 375 mg/L, 96h static (Pimephales promelas)	EC50 = 1224.6 mg/L 15 min	EC50: 1070 - 1933 mg/L, 48h Static (Daphnia magna) EC50: = 1300 mg/L, 48h (Daphnia magna)

Persistence and Degradability Soluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its water solubility.

Component	log Pow
Isobutyl alcohol	0.79

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

Component	RCRA - U Series Wastes	RCRA - P Series Wastes
Isobutyl alcohol - 78-83-1	U140	-

14. Transport information

DOT

UN-No	UN1212
Proper Shipping Name	ISOBUTANOL
Hazard Class	3
Packing Group	III

TDG

UN-No	UN1212
Proper Shipping Name	ISOBUTANOL
Hazard Class	3
Packing Group	III

IATA

UN-No	UN1212
Proper Shipping Name	ISOBUTANOL
Hazard Class	3
Packing Group	III

IMDG/IMO

UN-No	UN1212
Proper Shipping Name	ISOBUTANOL
Hazard Class	3
Packing Group	III

15. Regulatory information

United States of America Inventory

Component	CAS-No	TSCA	TSCA Inventory notification - Active/Inactive	TSCA - EPA Regulatory Flags
Isobutyl alcohol	78-83-1	X	ACTIVE	-

Legend:
TSCA - Toxic Substances Control Act, (40 CFR Part 710)
X - Listed
'-' - Not Listed

TSCA 12(b) - Notices of Export Not applicable

International Inventories
Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Australia (AICS), China (IECSC), Korea (ECL).

Component	CAS-No	DSL	NDSL	EINECS	PICCS	ENCS	AICS	IECSC	KECL
Isobutyl alcohol	78-83-1	X	-	201-148-0	X	X	X	X	KE-24894

U.S. Federal Regulations

SARA 313 Not applicable

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration

CERCLA This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302)

Component	Hazardous Substances RQs	CERCLA EHS RQs
Isobutyl alcohol	5000 lb	-

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Isobutyl alcohol	X	X	X	-	X

U.S. Department of Transportation
Reportable Quantity (RQ): Y
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade Serious risk, Grade 3

16. Other information

Prepared By	Health, Safety and Environmental Department Email: tech@alfa.com www.alfa.com
Creation Date	22-Jan-2009
Revision Date	14-Feb-2020
Print Date	14-Feb-2020
Revision Summary	SDS authoring systems update, replaces ChemGes SDS No. 78-83-1.

Disclaimer
The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS

26.2.4 Water

ThermoFisher SCIENTIFIC

SAFETY DATA SHEET

Creation Date 18-Jun-2009 **Revision Date** 23-Jan-2018 **Revision Number** 4

1. Identification

Product Name Water

Cat No. : AC615150025

CAS-No 7732-18-5
Synonyms No information available

Recommended Use Laboratory chemicals.
Uses advised against Not for food, drug, pesticide or biocidal product use

Details of the supplier of the safety data sheet

Company
Fisher Scientific
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number
For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US:**001-201-796-7100 / **Europe:** +32 14 57 52 99
CHEMTREC Tel. No.**US:**001-800-424-9300 / **Europe:**001-703-527-3887

2. Hazard(s) identification

Classification
Classification under 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Based on available data, the classification criteria are not met

Label Elements
None required

Hazards not otherwise classified (HNOC)
None identified

3. Composition/Information on Ingredients

Component	CAS-No	Weight %
Water	7732-18-5	100

4. First-aid measures

Eye Contact	Immediate medical attention is not required.
Skin Contact	Immediate medical attention is not required.
Inhalation	Immediate medical attention is not required.
Ingestion	Immediate medical attention is not required.
Most important symptoms and effects	No information available.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Substance is nonflammable; use agent most appropriate to extinguish surrounding fire.
Unsuitable Extinguishing Media	No information available
Flash Point	Not applicable
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical
None known.

Hazardous Combustion Products
None

Protective Equipment and Precautions for Firefighters
As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
0	0	0	N/A

6. Accidental release measures

Personal Precautions	No special precautions required. If spilled, take caution, as material can cause surfaces to become very slippery.
Environmental Precautions	No special environmental precautions required. See Section 12 for additional ecological information.
Methods for Containment and Clean Up	Soak up with inert absorbent material.

7. Handling and storage

Handling	No special handling advice required.
Storage	No special storage conditions required.

8. Exposure controls / personal protection

Exposure Guidelines	This product does not contain any hazardous materials with occupational exposure limitsestablished by the region specific regulatory bodies.

Engineering Measures	None under normal use conditions.
<u>Personal Protective Equipment</u>	
Eye/face Protection	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin and body protection	No special protective equipment required.
Respiratory Protection	No protective equipment is needed under normal use conditions.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Clear, Colorless
Odor	Odorless
Odor Threshold	No information available
pH	No information available
Melting Point/Range	No data available
Boiling Point/Range	100 °C / 212 °F
Flash Point	Not applicable
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	17.5 mmHg @ 20 °C
Vapor Density	No information available
Specific Gravity	1.000
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	H_2O
Molecular Weight	18.02

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	None known.
Incompatible Materials	None known
Hazardous Decomposition Products	None
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information No acute toxicity information is available for this product

Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Water	-	Not listed	Not listed

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
Water	7732-18-5	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known
STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects,both acute and delayed No information available

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity
Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

Persistence and Degradability No information available

Bioaccumulation/ Accumulation No information available.

Mobility .

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT Not regulated
TDG Not regulated
IATA Not regulated
IMDG/IMO Not regulated

15. Regulatory information

International Inventories

Component	TSCA	DSL	NDSL	EINECS	ELINCS	NLP	PICCS	ENCS	AICS	IECSC	KECL
Water	X	X	-	231-791-2	-		X	-	X	X	X

Legend:
X - Listed
E - Indicates a substance that is the subject of a Section 5(e) Consent order under TSCA.
F - Indicates a substance that is the subject of a Section 5(f) Rule under TSCA.
N - Indicates a polymeric substance containing no free-radical initiator in its inventory name but is considered to cover the designated polymer made with any free-radical initiator regardless of the amount used.
P - Indicates a commenced PMN substance
R - Indicates a substance that is the subject of a Section 6 risk management rule under TSCA.
S - Indicates a substance that is identified in a proposed or final Significant New Use Rule
T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.
XU - Indicates a substance exempt from reporting under the Inventory Update Rule, i.e. Partial Updating of the TSCA Inventory Data Base Production and Site Reports (40 CFR 710(B).
Y1 - Indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.
Y2 - Indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule.

U.S. Federal Regulations

TSCA 12(b) Not applicable

SARA 313 Not applicable

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA Occupational Safety and Health Administration
Not applicable

CERCLA Not applicable

California Proposition 65 This product does not contain any Proposition 65 chemicals

U.S. State Right-to-Know Regulations Not applicable

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Water	-	-	X	-	-

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security
This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

16. Other information

Prepared By Regulatory Affairs

Thermo Fisher Scientific
Email: EMSDS.RA@thermofisher.com

Creation Date	18-Jun-2009
Revision Date	23-Jan-2018
Print Date	23-Jan-2018
Revision Summary	This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

Disclaimer
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End of SDS

26.3 Engineering Calculations

26.3.1 Flare Gas Energy Calculations

Table 26.3.1 Composition and Energy Calculation for Flare Gas Byproduct

Substance	Flow Rate [mol/hr]	DeltaH [kJ/mol]	kJ/hr	BTU/hr
Methonal	2259	764	1725237	1635209
Hydrogen	21349	286	6101630	5783229
Propane	50	2219	110194	104443
C2H2	1325	1301	1723489	1633552
Isobutene	35	2868	99089	93918
N-Butene	286	2877	822684	779754
Trans	25	2707	66570	63096
Cis-2	98	2710	266056	252172
C2H2	426	1411	601033	569669
CH4	3175	890	2825465	2678024
			Total =	13593066.8

26.3.2 Reactor Size Calculation

The reactors were sized based on the original volume needed for the catalyst in the reference paper. This volume was scaled to produce the desired final reactor effluent flow rate, however assumptions were made that a 3x better catalyst could be used and the reactor size would need to be increased by 100%.

$$Volume\ of\ Catalyst\ (paper) = 0.0000314159\ m^3$$

$$Molar\ Flow\ of\ Isobutanol\ (paper) = 0.0000173562\ kmol/hr$$

$$Scale\ Up\ Factor = 12718654.59$$

$$Volume\ of\ Catalyst\ Needed = Volume\ of\ Catalyst\ (paper) * Scale\ Up\ Factor$$

$$Volume\ of\ Catalyst\ Needed = 399.568318\ m^3$$

$$Corrected\ for\ 3X\ Better\ Catalyst = 133.1894394\ m^3$$

$$Corrected\ for\ 100\%\ Oversizing = 266.37887\ m^3$$

Due to this large total reactor volume needed, it was determined that 5 reactors in series would be used, with an extra to account for decoking time.

$$Volume\ Required\ per\ Reactor = 53.27577\ m^3$$

$$Diameter\ of\ Reactor = 4.07830749\ m$$

$$Diameter\ of\ Reactor = 13.38027434\ ft$$

$$Catalyst\ Volume\ with\ Porosity\ of\ 0.45 = 7060\ ft^3$$

26.3.3 Pressure Drop Calculations with Ergun Equation

The pressure drop through all five reactors was estimated using the Ergun Equation for both the smaller reactor of the paper, and the larger series of reactors in this process. The data and the equation used are both shown below.

$$\Delta p = \frac{150 \mu u_0 L_b}{\Phi_s^2 D_p^2} \frac{(1-\varepsilon)^2}{\varepsilon^3} + \frac{1.75 \rho u_0^2 L_b}{\Phi_s D_p} \frac{(1-\varepsilon)}{\varepsilon^3}$$

FEED			
viscosity =	1.95E-05	kg/m sec	
density =	3.70E+00	kg/m^3	
flow rate =	3.94E-01	m/sec	
flow rate (paper) =	3.29E-05	m/sec	
ACTIVATED CARBON			
sphericity =	1.00E+00		
particle diameter =	1.00E-03	m	
porosity =	4.50E-01		
BED SIZE			
L	4.08E+00	m	
L (paper)	4.00E-01	m	
DELTA P			
29.23	psig	through all 5 reactors	
1.85E-05	psig	paper	

26.3.4 Distillation Column 1 Efficiency Analysis

The O'Connell Correlation, along with ASPEN calculations, were used to find the real number of trays and tray efficiency. The following calculations were done and are summarized in the table below.

$$Relative\ Volatility = \frac{K_1}{K_2}$$

$$Stage\ Efficiency = 0.492 * (relative\ volatility * viscosity)^{-0.245}$$

$$Real\ Trays\ Required = \frac{1}{Stage\ Efficiency}$$

Table 26.3.4 Data from O'Connell Correlation for DC-1

Theoretical Trays	Viscosity of Liquid from Stage	K2 Value Water	K2 Value Methanol	Realative Volitility (Alpha)	Stage Efficiency	Real Trays
1	0.45249	0.22536992	0.68581182	3.04304946	0.452988	COND'R
2	0.389338	0.3680756	0.99873846	2.71340575	0.390171	2.06004199
3	0.388069	0.37016374	1.00368889	2.71147271	0.39021	4.11807755
4	0.387399	0.37179267	1.00989494	2.7162852	0.392593	6.17613595
5	0.387793	0.37457287	1.02290881	2.7308673	0.399411	8.23740904
6	0.390565	0.38075957	1.05094566	2.76012929	0.412298	10.3076813
7	0.397939	0.39569482	1.11024006	2.80579882	0.427534	12.3958414
8	0.411137	0.42871619	1.22435478	2.85586318	0.437166	14.5099012
9	0.425777	0.48691273	1.40153766	2.87841656	0.439251	16.6462747
10	0.434544	0.56184586	1.59759511	2.84347582	0.437688	18.7869279
11	0.437408	0.63361705	1.74216705	2.74955836	0.436306	20.9134581
12	0.440966	0.69771093	1.80852853	2.59208856	0.439243	23.013647
13	0.43693	0.82747353	1.88938915	2.28332276	0.434186	25.0449972
14	0.433698	0.90836287	1.81790901	2.00130263	0.431297	27.0082103
15	0.432734	0.95452535	1.7060417	1.78731941	0.429729	28.9167385
16	0.433875	0.97401795	1.69100197	1.73610966	0.428466	30.812945
17	0.434873	0.982466	1.72209144	1.75282547	0.427174	32.7146785
18	0.434979	0.98868323	1.73584862	1.75571767	0.425786	34.617294
19	0.434448	0.99305695	1.7371677	1.74931327	0.424316	36.517638
20	0.433483	0.9960922	1.73014288	1.73693045	0.422779	38.4136442
21	0.432229	0.99820638	1.71769308	1.7207795	0.4212	40.3039735
22	0.43079	0.99969973	1.70181542	1.70232658	0.419592	42.1877765
23	0.429231	1.00077098	1.68387712	1.68257988	0.417963	44.0645344
24	0.427593	1.00153174	1.66492169	1.66237536	0.41631	45.9339938
25	0.425887	1.00201792	1.64598817	1.64267338	0.414663	47.7961755
26	0.424088	1.00215746	1.62866006	1.62515384	0.412425	49.6515465
27	0.428367	1.03272636	1.55332709	1.50410327	0.424297	REB'R

26.3.5 Distillation Column 2 Efficiency Analysis

The same calculations are shown in Section 26.3.4 were performed for DC-2. The resulting data is shown below.

Table 26.3.5 Data from O'Connell Correlation for DC-2

Theoretical Trays	Viscosity of Liquid from Stage	K2 Value Water	K2 Value Methanol	Realative Volitility (Alpha)	Stage Efficiency	Real Trays
1	0.366921	0.859902443	1.446009517	1.681597173	NA	COND'R
2	0.290718	0.79449838	15.18088782	19.10751261	0.323235807	3.093716661
3	0.278318	0.889552665	20.01126094	22.4958698	0.313897099	6.279474042
4	0.277121	0.894169488	20.2148858	22.60744309	0.313848087	9.465728922
5	0.276409	0.894351532	20.19459511	22.58015377	0.314138908	12.64903406
6	0.26783	0.974644339	23.77713296	24.39570211	0.310633171	15.86826528
7	0.26542	0.994415967	24.64176829	24.78014141	0.310131539	19.09270354
8	0.264421	0.998589827	24.80000000	24.90000000	0.310195488	22.31647707
9	0.263708	0.999569979	24.80000000	24.90000000	0.310398094	25.53814634
10	0.263059	0.999865998	24.80000000	24.80000000	0.310645916	28.75724548
					NA	REB'R

26.4 ASPEN PLUS Input File

```
;
;Input Summary created by Aspen Plus Rel. 37.0 at 14:26:01 Mon Apr 12,
2021
;Directory C:\Users\novak\Desktop\ASPEN Files\Final Process Flowsheet
(updated 3-30)  Filename C:\Users\novak\AppData\Local\Temp\~ap797b.txt
;


DYNAMICS
    DYNAMICS RESULTS=ON

IN-UNITS ENG PRESSURE=psig TEMPERATURE=C DELTA-T=C PDROP=psi  &
        SHORT-LENGTH=in

DEF-STREAMS CONVEN ALL

SIM-OPTIONS MASS-BAL-CHE=YES FLASH-MAXIT=500

MODEL-OPTION

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
    METHANOL CH4O /
    ETHANOL C2H6O-2 /
    IB-ALDEH C4H8O-2 /
    PROPANOL C3H8O-1 /
    ISBUT-OH C4H10O-3 /
    2-ME1BOH C5H12O-2 /
    H2 H2 /
    CO2 CO2 /
    PROPANE C3H8 /
    C2H2 C2H2 /
    ISOBU-01 C4H10-2 /
    N-BUT-01 C4H10-1 /
    TRANS-01 C4H8-3 /
    CIS-2-01 C4H8-2 /
```

```
    C2H4 C2H4 /
    O2 O2 /
    CH4 CH4 /
    CO CO /
    WATER H2O /
    IBUTENE C4H8-5 /
    PROPENE C3H6-2 /
    2ME1BENE C5H10-5

HENRY-COMPS HC-1 H2 CO2 O2 CO

SOLVE
    RUN-MODE MODE=SIM

FLOWSHEET
    BLOCK R-5 IN=24 OUT=25
    BLOCK R-4 IN=19 OUT=20
    BLOCK R-3 IN=15 OUT=16
    BLOCK R-2 IN=11 OUT=12
    BLOCK DC-2 IN=49 OUT=52 51
    BLOCK FH-1 IN=6 OUT=7
    BLOCK ST-1 IN=25 5 OUT=26 6
    BLOCK FD-2 IN=39 OUT=40 41
    BLOCK M-3 IN=35 34 OUT=36
    BLOCK B-1 IN=31 OUT=35
    BLOCK FD-1 IN=29 OUT=34 30
    BLOCK R-1 IN=7 OUT=8
    BLOCK DC-1 IN=30 OUT=31 32 33
    BLOCK M-1 IN=42 43 3 4 OUT=5
    BLOCK M-4 IN=44 53 OUT=45
    BLOCK KR-1 IN=8 9 OUT=11 10
    BLOCK KR-2 IN=12 13 OUT=15 14
    BLOCK KR-3 IN=16 17 OUT=19 18
    BLOCK KR-4 IN=20 21 OUT=24 22
    BLOCK M-2 IN=10 14 18 22 OUT=23
    BLOCK P-3 IN=32 OUT=43
    BLOCK P-4 IN=41 OUT=42
    BLOCK ST-2 IN=26 27 OUT=29 28
    BLOCK ST-3 IN=36 37 OUT=39 38
    BLOCK ST-5 IN=45 46 OUT=48 47
    BLOCK P-5 IN=33 OUT=44
    BLOCK P-6 IN=52 OUT=53
    BLOCK P-1 IN=1 OUT=3
    BLOCK P-2 IN=2 OUT=4
    BLOCK ST-7 IN=55 56 OUT=58 57
```

```
    BLOCK R-6 IN=54 OUT=55
    BLOCK FH-2 IN=50 OUT=54
    BLOCK DEC-1 IN=48 OUT=50 49

PROPERTIES NRTL HENRY-COMPS=HC-1

PROP-DATA HENRY-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 MOLE-DENSITY='kmol/cum'  &
        MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol'  &
        MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l'  &
        PDROP=bar SHORT-LENGTH=mm
    PROP-LIST HENRY
    BPVAL H2 METHANOL -61.43472446 1867.400024 12.64300000  &
        -.0271870000 -60.00000000 69.85000000 0.0
    BPVAL H2 ETHANOL -39.88522446 1472.400024 8.548600000  &
        -.0176990000 -60.00000000 50.00000000 0.0
    BPVAL H2 PROPANOL -66.36592646 2023.300049 13.38100000  &
        -.0276820000 -60.00000000 25.00000000 0.0
    BPVAL H2 WATER 180.0660745 -6993.510000 -26.31190000  &
        .0150431000 .8500000000 65.85000000 0.0
    BPVAL CO2 METHANOL 15.46987454 -3426.699951 1.510800000  &
        -.0254510000 0.0 20.00000000 0.0
    BPVAL CO2 ETHANOL 89.58307554 -5018.799805 -11.89100000 0.0  &
        10.00000000 40.00000000 0.0
    BPVAL CO2 PROPANOL 82.59207754 -4594.600098 -10.91400000  &
        0.0 10.00000000 40.00000000 0.0
    BPVAL CO2 ISBUT-OH -5.302305465 -628.3699950 2.179000000  &
        -9.5000000E-5 .8300000000 54.85000000 0.0
    BPVAL CO2 WATER 159.8650745 -8741.550000 -21.66900000  &
        1.10259000E-3 -.1500000000 79.85000000 0.0
    BPVAL O2 METHANOL 26.69817654 -767.5700070 -2.977400000  &
        2.19200000E-3 -25.00000000 50.00000000 0.0
    BPVAL O2 ETHANOL -30.29762546 651.8400270 7.021200000  &
        -.0149260000 -25.00000000 50.00000000 0.0
    BPVAL O2 PROPANOL 7.094574535 59.15800100 0.0 0.0 0.0  &
        40.00000000 0.0
    BPVAL O2 ISBUT-OH -.7656254650 667.8300170 .5361900000  &
        8.58000000E-3 .9400000000 54.81000000 0.0
    BPVAL O2 WATER 144.4080745 -7775.060000 -18.39740000  &
        -9.4435400E-3 .8500000000 74.85000000 0.0
    BPVAL CO METHANOL 4.211874535 1144.400024 0.0 0.0  &
        20.00000000 25.00000000 0.0
    BPVAL CO ETHANOL 7.640474535 10.70800000 0.0 0.0  &
```

```
        20.00000000 25.00000000 0.0
    BPVAL CO PROPANOL 7.593474535 0.0 0.0 0.0 25.00000000  &
        25.00000000 0.0
    BPVAL CO ISBUT-OH 59.76217554 -783.5200200 -10.16300000  &
        .0271770000 .9000000000 54.83000000 0.0
    BPVAL CO WATER 171.7750745 -8296.750000 -23.33720000 0.0  &
        -.1500000000 79.85000000 0.0

PROP-DATA NRTL-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 MOLE-DENSITY='kmol/cum'  &
        MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol'  &
        MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l'  &
        PDROP=bar SHORT-LENGTH=mm
    PROP-LIST NRTL
    BPVAL METHANOL ETHANOL 4.711900000 -1162.294900 .3000000000  &
        0.0 0.0 0.0 20.00000000 78.40000000
    BPVAL ETHANOL METHANOL -2.312700000 483.8436000 .3000000000  &
        0.0 0.0 0.0 20.00000000 78.40000000
    BPVAL METHANOL PROPANOL 0.0 19.55470000 .3000000000 0.0  &
        0.0 0.0 60.02000000 97.12000000
    BPVAL PROPANOL METHANOL 0.0 -8.886700000 .3000000000 0.0  &
        0.0 0.0 60.02000000 97.12000000
    BPVAL METHANOL ISBUT-OH -16.04110000 5443.772500 .3000000000  &
        0.0 0.0 0.0 40.00000000 70.00000000
    BPVAL ISBUT-OH METHANOL 14.32890000 -4751.367700 .3000000000  &
        0.0 0.0 0.0 40.00000000 70.00000000
    BPVAL METHANOL N-BUT-01 0.0 380.4331000 .3000000000 0.0  &
        0.0 0.0 50.00000000 50.00000000
    BPVAL N-BUT-01 METHANOL 0.0 551.7243000 .3000000000 0.0  &
        0.0 0.0 50.00000000 50.00000000
    BPVAL METHANOL WATER -.6930000000 172.9871000 .3000000000  &
        0.0 0.0 0.0 24.99000000 100.0000000
    BPVAL WATER METHANOL 2.732200000 -617.2687000 .3000000000  &
        0.0 0.0 0.0 24.99000000 100.0000000
    BPVAL ETHANOL PROPANOL 8.260600000 -2846.682900 .3000000000  &
        0.0 0.0 0.0 40.00000000 97.16000000
    BPVAL PROPANOL ETHANOL -9.721000000 3409.686300 .3000000000  &
        0.0 0.0 0.0 40.00000000 97.16000000
    BPVAL ETHANOL ISBUT-OH -.3474000000 167.9138000 .3000000000  &
        0.0 0.0 0.0 40.00000000 105.9000000
    BPVAL ISBUT-OH ETHANOL -.8327000000 252.5334000 .3000000000  &
        0.0 0.0 0.0 40.00000000 105.9000000
    BPVAL ETHANOL WATER -.8009000000 246.1800000 .3000000000  &
```

```
    0.0 0.0 0.0 24.99000000 100.0000000
BPVAL WATER ETHANOL 3.457800000 -586.0809000 .3000000000  &
    0.0 0.0 0.0 24.99000000 100.0000000
BPVAL IB-ALDEH ISBUT-OH 0.0 504.1191000 .3000000000 0.0  &
    0.0 0.0 63.30000000 107.3000000
BPVAL ISBUT-OH IB-ALDEH 0.0 -282.9924000 .3000000000 0.0  &
    0.0 0.0 63.30000000 107.3000000
BPVAL IB-ALDEH WATER -2.334400000 987.1738000 .2000000000  &
    0.0 0.0 0.0 26.45000000 67.95000000
BPVAL WATER IB-ALDEH 8.240800000 -1408.577100 .2000000000  &
    0.0 0.0 0.0 26.45000000 67.95000000
BPVAL PROPANOL ISBUT-OH -.9906000000 110.2754000 .3000000000  &
    0.0 0.0 0.0 40.00000000 106.8000000
BPVAL ISBUT-OH PROPANOL .7245000000 69.23220000 .3000000000  &
    0.0 0.0 0.0 40.00000000 106.8000000
BPVAL PROPANOL N-BUT-01 0.0 193.2439000 .3000000000 0.0  &
    0.0 0.0 10.00000000 40.00000000
BPVAL N-BUT-01 PROPANOL 0.0 314.7243000 .3000000000 0.0  &
    0.0 0.0 10.00000000 40.00000000
BPVAL PROPANOL WATER -1.741100000 576.4458000 .3000000000  &
    0.0 0.0 0.0 25.00000000 100.0000000
BPVAL WATER PROPANOL 5.448600000 -861.1792000 .3000000000  &
    0.0 0.0 0.0 25.00000000 100.0000000
BPVAL ISBUT-OH WATER 0.0 -23.09940000 .3000000000 0.0 0.0  &
    0.0 89.67000000 106.6000000
BPVAL WATER ISBUT-OH 0.0 1343.689600 .3000000000 0.0 0.0  &
    0.0 89.67000000 106.6000000
BPVAL 2-ME1BOH WATER -1.893500000 410.6462000 .2000000000  &
    0.0 0.0 0.0 20.00000000 30.00000000
BPVAL WATER 2-ME1BOH 9.920600000 -1319.318800 .2000000000  &
    0.0 0.0 0.0 20.00000000 30.00000000
BPVAL N-BUT-01 TRANS-01 0.0 -167.7039000 .3000000000 0.0  &
    0.0 0.0 5.000000000 5.000000000
BPVAL TRANS-01 N-BUT-01 0.0 227.2447000 .3000000000 0.0  &
    0.0 0.0 5.000000000 5.000000000
BPVAL N-BUT-01 CIS-2-01 0.0 -182.7351000 .3000000000 0.0  &
    0.0 0.0 5.000000000 5.000000000
BPVAL CIS-2-01 N-BUT-01 0.0 260.7721000 .3000000000 0.0  &
    0.0 0.0 5.000000000 5.000000000
BPVAL TRANS-01 CIS-2-01 0.0 147.1440000 .3000000000 0.0  &
    0.0 0.0 5.000000000 5.000000000
BPVAL CIS-2-01 TRANS-01 0.0 -126.6744000 .3000000000 0.0  &
    0.0 0.0 5.000000000 5.000000000
BPVAL METHANOL IBUTENE 0.0 412.2995000 .4700000000 0.0 0.0  &
    0.0 50.00000000 50.00000000
```

```
    BPVAL IBUTENE METHANOL 0.0 840.5508000 .4700000000 0.0 0.0  &
        0.0 50.00000000 50.00000000
    BPVAL METHANOL PROPENE 0.0 207.6027000 .3000000000 0.0 0.0  &
        0.0 25.00000000 25.00000000
    BPVAL PROPENE METHANOL 0.0 660.5184000 .3000000000 0.0 0.0  &
        0.0 25.00000000 25.00000000
    BPVAL METHANOL 2ME1BENE 0.0 520.3923000 .4700000000 0.0  &
        0.0 0.0 27.38000000 44.70000000
    BPVAL 2ME1BENE METHANOL 0.0 755.7555000 .4700000000 0.0  &
        0.0 0.0 27.38000000 44.70000000

DEF-STREAMS LOAD

STREAM-NAMES
    NAMES 27 "see Comments below..."

STREAM 1
    SUBSTREAM MIXED TEMP=23. PRES=5.304051224
    MOLE-FLOW METHANOL 1022.605643

STREAM 2
    SUBSTREAM MIXED TEMP=23. PRES=5.304051224
    MOLE-FLOW ETHANOL 542.7709930

STREAM 8
    SUBSTREAM MIXED TEMP=392.18059145 PRES=40.76945122
    MOLE-FLOW METHANOL 3612.471906 / ETHANOL 382.4609698 /  &
        IB-ALDEH 1.413011209 / PROPANOL 5.652051378 / ISBUT-OH  &
        147.8010027 / 2-ME1BOH 1.413011418 / H2 14.13032692 /  &
        CO2 1.884031927 / PROPANE .1413000000 / C2H2  &
        1.318805507 / ISOBU-01 .2449209658 / N-BUT-01  &
        .5181026922 / TRANS-01 .2637607004 / CIS-2-01  &
        1.158663307 / C2H4 .3768016922 / O2 1.648538867 /  &
        CH4 2.166615191 / CO 2.760099857 / WATER 310.2367495

STREAM 9
    SUBSTREAM MIXED TEMP=185.5555556 PRES=151.4200000  &
        MASS-FLOW=8626.38273
    MASS-FRAC WATER 1.

STREAM 13
    SUBSTREAM MIXED TEMP=185.5555556 PRES=151.4200000  &
        MASS-FLOW=6592.3220537
    MASS-FRAC WATER 1.
```

```
STREAM 17
    SUBSTREAM MIXED TEMP=185.5555556 PRES=151.4200000  &
        MASS-FLOW=5263.34889
    MASS-FRAC WATER 1.

STREAM 21
    SUBSTREAM MIXED TEMP=185.5555556 PRES=151.4200000  &
        MASS-FLOW=3771.7153
    MASS-FRAC WATER 1.

STREAM 26
    SUBSTREAM MIXED TEMP=110. PRES=4.214051224
    MOLE-FLOW METHANOL 2883.538980 / ETHANOL 0.0 / IB-ALDEH  &
        4.709879518 / PROPANOL 18.83954575 / ISBUT-OH  &
        492.6537141 / 2-ME1BOH 4.709878886 / H2 47.09955715 /  &
        CO2 6.279902185 / PROPANE .4709876976 / C2H2  &
        4.395861397 / ISOBU-01 .8163753571 / N-BUT-01  &
        1.726949269 / TRANS-01 .8791723646 / CIS-2-01  &
        3.862083309 / C2H4 1.255965901 / O2 5.494952562 /  &
        CH4 7.221824362 / CO 9.200019642 / WATER 1034.088305

;water flow rate to rise to 120F = 2852406.667 lb/hr, water flow rate
to rise to 103F = 6621966 lb/hr
;

STREAM 27
    SUBSTREAM MIXED TEMP=32.22222222 PRES=7.304051224  &
        MASS-FLOW=6621966.
    MASS-FRAC WATER 1.

STREAM 37
    SUBSTREAM MIXED TEMP=2. PRES=3.304051224  &
        MASS-FLOW=52188.603049
    MASS-FRAC WATER 1.

STREAM 46
    SUBSTREAM MIXED TEMP=32.22222222 PRES=3.304051224  &
        MASS-FLOW=424649.18604
    MASS-FRAC WATER 1.

STREAM 52
    SUBSTREAM MIXED TEMP=90.162342624 PRES=.1040512245
    MOLE-FLOW METHANOL .2710076921 / ETHANOL 0.0 / IB-ALDEH  &
        0.0 / PROPANOL 1.145111399 / ISBUT-OH 8.073943648 /  &
        2-ME1BOH .0396846691 / H2 0.0 / CO2 0.0 / PROPANE  &
```

```
        0.0 / C2H2 0.0 / ISOBU-01 0.0 / N-BUT-01 0.0 /  &
        TRANS-01 0.0 / CIS-2-01 0.0 / C2H4 0.0 / O2 0.0 /  &
        CH4 0.0 / CO 0.0 / WATER 34.56270585

STREAM 56
    SUBSTREAM MIXED TEMP=32.22222222 PRES=9.304051224  &
        MASS-FLOW=500774.42246
    MASS-FRAC WATER 1.

BLOCK M-1 MIXER
    PARAM

BLOCK M-2 MIXER
    PARAM

BLOCK M-3 MIXER
    PARAM

BLOCK M-4 MIXER
    PARAM NPHASE=2 T-EST=90.
    BLOCK-OPTION FREE-WATER=NO

BLOCK FH-1 HEATER
    PARAM TEMP=332. PRES=-2.000000000 <psi> DPPARMOPT=NO

BLOCK FH-2 HEATER
    PARAM TEMP=325. PRES=13.30405122 DPPARMOPT=NO

BLOCK FD-1 FLASH2
    PARAM TEMP=40. PRES=5.304051224

BLOCK FD-2 FLASH2
    PARAM TEMP=10. PRES=1.304051224

BLOCK DEC-1 DECANTER
    PARAM TEMP=40. PRES=3.304051224 L2-COMPS=WATER ISBUT-OH

BLOCK KR-1 HEATX
    DESCRIPTION "Hot stream outlet T = 338 C"
    PARAM DUTY=7392810. CALC-TYPE=DESIGN  &
        PRES-HOT=-2.800000000 <psi> PRES-COLD=-1.090000000 <psi>  &
        U-OPTION=CONSTANT F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
    FEEDS HOT=8 COLD=9
    OUTLETS-HOT 11
    OUTLETS-COLD 10
```

```
    HEAT-TR-COEF U=101.3500000
    HOT-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    COLD-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    TQ-PARAM CURVE=YES

BLOCK KR-2 HEATX
    PARAM DUTY=5649620. PRES-HOT=-2.000000000 <psi>  &
        PRES-COLD=-13.58594878 U-OPTION=CONSTANT  &
        CALC-METHOD=SHORTCUT
    FEEDS HOT=12 COLD=13
    OUTLETS-HOT 15
    OUTLETS-COLD 14
    HEAT-TR-COEF U=12.22752377
    HOT-SIDE DPPARMOPT=NO
    COLD-SIDE DPPARMOPT=NO
    TQ-PARAM CURVE=YES

BLOCK KR-3 HEATX
    PARAM DUTY=4510690. PRES-HOT=-2.000000000 <psi>  &
        PRES-COLD=-1.110000000 <psi> U-OPTION=CONSTANT
    FEEDS HOT=16 COLD=17
    OUTLETS-HOT 19
    OUTLETS-COLD 18
    HEAT-TR-COEF U=59.70000000
    HOT-SIDE DPPARMOPT=NO
    COLD-SIDE DPPARMOPT=NO
    TQ-PARAM CURVE=YES

BLOCK KR-4 HEATX
    PARAM DUTY=3232360. PRES-HOT=-2.000000000 <psi>  &
        PRES-COLD=-1.110000000 <psi> U-OPTION=CONSTANT
    FEEDS HOT=20 COLD=21
    OUTLETS-HOT 24
    OUTLETS-COLD 22
    HEAT-TR-COEF U=59.70000000
    HOT-SIDE DPPARMOPT=NO
    COLD-SIDE DPPARMOPT=NO
    TQ-PARAM CURVE=YES

BLOCK ST-1 HEATX
    DESCRIPTION "Hot stream outlet T = 110 C"
    PARAM T-HOT=110. CALC-TYPE=DESIGN TYPE=COUNTERCURRE  &
        PRES-HOT=-1.930000000 <psi> PRES-COLD=-.7300000000 <psi>  &
        U-OPTION=CONSTANT F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
    FEEDS HOT=25 COLD=5
```

```
    OUTLETS-HOT 26
    OUTLETS-COLD 6
    HEAT-TR-COEF U=29.47000000
    FLASH-SPECS 26 NPHASE=1 PHASE=V FREE-WATER=NO
    HOT-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    COLD-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    TQ-PARAM CURVE=YES PRES-PROF=INLET

BLOCK ST-2 HEATX
    PARAM T-HOT=40. CALC-TYPE=DESIGN PRES-HOT=-1.410000000 <psi>  &
        PRES-COLD=-5.050000000 <psi> U-OPTION=CONSTANT  &
        F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
    FEEDS HOT=26 COLD=27
    OUTLETS-HOT 29
    OUTLETS-COLD 28
    HEAT-TR-COEF U=103.5700000
    HOT-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    COLD-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    TQ-PARAM CURVE=YES

BLOCK ST-3 HEATX
    PARAM T-HOT=10. CALC-TYPE=DESIGN PRES-HOT=-1.120000000 <psi>  &
        PRES-COLD=-.5800000000 <psi> U-OPTION=CONSTANT  &
        F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
    FEEDS HOT=36 COLD=37
    OUTLETS-HOT 39
    OUTLETS-COLD 38
    HEAT-TR-COEF U=99.13000000
    HOT-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    COLD-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    TQ-PARAM CURVE=YES

BLOCK ST-5 HEATX
    PARAM T-HOT=40. CALC-TYPE=DESIGN PRES-HOT=-1.620000000 <psi>  &
        PRES-COLD=-1.340000000 <psi> U-OPTION=CONSTANT  &
        F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
    FEEDS HOT=45 COLD=46
    OUTLETS-HOT 48
    OUTLETS-COLD 47
    HEAT-TR-COEF U=115.6200000
    HOT-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    COLD-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    TQ-PARAM CURVE=YES

BLOCK ST-7 HEATX
```

```
    PARAM T-HOT=90. CALC-TYPE=DESIGN PRES-HOT=-1.500000000 <psi>  &
        PRES-COLD=-1.860000000 <psi> U-OPTION=CONSTANT  &
        F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
    FEEDS HOT=55 COLD=56
    OUTLETS-HOT 58
    OUTLETS-COLD 57
    HEAT-TR-COEF U=238.6700000
    HOT-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    COLD-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    TQ-PARAM CURVE=YES

;2.8 RR up from 2.1 as safety to deal with fuctuations in actual RR

BLOCK DC-1 RADFRAC
    SUBOBJECTS INTERNALS = CS-1
    PARAM NSTAGE=27 ALGORITHM=STANDARD HYDRAULIC=NO MAXOL=200  &
        NPHASE=3 DAMPING=NONE
    PARAM2 STATIC-DP=YES
    COL-CONFIG CONDENSER=PARTIAL-V-L CA-CONFIG=INT-1
    FEEDS 30 12
    PRODUCTS 33 27 L / 32 1 L / 31 1 V
    P-SPEC 1 -7.695948776
    COL-SPECS DP-STAGE=0.14 MOLE-RDV=0.005 MOLE-D=2888.055635  &
        MOLE-RR=2.8 DP-COND=1.4
    L2-COMPS ISBUT-OH WATER
    L2-STAGES 1 27
    BLOCK-OPTION FREE-WATER=NO
    REPORT NOHYDRAULIC
    INTERNALS CS-1 STAGE1=2 STAGE2=26 P-UPDATE=NO
    TRAY-SIZE 1 2 26 SIEVE

BLOCK DC-2 RADFRAC
    SUBOBJECTS INTERNALS = CS-1
    PARAM NSTAGE=10 ALGORITHM=STANDARD HYDRAULIC=NO MAXOL=25  &
        NPHASE=3 DAMPING=NONE
    PARAM2 STATIC-DP=YES
    COL-CONFIG CONDENSER=TOTAL CA-CONFIG=INT-1
    FEEDS 49 5
    PRODUCTS 52 1 L / 51 10 L
    P-SPEC 1 1.304051224
    COL-SPECS DP-STAGE=.1400000000 MOLE-D=44.09245244 MOLE-RR=1.  &
        DP-COND=0.59
    L2-COMPS ISBUT-OH WATER
    L2-STAGES 1 10
    BLOCK-OPTION FREE-WATER=NO
```

```
    REPORT NOHYDRAULIC
    INTERNALS CS-1 STAGE1=2 STAGE2=9 P-UPDATE=NO
    TRAY-SIZE 1 2 9 SIEVE

BLOCK R-6 RSTOIC
    PARAM PRES=-5.000000000 <psi> DUTY=0. SERIES=NO  &
        COMBUSTION=NO
    STOIC 1 MIXED ISBUT-OH -1. / WATER 1. / IBUTENE 1.
    STOIC 2 MIXED PROPANOL -1. / WATER 1. / PROPENE 1.
    STOIC 3 MIXED 2-ME1BOH -1. / WATER 1. / 2ME1BENE 1.
    CONV 1 MIXED ISBUT-OH 1.
    CONV 2 MIXED PROPANOL 1.
    CONV 3 MIXED 2-ME1BOH 1.

BLOCK R-1 RYIELD
    PARAM PRES=-5.846345717 <psi> DUTY=0.0 NPHASE=1 PHASE=V
    MASS-YIELD MIXED METHANOL 0.766916384 / ETHANOL  &
        0.116739556 / IB-ALDEH 0.000675063 / PROPANOL  &
        0.002250468 / ISBUT-OH 0.07258568 / 2-ME1BOH  &
        0.000825255 / H2 0.000188729 / CO2 0.000549363 /  &
        PROPANE 4.12829E-05 / C2H2 0.000227514 / ISOBU-01  &
        9.43189E-05 / N-BUT-01 0.000199521 / TRANS-01  &
        9.80512E-05 / CIS-2-01 0.000430725 / C2H4 7.00367E-05 /  &
        O2 0.000349506 / CH4 0.000230294 / CO 0.000512231 /  &
        WATER 0.037030196
    BLOCK-OPTION FREE-WATER=NO

BLOCK R-2 RYIELD
    PARAM PRES=-5.846345717 <psi> DUTY=0.0 NPHASE=1 PHASE=V
    MASS-YIELD MIXED METHANOL 0.7116557 / ETHANOL 0.075046857 /  &
        IB-ALDEH 0.001237615 / PROPANOL 0.004125858 / ISBUT-OH  &
        0.133073746 / 2-ME1BOH 0.001512967 / H2 0.000346004 /  &
        CO2 0.001007166 / PROPANE 7.56852E-05 / C2H2  &
        0.000417108 / ISOBU-01 0.000172918 / N-BUT-01  &
        0.000365788 / TRANS-01 0.000179761 / CIS-2-01  &
        0.000789662 / C2H4 0.000128401 / O2 0.000640761 / CH4  &
        0.000422206 / CO 0.000939089 / WATER 0.067888693
    BLOCK-OPTION FREE-WATER=NO

BLOCK R-3 RYIELD
    PARAM PRES=-5.846345717 <psi> DUTY=0.0 NPHASE=1 PHASE=V
    MASS-YIELD MIXED METHANOL 0.667447152 / ETHANOL  &
        0.041692699 / IB-ALDEH 0.001687657 / PROPANOL  &
        0.00562617 / ISBUT-OH 0.181464199 / 2-ME1BOH  &
        0.002063136 / H2 0.000471823 / CO2 0.001373408 /  &
```

```
        PROPANE 0.000103207 / C2H2 0.000568784 / ISOBU-01  &
        0.000235797 / N-BUT-01 0.000498802 / TRANS-01  &
        0.000245128 / CIS-2-01 0.001076812 / C2H4 0.000175092 /  &
        O2 0.000873766 / CH4 0.000575736 / CO 0.001280576 /  &
        WATER 0.09257549
    BLOCK-OPTION FREE-WATER=NO

BLOCK R-4 RYIELD
    PARAM PRES=-5.846345717 <psi> DUTY=0.0 NPHASE=1 PHASE=V
    MASS-YIELD MIXED METHANOL 0.634290742 / ETHANOL  &
        0.016677079 / IB-ALDEH 0.002025188 / PROPANOL  &
        0.006751403 / ISBUT-OH 0.217757039 / 2-ME1BOH  &
        0.002475764 / H2 0.000566188 / CO2 0.00164809 /  &
        PROPANE 0.000123849 / C2H2 0.000682541 / ISOBU-01  &
        0.000282957 / N-BUT-01 0.000598562 / TRANS-01  &
        0.000294154 / CIS-2-01 0.001292175 / C2H4 0.00021011 /  &
        O2 0.001048519 / CH4 0.000690883 / CO 0.001536692 /  &
        WATER 0.111090588
    BLOCK-OPTION FREE-WATER=NO

BLOCK R-5 RYIELD
    PARAM PRES=-5.846345717 <psi> DUTY=0.0 NPHASE=1 PHASE=V
    MASS-YIELD MIXED METHANOL 0.612186468 / ETHANOL 0. /  &
        IB-ALDEH 0.002250209 / PROPANOL 0.007501559 / ISBUT-OH  &
        0.241952265 / 2-ME1BOH 0.002750848 / H2 0.000629097 /  &
        CO2 0.001831211 / PROPANE 0.00013761 / C2H2  &
        0.000758378 / ISOBU-01 0.000314396 / N-BUT-01  &
        0.000665069 / TRANS-01 0.000326837 / CIS-2-01  &
        0.00143575 / C2H4 0.000233456 / O2 0.001165021 / CH4  &
        0.000767648 / CO 0.001707435 / WATER 0.123433987
    BLOCK-OPTION FREE-WATER=NO

BLOCK P-1 PUMP
    PARAM PRES=60.30405122

BLOCK P-2 PUMP
    PARAM PRES=60.30405122

BLOCK P-3 PUMP
    DESCRIPTION  &
        "edit this outlet P and other feed P's will adjust
accordingly"
    PARAM PRES=52.60575122

BLOCK P-4 PUMP
```

```
    PARAM PRES=60.30405122

BLOCK P-5 PUMP
    PARAM PRES=5.304051224

BLOCK P-6 PUMP
    PARAM PRES=5.304051224

BLOCK B-1 COMPR
    PARAM TYPE=ISENTROPIC PRES=5.304051224 SB-MAXIT=30  &
        SB-TOL=0.0001

EO-CONV-OPTI

CALCULATOR FEEDPRES
;  "Sets other feed streams to appropriate P based on large MEOH rec"

    DEFINE BIGRECY BLOCK-VAR BLOCK=P-3 VARIABLE=PRES  &
        SENTENCE=PARAM UOM="psia"
    DEFINE SMALRECY BLOCK-VAR BLOCK=P-4 VARIABLE=PRES  &
        SENTENCE=PARAM UOM="psia"
    DEFINE MEOHFEED BLOCK-VAR BLOCK=P-1 VARIABLE=PRES  &
        SENTENCE=PARAM UOM="psia"
    DEFINE ETOHFEED BLOCK-VAR BLOCK=P-2 VARIABLE=PRES  &
        SENTENCE=PARAM UOM="psia"
F     SMALRECY = BIGRECY + 10
F     MEOHFEED = BIGRECY + 10
F     ETOHFEED = BIGRECY + 10
    EXECUTE FIRST

CALCULATOR MEOHCALC
    DEFINE FRSHMEOH MOLE-FLOW STREAM=1 SUBSTREAM=MIXED  &
        COMPONENT=METHANOL UOM="kmol/hr"
    DEFINE MEOHVAPR MOLE-FLOW STREAM=41 SUBSTREAM=MIXED  &
        COMPONENT=METHANOL UOM="kmol/hr"
    DEFINE MEOHLIQR MOLE-FLOW STREAM=32 SUBSTREAM=MIXED  &
        COMPONENT=METHANOL UOM="kmol/hr"
F     FRSHMEOH = 1768.655037 - MEOHVAPR - MEOHLIQR
    EXECUTE BEFORE BLOCK M-1

CALCULATOR RHXDELP
;  "Sets deltaP of Guerbet sequence kettle reboilers appropriately."

    DEFINE RHX1DPS BLOCK-VAR BLOCK=KR-1 VARIABLE=PRES-COLD  &
        SENTENCE=PARAM UOM="psia"
```

```
    DEFINE RHX1DPT BLOCK-VAR BLOCK=KR-1 VARIABLE=PRES-HOT  &
        SENTENCE=PARAM UOM="psia"
    DEFINE RHX2DPS BLOCK-VAR BLOCK=KR-2 VARIABLE=PRES-COLD  &
        SENTENCE=PARAM UOM="psia"
    DEFINE RHX2DPT BLOCK-VAR BLOCK=KR-2 VARIABLE=PRES-HOT  &
        SENTENCE=PARAM UOM="psia"
    DEFINE RHX3DPS BLOCK-VAR BLOCK=KR-3 VARIABLE=PRES-COLD  &
        SENTENCE=PARAM UOM="psia"
    DEFINE RHX3DPT BLOCK-VAR BLOCK=KR-3 VARIABLE=PRES-HOT  &
        SENTENCE=PARAM UOM="psia"
    DEFINE RHX4DPS BLOCK-VAR BLOCK=KR-4 VARIABLE=PRES-COLD  &
        SENTENCE=PARAM UOM="psia"
    DEFINE RHX4DPT BLOCK-VAR BLOCK=KR-4 VARIABLE=PRES-HOT  &
        SENTENCE=PARAM UOM="psia"
    DEFINE DELPR1 BLOCK-VAR BLOCK=R-1 VARIABLE=PRES  &
        SENTENCE=PARAM UOM="psi"
    DEFINE DELPR2 BLOCK-VAR BLOCK=R-2 VARIABLE=PRES  &
        SENTENCE=PARAM UOM="psi"
    DEFINE DELPR3 BLOCK-VAR BLOCK=R-3 VARIABLE=PRES  &
        SENTENCE=PARAM UOM="psi"
    DEFINE DELPR4 BLOCK-VAR BLOCK=R-4 VARIABLE=PRES  &
        SENTENCE=PARAM UOM="psi"
    DEFINE DELPR5 BLOCK-VAR BLOCK=R-5 VARIABLE=PRES  &
        SENTENCE=PARAM UOM="psi"
F     RHX2DPT = RHX1DPT
F     RHX3DPT = RHX1DPT
F     RHX4DPT = RHX1DPT
F     RHX2DPS = RHX1DPS * 25 / 30
F     RHX3DPS = RHX1DPS * 20 / 30
F     RHX4DPS = RHX1DPS * 15 / 30
F     DELPR2 = DELPR1
F     DELPR3 = DELPR1
F     DELPR4 = DELPR1
F     DELPR5 = DELPR1
F
    EXECUTE FIRST

CONV-OPTIONS
    PARAM TOL=1E-05
    WEGSTEIN MAXIT=200

REPORT NOINPUT

BLOCK-REPORT NEWPAGE
```

```
STREAM-REPOR NOSORT MOLEFLOW MASSFLOW MASSFRAC INCL-STREAMS=1 2  &
        3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19  &
        20 21 22 23 24 25 26 27 28 29 30 31 32 33 34  &
        35 36 37 38 39 40 41 42 43 44 45 46 47 48 49  &
        50 51 52 53 54 55 56 57 58

PROPERTY-REP PCES
;
;
;
;
;
```

26.5 ASPEN PLUS Report File

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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 13, 2021
VERSION: 37.0   Build 395                               TUESDAY
INSTALLATION:                                           12:50:22 P.M.
```

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```
                             RUN CONTROL SECTION

RUN CONTROL INFORMATION
-----------------------

THIS COPY OF ASPEN PLUS LICENSED TO UNIVERSITY OF PENNSYLVAN

TYPE OF RUN: NEW

INPUT FILE NAME: _4545hey.inm

OUTPUT PROBLEM DATA FILE NAME: _4545hey
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
```

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
9	----	KR-1	13	----	KR-2
17	----	KR-3	21	----	KR-4
27	----	ST-2	37	----	ST-3
46	----	ST-5	1	----	P-1
2	----	P-2	56	----	ST-7
25	R-5	ST-1	20	R-4	KR-4
16	R-3	KR-3	12	R-2	KR-2
52	DC-2	P-6	51	DC-2	----
7	FH-1	R-1	26	ST-1	ST-2
6	ST-1	FH-1	40	FD-2	----
41	FD-2	P-4	36	M-3	ST-3
35	B-1	M-3	34	FD-1	M-3
30	FD-1	DC-1	8	R-1	KR-1
31	DC-1	B-1	32	DC-1	P-3
33	DC-1	P-5	5	M-1	ST-1
45	M-4	ST-5	11	KR-1	R-2
10	KR-1	M-2	15	KR-2	R-3
14	KR-2	M-2	19	KR-3	R-4
18	KR-3	M-2	24	KR-4	R-5
22	KR-4	M-2	23	M-2	----
43	P-3	M-1	42	P-4	M-1
29	ST-2	FD-1	28	ST-2	----
39	ST-3	FD-2	38	ST-3	----
48	ST-5	DEC-1	47	ST-5	----

44	P-5	M-4	53	P-6	M-4
3	P-1	M-1	4	P-2	M-1
58	ST-7	----	57	ST-7	----
55	R-6	ST-7	54	FH-2	R-6
50	DEC-1	FH-2	49	DEC-1	DC-2

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
R-5	24	25
R-4	19	20
R-3	15	16
R-2	11	12
DC-2	49	52 51
FH-1	6	7
ST-1	25 5	26 6
FD-2	39	40 41
M-3	35 34	36
B-1	31	35
FD-1	29	34 30
R-1	7	8
DC-1	30	31 32 33
M-1	42 43 3 4	5
M-4	44 53	45
KR-1	8 9	11 10
KR-2	12 13	15 14
KR-3	16 17	19 18

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY BLOCKS (CONTINUED)

KR-4	20 21	24 22
M-2	10 14 18 22	23
P-3	32	43
P-4	41	42
ST-2	26 27	29 28
ST-3	36 37	39 38
ST-5	45 46	48 47
P-5	33	44
P-6	52	53
P-1	1	3
P-2	2	4
ST-7	55 56	58 57
R-6	54	55
FH-2	50	54
DEC-1	48	50 49

CONVERGENCE STATUS SUMMARY

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

STREAM ID	VARIABLE ID	MAXIMUM ERR/TOL	MAX. ERR. RELATIVE	ABSOLUTE ERROR	STAT	CONV BLOCK
26	PROPANOLMOLEFLOW	0.11943E-01	-0.11943E-06	0.28336E-09	#	$OLVER01

```
  8        MASS ENTHALPY     0.89360     -0.89360E-05  0.49251E-06  #    $OLVER01
  52       METHANOLMOLEFLOW  0.16222     -0.16222E-05  0.32839E-10  #    $OLVER02

  #  = CONVERGED
  *  = NOT CONVERGED

CALCULATOR BLOCK:   FEEDPRES
----------------------------

  SAMPLED VARIABLES:
    BIGRECY  : SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK P-3
    SMALRECY : SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK P-4
    MEOHFEED : SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK P-1
    ETOHFEED : SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK P-2

  FORTRAN STATEMENTS:
        SMALRECY = BIGRECY + 10
        MEOHFEED = BIGRECY + 10
        ETOHFEED = BIGRECY + 10

  EXECUTE FIRST

  VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:
    VARIABLE        VALUE READ      VALUE WRITTEN    UNITS
    --------        ----------      -------------    -----
    BIGRECY          67.3017          67.3017        PSIA
    SMALRECY         75.0000          77.3017        PSIA
    MEOHFEED         75.0000          77.3017        PSIA
```

```
CALCULATOR BLOCK:   FEEDPRES (CONTINUED)
    ETOHFEED          75.0000          77.3017        PSIA

CALCULATOR BLOCK:   MEOHCALC
----------------------------

  SAMPLED VARIABLES:
    FRSHMEOH : METHANOLMOLEFLOW IN STREAM 1 SUBSTREAM MIXED
    MEOHVAPR : METHANOLMOLEFLOW IN STREAM 41 SUBSTREAM MIXED
    MEOHLIQR : METHANOLMOLEFLOW IN STREAM 32 SUBSTREAM MIXED

  FORTRAN STATEMENTS:
        FRSHMEOH = 1768.655037 - MEOHVAPR - MEOHLIQR

  EXECUTE BEFORE BLOCK M-1

  VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:
    VARIABLE        VALUE READ      VALUE WRITTEN    UNITS
    --------        ----------      -------------    -----
    FRSHMEOH         463.808          463.837        KMOL/HR
    MEOHVAPR         9.09965          9.09965        KMOL/HR
    MEOHLIQR         1295.72          1295.72        KMOL/HR

CALCULATOR BLOCK:   RHXDELP
---------------------------

  SAMPLED VARIABLES:
    RHX1DPS  : SENTENCE=PARAM VARIABLE=PRES-COLD IN UOS BLOCK KR-1
```

```
  RHX1DPT  : SENTENCE=PARAM VARIABLE=PRES-HOT IN UOS BLOCK KR-1
  RHX2DPS  : SENTENCE=PARAM VARIABLE=PRES-COLD IN UOS BLOCK KR-2
  RHX2DPT  : SENTENCE=PARAM VARIABLE=PRES-HOT IN UOS BLOCK KR-2
  RHX3DPS  : SENTENCE=PARAM VARIABLE=PRES-COLD IN UOS BLOCK KR-3
  RHX3DPT  : SENTENCE=PARAM VARIABLE=PRES-HOT IN UOS BLOCK KR-3
  RHX4DPS  : SENTENCE=PARAM VARIABLE=PRES-COLD IN UOS BLOCK KR-4
  RHX4DPT  : SENTENCE=PARAM VARIABLE=PRES-HOT IN UOS BLOCK KR-4
  DELPR1   : SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK R-1
  DELPR2   : SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK R-2
  DELPR3   : SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK R-3
  DELPR4   : SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK R-4
  DELPR5   : SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK R-5

FORTRAN STATEMENTS:
      RHX2DPT = RHX1DPT
      RHX3DPT = RHX1DPT
      RHX4DPT = RHX1DPT
      RHX2DPS = RHX1DPS * 25 / 30
      RHX3DPS = RHX1DPS * 20 / 30
      RHX4DPS = RHX1DPS * 15 / 30
      DELPR2 = DELPR1
      DELPR3 = DELPR1
      DELPR4 = DELPR1
      DELPR5 = DELPR1
```

FLOWSHEET SECTION

CALCULATOR BLOCK: RHXDELP (CONTINUED)

EXECUTE FIRST

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE READ	VALUE WRITTEN	UNITS
RHX1DPS	-1.09000	-1.09000	PSIA
RHX1DPT	-2.80000	-2.80000	PSIA
RHX2DPS	1.11000	-0.908333	PSIA
RHX2DPT	-2.00000	-2.80000	PSIA
RHX3DPS	-1.11000	-0.726667	PSIA
RHX3DPT	-2.00000	-2.80000	PSIA
RHX4DPS	-1.11000	-0.545000	PSIA
RHX4DPT	-2.00000	-2.80000	PSIA
DELPR1	-5.84635	-5.84635	PSI
DELPR2	-5.84635	-5.84635	PSI
DELPR3	-5.84635	-5.84635	PSI
DELPR4	-5.84635	-5.84635	PSI
DELPR5	-5.84635	-5.84635	PSI

CONVERGENCE BLOCK: $OLVER01

Tear Stream : 26   8
Tolerance used: 0.100D-04 0.100D-04
Trace molefrac: 0.100D-06 0.100D-06

MAXIT= 200 WAIT   1 ITERATIONS BEFORE ACCELERATING

QMAX = 0.0 QMIN = -5.0
METHOD: WEGSTEIN STATUS: CONVERGED
TOTAL NUMBER OF ITERATIONS: 7

*** FINAL VALUES ***

VAR#	TEAR STREAM VAR	STREAM	SUBSTREA	COMPONEN	UNIT	VALUE	PREV VALUE	ERR/TOL
1	TOTAL MOLEFLOW	26	MIXED		LBMOL/HR	4524.9790	4524.9795	-1.1943-02
2	TOTAL MOLEFLOW	8	MIXED		LBMOL/HR	4485.7911	4485.8153	-0.5385
3	MOLE-FLOW	26	MIXED	METHANOL	LBMOL/HR	2882.0963	2882.0967	-1.1943-02
4	MOLE-FLOW	26	MIXED	ETHANOL	LBMOL/HR	0.0	0.0	0.0
5	MOLE-FLOW	26	MIXED	IB-ALDEH	LBMOL/HR	4.7075	4.7075	-1.1943-02
6	MOLE-FLOW	26	MIXED	PROPANOL	LBMOL/HR	18.8301	18.8301	-1.1943-02
7	MOLE-FLOW	26	MIXED	ISBUT-OH	LBMOL/HR	492.4072	492.4073	-1.1943-02
8	MOLE-FLOW	26	MIXED	2-ME1BOH	LBMOL/HR	4.7075	4.7075	-1.1943-02
9	MOLE-FLOW	26	MIXED	H2	LBMOL/HR	47.0760	47.0760	-1.1943-02
10	MOLE-FLOW	26	MIXED	CO2	LBMOL/HR	6.2768	6.2768	-1.1943-02
11	MOLE-FLOW	26	MIXED	PROPANE	LBMOL/HR	0.4708	0.4708	-1.1943-02
12	MOLE-FLOW	26	MIXED	C2H2	LBMOL/HR	4.3937	4.3937	-1.1943-02
13	MOLE-FLOW	26	MIXED	ISOBU-01	LBMOL/HR	0.8160	0.8160	-1.1943-02
14	MOLE-FLOW	26	MIXED	N-BUT-01	LBMOL/HR	1.7261	1.7261	-1.1943-02
15	MOLE-FLOW	26	MIXED	TRANS-01	LBMOL/HR	0.8787	0.8787	-1.1943-02
16	MOLE-FLOW	26	MIXED	CIS-2-01	LBMOL/HR	3.8602	3.8602	-1.1943-02
17	MOLE-FLOW	26	MIXED	C2H4	LBMOL/HR	1.2553	1.2553	-1.1943-02
18	MOLE-FLOW	26	MIXED	O2	LBMOL/HR	5.4922	5.4922	-1.1943-02
19	MOLE-FLOW	26	MIXED	CH4	LBMOL/HR	7.2182	7.2182	-1.1943-02
20	MOLE-FLOW	26	MIXED	CO	LBMOL/HR	9.1954	9.1954	-1.1943-02

FLOWSHEET SECTION

CONVERGENCE BLOCK: $OLVER01 (CONTINUED)

21	MOLE-FLOW	26	MIXED	WATER	LBMOL/HR	1033.5710	1033.5711	-1.1943-02
22	MOLE-FLOW	26	MIXED	IBUTENE	LBMOL/HR	0.0	0.0	0.0
23	MOLE-FLOW	26	MIXED	PROPENE	LBMOL/HR	0.0	0.0	0.0
24	MOLE-FLOW	26	MIXED	2ME1BENE	LBMOL/HR	0.0	0.0	0.0
25	PRESSURE	26	MIXED		PSIG	7.5140	7.5140	0.0
26	MASS ENTHALPY	26	MIXED		BTU/LB	-2732.9543	-2732.9543	0.0
27	MOLE-FLOW	8	MIXED	METHANOL	LBMOL/HR	3610.6451	3610.6646	-0.5385
28	MOLE-FLOW	8	MIXED	ETHANOL	LBMOL/HR	382.2676	382.2696	-0.5385
29	MOLE-FLOW	8	MIXED	IB-ALDEH	LBMOL/HR	1.4123	1.4123	-0.5385
30	MOLE-FLOW	8	MIXED	PROPANOL	LBMOL/HR	5.6492	5.6492	-0.5385
31	MOLE-FLOW	8	MIXED	ISBUT-OH	LBMOL/HR	147.7263	147.7271	-0.5385
32	MOLE-FLOW	8	MIXED	2-ME1BOH	LBMOL/HR	1.4123	1.4123	-0.5385
33	MOLE-FLOW	8	MIXED	H2	LBMOL/HR	14.1232	14.1233	-0.5385
34	MOLE-FLOW	8	MIXED	CO2	LBMOL/HR	1.8831	1.8831	-0.5385
35	MOLE-FLOW	8	MIXED	PROPANE	LBMOL/HR	0.1412	0.1412	-0.5385
36	MOLE-FLOW	8	MIXED	C2H2	LBMOL/HR	1.3181	1.3181	-0.5385
37	MOLE-FLOW	8	MIXED	ISOBU-01	LBMOL/HR	0.2448	0.2448	-0.5385
38	MOLE-FLOW	8	MIXED	N-BUT-01	LBMOL/HR	0.5178	0.5178	-0.5385
39	MOLE-FLOW	8	MIXED	TRANS-01	LBMOL/HR	0.2636	0.2636	-0.5385
40	MOLE-FLOW	8	MIXED	CIS-2-01	LBMOL/HR	1.1581	1.1581	-0.5385
41	MOLE-FLOW	8	MIXED	C2H4	LBMOL/HR	0.3766	0.3766	-0.5385
42	MOLE-FLOW	8	MIXED	O2	LBMOL/HR	1.6477	1.6477	-0.5385
43	MOLE-FLOW	8	MIXED	CH4	LBMOL/HR	2.1655	2.1655	-0.5385
44	MOLE-FLOW	8	MIXED	CO	LBMOL/HR	2.7587	2.7587	-0.5385
45	MOLE-FLOW	8	MIXED	WATER	LBMOL/HR	310.0799	310.0815	-0.5385
46	MOLE-FLOW	8	MIXED	IBUTENE	LBMOL/HR	0.0	0.0	0.0
47	MOLE-FLOW	8	MIXED	PROPENE	LBMOL/HR	0.0	0.0	0.0

48	MOLE-FLOW	8	MIXED	2ME1BENE	LBMOL/HR	0.0	0.0	0.0
49	PRESSURE	8	MIXED		PSIG	44.0294	44.0294	0.0
50	MASS ENTHALPY	8	MIXED		BTU/LB	-2369.5618	-2369.5406	-0.8936

*** ITERATION HISTORY ***

TEAR STREAMS AND TEAR VARIABLES:

ITERATION	MAX-ERR/TOL	VAR#	STREAM ID	VAR DESCRIPTION	SUBSTREA	COMPONEN	ATTRIBUT	ELEMENT
1	5877.	49	8	PRESSURE	MIXED			
2	0.1720E+05	25	26	PRESSURE	MIXED			
3	-15.29	50	8	MASS ENT	MIXED			
4	-9.259	8	26	MOLE-FLO	MIXED	2-ME1BOH		
5	-3.676	50	8	MASS ENT	MIXED			
6	-2.209	17	26	MOLE-FLO	MIXED	C2H4		
7	-0.8936	50	8	MASS ENT	MIXED			

CONVERGENCE BLOCK: $OLVER02

Tear Stream : 52
Tolerance used: 0.100D-04
Trace molefrac: 0.100D-06

FLOWSHEET SECTION

CONVERGENCE BLOCK: $OLVER02 (CONTINUED)
MAXIT= 200 WAIT 1 ITERATIONS BEFORE ACCELERATING
QMAX = 0.0 QMIN = -5.0
METHOD: WEGSTEIN STATUS: CONVERGED
TOTAL NUMBER OF ITERATIONS: 6

*** FINAL VALUES ***

VAR#	TEAR STREAM VAR	STREAM	SUBSTREA	COMPONEN	UNIT	VALUE	PREV VALUE	ERR/TOL
1	TOTAL MOLEFLOW	52	MIXED		LBMOL/HR	44.0925	44.0925	4.8361-04
2	MOLE-FLOW	52	MIXED	METHANOL	LBMOL/HR	0.1607	0.1607	-0.1622
3	MOLE-FLOW	52	MIXED	ETHANOL	LBMOL/HR	0.0	0.0	0.0
4	MOLE-FLOW	52	MIXED	IB-ALDEH	LBMOL/HR	0.0	0.0	0.0
5	MOLE-FLOW	52	MIXED	PROPANOL	LBMOL/HR	1.1603	1.1603	-2.5892-02
6	MOLE-FLOW	52	MIXED	ISBUT-OH	LBMOL/HR	8.1097	8.1097	-3.0754-02
7	MOLE-FLOW	52	MIXED	2-ME1BOH	LBMOL/HR	3.9798-02	3.9798-02	-3.9422-02
8	MOLE-FLOW	52	MIXED	H2	LBMOL/HR	0.0	0.0	0.0
9	MOLE-FLOW	52	MIXED	CO2	LBMOL/HR	0.0	0.0	0.0
10	MOLE-FLOW	52	MIXED	PROPANE	LBMOL/HR	0.0	0.0	0.0
11	MOLE-FLOW	52	MIXED	C2H2	LBMOL/HR	0.0	0.0	0.0
12	MOLE-FLOW	52	MIXED	ISOBU-01	LBMOL/HR	0.0	0.0	0.0
13	MOLE-FLOW	52	MIXED	N-BUT-01	LBMOL/HR	0.0	0.0	0.0
14	MOLE-FLOW	52	MIXED	TRANS-01	LBMOL/HR	0.0	0.0	0.0
15	MOLE-FLOW	52	MIXED	CIS-2-01	LBMOL/HR	0.0	0.0	0.0
16	MOLE-FLOW	52	MIXED	C2H4	LBMOL/HR	0.0	0.0	0.0
17	MOLE-FLOW	52	MIXED	O2	LBMOL/HR	0.0	0.0	0.0

18	MOLE-FLOW	52	MIXED	CH4	LBMOL/HR	0.0	0.0	0.0
19	MOLE-FLOW	52	MIXED	CO	LBMOL/HR	0.0	0.0	0.0
20	MOLE-FLOW	52	MIXED	WATER	LBMOL/HR	34.6220	34.6220	9.4854-03
21	MOLE-FLOW	52	MIXED	IBUTENE	LBMOL/HR	0.0	0.0	0.0
22	MOLE-FLOW	52	MIXED	PROPENE	LBMOL/HR	0.0	0.0	0.0
23	MOLE-FLOW	52	MIXED	2ME1BENE	LBMOL/HR	0.0	0.0	0.0
24	PRESSURE	52	MIXED		PSIG	1.3041	1.3041	0.0
25	MASS ENTHALPY	52	MIXED		BTU/LB	-4180.0123	-4180.0118	-1.1843-02

*** ITERATION HISTORY ***

TEAR STREAMS AND TEAR VARIABLES:

ITERATION	MAX-ERR/TOL	VAR#	STREAM ID	VAR DESCRIPTION	SUBSTREA	COMPONEN	ATTRIBUT	ELEMENT
1	-0.3058E+05	2	52	MOLE-FLO	MIXED	METHANOL		
2	-0.1097E+05	2	52	MOLE-FLO	MIXED	METHANOL		
3	-168.9	20	52	MOLE-FLO	MIXED	WATER		
4	15.58	20	52	MOLE-FLO	MIXED	WATER		
5	1.229	25	52	MASS ENT	MIXED			
6	-0.1622	2	52	MOLE-FLO	MIXED	METHANOL		

FLOWSHEET SECTION

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:

```
   RHXDELP FEEDPRES P-2 P-1
   $OLVER01 ST-2 FD-1 DC-1 B-1 M-3 ST-3 FD-2 P-4 P-3 MEOHCALC M-1 KR-1
   |  *R-2 KR-2 *R-3 KR-3 *R-4 KR-4 *R-5 ST-1 FH-1 *R-1
   (RETURN $OLVER01)
   P-5
   $OLVER02 P-6 M-4 ST-5 DEC-1 DC-2
   (RETURN $OLVER02)
   FH-2 R-6 ST-7 M-2
```

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
CONVENTIONAL COMPONENTS				
(LBMOL/HR)				
METHANOL	1022.59	5.46483	-1017.16	-0.394986E-04
ETHANOL	542.771	0.00000	-542.773	-0.379290E-05
IB-ALDEH	0.00000	0.215745E-01	0.215663E-01	-0.378598E-03
PROPANOL	0.00000	0.855108E-03	0.822536E-03	-0.380913E-01
ISBUT-OH	0.00000	0.178637E-02	0.940870E-03	-0.473307
2-ME1BOH	0.00000	0.573092E-05	-0.234259E-05	-1.40876
H2	0.00000	47.0672	47.0671	-0.173538E-05
CO2	0.00000	5.77751	5.77750	-0.188413E-05

PROPANE	0.00000	0.109480	0.109479	-0.745844E-05
C2H2	0.00000	2.92034	2.92033	-0.260866E-05
ISOBU-01	0.00000	0.761696E-01	0.761682E-01	-0.185849E-04
N-BUT-01	0.00000	0.630415	0.630412	-0.474748E-05
TRANS-01	0.00000	0.542234E-01	0.542218E-01	-0.281162E-04
CIS-2-01	0.00000	0.216456	0.216450	-0.309403E-04
C2H4	0.00000	0.938954	0.938951	-0.231809E-05
O2	0.00000	5.48661	5.48660	-0.173675E-05
CH4	0.00000	6.99896	6.99895	-0.178872E-05
CO	0.00000	9.18764	9.18762	-0.173646E-05
WATER	0.00000	424731.	424731.	-0.424259E-08
IBUTENE	0.00000	491.969	491.969	0.00000
PROPENE	0.00000	18.7587	18.7587	0.00000
2ME1BENE	0.00000	4.70639	4.70639	0.00000
TOTAL BALANCE				
MOLE(LBMOL/HR)	424752.	425331.	578.951	-0.106504E-06
MASS(LB/HR)	0.768160E+07	0.768160E+07		-0.193976E-06
ENTHALPY(BTU/HR)	-0.520649E+11	-0.519528E+11		-0.215421E-02

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	LB/HR
PRODUCT STREAMS CO2E	3061.33	LB/HR
NET STREAMS CO2E PRODUCTION	3061.33	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	3061.33	LB/HR

PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME
METHANOL	C	CH4O	METHANOL
ETHANOL	C	C2H6O-2	ETHANOL
IB-ALDEH	C	C4H8O-2	ISOBUTYRALDEHYDE
PROPANOL	C	C3H8O-1	1-PROPANOL
ISBUT-OH	C	C4H10O-3	ISOBUTANOL
2-ME1BOH	C	C5H12O-2	2-METHYL-1-BUTANOL
H2	C	H2	HYDROGEN
CO2	C	CO2	CARBON-DIOXIDE
PROPANE	C	C3H8	PROPANE
C2H2	C	C2H2	ACETYLENE
ISOBU-01	C	C4H10-2	ISOBUTANE
N-BUT-01	C	C4H10-1	N-BUTANE
TRANS-01	C	C4H8-3	TRANS-2-BUTENE
CIS-2-01	C	C4H8-2	CIS-2-BUTENE
C2H4	C	C2H4	ETHYLENE
O2	C	O2	OXYGEN
CH4	C	CH4	METHANE
CO	C	CO	CARBON-MONOXIDE
WATER	C	H2O	WATER
IBUTENE	C	C4H8-5	ISOBUTYLENE
PROPENE	C	C3H6-2	PROPYLENE
2ME1BENE	C	C5H10-5	2-METHYL-1-BUTENE

LISTID   SUPERCRITICAL COMPONENT LIST

HC-1 H2 CO2 O2 CO

U-O-S BLOCK SECTION

BLOCK: B-1 MODEL: COMPR

INLET STREAM: 31
OUTLET STREAM: 35
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	14.4403	14.4403	0.00000
MASS(LB/HR)	454.711	454.711	0.162513E-14
ENTHALPY(BTU/HR)	-975989.	-950195.	-0.264283E-01

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	424.284	LB/HR
PRODUCT STREAMS CO2E	424.284	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

*** INPUT DATA ***

ISENTROPIC CENTRIFUGAL COMPRESSOR

OUTLET PRESSURE PSIG	5.30405
ISENTROPIC EFFICIENCY	0.72000
MECHANICAL EFFICIENCY	1.00000

U-O-S BLOCK SECTION

BLOCK: B-1   MODEL: COMPR (CONTINUED)

*** RESULTS ***

INDICATED HORSEPOWER REQUIREMENT	HP	10.1373
BRAKE HORSEPOWER REQUIREMENT	HP	10.1373
NET WORK REQUIRED	HP	10.1373
POWER LOSSES	HP	0.0
ISENTROPIC HORSEPOWER REQUIREMENT	HP	7.29888
CALCULATED OUTLET TEMP	C	124.289
ISENTROPIC TEMPERATURE	C	101.431
EFFICIENCY (POLYTR/ISENTR) USED		0.72000
OUTLET VAPOR FRACTION		1.00000
HEAD DEVELOPED,	FT-LBF/LB	31,782.4
MECHANICAL EFFICIENCY USED		1.00000
INLET HEAT CAPACITY RATIO		1.22507
INLET VOLUMETRIC FLOW RATE ,	CUFT/HR	12,422.3
OUTLET VOLUMETRIC FLOW RATE,	CUFT/HR	5,543.01
INLET COMPRESSIBILITY FACTOR		1.00000
OUTLET COMPRESSIBILITY FACTOR		1.00000
AV. ISENT. VOL. EXPONENT		1.21200
AV. ISENT. TEMP EXPONENT		1.21200
AV. ACTUAL VOL. EXPONENT		1.30096
AV. ACTUAL TEMP EXPONENT		1.30096

BLOCK: DC-1   MODEL: RADFRAC

INLETS   - 30   STAGE 12

```
 OUTLETS  - 31       STAGE   1
            32       STAGE   1
            33       STAGE  27
PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID:        HC-1

                  ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
 TOTAL BALANCE
    MOLE(LBMOL/HR)           4432.40         4432.40         0.00000
    MASS(LB/HR   )           149373.         149373.       -0.340189E-12
    ENTHALPY(BTU/HR  )     -0.495014E+09   -0.488323E+09   -0.135162E-01

                  ***  CO2 EQUIVALENT SUMMARY ***
 FEED STREAMS CO2E            530.545      LB/HR
 PRODUCT STREAMS CO2E         530.545      LB/HR
 NET STREAMS CO2E PRODUCTION -0.229490E-05  LB/HR
 UTILITIES CO2E PRODUCTION     0.00000      LB/HR
 TOTAL CO2E PRODUCTION       -0.229490E-05  LB/HR
```

U-O-S BLOCK SECTION

BLOCK: DC-1   MODEL: RADFRAC (CONTINUED)

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

****   INPUT PARAMETERS   ****

NUMBER OF STAGES	27
ALGORITHM OPTION	3-PHASE
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	BROYDEN
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	200
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	500
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

****   COL-SPECS   ****

MOLAR VAPOR DIST / TOTAL DIST		0.0050000
MOLAR REFLUX RATIO		2.80000
MOLAR DISTILLATE RATE	LBMOL/HR	2,888.06

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

 TWO LIQUID PHASE CALCULATIONS ARE PERFORMED FOR    STAGE  TO  STAGE
                                                       1         27

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

 KEY COMPONENTS IN THE SECOND LIQUID PHASE        COMPONENT
                                                   ISBUT-OH
                                                   WATER

****    PROFILES   ****

 P-SPEC          STAGE   1  PRES, PSIG                  -7.69595
```

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

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

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS		
	31	32	33
COMPONENT:			
METHANOL	.34337E-02	.99640	.16894E-03
IB-ALDEH	.41678E-02	.99583	.10165E-14
PROPANOL	.18643E-05	.26755E-02	.99732
ISBUT-OH	.69015E-08	.15156E-04	.99998
2-ME1BOH	.17015E-14	.12672E-10	1.0000
H2	.98392	.16081E-01	0.0000
CO2	.66850	.33150	0.0000
PROPANE	.12123	.87877	0.0000
C2H2	.40608	.59392	0.0000
ISOBU-01	.50527E-01	.94947	0.0000
N-BUT-01	.26365	.73635	0.0000
TRANS-01	.35360E-01	.96464	.75867E-14
CIS-2-01	.32685E-01	.96731	.22789E-13
C2H4	.48253	.51747	0.0000
O2	.96297	.37029E-01	0.0000

```
 CH4          .81780       .18220       0.0000
 CO           .96481       .35191E-01   0.0000
 WATER        .36349E-05   .32096E-02   .99679


***    SUMMARY OF KEY RESULTS    ***

 TOP STAGE TEMPERATURE          C                             38.5929
 BOTTOM STAGE TEMPERATURE       C                             84.9594
 TOP STAGE LIQUID FLOW          LBMOL/HR                  10,960.2
 BOTTOM STAGE LIQUID FLOW       LBMOL/HR                   1,544.34
 TOP STAGE VAPOR FLOW           LBMOL/HR                      14.4403
 BOILUP VAPOR FLOW              LBMOL/HR                  10,057.6
 MOLAR REFLUX RATIO                                            2.80000
 MOLAR BOILUP RATIO                                            6.51257
 CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                        -0.175688+09
 REBOILER DUTY                  BTU/HR                         0.182379+09

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

 DEW POINT                       0.13012E-04  STAGE= 16 PHASE=L1
 BUBBLE POINT                    0.61177E-04  STAGE= 16 PHASE=L2
 COMPONENT MASS BALANCE          0.25498E-05  STAGE= 11 COMP=C2H2
 ENERGY BALANCE                  0.38480E-04  STAGE=  8
```

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

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

STAGE	TEMPERATURE C	PRESSURE PSIG	ENTHALPY BTU/LBMOL LIQUID	ENTHALPY BTU/LBMOL VAPOR	HEAT DUTY BTU/HR
1	38.593	-7.6959	-0.10170E+06	-67588.	-.17569+09
2	50.939	-6.2959	-0.10147E+06	-85647.	
3	51.433	-6.1559	-0.10155E+06	-85835.	
4	51.948	-6.0159	-0.10172E+06	-85891.	
10	65.571	-5.1759	-0.11417E+06	-91849.	
11	68.781	-5.0359	-0.11633E+06	-94006.	
12	70.948	-4.8959	-0.11768E+06	-95563.	
13	75.285	-4.7559	-0.12033E+06	-99762.	
26	84.617	-2.9359	-0.12596E+06	-0.10773E+06	
27	84.959	-2.7959	-0.12633E+06	-0.10777E+06	.18238+09

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.1096E+05	14.44				2873.6153	14.4402
2	8340.	0.1097E+05					
3	8335.	0.1123E+05					

4	8320.	0.1122E+05			
10	7637.	0.1061E+05			
11	7627.	0.1053E+05		1.5990	
12	0.1247E+05	0.1051E+05	4430.7967		
13	0.1236E+05	0.1093E+05			
26	0.1160E+05	0.1006E+05			
27	1544.	0.1006E+05			1544.3401

STAGE	FLOW RATE LBMOL/HR		ENTHALPY BTU/LBMO	
	LIQUID1	LIQUID2	LIQUID1	LIQUID2
1	0.1096E+05	0.000	-0.10170E+06	-0.10170E+06
2	8340.	0.000	-0.10147E+06	-0.10147E+06
3	8335.	0.000	-0.10155E+06	-0.10155E+06
4	8320.	0.000	-0.10172E+06	-0.10172E+06
10	7637.	0.000	-0.11417E+06	-0.11417E+06
11	0.000	7627.	-0.11633E+06	-0.11633E+06
12	0.000	0.1247E+05	-0.11768E+06	-0.11768E+06
13	0.000	0.1236E+05	-0.12033E+06	-0.12033E+06
26	7038.	4564.	-0.12900E+06	-0.12127E+06
27	996.7	547.7	-0.12912E+06	-0.12125E+06

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.3523E+06	454.7				.92368+05	454.7107
2	0.2674E+06	0.3528E+06					
3	0.2668E+06	0.3602E+06					
4	0.2655E+06	0.3596E+06					
10	0.2419E+06	0.3348E+06					
11	0.2453E+06	0.3347E+06		39.2907			
12	0.4144E+06	0.3381E+06	.14933+06				
13	0.4159E+06	0.3578E+06					
26	0.4112E+06	0.3545E+06					
27	0.5655E+05	0.3546E+06				.56551+05	

STAGE	FLOW RATE LB/HR	
	LIQUID1	LIQUID2
1	0.3523E+06	0.000
2	0.2674E+06	0.000
3	0.2668E+06	0.000
4	0.2655E+06	0.000
10	0.2419E+06	0.000
11	0.000	0.2453E+06
12	0.000	0.4144E+06

13	0.000	0.4159E+06
26	0.3216E+06	0.8961E+05
27	0.4581E+05	0.1074E+05

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
1	0.99407	0.16144E-02	0.17513E-04	0.25948E-05	0.20754E-13
2	0.99507	0.14440E-02	0.76353E-04	0.13681E-04	0.42132E-12
3	0.99104	0.13187E-02	0.26379E-03	0.56214E-04	0.63653E-11
4	0.98220	0.12145E-02	0.84938E-03	0.21576E-03	0.92743E-10
10	0.42643	0.16168E-03	0.79987E-01	0.76529E-01	0.53719E-04
11	0.33204	0.11039E-03	0.79827E-01	0.10884	0.18512E-03
12	0.28201	0.94747E-04	0.73052E-01	0.14493	0.56496E-03
13	0.16851	0.14291E-04	0.80600E-01	0.17525	0.62074E-03
26	0.48665E-03	0.23806E-16	0.14876E-01	0.29735	0.15496E-02
27	0.31362E-03	0.30662E-17	0.12147E-01	0.31856	0.30475E-02

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
1	0.23900E-05	0.16845E-03	0.12380E-03	0.50317E-03	0.25361E-03
2	0.42976E-08	0.60208E-06	0.42458E-05	0.40557E-05	0.21272E-04
3	0.40798E-08	0.30637E-06	0.13098E-05	0.15180E-05	0.70170E-05
4	0.41240E-08	0.30539E-06	0.12491E-05	0.15211E-05	0.61853E-05
10	0.31032E-08	0.20514E-06	0.14374E-05	0.17962E-05	0.68164E-05
11	0.28159E-08	0.19735E-06	0.14767E-05	0.18555E-05	0.69516E-05
12	0.54809E-09	0.18088E-06	0.14918E-05	0.18396E-05	0.70151E-05

U-O-S BLOCK SECTION

BLOCK: DC-1   MODEL: RADFRAC (CONTINUED)

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
13	0.35371E-13	0.29324E-09	0.67642E-07	0.18017E-07	0.74861E-06
26	0.23028E-70	0.84464E-45	0.49338E-24	0.34537E-33	0.30812E-18
27	0.62579E-75	0.17221E-47	0.23543E-25	0.36438E-35	0.33631E-19

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

STAGE	N-BUT-01	TRANS-01	CIS-2-01	C2H4	O2
1	0.37539E-03	0.28266E-03	0.12492E-02	0.10805E-03	0.17208E-05
2	0.52655E-05	0.33396E-04	0.15914E-03	0.70290E-06	0.30872E-08
3	0.17550E-05	0.11760E-04	0.57044E-04	0.28542E-06	0.27627E-08
4	0.17712E-05	0.99377E-05	0.47739E-04	0.28732E-06	0.27771E-08
10	0.57259E-05	0.10565E-04	0.50371E-04	0.35407E-06	0.21046E-08
11	0.70610E-05	0.10710E-04	0.51021E-04	0.36927E-06	0.20793E-08
12	0.79725E-05	0.10775E-04	0.51309E-04	0.36486E-06	0.91167E-09
13	0.64574E-06	0.15565E-05	0.79440E-05	0.29435E-08	0.18012E-12
26	0.11065E-17	0.28562E-16	0.35378E-15	0.57787E-35	0.38928E-59
27	0.15365E-18	0.41366E-17	0.54761E-16	0.51590E-37	0.11957E-62

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

STAGE	CH4	CO	WATER
1	0.73715E-04	0.24621E-05	0.11524E-02
2	0.18825E-06	0.51678E-08	0.31670E-02
3	0.12345E-06	0.46716E-08	0.72416E-02
4	0.12531E-06	0.47164E-08	0.15447E-01
10	0.16695E-06	0.31592E-08	0.41676

11	0.17718E-06	0.30043E-08	0.47892
12	0.15538E-06	0.12065E-08	0.49926
13	0.32242E-09	0.21028E-12	0.57499
26	0.21286E-43	0.29117E-60	0.68573
27	0.51377E-46	0.72028E-64	0.66593

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
1	0.99407	0.16144E-02	0.17513E-04	0.25948E-05	0.20754E-13
2	0.99507	0.14440E-02	0.76353E-04	0.13681E-04	0.42132E-12
3	0.99104	0.13187E-02	0.26379E-03	0.56214E-04	0.63653E-11
4	0.98220	0.12145E-02	0.84938E-03	0.21576E-03	0.92743E-10
10	0.42643	0.16168E-03	0.79987E-01	0.76529E-01	0.53719E-04
11	0.33204	0.11039E-03	0.79827E-01	0.10884	0.18512E-03
12	0.28201	0.94747E-04	0.73052E-01	0.14493	0.56496E-03
13	0.16851	0.14291E-04	0.80600E-01	0.17525	0.62074E-03
26	0.65607E-03	0.38271E-16	0.22955E-01	0.47267	0.25303E-02
27	0.41000E-03	0.46524E-17	0.17805E-01	0.47881	0.46851E-02

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
1	0.23900E-05	0.16845E-03	0.12380E-03	0.50317E-03	0.25361E-03
2	0.42976E-08	0.60208E-06	0.42458E-05	0.40557E-05	0.21272E-04
3	0.40798E-08	0.30637E-06	0.13098E-05	0.15180E-05	0.70170E-05
4	0.41240E-08	0.30539E-06	0.12491E-05	0.15211E-05	0.61853E-05
10	0.31032E-08	0.20514E-06	0.14374E-05	0.17962E-05	0.68164E-05
11	0.28159E-08	0.19735E-06	0.14767E-05	0.18555E-05	0.69516E-05
12	0.54809E-09	0.18088E-06	0.14918E-05	0.18396E-05	0.70151E-05

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
13	0.35371E-13	0.29324E-09	0.67642E-07	0.18017E-07	0.74861E-06
26	0.28715E-70	0.12954E-44	0.56611E-24	0.39629E-33	0.35354E-18
27	0.75168E-75	0.25105E-47	0.26629E-25	0.41214E-35	0.38039E-19

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

STAGE	N-BUT-01	TRANS-01	CIS-2-01	C2H4	O2
1	0.37539E-03	0.28266E-03	0.12492E-02	0.10805E-03	0.17208E-05
2	0.52655E-05	0.33396E-04	0.15914E-03	0.70290E-06	0.30872E-08
3	0.17550E-05	0.11760E-04	0.57044E-04	0.28542E-06	0.27627E-08
4	0.17712E-05	0.99377E-05	0.47739E-04	0.28732E-06	0.27771E-08
10	0.57259E-05	0.10565E-04	0.50371E-04	0.35407E-06	0.21046E-08
11	0.70610E-05	0.10710E-04	0.51021E-04	0.36927E-06	0.20793E-08
12	0.79725E-05	0.10775E-04	0.51309E-04	0.36486E-06	0.91167E-09
13	0.64574E-06	0.15565E-05	0.79440E-05	0.29435E-08	0.18012E-12
26	0.12526E-17	0.32772E-16	0.40593E-15	0.66306E-35	0.61995E-59
27	0.17219E-18	0.46788E-17	0.61938E-16	0.58352E-37	0.17999E-62

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

STAGE	CH4	CO	WATER
1	0.73715E-04	0.24621E-05	0.11524E-02
2	0.18825E-06	0.51678E-08	0.31670E-02
3	0.12345E-06	0.46716E-08	0.72416E-02
4	0.12531E-06	0.47164E-08	0.15447E-01
10	0.16695E-06	0.31592E-08	0.41676

11	0.17718E-06	0.30043E-08	0.47892
12	0.15538E-06	0.12065E-08	0.49926
13	0.32242E-09	0.21028E-12	0.57499
26	0.24424E-43	0.46395E-60	0.50119
27	0.58111E-46	0.10847E-63	0.49829

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
1	0.99407	0.16144E-02	0.17513E-04	0.25948E-05	0.20754E-13
2	0.99507	0.14440E-02	0.76353E-04	0.13681E-04	0.42132E-12
3	0.99104	0.13187E-02	0.26379E-03	0.56214E-04	0.63653E-11
4	0.98220	0.12145E-02	0.84938E-03	0.21576E-03	0.92743E-10
10	0.42643	0.16168E-03	0.79987E-01	0.76529E-01	0.53719E-04
11	0.33204	0.11039E-03	0.79827E-01	0.10884	0.18512E-03
12	0.28201	0.94747E-04	0.73052E-01	0.14493	0.56496E-03
13	0.16851	0.14291E-04	0.80600E-01	0.17525	0.62074E-03
26	0.22537E-03	0.14986E-17	0.24165E-02	0.26980E-01	0.37198E-04
27	0.13823E-03	0.17944E-18	0.18489E-02	0.26940E-01	0.67239E-04

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
1	0.23900E-05	0.16845E-03	0.12380E-03	0.50317E-03	0.25361E-03
2	0.42976E-08	0.60208E-06	0.42458E-05	0.40557E-05	0.21272E-04
3	0.40798E-08	0.30637E-06	0.13098E-05	0.15180E-05	0.70170E-05
4	0.41240E-08	0.30539E-06	0.12491E-05	0.15211E-05	0.61853E-05
10	0.31032E-08	0.20514E-06	0.14374E-05	0.17962E-05	0.68164E-05
11	0.28159E-08	0.19735E-06	0.14767E-05	0.18555E-05	0.69516E-05
12	0.54809E-09	0.18088E-06	0.14918E-05	0.18396E-05	0.70151E-05

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
13	0.35371E-13	0.29324E-09	0.67642E-07	0.18017E-07	0.74861E-06
26	0.14257E-70	0.14948E-45	0.38121E-24	0.26685E-33	0.23806E-18
27	0.39669E-75	0.28730E-48	0.17927E-25	0.27746E-35	0.25608E-19

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

STAGE	N-BUT-01	TRANS-01	CIS-2-01	C2H4	O2
1	0.37539E-03	0.28266E-03	0.12492E-02	0.10805E-03	0.17208E-05
2	0.52655E-05	0.33396E-04	0.15914E-03	0.70290E-06	0.30872E-08
3	0.17550E-05	0.11760E-04	0.57044E-04	0.28542E-06	0.27627E-08
4	0.17712E-05	0.99377E-05	0.47739E-04	0.28732E-06	0.27771E-08
10	0.57259E-05	0.10565E-04	0.50371E-04	0.35407E-06	0.21046E-08
11	0.70610E-05	0.10710E-04	0.51021E-04	0.36927E-06	0.20793E-08
12	0.79725E-05	0.10775E-04	0.51309E-04	0.36486E-06	0.91167E-09
13	0.64574E-06	0.15565E-05	0.79440E-05	0.29435E-08	0.18012E-12
26	0.88113E-18	0.22068E-16	0.27334E-15	0.44649E-35	0.33519E-60
27	0.11991E-18	0.31498E-17	0.41698E-16	0.39283E-37	0.96164E-64

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

STAGE	CH4	CO	WATER
1	0.73715E-04	0.24621E-05	0.11524E-02
2	0.18825E-06	0.51678E-08	0.31670E-02
3	0.12345E-06	0.46716E-08	0.72416E-02
4	0.12531E-06	0.47164E-08	0.15447E-01
10	0.16695E-06	0.31592E-08	0.41676

11	0.17718E-06	0.30043E-08	0.47892
12	0.15538E-06	0.12065E-08	0.49926
13	0.32242E-09	0.21028E-12	0.57499
26	0.16447E-43	0.24703E-61	0.97034
27	0.39121E-46	0.57044E-65	0.97101

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
1	0.68171	0.13446E-02	0.24284E-05	0.23513E-06	0.55456E-15
2	0.99366	0.16140E-02	0.17493E-04	0.25917E-05	0.20727E-13
3	0.99441	0.14875E-02	0.61198E-04	0.10827E-04	0.31826E-12
4	0.99142	0.13945E-02	0.20040E-03	0.42413E-04	0.47326E-11
10	0.68386	0.64437E-03	0.47773E-01	0.33292E-01	0.86106E-05
11	0.58175	0.55991E-03	0.58044E-01	0.55531E-01	0.38979E-04
12	0.51347	0.52302E-03	0.57915E-01	0.78954E-01	0.13429E-03
13	0.32183	0.10814E-03	0.81659E-01	0.12039	0.21412E-03
26	0.83533E-03	0.22346E-15	0.19786E-01	0.29125	0.71521E-03
27	0.51322E-03	0.26991E-16	0.15295E-01	0.29410	0.13196E-02

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
1	0.29100E-01	0.67599E-01	0.33987E-02	0.68463E-01	0.26857E-02
2	0.40677E-04	0.25717E-03	0.12811E-03	0.59259E-03	0.25681E-03
3	0.38042E-04	0.13050E-03	0.39211E-04	0.21985E-03	0.84163E-04
4	0.38057E-04	0.13033E-03	0.37045E-04	0.21805E-03	0.73602E-04
10	0.40261E-04	0.13780E-03	0.39173E-04	0.23074E-03	0.77193E-04
11	0.40579E-04	0.13888E-03	0.39506E-04	0.23260E-03	0.77869E-04
12	0.83763E-05	0.12457E-03	0.39359E-04	0.22653E-03	0.77888E-04

U-O-S BLOCK SECTION

BLOCK: DC-1   MODEL: RADFRAC (CONTINUED)

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
13	0.62555E-09	0.20645E-06	0.17026E-05	0.20995E-05	0.80065E-05
26	0.95894E-66	0.50746E-42	0.12056E-22	0.38385E-31	0.32621E-17
27	0.26564E-70	0.97407E-45	0.56552E-24	0.39785E-33	0.35026E-18

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

STAGE	N-BUT-01	TRANS-01	CIS-2-01	C2H4	O2
1	0.26748E-01	0.20619E-02	0.83997E-02	0.20051E-01	0.89056E-02
2	0.41009E-03	0.28500E-03	0.12586E-02	0.13430E-03	0.13436E-04
3	0.13439E-03	0.99802E-04	0.44873E-03	0.53966E-04	0.11897E-04
4	0.13184E-03	0.83761E-04	0.37302E-03	0.53678E-04	0.11901E-04
10	0.14122E-03	0.86935E-04	0.38591E-03	0.56807E-04	0.12590E-04
11	0.14334E-03	0.87666E-04	0.38912E-03	0.57266E-04	0.12689E-04
12	0.14360E-03	0.87739E-04	0.38949E-03	0.55228E-04	0.52626E-05
13	0.90991E-05	0.12298E-04	0.58560E-04	0.41642E-06	0.10405E-08
26	0.92413E-17	0.22668E-15	0.26234E-14	0.75985E-33	0.15687E-55
27	0.12528E-17	0.32312E-16	0.39969E-15	0.66581E-35	0.44903E-59

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

STAGE	CH4	CO	WATER
1	0.65842E-01	0.13433E-01	0.25971E-03
2	0.16025E-03	0.20134E-04	0.11512E-02
3	0.10369E-03	0.17911E-04	0.26477E-02
4	0.10368E-03	0.17918E-04	0.56735E-02
10	0.10970E-03	0.18954E-04	0.23308

11	0.11058E-03	0.19104E-04	0.30272
12	0.93561E-04	0.74222E-05	0.34774
13	0.17734E-06	0.13770E-08	0.47571
26	0.10380E-40	0.14585E-56	0.68742
27	0.24547E-43	0.33587E-60	0.68877

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH	H2
1	0.6858	0.8329	0.1387	9.0616-02	2.6721-02	1.2176+04
2	0.9986	1.1178	0.2291	0.1894	4.9196-02	9465.0829
3	1.0034	1.1280	0.2320	0.1926	4.9999-02	9324.4265
4	1.0094	1.1482	0.2359	0.1966	5.1029-02	9228.3792
10	1.6039	3.9866	0.5974	0.4351	0.1603	1.2979+04
11	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
12	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
13	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
26	1.2732	5.8390	0.8620	0.6162	0.2827	3.3394+04
27	1.2518	5.8015	0.8590	0.6142	0.2817	3.5340+04

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

STAGE	CO2	PROPANE	C2H2	ISOBU-01	N-BUT-01	TRANS-01
1	401.3020	27.4522	136.0644	10.5900	71.2519	7.2945
2	427.1385	30.1740	146.1135	12.0727	77.8826	8.5340
3	425.9582	29.9366	144.8313	11.9942	76.5775	8.4869
4	426.7865	29.6582	143.3477	11.8995	74.4325	8.4286
10	672.0479	27.2575	128.4860	11.3266	24.6709	8.2301
11	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
12	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

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

STAGE	CO2	PROPANE	C2H2	ISOBU-01	N-BUT-01	TRANS-01
13	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
26	391.7451	21.2958	96.8619	9.2271	7.3779	6.9169
27	387.9972	21.2371	96.5312	9.2080	7.2755	6.9061

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

STAGE	CIS-2-01	C2H4	O2	CH4	CO	WATER
1	6.7241	185.5667	5175.1640	893.1863	5455.8491	0.2254
2	7.9086	191.0587	4352.2889	851.2758	3896.0919	0.3635
3	7.8664	189.0756	4306.1732	839.9407	3833.9775	0.3656
4	7.8138	186.8243	4285.4754	827.3818	3799.0681	0.3673
10	7.6625	160.4696	5985.8692	657.2194	6002.6182	0.5592
11	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
12	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
13	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
26	6.4628	114.5990	2530.3508	424.9746	3143.7278	1.3716
27	6.4530	114.1025	2494.7387	422.4186	3096.3462	1.3823

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH	H2
1	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
2	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
3	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
4	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
10	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING

11	1.7522	5.0730	0.7272	0.5103	0.2106	1.4416+04
12	1.8209	5.5209	0.7929	0.5448	0.2377	1.5287+04
13	1.9102	7.5673	1.0132	0.6870	0.3450	1.7691+04
26	3.7065	149.1120	8.1879	10.7949	19.2268	6.7260+04
27	3.7129	150.4140	8.2725	10.9168	19.6257	6.6964+04

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

STAGE	CO2	PROPANE	C2H2	ISOBU-01	N-BUT-01	TRANS-01
1	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
2	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
3	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
4	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
10	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
11	703.9724	26.7571	125.3830	11.2035	20.3058	8.1864
12	688.8674	26.3885	123.1611	11.1045	18.0160	8.1441
13	704.2385	25.1763	116.5582	10.6976	14.0958	7.9024
26	3394.8008	31.6253	143.8445	13.7027	10.4880	10.2719
27	3390.3851	31.5457	143.3875	13.6776	10.4480	10.2583

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

STAGE	CIS-2-01	C2H4	O2	CH4	CO	WATER
1	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
2	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
3	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
4	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
10	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
11	7.6278	155.1065	6105.5772	624.2252	6361.0580	0.6320
12	7.5922	151.3945	5774.4972	602.2361	6153.5920	0.6964

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

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

STAGE	CIS-2-01	C2H4	O2	CH4	CO	WATER
13	7.3733	141.5040	5778.9410	550.1712	6549.9533	0.8273
26	9.5976	170.1848	4.6801+04	631.1070	5.9042+04	0.7084
27	9.5853	169.4879	4.6695+04	627.4609	5.8879+04	0.7093

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH	H2
1	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
2	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
3	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
4	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
10	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
11	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
12	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
13	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
26	0.3435	3.9159-02	0.1053	5.7080-02	1.4701-02	0.4965
27	0.3371	3.8570-02	0.1038	5.6265-02	1.4352-02	0.5277

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

STAGE	CO2	PROPANE	C2H2	ISOBU-01	N-BUT-01	TRANS-01
1	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
2	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
3	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
4	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
10	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING

11	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
12	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
13	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
26	0.1154	0.6734	0.6734	0.6734	0.7035	0.6734
27	0.1144	0.6732	0.6732	0.6732	0.6964	0.6732

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

STAGE	CIS-2-01	C2H4	O2	CH4	CO	WATER
1	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
2	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
3	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
4	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
10	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
11	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
12	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
13	MISSING	MISSING	MISSING	MISSING	MISSING	MISSING
26	0.6734	0.6734	5.4066-02	0.6734	5.3246-02	1.9361
27	0.6732	0.6732	5.3427-02	0.6732	5.2589-02	1.9487

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
1	0.99094	0.36215E-02	0.32742E-04	0.59837E-05	0.56914E-13
2	0.99440	0.32473E-02	0.14311E-03	0.31628E-04	0.11583E-11
3	0.99219	0.29711E-02	0.49532E-03	0.13019E-03	0.17531E-10
4	0.98631	0.27446E-02	0.15997E-02	0.50121E-03	0.25621E-09
10	0.43141	0.36808E-03	0.15177	0.17910	0.14951E-03
11	0.33082	0.24751E-03	0.14917	0.25084	0.50741E-03
12	0.27198	0.20563E-03	0.13213	0.32333	0.14989E-02

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
13	0.16047	0.30626E-04	0.14395	0.38606	0.16262E-02
26	0.43998E-03	0.48436E-16	0.25225E-01	0.62191	0.38543E-02
27	0.27443E-03	0.60378E-17	0.19935E-01	0.64483	0.73361E-02

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
1	0.14989E-06	0.23063E-03	0.16984E-03	0.40759E-03	0.45859E-03
2	0.27019E-09	0.82640E-06	0.58392E-05	0.32935E-05	0.38560E-04
3	0.25697E-09	0.42129E-06	0.18047E-05	0.12349E-05	0.12743E-04
4	0.26054E-09	0.42121E-06	0.17262E-05	0.12413E-05	0.11267E-04
10	0.19752E-09	0.28505E-06	0.20013E-05	0.14767E-05	0.12509E-04
11	0.17651E-09	0.27006E-06	0.20248E-05	0.15022E-05	0.12564E-04
12	0.33255E-10	0.23960E-06	0.19799E-05	0.14417E-05	0.12272E-04
13	0.21191E-14	0.38354E-09	0.88645E-07	0.13942E-07	0.12931E-05
26	0.13099E-71	0.10489E-44	0.61388E-24	0.25374E-33	0.50532E-18
27	0.34450E-76	0.20697E-47	0.28351E-25	0.25910E-35	0.53381E-19

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

STAGE	N-BUT-01	TRANS-01	CIS-2-01	C2H4	O2
1	0.67881E-03	0.49340E-03	0.21805E-02	0.94306E-04	0.17131E-05
2	0.95451E-05	0.58439E-04	0.27848E-03	0.61499E-06	0.30810E-08
3	0.31871E-05	0.20616E-04	0.10000E-03	0.25018E-06	0.27621E-08
4	0.32263E-05	0.17474E-04	0.83943E-04	0.25261E-06	0.27850E-08
10	0.10508E-04	0.18716E-04	0.89234E-04	0.31362E-06	0.21263E-08

11	0.12761E-04	0.18686E-04	0.89013E-04	0.32212E-06	0.20688E-08
12	0.13947E-04	0.18196E-04	0.86647E-04	0.30807E-06	0.87804E-09
13	0.11154E-05	0.25955E-05	0.13246E-04	0.24541E-08	0.17129E-12
26	0.18146E-17	0.45217E-16	0.56008E-15	0.45742E-35	0.35147E-59
27	0.24388E-18	0.63382E-17	0.83906E-16	0.39523E-37	0.10449E-62

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

STAGE	CH4	CO	WATER
1	0.36791E-04	0.21456E-05	0.64587E-03
2	0.94189E-07	0.45145E-08	0.17794E-02
3	0.61878E-07	0.40885E-08	0.40762E-02
4	0.63004E-07	0.41402E-08	0.87213E-02
10	0.84568E-07	0.27939E-08	0.23706
11	0.88382E-07	0.26166E-08	0.26828
12	0.75028E-07	0.10171E-08	0.27071
13	0.15372E-09	0.17505E-12	0.30785
26	0.96356E-44	0.23013E-60	0.34857
27	0.22508E-46	0.55097E-64	0.32762

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
1	0.99094	0.36215E-02	0.32742E-04	0.59837E-05	0.56914E-13
2	0.99440	0.32473E-02	0.14311E-03	0.31628E-04	0.11583E-11
3	0.99219	0.29711E-02	0.49532E-03	0.13019E-03	0.17531E-10
4	0.98631	0.27446E-02	0.15997E-02	0.50121E-03	0.25621E-09
10	0.43141	0.36808E-03	0.15177	0.17910	0.14951E-03
11	0.33082	0.24751E-03	0.14917	0.25084	0.50741E-03
12	0.27198	0.20563E-03	0.13213	0.32333	0.14989E-02

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
13	0.16047	0.30626E-04	0.14395	0.38606	0.16262E-02
26	0.46012E-03	0.60401E-16	0.30194E-01	0.76684	0.48819E-02
27	0.28582E-03	0.72986E-17	0.23280E-01	0.77215	0.89852E-02

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
1	0.14989E-06	0.23063E-03	0.16984E-03	0.40759E-03	0.45859E-03
2	0.27019E-09	0.82640E-06	0.58392E-05	0.32935E-05	0.38560E-04
3	0.25697E-09	0.42129E-06	0.18047E-05	0.12349E-05	0.12743E-04
4	0.26054E-09	0.42121E-06	0.17262E-05	0.12413E-05	0.11267E-04
10	0.19752E-09	0.28505E-06	0.20013E-05	0.14767E-05	0.12509E-04
11	0.17651E-09	0.27006E-06	0.20248E-05	0.15022E-05	0.12564E-04
12	0.33255E-10	0.23960E-06	0.19799E-05	0.14417E-05	0.12272E-04
13	0.21191E-14	0.38354E-09	0.88645E-07	0.13942E-07	0.12931E-05
26	0.12670E-71	0.12478E-44	0.54639E-24	0.22585E-33	0.44976E-18
27	0.32967E-76	0.24038E-47	0.25547E-25	0.23348E-35	0.48102E-19

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

STAGE	N-BUT-01	TRANS-01	CIS-2-01	C2H4	O2
1	0.67881E-03	0.49340E-03	0.21805E-02	0.94306E-04	0.17131E-05
2	0.95451E-05	0.58439E-04	0.27848E-03	0.61499E-06	0.30810E-08
3	0.31871E-05	0.20616E-04	0.10000E-03	0.25018E-06	0.27621E-08
4	0.32263E-05	0.17474E-04	0.83943E-04	0.25261E-06	0.27850E-08
10	0.10508E-04	0.18716E-04	0.89234E-04	0.31362E-06	0.21263E-08

11	0.12761E-04	0.18686E-04	0.89013E-04	0.32212E-06	0.20688E-08
12	0.13947E-04	0.18196E-04	0.86647E-04	0.30807E-06	0.87804E-09
13	0.11154E-05	0.25955E-05	0.13246E-04	0.24541E-08	0.17129E-12
26	0.15935E-17	0.40246E-16	0.49850E-15	0.40713E-35	0.43420E-59
27	0.21774E-18	0.57114E-17	0.75608E-16	0.35615E-37	0.12531E-62

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

STAGE	CH4	CO	WATER
1	0.36791E-04	0.21456E-05	0.64587E-03
2	0.94189E-07	0.45145E-08	0.17794E-02
3	0.61878E-07	0.40885E-08	0.40762E-02
4	0.63004E-07	0.41402E-08	0.87213E-02
10	0.84568E-07	0.27939E-08	0.23706
11	0.88382E-07	0.26166E-08	0.26828
12	0.75028E-07	0.10171E-08	0.27071
13	0.15372E-09	0.17505E-12	0.30785
26	0.85763E-44	0.28444E-60	0.19762
27	0.20283E-46	0.66104E-64	0.19530

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
1	0.99094	0.36215E-02	0.32742E-04	0.59837E-05	0.56914E-13
2	0.99440	0.32473E-02	0.14311E-03	0.31628E-04	0.11583E-11
3	0.99219	0.29711E-02	0.49532E-03	0.13019E-03	0.17531E-10
4	0.98631	0.27446E-02	0.15997E-02	0.50121E-03	0.25621E-09
10	0.43141	0.36808E-03	0.15177	0.17910	0.14951E-03
11	0.33082	0.24751E-03	0.14917	0.25084	0.50741E-03
12	0.27198	0.20563E-03	0.13213	0.32333	0.14989E-02

U-O-S BLOCK SECTION

BLOCK: DC-1   MODEL: RADFRAC (CONTINUED)

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
13	0.16047	0.30626E-04	0.14395	0.38606	0.16262E-02
26	0.36774E-03	0.55031E-17	0.73955E-02	0.10184	0.16699E-03
27	0.22584E-03	0.65978E-18	0.56657E-02	0.10182	0.30223E-03

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
1	0.14989E-06	0.23063E-03	0.16984E-03	0.40759E-03	0.45859E-03
2	0.27019E-09	0.82640E-06	0.58392E-05	0.32935E-05	0.38560E-04
3	0.25697E-09	0.42129E-06	0.18047E-05	0.12349E-05	0.12743E-04
4	0.26054E-09	0.42121E-06	0.17262E-05	0.12413E-05	0.11267E-04
10	0.19752E-09	0.28505E-06	0.20013E-05	0.14767E-05	0.12509E-04
11	0.17651E-09	0.27006E-06	0.20248E-05	0.15022E-05	0.12564E-04
12	0.33255E-10	0.23960E-06	0.19799E-05	0.14417E-05	0.12272E-04
13	0.21191E-14	0.38354E-09	0.88645E-07	0.13942E-07	0.12931E-05
26	0.14637E-71	0.33502E-45	0.85606E-24	0.35384E-33	0.70466E-18
27	0.40777E-76	0.64474E-48	0.40310E-25	0.36839E-35	0.75898E-19

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

STAGE	N-BUT-01	TRANS-01	CIS-2-01	C2H4	O2
1	0.67881E-03	0.49340E-03	0.21805E-02	0.94306E-04	0.17131E-05
2	0.95451E-05	0.58439E-04	0.27848E-03	0.61499E-06	0.30810E-08
3	0.31871E-05	0.20616E-04	0.10000E-03	0.25018E-06	0.27621E-08
4	0.32263E-05	0.17474E-04	0.83943E-04	0.25261E-06	0.27850E-08
10	0.10508E-04	0.18716E-04	0.89234E-04	0.31362E-06	0.21263E-08

11	0.12761E-04	0.18686E-04	0.89013E-04	0.32212E-06	0.20688E-08
12	0.13947E-04	0.18196E-04	0.86647E-04	0.30807E-06	0.87804E-09
13	0.11154E-05	0.25955E-05	0.13246E-04	0.24541E-08	0.17129E-12
26	0.26081E-17	0.63055E-16	0.78103E-15	0.63787E-35	0.54620E-60
27	0.35537E-18	0.90117E-17	0.11930E-15	0.56195E-37	0.15691E-63

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

STAGE	CH4	CO	WATER
1	0.36791E-04	0.21456E-05	0.64587E-03
2	0.94189E-07	0.45145E-08	0.17794E-02
3	0.61878E-07	0.40885E-08	0.40762E-02
4	0.63004E-07	0.41402E-08	0.87213E-02
10	0.84568E-07	0.27939E-08	0.23706
11	0.88382E-07	0.26166E-08	0.26828
12	0.75028E-07	0.10171E-08	0.27071
13	0.15372E-09	0.17505E-12	0.30785
26	0.13437E-43	0.35238E-61	0.89023
27	0.32003E-46	0.81475E-65	0.89198

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
1	0.69368	0.30789E-02	0.46344E-05	0.55348E-06	0.15524E-14
2	0.99056	0.36208E-02	0.32706E-04	0.59767E-05	0.56843E-13
3	0.99314	0.33430E-02	0.11463E-03	0.25013E-04	0.87442E-12
4	0.99149	0.31383E-02	0.37588E-03	0.98120E-04	0.13021E-10
10	0.69443	0.14725E-02	0.90984E-01	0.78203E-01	0.24054E-04
11	0.58618	0.12696E-02	0.10969	0.12944	0.10805E-03
12	0.51166	0.11728E-02	0.10824	0.18200	0.36814E-03

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

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

STAGE	METHANOL	IB-ALDEH	PROPANOL	ISBUT-OH	2-ME1BOH
13	0.31492	0.23813E-03	0.14987	0.27252	0.57642E-03
26	0.75929E-03	0.45711E-15	0.33732E-01	0.61241	0.17885E-02
27	0.46639E-03	0.55197E-16	0.26069E-01	0.61825	0.32990E-02

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

STAGE	H2	CO2	PROPANE	C2H2	ISOBU-01
1	0.18630E-02	0.94477E-01	0.47595E-02	0.56611E-01	0.49573E-02
2	0.25511E-05	0.35212E-03	0.17576E-03	0.48004E-03	0.46439E-03
3	0.23903E-05	0.17901E-03	0.53894E-04	0.17842E-03	0.15247E-03
4	0.23945E-05	0.17903E-03	0.50986E-04	0.17720E-03	0.13352E-03
10	0.25721E-05	0.19220E-03	0.54742E-04	0.19040E-03	0.14219E-03
11	0.25723E-05	0.19220E-03	0.54782E-04	0.19045E-03	0.14233E-03
12	0.52512E-06	0.17049E-03	0.53974E-04	0.18343E-03	0.14079E-03
13	0.38511E-10	0.27747E-06	0.22928E-05	0.16695E-05	0.14212E-04
26	0.54839E-67	0.63355E-42	0.15081E-22	0.28353E-31	0.53788E-17
27	0.15187E-71	0.12158E-44	0.70725E-24	0.29379E-33	0.57738E-18

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

STAGE	N-BUT-01	TRANS-01	CIS-2-01	C2H4	O2
1	0.49372E-01	0.36739E-02	0.14967E-01	0.17864E-01	0.90498E-02
2	0.74158E-03	0.49750E-03	0.21970E-02	0.11721E-03	0.13376E-04
3	0.24347E-03	0.17454E-03	0.78474E-03	0.47188E-04	0.11865E-04
4	0.23917E-03	0.14668E-03	0.65323E-03	0.47000E-04	0.11886E-04
10	0.26012E-03	0.15458E-03	0.68619E-03	0.50504E-04	0.12767E-04

11	0.26199E-03	0.15467E-03	0.68655E-03	0.50519E-04	0.12768E-04
12	0.25956E-03	0.15309E-03	0.67960E-03	0.48183E-04	0.52368E-05
13	0.16151E-04	0.21072E-04	0.10034E-03	0.35676E-06	0.10168E-08
26	0.15238E-16	0.36080E-15	0.41756E-14	0.60471E-33	0.14240E-55
27	0.20651E-17	0.51417E-16	0.63601E-15	0.52974E-35	0.40750E-59

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

STAGE	CH4	CO	WATER
1	0.33544E-01	0.11949E-01	0.14858E-03
2	0.79984E-04	0.17546E-04	0.64522E-03
3	0.51847E-04	0.15637E-04	0.14867E-02
4	0.51915E-04	0.15664E-04	0.31901E-02
10	0.55774E-04	0.16825E-04	0.13307
11	0.55784E-04	0.16827E-04	0.17150
12	0.46678E-04	0.64653E-05	0.19482
13	0.86886E-07	0.11779E-08	0.26172
26	0.47238E-41	0.11590E-56	0.35131
27	0.11169E-43	0.26681E-60	0.35192

U-O-S BLOCK SECTION

BLOCK: DC-1   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	38.593	50.939

2	50.939	51.433
3	51.433	51.948
4	51.948	52.609
10	65.571	68.781
11	68.781	70.944
12	70.948	75.285
13	75.285	77.789
26	84.617	84.959
27	84.959	84.959

	MASS FLOW LB/HR		VOLUME FLOW CUFT/HR		MOLECULAR WEIGHT	
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	0.35230E+06	0.35275E+06	7273.9	0.81790E+07	32.143	32.142
2	0.26740E+06	0.36022E+06	5624.2	0.82430E+07	32.064	32.083
3	0.26676E+06	0.35959E+06	5612.8	0.81196E+07	32.005	32.040
4	0.26549E+06	0.35831E+06	5585.7	0.79965E+07	31.909	31.968
10	0.24189E+06	0.33471E+06	4870.7	0.71967E+07	31.672	31.800
11	0.24529E+06	0.33811E+06	4906.1	0.72350E+07	32.160	32.155
12	0.41438E+06	0.35783E+06	8279.9	0.73994E+07	33.225	32.745
13	0.41585E+06	0.35930E+06	8252.0	0.72728E+07	33.648	33.224
26	0.41118E+06	0.35463E+06	8130.4	0.58465E+07	35.441	35.260
27	56551.	0.0000	1123.3	0.0000	36.618	

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

STAGE	DENSITY LB/CUFT LIQUID FROM	DENSITY LB/CUFT VAPOR TO	VISCOSITY CP LIQUID FROM	VISCOSITY CP VAPOR TO	SURFACE TENSION DYNE/CM LIQUID FROM
1	48.433	0.43129E-01	0.45248	0.10526E-01	21.132
2	47.544	0.43700E-01	0.39600	0.10548E-01	20.223
3	47.528	0.44286E-01	0.39459	0.10569E-01	20.376
4	47.530	0.44809E-01	0.39380	0.10598E-01	20.722
10	49.663	0.46509E-01	0.44355	0.11106E-01	38.140
11	49.996	0.46732E-01	0.44676	0.11140E-01	40.581
12	50.047	0.48359E-01	0.45058	0.11182E-01	41.223
13	50.394	0.49403E-01	0.44661	0.11185E-01	44.066
26	50.573	0.60657E-01	0.43196	0.11242E-01	47.579
27	50.342		0.43655		46.666

STAGE	MARANGONI INDEX DYNE/CM	FLOW PARAM	QR CUFT/HR	REDUCED F-FACTOR (LB-CUFT)**.5/HR
1		0.29802E-01	0.24418E+06	0.16986E+07
2	-.90875	0.22505E-01	0.25002E+06	0.17232E+07
3	0.15286	0.22646E-01	0.24797E+06	0.17087E+07
4	0.34582	0.22750E-01	0.24564E+06	0.16927E+07
10	4.0207	0.22116E-01	0.22034E+06	0.15520E+07
11	2.4415	0.22180E-01	0.22130E+06	0.15640E+07
12	3.2934	0.35998E-01	0.23012E+06	0.16272E+07
13	2.8437	0.36238E-01	0.22783E+06	0.16165E+07

26	-.45626E-02	0.40155E-01	0.20260E+06	0.14399E+07
27	-.91247		0.0000	0.0000

U-O-S BLOCK SECTION

BLOCK: DC-1   MODEL: RADFRAC (CONTINUED)

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


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

   STARTING STAGE NUMBER                                           2
   ENDING STAGE NUMBER                                            26
   FLOODING CALCULATION METHOD                                 GLITSCH6

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

   TRAY SPECIFICATIONS
   -------------------
```

TRAY TYPE		SIEVE
NUMBER OF PASSES		1
TRAY SPACING	FT	2.00000

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

STAGE WITH MAXIMUM DIAMETER		2
COLUMN DIAMETER	FT	19.9832
DC AREA/COLUMN AREA		0.100000
DOWNCOMER VELOCITY	FT/SEC	0.049813
FLOW PATH LENGTH PER PANEL	FT	13.7294
SIDE DOWNCOMER WIDTH	FT	3.12688
SIDE WEIR LENGTH	FT	14.5200
CENTER DOWNCOMER WIDTH	FT	0.0
CENTER WEIR LENGTH	FT	MISSING
OFF-CENTER DOWNCOMER WIDTH	FT	0.0
OFF-CENTER SHORT WEIR LENGTH	FT	MISSING
OFF-CENTER LONG WEIR LENGTH	FT	MISSING
TRAY CENTER TO OCDC CENTER	FT	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA	SIDE DC AREA
	FT	SQFT	SQFT	SQFT
2	19.983	313.63	250.90	31.363
3	19.983	313.63	250.90	31.363
4	19.983	313.63	250.90	31.363
5	19.983	313.63	250.90	31.363
6	19.983	313.63	250.90	31.363
7	19.983	313.63	250.90	31.363

8	19.983	313.63	250.90	31.363
9	19.983	313.63	250.90	31.363
10	19.983	313.63	250.90	31.363
11	19.983	313.63	250.90	31.363

U-O-S BLOCK SECTION

BLOCK: DC-1   MODEL: RADFRAC (CONTINUED)

STAGE	DIAMETER FT	TOTAL AREA SQFT	ACTIVE AREA SQFT	SIDE DC AREA SQFT
12	19.983	313.63	250.90	31.363
13	19.983	313.63	250.90	31.363
14	19.983	313.63	250.90	31.363
15	19.983	313.63	250.90	31.363
16	19.983	313.63	250.90	31.363
17	19.983	313.63	250.90	31.363
18	19.983	313.63	250.90	31.363
19	19.983	313.63	250.90	31.363
20	19.983	313.63	250.90	31.363
21	19.983	313.63	250.90	31.363
22	19.983	313.63	250.90	31.363
23	19.983	313.63	250.90	31.363
24	19.983	313.63	250.90	31.363
25	19.983	313.63	250.90	31.363
26	19.983	313.63	250.90	31.363

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP PSI	DC BACKUP FT	DC BACKUP/ (TSPC+WHT)
2	80.00	0.1082	0.7522	34.72
3	79.22	0.1072	0.7479	34.52

4	78.37	0.1061	0.7427	34.28
5	77.35	0.1048	0.7356	33.95
6	76.05	0.1033	0.7255	33.48
7	74.34	0.1016	0.7117	32.85
8	72.36	0.1001	0.6966	32.15
9	70.65	0.9953E-01	0.6853	31.63
10	69.64	0.9982E-01	0.6808	31.42
11	69.91	0.1012	0.6848	31.61
12	77.32	0.1120	0.8489	39.18
13	76.37	0.1120	0.8453	39.01
14	75.01	0.1109	0.8375	38.65
15	73.90	0.1099	0.8330	38.45
16	72.67	0.1086	0.8271	38.17
17	71.61	0.1075	0.8223	37.95
18	70.76	0.1066	0.8187	37.79
19	70.06	0.1058	0.8162	37.67
20	69.46	0.1052	0.8143	37.58
21	68.94	0.1046	0.8129	37.52
22	68.47	0.1042	0.8118	37.47
23	68.03	0.1037	0.8109	37.42
24	67.62	0.1033	0.8101	37.39
25	67.23	0.1029	0.8094	37.35
26	66.84	0.1025	0.8085	37.32

U-O-S BLOCK SECTION

BLOCK: DC-1 MODEL: RADFRAC (CONTINUED)

STAGE	HEIGHT OVER WEIR FT	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.3131	0.6071	0.1925	42.70
3	0.3116	0.6071	0.1934	42.27
4	0.3095	0.6071	0.1944	41.70
5	0.3060	0.6071	0.1957	40.88
6	0.3003	0.6071	0.1973	39.62
7	0.2920	0.6072	0.1995	37.81
8	0.2823	0.6073	0.2019	35.63
9	0.2749	0.6074	0.2038	33.69
10	0.2719	0.6075	0.2046	32.46
11	0.2742	0.6076	0.2037	32.15
12	0.4002	0.6076	0.1989	33.35
13	0.3982	0.6077	0.1997	32.53
14	0.3937	0.6077	0.2013	31.76
15	0.3912	0.6077	0.2028	31.25
16	0.3877	0.6077	0.2047	30.72
17	0.3847	0.6077	0.2063	30.27
18	0.3824	0.6077	0.2077	29.92
19	0.3807	0.6077	0.2089	29.65
20	0.3794	0.6077	0.2099	29.42
21	0.3783	0.6077	0.2108	29.22
22	0.3775	0.6077	0.2117	29.05
23	0.3768	0.6077	0.2124	28.89
24	0.3761	0.6077	0.2132	28.74

```
 25    0.3755      0.6077      0.2139       28.60
 26    0.3747      0.6077      0.2146       28.46

BLOCK:  DC-2     MODEL: RADFRAC
-------------------------------
   INLETS   - 49       STAGE   5
   OUTLETS  - 52       STAGE   1
              51       STAGE  10
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           603.767         603.767        0.353173E-09
      MASS(LB/HR   )           11386.0         11386.0       -0.134864E-07
      ENTHALPY(BTU/HR  )     -0.740322E+08   -0.727089E+08   -0.178749E-01
```

U-O-S BLOCK SECTION

BLOCK: DC-2 MODEL: RADFRAC (CONTINUED)

*** CO2 EQUIVALENT SUMMARY ***

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

****

**** INPUT DATA ****

****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	10
ALGORITHM OPTION	3-PHASE
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	BROYDEN
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	500
FLASH TOLERANCE	0.000100000

```
 OUTSIDE LOOP CONVERGENCE TOLERANCE                         0.000100000

**** COL-SPECS ****

 MOLAR VAPOR DIST / TOTAL DIST                              0.0
 MOLAR REFLUX RATIO                                         1.00000
 MOLAR DISTILLATE RATE          LBMOL/HR                   44.0925

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

 TWO LIQUID PHASE CALCULATIONS ARE PERFORMED FOR    STAGE  TO  STAGE
                                                      1         10

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

 KEY COMPONENTS IN THE SECOND LIQUID PHASE        COMPONENT
                                                   ISBUT-OH
                                                   WATER
```

U-O-S BLOCK SECTION

BLOCK: DC-2   MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

P-SPEC   STAGE   1 PRES, PSIG   1.30405

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

*** COMPONENT SPLIT FRACTIONS ***

COMPONENT:	OUTLET STREAMS 52	51
METHANOL	.97000	.30004E-01
PROPANOL	.99987	.13332E-03
ISBUT-OH	.99995	.49277E-04
2-ME1BOH	1.0000	.49887E-07
WATER	.58258E-01	.94174

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	C	92.2267
BOTTOM STAGE TEMPERATURE	C	105.332

```
 TOP STAGE LIQUID FLOW          LBMOL/HR                   88.1849
 BOTTOM STAGE LIQUID FLOW       LBMOL/HR                  559.674
 TOP STAGE VAPOR FLOW           LBMOL/HR                    0.0
 BOILUP VAPOR FLOW              LBMOL/HR                  166.059
 MOLAR REFLUX RATIO                                         1.00000
 MOLAR BOILUP RATIO                                         0.29671
 CONDENSER DUTY (W/O SUBCOOL)   BTU/HR            -1,569,540.
 REBOILER DUTY                  BTU/HR             2,892,860.

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

 DEW POINT                       0.17859E-09  STAGE=  1 PHASE=L1
 BUBBLE POINT                    0.21955E-09  STAGE=  1 PHASE=L1
 COMPONENT MASS BALANCE          0.85915E-10  STAGE=  2 COMP=2-ME1BOH
 ENERGY BALANCE                  0.12680E-10  STAGE=  2
```

U-O-S BLOCK SECTION

BLOCK: DC-2 MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

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

STAGE	TEMPERATURE C	PRESSURE PSIG	ENTHALPY BTU/LBMOL LIQUID	ENTHALPY BTU/LBMOL VAPOR	HEAT DUTY BTU/HR
1	92.227	1.3041	-0.12355E+06	-0.10723E+06	-.15695+07
2	97.020	1.8941	-0.12061E+06	-0.10575E+06	
3	100.41	2.0341	-0.12041E+06	-0.10435E+06	
4	100.78	2.1741	-0.12039E+06	-0.10429E+06	
5	101.02	2.3141	-0.12038E+06	-0.10428E+06	
6	103.70	2.4541	-0.12024E+06	-0.10311E+06	
8	104.84	2.7341	-0.12020E+06	-0.10281E+06	
9	105.10	2.8741	-0.12019E+06	-0.10280E+06	
10	105.33	3.0141	-0.12018E+06	-0.10279E+06	.28929+07

STAGE	FLOW RATE LBMOL/HR LIQUID	FLOW RATE LBMOL/HR VAPOR	FEED RATE LBMOL/HR LIQUID	FEED RATE LBMOL/HR VAPOR	FEED RATE LBMOL/HR MIXED	PRODUCT RATE LBMOL/HR LIQUID	PRODUCT RATE LBMOL/HR VAPOR
1	88.18	0.000				44.0924	
2	44.48	88.18					
3	44.69	88.57					
4	44.70	88.78					

5	720.6	88.79	603.7666	
6	723.9	161.0		
8	725.4	165.3		
9	725.7	165.7		
10	559.7	166.1		559.6742

STAGE	FLOW RATE LBMOL/HR		ENTHALPY BTU/LBMO	
	LIQUID1	LIQUID2	LIQUID1	LIQUID2
1	35.80	52.39	-0.12726E+06	-0.12101E+06
2	0.000	44.48	-0.12061E+06	-0.12061E+06
3	0.000	44.69	-0.12041E+06	-0.12041E+06
4	0.000	44.70	-0.12039E+06	-0.12039E+06
5	0.000	720.6	-0.12038E+06	-0.12038E+06
6	0.000	723.9	-0.12024E+06	-0.12024E+06
8	0.000	725.4	-0.12020E+06	-0.12020E+06
9	0.000	725.7	-0.12019E+06	-0.12019E+06
10	0.000	559.7	-0.12018E+06	-0.12018E+06

U-O-S BLOCK SECTION

BLOCK: DC-2 MODEL: RADFRAC (CONTINUED)

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	2606.	0.000				1303.2221	
2	835.2	2606.					
3	819.0	2138.					
4	818.5	2122.					
5	0.1320E+05	2122.	.11386+05				
6	0.1308E+05	3113.					
8	0.1307E+05	2986.					
9	0.1307E+05	2987.					
10	0.1008E+05	2992.				.10083+05	

STAGE	FLOW RATE LB/HR	
	LIQUID1	LIQUID2
1	1558.	1048.
2	0.000	835.2
3	0.000	819.0
4	0.000	818.5
5	0.000	0.1320E+05
6	0.000	0.1308E+05
8	0.000	0.1307E+05
9	0.000	0.1307E+05

10 0.000 0.1008E+05

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER
1	0.36438E-02	0.26314E-01	0.18392	0.90259E-03	0.78521
2	0.73709E-03	0.20747E-02	0.11853E-01	0.23442E-04	0.98531
3	0.34351E-03	0.84750E-03	0.48215E-02	0.79721E-05	0.99398
4	0.30895E-03	0.79962E-03	0.45948E-02	0.76776E-05	0.99429
5	0.30634E-03	0.79734E-03	0.45937E-02	0.76516E-05	0.99429
6	0.17638E-03	0.17722E-03	0.85909E-03	0.44918E-06	0.99879
8	0.48595E-04	0.77088E-05	0.26829E-04	0.13136E-08	0.99992
9	0.22994E-04	0.15518E-05	0.46174E-05	0.69737E-10	0.99997
10	0.88796E-05	0.27642E-06	0.71406E-06	0.35474E-11	0.99999

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER
1	0.62633E-02	0.55194E-01	0.40907	0.21649E-02	0.52731
2	0.73709E-03	0.20747E-02	0.11853E-01	0.23442E-04	0.98531
3	0.34351E-03	0.84750E-03	0.48215E-02	0.79721E-05	0.99398
4	0.30895E-03	0.79962E-03	0.45948E-02	0.76776E-05	0.99429
5	0.30634E-03	0.79734E-03	0.45937E-02	0.76516E-05	0.99429
6	0.17638E-03	0.17722E-03	0.85909E-03	0.44918E-06	0.99879
8	0.48595E-04	0.77088E-05	0.26829E-04	0.13136E-08	0.99992
9	0.22994E-04	0.15518E-05	0.46174E-05	0.69737E-10	0.99997
10	0.88796E-05	0.27642E-06	0.71406E-06	0.35474E-11	0.99999

U-O-S BLOCK SECTION

BLOCK: DC-2 MODEL: RADFRAC (CONTINUED)

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER
1	0.18540E-02	0.65817E-02	0.30089E-01	0.40075E-04	0.96143
2	0.73709E-03	0.20747E-02	0.11853E-01	0.23442E-04	0.98531
3	0.34351E-03	0.84750E-03	0.48215E-02	0.79721E-05	0.99398
4	0.30895E-03	0.79962E-03	0.45948E-02	0.76776E-05	0.99429
5	0.30634E-03	0.79734E-03	0.45937E-02	0.76516E-05	0.99429
6	0.17638E-03	0.17722E-03	0.85909E-03	0.44918E-06	0.99879
8	0.48595E-04	0.77088E-05	0.26829E-04	0.13136E-08	0.99992
9	0.22994E-04	0.15518E-05	0.46174E-05	0.69737E-10	0.99997
10	0.88796E-05	0.27642E-06	0.71406E-06	0.35474E-11	0.99999

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER
1	0.59387E-02	0.49463E-01	0.27068	0.67886E-03	0.67324
2	0.36438E-02	0.26314E-01	0.18392	0.90259E-03	0.78521
3	0.21842E-02	0.14142E-01	0.97517E-01	0.46112E-03	0.88570
4	0.19825E-02	0.13495E-01	0.93770E-01	0.45227E-03	0.89030
5	0.19650E-02	0.13470E-01	0.93647E-01	0.45208E-03	0.89047
6	0.13405E-02	0.35686E-02	0.20563E-01	0.34255E-04	0.97449
8	0.38569E-03	0.16261E-03	0.66811E-03	0.10753E-06	0.99878
9	0.18272E-03	0.32810E-04	0.11503E-03	0.57379E-08	0.99967
10	0.70566E-04	0.58504E-05	0.17773E-04	0.29282E-09	0.99991

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER

1	0.9482	0.8962	0.6617	0.3136	1.2767
2	MISSING	MISSING	MISSING	MISSING	MISSING
3	MISSING	MISSING	MISSING	MISSING	MISSING
4	MISSING	MISSING	MISSING	MISSING	MISSING
5	MISSING	MISSING	MISSING	MISSING	MISSING
6	MISSING	MISSING	MISSING	MISSING	MISSING
8	MISSING	MISSING	MISSING	MISSING	MISSING
9	MISSING	MISSING	MISSING	MISSING	MISSING
10	MISSING	MISSING	MISSING	MISSING	MISSING

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER
1	3.2032	7.5152	8.9959	16.9399	0.7002
2	4.9435	12.6831	15.5167	38.5040	0.7969
3	6.3583	16.6868	20.2257	57.8416	0.8911
4	6.4170	16.8767	20.4079	58.9072	0.8954
5	6.4144	16.8932	20.3857	59.0821	0.8956
6	7.6001	20.1368	23.9354	76.2617	0.9757
8	7.9370	21.0947	24.9021	81.8618	0.9989
9	7.9464	21.1424	24.9116	82.2784	0.9997
10	7.9470	21.1647	24.8904	82.5451	0.9999

U-O-S BLOCK SECTION

BLOCK: DC-2 MODEL: RADFRAC (CONTINUED)

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER
1	0.2960	0.1192	7.3555-02	1.8511-02	1.8233
2	MISSING	MISSING	MISSING	MISSING	MISSING
3	MISSING	MISSING	MISSING	MISSING	MISSING
4	MISSING	MISSING	MISSING	MISSING	MISSING
5	MISSING	MISSING	MISSING	MISSING	MISSING
6	MISSING	MISSING	MISSING	MISSING	MISSING
8	MISSING	MISSING	MISSING	MISSING	MISSING
9	MISSING	MISSING	MISSING	MISSING	MISSING
10	MISSING	MISSING	MISSING	MISSING	MISSING

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER
1	0.39502E-02	0.53503E-01	0.46125	0.26919E-02	0.47860
2	0.12576E-02	0.66393E-02	0.46785E-01	0.11003E-03	0.94521
3	0.60059E-03	0.27791E-02	0.19500E-01	0.38345E-04	0.97708
4	0.54061E-03	0.26242E-02	0.18599E-01	0.36959E-04	0.97820
5	0.53604E-03	0.26168E-02	0.18595E-01	0.36834E-04	0.97822
6	0.31271E-03	0.58926E-03	0.35233E-02	0.21908E-05	0.99557
8	0.86419E-04	0.25712E-04	0.11037E-03	0.64265E-08	0.99978
9	0.40897E-04	0.51765E-05	0.18998E-04	0.34121E-09	0.99993
10	0.15793E-04	0.92209E-06	0.29379E-05	0.17357E-10	0.99998

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER

1	0.46104E-02	0.76199E-01	0.69657	0.43841E-02	0.21823
2	0.12576E-02	0.66393E-02	0.46785E-01	0.11003E-03	0.94521
3	0.60059E-03	0.27791E-02	0.19500E-01	0.38345E-04	0.97708
4	0.54061E-03	0.26242E-02	0.18599E-01	0.36959E-04	0.97820
5	0.53604E-03	0.26168E-02	0.18595E-01	0.36834E-04	0.97822
6	0.31271E-03	0.58926E-03	0.35233E-02	0.21908E-05	0.99557
8	0.86419E-04	0.25712E-04	0.11037E-03	0.64265E-08	0.99978
9	0.40897E-04	0.51765E-05	0.18998E-04	0.34121E-09	0.99993
10	0.15793E-04	0.92209E-06	0.29379E-05	0.17357E-10	0.99998

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER
1	0.29689E-02	0.19768E-01	0.11146	0.17655E-03	0.86562
2	0.12576E-02	0.66393E-02	0.46785E-01	0.11003E-03	0.94521
3	0.60059E-03	0.27791E-02	0.19500E-01	0.38345E-04	0.97708
4	0.54061E-03	0.26242E-02	0.18599E-01	0.36959E-04	0.97820
5	0.53604E-03	0.26168E-02	0.18595E-01	0.36834E-04	0.97822
6	0.31271E-03	0.58926E-03	0.35233E-02	0.21908E-05	0.99557
8	0.86419E-04	0.25712E-04	0.11037E-03	0.64265E-08	0.99978
9	0.40897E-04	0.51765E-05	0.18998E-04	0.34121E-09	0.99993
10	0.15793E-04	0.92209E-06	0.29379E-05	0.17357E-10	0.99998

U-O-S BLOCK SECTION

BLOCK: DC-2 MODEL: RADFRAC (CONTINUED)

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

STAGE	METHANOL	PROPANOL	ISBUT-OH	2-ME1BOH	WATER
1	0.53731E-02	0.83934E-01	0.56653	0.16897E-02	0.34247
2	0.39502E-02	0.53503E-01	0.46125	0.26919E-02	0.47860
3	0.28986E-02	0.35199E-01	0.29937	0.16835E-02	0.66085
4	0.26575E-02	0.33927E-01	0.29077	0.16678E-02	0.67098
5	0.26349E-02	0.33875E-01	0.29049	0.16677E-02	0.67134
6	0.22209E-02	0.11089E-01	0.78808E-01	0.15613E-03	0.90773
8	0.68411E-03	0.54096E-03	0.27413E-02	0.52471E-06	0.99603
9	0.32480E-03	0.10938E-03	0.47300E-03	0.28059E-07	0.99909
10	0.12549E-03	0.19514E-04	0.73117E-04	0.14326E-08	0.99978

****
***** 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	92.227	97.020
2	97.020	100.41
3	100.41	100.78
4	100.78	101.02
5	101.02	103.70
6	103.70	104.50
8	104.84	105.10
9	105.10	105.33
10	105.33	105.33

U-O-S BLOCK SECTION

BLOCK: DC-2 MODEL: RADFRAC (CONTINUED)

	MASS FLOW LB/HR		VOLUME FLOW CUFT/HR		MOLECULAR WEIGHT	
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	2606.4	2606.4	50.747	38008.	29.557	29.557
2	835.22	2138.4	14.722	38200.	18.780	24.145
3	819.04	2122.3	14.378	38013.	18.327	23.904
4	818.52	2121.7	14.371	37728.	18.312	23.896
5	13196.	3113.3	231.76	68326.	18.311	19.340
6	13084.	3001.0	229.48	69299.	18.073	18.271
8	13070.	2987.2	229.29	68913.	18.018	18.026
9	13075.	2992.0	229.43	68552.	18.016	18.018
10	10083.	0.0000	176.98	0.0000	18.015	

	DENSITY LB/CUFT		VISCOSITY CP		SURFACE TENSION DYNE/CM
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM
1	51.362	0.68576E-01	0.35700	0.12008E-01	50.627
2	56.731	0.55980E-01	0.29153	0.12417E-01	58.208
3	56.963	0.55829E-01	0.27924	0.12441E-01	57.919
4	56.955	0.56237E-01	0.27805	0.12450E-01	57.860
5	56.939	0.45565E-01	0.27733	0.12698E-01	57.814
6	57.015	0.43306E-01	0.26874	0.12743E-01	57.482
8	57.002	0.43347E-01	0.26536	0.12767E-01	57.307
9	56.988	0.43645E-01	0.26465	0.12776E-01	57.260

10	56.973	0.26399	57.215

STAGE	MARANGONI INDEX DYNE/CM	FLOW PARAM	QR CUFT/HR	REDUCED F-FACTOR (LB-CUFT)**.5/HR
1		0.36540E-01	1389.7	9953.2
2	7.5812	0.12269E-01	1200.6	9038.2
3	-.28890	0.12082E-01	1190.6	8981.9
4	-.58996E-01	0.12122E-01	1186.1	8947.1
5	-10.408	0.11991	1933.6	14585.
6	-.33231	0.12015	1910.6	14421.
8	-.58698E-01	0.12066	1901.1	14348.
9	-.47309E-01	0.12094	1897.9	14322.
10	-.45012E-01		0.0000	0.0000

U-O-S BLOCK SECTION

BLOCK: DC-2   MODEL: RADFRAC (CONTINUED)

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


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

   STARTING STAGE NUMBER                                        2
   ENDING STAGE NUMBER                                          9
   FLOODING CALCULATION METHOD                            GLITSCH6

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

   TRAY SPECIFICATIONS
   -------------------
```

TRAY TYPE		SIEVE
NUMBER OF PASSES		1
TRAY SPACING	FT	2.00000

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

STAGE WITH MAXIMUM DIAMETER		5
COLUMN DIAMETER	FT	1.69596
DC AREA/COLUMN AREA		0.100000
DOWNCOMER VELOCITY	FT/SEC	0.28498
FLOW PATH LENGTH PER PANEL	FT	1.16521
SIDE DOWNCOMER WIDTH	FT	0.26538
SIDE WEIR LENGTH	FT	1.23231
CENTER DOWNCOMER WIDTH	FT	0.0
CENTER WEIR LENGTH	FT	MISSING
OFF-CENTER DOWNCOMER WIDTH	FT	0.0
OFF-CENTER SHORT WEIR LENGTH	FT	MISSING
OFF-CENTER LONG WEIR LENGTH	FT	MISSING
TRAY CENTER TO OCDC CENTER	FT	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA	SIDE DC AREA
	FT	SQFT	SQFT	SQFT
2	1.6960	2.2590	1.8072	0.22590
3	1.6960	2.2590	1.8072	0.22590
4	1.6960	2.2590	1.8072	0.22590
5	1.6960	2.2590	1.8072	0.22590
6	1.6960	2.2590	1.8072	0.22590
7	1.6960	2.2590	1.8072	0.22590

8	1.6960	2.2590	1.8072	0.22590
9	1.6960	2.2590	1.8072	0.22590

U-O-S BLOCK SECTION

BLOCK: DC-2 MODEL: RADFRAC (CONTINUED)

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP PSI	DC BACKUP FT	DC BACKUP/ (TSPC+WHT)
2	45.64	0.7679E-01	0.4362	20.13
3	45.28	0.7656E-01	0.4346	20.06
4	45.05	0.7635E-01	0.4341	20.04
5	80.00	0.1375	0.6988	32.25
6	79.73	0.1354	0.6904	31.86
7	79.55	0.1349	0.6884	31.77
8	79.34	0.1345	0.6873	31.72
9	79.12	0.1342	0.6863	31.68

STAGE	HEIGHT OVER WEIR FT	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.2690E-01	0.6082	0.2359	22.84
3	0.2639E-01	0.6082	0.2369	22.70
4	0.2633E-01	0.6082	0.2376	22.62
5	0.3032	0.6082	0.1780	37.01
6	0.3002	0.6082	0.1789	36.62
7	0.2997	0.6082	0.1791	36.52
8	0.2996	0.6082	0.1793	36.46
9	0.2996	0.6082	0.1794	36.41

U-O-S BLOCK SECTION

```
BLOCK:  DEC-1    MODEL: DECANTER
--------------------------------
  INLET STREAM:           48
  FIRST LIQUID OUTLET:    50
  SECOND LIQUID OUTLET:   49
  PROPERTY OPTION SET:    NRTL       RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:         HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1588.43         1588.43       -0.286287E-15
      MASS(LB/HR   )           57854.4         57854.4        0.114544E-07
      ENTHALPY(BTU/HR  )     -0.204642E+09   -0.204758E+09    0.564878E-03

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

                        ***  INPUT DATA  ***

  LIQUID-LIQUID SPLIT, TP SPECIFICATION
  SPECIFIED TEMPERATURE              C                          40.0000
  SPECIFIED PRESSURE                 PSIG                     3.30405
  CONVERGENCE TOLERANCE ON EQUILIBRIUM                       0.10000E-03
```

MAXIMUM NO ITERATIONS ON EQUILIBRIUM	500
EQUILIBRIUM METHOD	EQUATION-SOLVING
KLL COEFFICIENTS FROM	OPTION SET OR EOS
KLL BASIS	MOLE

KEY COMPONENT(S): WATER ISBUT-OH

U-O-S BLOCK SECTION

BLOCK: DEC-1 MODEL: DECANTER (CONTINUED)

*** RESULTS ***

OUTLET TEMPERATURE	C	40.000
OUTLET PRESSURE	PSIG	3.3041
CALCULATED HEAT DUTY	BTU/HR	-0.11566E+06
MOLAR RATIO 1ST LIQUID / TOTAL LIQUID		0.61990

L1-L2 PHASE EQUILIBRIUM :

COMP	F	X1	X2	K
METHANOL	0.00040606	0.00048683	0.00027433	0.56351
PROPANOL	0.012540	0.019051	0.0019220	0.10089
ISBUT-OH	0.31483	0.49963	0.013433	0.026885
2-ME1BOH	0.0029880	0.0047797	0.659154-04	0.013791
WATER	0.66924	0.47605	0.98431	2.06764

U-O-S BLOCK SECTION

```
BLOCK:  FD-1     MODEL: FLASH2
------------------------------
  INLET STREAM:          29
  OUTLET VAPOR STREAM:   34
  OUTLET LIQUID STREAM:  30
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                  ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          4524.98         4524.98       -0.119434E-06
      MASS(LB/HR   )          150858.         150858.       -0.119434E-06
      ENTHALPY(BTU/HR  )    -0.497822E+09   -0.497806E+09   -0.310301E-04

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           3171.24      LB/HR
   PRODUCT STREAMS CO2E        3171.24      LB/HR
   NET STREAMS CO2E PRODUCTION  0.378753E-03  LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION       0.378753E-03  LB/HR

                      ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE C                             40.0000
  SPECIFIED PRESSURE    PSIG                           5.30405
  MAXIMUM NO. ITERATIONS                             500
  CONVERGENCE TOLERANCE                                0.000100000
```

*** RESULTS ***

OUTLET TEMPERATURE	C	40.000
OUTLET PRESSURE	PSIG	5.3041
HEAT DUTY	BTU/HR	15507.
VAPOR FRACTION		0.20461E-01

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
METHANOL	0.63693	0.64681	0.16415	0.25379
IB-ALDEH	0.10403E-02	0.10510E-02	0.52909E-03	0.50340
PROPANOL	0.41614E-02	0.42436E-02	0.22612E-03	0.53285E-01
ISBUT-OH	0.10882	0.11100	0.46446E-02	0.41845E-01
2-ME1BOH	0.10403E-02	0.10618E-02	0.12252E-04	0.11539E-01
H2	0.10404E-01	0.96355E-04	0.50386	5229.1
CO2	0.13871E-02	0.32944E-03	0.52024E-01	157.92

U-O-S BLOCK SECTION

BLOCK: FD-1   MODEL: FLASH2 (CONTINUED)

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
PROPANE	0.10403E-03	0.91337E-04	0.71188E-03	7.7939
C2H2	0.97098E-03	0.54926E-03	0.21160E-01	38.525
ISOBU-01	0.18033E-03	0.17317E-03	0.52294E-03	3.0198
N-BUT-01	0.38146E-03	0.33052E-03	0.28202E-02	8.5326
TRANS-01	0.19420E-03	0.18997E-03	0.39635E-03	2.0864
CIS-2-01	0.85308E-03	0.83724E-03	0.16113E-02	1.9245
C2H4	0.27742E-03	0.13538E-03	0.70778E-02	52.281
O2	0.12138E-02	0.30129E-04	0.57879E-01	1921.0
CH4	0.15952E-02	0.26230E-03	0.65407E-01	249.36
CO	0.20321E-02	0.45360E-04	0.97148E-01	2141.7
WATER	0.22841	0.23277	0.19821E-01	0.85152E-01

U-O-S BLOCK SECTION

```
BLOCK:  FD-2     MODEL: FLASH2
------------------------------
  INLET STREAM:           39
  OUTLET VAPOR STREAM:    40
  OUTLET LIQUID STREAM:   41
  PROPERTY OPTION SET:    NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:         HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            107.024         107.024         0.00000
      MASS(LB/HR   )            1938.79         1938.79       -0.117276E-15
      ENTHALPY(BTU/HR  )      -0.422180E+07   -0.420803E+07   -0.326039E-02

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             3064.98      LB/HR
   PRODUCT STREAMS CO2E          3064.98      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         0.00000      LB/HR

                        ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE C                                 10.0000
  SPECIFIED PRESSURE    PSIG                               1.30405
  MAXIMUM NO. ITERATIONS                                 500
  CONVERGENCE TOLERANCE                                    0.000100000
```

*** RESULTS ***

OUTLET TEMPERATURE	C	10.000
OUTLET PRESSURE	PSIG	1.3041
HEAT DUTY	BTU/HR	13765.
VAPOR FRACTION		0.79027

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
METHANOL	0.23398	0.89376	0.58886E-01	0.65886E-01
IB-ALDEH	0.63911E-03	0.20862E-02	0.25508E-03	0.12227
PROPANOL	0.19594E-03	0.90303E-03	0.82811E-05	0.91703E-02
ISBUT-OH	0.40179E-02	0.19096E-01	0.16396E-04	0.85860E-03
2-ME1BOH	0.10599E-04	0.50280E-04	0.67735E-07	0.13472E-02
H2	0.43980	0.86758E-04	0.55649	6414.3
CO2	0.54125E-01	0.67694E-03	0.68310E-01	100.91

U-O-S BLOCK SECTION

BLOCK: FD-2 MODEL: FLASH2 (CONTINUED)

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
PROPANE	0.10744E-02	0.24533E-03	0.12944E-02	5.2762
C2H2	0.27543E-01	0.12210E-02	0.34528E-01	28.278
ISOBU-01	0.81475E-03	0.49132E-03	0.90058E-03	1.8330
N-BUT-01	0.60486E-02	0.75428E-03	0.74536E-02	9.8818
TRANS-01	0.62108E-03	0.54562E-03	0.64110E-03	1.1750
CIS-2-01	0.25272E-02	0.24064E-02	0.25592E-02	1.0635
C2H4	0.88282E-02	0.26188E-03	0.11102E-01	42.392
O2	0.51271E-01	0.29140E-04	0.64870E-01	2226.2
CH4	0.65466E-01	0.33048E-03	0.82752E-01	250.40
CO	0.85853E-01	0.31506E-04	0.10863	3447.9
WATER	0.17182E-01	0.77023E-01	0.13005E-02	0.16885E-01

U-O-S BLOCK SECTION

BLOCK: FH-1 MODEL: HEATER

INLET STREAM: 6
OUTLET STREAM: 7
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	4461.44	4461.44	0.00000
MASS(LB/HR)	150857.	150857.	0.00000
ENTHALPY(BTU/HR)	-0.430224E+09	-0.357464E+09	-0.169121

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	109.905	LB/HR
PRODUCT STREAMS CO2E	109.905	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

*** INPUT DATA ***

TWO PHASE TP FLASH

SPECIFIED TEMPERATURE	C	332.000
PRESSURE DROP	PSI	2.00000
MAXIMUM NO. ITERATIONS		500
CONVERGENCE TOLERANCE		0.000100000

*** RESULTS ***

OUTLET TEMPERATURE	C	332.00
OUTLET PRESSURE	PSIG	49.876
HEAT DUTY	BTU/HR	0.72760E+08
OUTLET VAPOR FRACTION		1.0000

U-O-S BLOCK SECTION

BLOCK: FH-1 MODEL: HEATER (CONTINUED)

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
METHANOL	0.87399	0.66582	0.87399	69.510
ETHANOL	0.12166	0.18634	0.12166	33.937
IB-ALDEH	0.10503E-02	0.20986E-02	0.10503E-02	26.600
PROPANOL	0.15823E-04	0.24957E-02	0.15823E-04	0.39352
ISBUT-OH	0.97745E-04	0.14122	0.97745E-04	0.37451E-01
2-ME1BOH	0.25297E-06	0.97825E-06	0.25297E-06	13.774
H2	0.19759E-05	0.46256E-06	0.19759E-05	227.57
CO2	0.11190E-03	0.99487E-06	0.11190E-03	6003.1
PROPANE	0.80977E-04	0.36124E-04	0.80977E-04	119.41
C2H2	0.33023E-03	0.44447E-04	0.33023E-03	395.77
ISOBU-01	0.16582E-03	0.11797E-03	0.16582E-03	74.870
N-BUT-01	0.24559E-03	0.90576E-04	0.24559E-03	145.74
TRANS-01	0.18481E-03	0.13443E-03	0.18481E-03	73.228
CIS-2-01	0.81671E-03	0.65262E-03	0.81671E-03	66.660
C2H4	0.70915E-04	0.11958E-04	0.70915E-04	315.90
O2	0.12550E-05	0.10020E-06	0.12550E-05	669.72
CH4	0.49143E-04	0.46005E-05	0.49143E-04	569.00
CO	0.17444E-05	0.12258E-05	0.17444E-05	75.603
WATER	0.11298E-02	0.93309E-03	0.11298E-02	64.104

U-O-S BLOCK SECTION

```
BLOCK:  FH-2     MODEL: HEATER
------------------------------
  INLET STREAM:          50
  OUTLET STREAM:         54
  PROPERTY OPTION SET:   NRTL       RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          984.666         984.666         0.00000
      MASS(LB/HR   )          46468.4         46468.4       -0.313157E-15
      ENTHALPY(BTU/HR  )    -0.130726E+09   -0.993411E+08   -0.240079

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

                        ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE             C                      325.000
  SPECIFIED PRESSURE                PSIG                    13.3041
  MAXIMUM NO. ITERATIONS                                   500
  CONVERGENCE TOLERANCE                                      0.000100000
```

*** RESULTS ***

OUTLET TEMPERATURE	C	325.00
OUTLET PRESSURE	PSIG	13.304
HEAT DUTY	BTU/HR	0.31384E+08
OUTLET VAPOR FRACTION		1.0000

U-O-S BLOCK SECTION

BLOCK: FH-2   MODEL: HEATER (CONTINUED)

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
METHANOL	0.48683E-03	0.14393	0.48683E-03	0.30967E-01
PROPANOL	0.19051E-01	0.11115E-02	0.19051E-01	156.92
ISBUT-OH	0.49963	0.82495	0.49963	5.5448
2-ME1BOH	0.47797E-02	0.12587E-02	0.47797E-02	34.765
WATER	0.47605	0.28748E-01	0.47605	151.60

U-O-S BLOCK SECTION

```
BLOCK:  KR-1     MODEL: HEATX
-----------------------------
HOT STREAM OUTLET T = 338 C
  HOT SIDE:
  ---------
  INLET STREAM:              8
  OUTLET STREAM:             11
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
  COLD SIDE:
  ----------
  INLET STREAM:              9
  OUTLET STREAM:             10
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           4964.65         4964.65         0.00000
      MASS(LB/HR   )           159484.         159484.         0.00000
      ENTHALPY(BTU/HR  )      -0.413508E+09   -0.413508E+09     0.00000

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            951.402      LB/HR
   PRODUCT STREAMS CO2E         951.402      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
```

```
 TOTAL CO2E PRODUCTION         0.00000      LB/HR

                       ***  INPUT DATA  ***

FLASH SPECS FOR HOT SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                      500
CONVERGENCE TOLERANCE                                         0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                      500
CONVERGENCE TOLERANCE                                         0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED EXCHANGER DUTY
  SPECIFIED VALUE                BTU/HR             7392810.0000
  LMTD CORRECTION FACTOR                                  1.00000
```

U-O-S BLOCK SECTION

BLOCK: KR-1   MODEL: HEATX (CONTINUED)

```
  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                          2.8000
    COLD SIDE PRESSURE DROP        PSI                          1.0900

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT            BTU/HR-SQFT-R              101.3500

                       ***  OVERALL RESULTS  ***

  STREAMS:
                --------------------------------------
                |                                    |
  8        ----->|               HOT                  |-----> 11
  T=  3.9377D+02  |                                    |       T=  3.4298D+02
  P=  4.4029D+01  |                                    |       P=  4.1229D+01
  V=  1.0000D+00  |                                    |       V=  1.0000D+00
                |                                    |
  10       <-----|               COLD                 |<----- 9
  T=  1.8582D+02  |                                    |       T=  1.8556D+02
  P=  1.5033D+02  |                                    |       P=  1.5142D+02
  V=  1.0000D+00  |                                    |       V=  0.0000D+00
                --------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR                 7392810.0000
    CALCULATED (REQUIRED) AREA     SQFT                       223.2386
```

ACTUAL EXCHANGER AREA	SQFT	223.2386
PER CENT OVER-DESIGN		0.0000
HEAT TRANSFER COEFFICIENT:		
AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	101.3500
UA (DIRTY)	BTU/HR-R	22625.2351
LOG-MEAN TEMPERATURE DIFFERENCE:		
LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	181.5281
NUMBER OF SHELLS IN SERIES		1
PRESSURE DROP:		
HOTSIDE, TOTAL	PSI	2.8000
COLDSIDE, TOTAL	PSI	1.0900

U-O-S BLOCK SECTION

HEATX COLD-TQCU KR-1 TQCURV INLET

```
  PRESSURE PROFILE:      CONSTANT2
  PRESSURE DROP:         -1.0900     PSI
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
```

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	151.4200	185.9604	0.9999
3.5204+05	151.4200	185.9604	0.9522
7.0408+05	151.4200	185.9604	0.9045
1.0561+06	151.4200	185.9604	0.8569
1.4082+06	151.4200	185.9604	0.8092
1.7602+06	151.4200	185.9604	0.7615
2.1122+06	151.4200	185.9604	0.7139
2.4643+06	151.4200	185.9604	0.6662
2.8163+06	151.4200	185.9604	0.6185
3.1683+06	151.4200	185.9604	0.5709
3.5204+06	151.4200	185.9604	0.5232

3.8724+06	151.4200	185.9604	0.4755
4.2245+06	151.4200	185.9604	0.4279
4.5765+06	151.4200	185.9604	0.3802
4.9285+06	151.4200	185.9604	0.3325
5.2806+06	151.4200	185.9604	0.2849
5.6326+06	151.4200	185.9604	0.2372
5.9847+06	151.4200	185.9604	0.1895
6.3367+06	151.4200	185.9604	0.1419
6.6887+06	151.4200	185.9604	9.4193-02
7.0408+06	151.4200	185.9604	4.6526-02
7.3844+06	151.4200	185.9604	BUB>0.0
7.3928+06	151.4200	185.5556	0.0

U-O-S BLOCK SECTION

HEATX HOT-TQCUR KR-1 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	44.0294	393.7873	1.0000
3.5204+05	44.0294	391.4210	1.0000
7.0408+05	44.0294	389.0498	1.0000
1.0561+06	44.0294	386.6734	1.0000
1.4082+06	44.0294	384.2921	1.0000
1.7602+06	44.0294	381.9056	1.0000
2.1122+06	44.0294	379.5139	1.0000
2.4643+06	44.0294	377.1170	1.0000
2.8163+06	44.0294	374.7148	1.0000
3.1683+06	44.0294	372.3074	1.0000
3.5204+06	44.0294	369.8945	1.0000

3.8724+06	44.0294	367.4763	1.0000
4.2245+06	44.0294	365.0526	1.0000
4.5765+06	44.0294	362.6233	1.0000
4.9285+06	44.0294	360.1885	1.0000
5.2806+06	44.0294	357.7480	1.0000
5.6326+06	44.0294	355.3019	1.0000
5.9847+06	44.0294	352.8500	1.0000
6.3367+06	44.0294	350.3923	1.0000
6.6887+06	44.0294	347.9287	1.0000
7.0408+06	44.0294	345.4593	1.0000
7.3844+06	44.0294	343.0431	1.0000
7.3928+06	44.0294	342.9838	1.0000

U-O-S BLOCK SECTION

```
BLOCK:  KR-2     MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:             12
  OUTLET STREAM:            15
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
  COLD SIDE:
  ----------
  INLET STREAM:             13
  OUTLET STREAM:            14
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                   ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           4865.73         4865.73         0.00000
      MASS(LB/HR   )           157450.         157450.         0.00000
      ENTHALPY(BTU/HR  )      -0.407686E+09   -0.407686E+09    0.438607E-15

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            1744.22      LB/HR
   PRODUCT STREAMS CO2E         1744.22      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         0.00000      LB/HR
```

```
                       ***  INPUT DATA  ***

FLASH SPECS FOR HOT SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                    500
CONVERGENCE TOLERANCE                                       0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                    500
CONVERGENCE TOLERANCE                                       0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED EXCHANGER DUTY
  SPECIFIED VALUE                BTU/HR             5649620.0000
  LMTD CORRECTION FACTOR                                  1.00000
```

U-O-S BLOCK SECTION

BLOCK: KR-2   MODEL: HEATX (CONTINUED)

```
  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                         2.8000
    COLD SIDE PRESSURE DROP        PSI                         0.9083

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT            BTU/HR-SQFT-R              12.2275

                       ***  OVERALL RESULTS  ***

  STREAMS:
                 --------------------------------------
                |                                      |
  12       ----->|                HOT                   |-----> 15
  T=  3.8650D+02 |                                      |       T=  3.4786D+02
  P=  3.5383D+01 |                                      |       P=  3.2583D+01
  V=  1.0000D+00 |                                      |       V=  1.0000D+00
                |                                      |
  14       <-----|                COLD                  |<----- 13
  T=  1.8582D+02 |                                      |       T=  1.8556D+02
  P=  1.5051D+02 |                                      |       P=  1.5142D+02
  V=  1.0000D+00 |                                      |       V=  0.0000D+00
                 --------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR               5649620.0000
    CALCULATED (REQUIRED) AREA     SQFT                    1419.6507
```

ACTUAL EXCHANGER AREA	SQFT	1419.6507
PER CENT OVER-DESIGN		0.0000
HEAT TRANSFER COEFFICIENT:		
AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	12.2275
UA (DIRTY)	BTU/HR-R	17358.8130
LOG-MEAN TEMPERATURE DIFFERENCE:		
LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	180.8118
NUMBER OF SHELLS IN SERIES		1
PRESSURE DROP:		
HOTSIDE, TOTAL	PSI	2.8000
COLDSIDE, TOTAL	PSI	0.9083

U-O-S BLOCK SECTION

HEATX COLD-TQCU KR-2 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -0.9083 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	151.4200	185.9604	0.9999
2.6903+05	151.4200	185.9604	0.9522
5.3806+05	151.4200	185.9604	0.9045
8.0709+05	151.4200	185.9604	0.8569
1.0761+06	151.4200	185.9604	0.8092
1.3451+06	151.4200	185.9604	0.7615
1.6142+06	151.4200	185.9604	0.7139
1.8832+06	151.4200	185.9604	0.6662
2.1522+06	151.4200	185.9604	0.6185
2.4213+06	151.4200	185.9604	0.5709
2.6903+06	151.4200	185.9604	0.5232

2.9593+06	151.4200	185.9604	0.4755
3.2284+06	151.4200	185.9604	0.4279
3.4974+06	151.4200	185.9604	0.3802
3.7664+06	151.4200	185.9604	0.3325
4.0354+06	151.4200	185.9604	0.2849
4.3045+06	151.4200	185.9604	0.2372
4.5735+06	151.4200	185.9604	0.1895
4.8425+06	151.4200	185.9604	0.1419
5.1116+06	151.4200	185.9604	9.4193-02
5.3806+06	151.4200	185.9604	4.6526-02
5.6432+06	151.4200	185.9604	BUB>0.0
5.6496+06	151.4200	185.5556	0.0

HEATX HOT-TQCUR KR-2 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	35.3831	386.4972	1.0000
2.6903+05	35.3831	384.6875	1.0000
5.3806+05	35.3831	382.8748	1.0000
8.0709+05	35.3831	381.0593	1.0000
1.0761+06	35.3831	379.2408	1.0000
1.3451+06	35.3831	377.4193	1.0000
1.6142+06	35.3831	375.5949	1.0000
1.8832+06	35.3831	373.7674	1.0000
2.1522+06	35.3831	371.9370	1.0000
2.4213+06	35.3831	370.1035	1.0000
2.6903+06	35.3831	368.2669	1.0000

2.9593+06	35.3831	366.4273	1.0000
3.2284+06	35.3831	364.5845	1.0000
3.4974+06	35.3831	362.7386	1.0000
3.7664+06	35.3831	360.8895	1.0000
4.0354+06	35.3831	359.0373	1.0000
4.3045+06	35.3831	357.1818	1.0000
4.5735+06	35.3831	355.3231	1.0000
4.8425+06	35.3831	353.4612	1.0000
5.1116+06	35.3831	351.5960	1.0000
5.3806+06	35.3831	349.7275	1.0000
5.6432+06	35.3831	347.9005	1.0000
5.6496+06	35.3831	347.8557	1.0000

U-O-S BLOCK SECTION

BLOCK: KR-3   MODEL: HEATX

```
  HOT SIDE:
  ---------
  INLET STREAM:             16
  OUTLET STREAM:            19
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
  COLD SIDE:
  ----------
  INLET STREAM:             17
  OUTLET STREAM:            18
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
```

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	4803.15	4803.15	0.00000
MASS(LB/HR)	156121.	156121.	0.00000
ENTHALPY(BTU/HR)	-0.404701E+09	-0.404701E+09	-0.589123E-15

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	2378.46	LB/HR
PRODUCT STREAMS CO2E	2378.46	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

```
                       ***  INPUT DATA  ***

FLASH SPECS FOR HOT SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                   500
CONVERGENCE TOLERANCE                                      0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                   500
CONVERGENCE TOLERANCE                                      0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED EXCHANGER DUTY
  SPECIFIED VALUE               BTU/HR             4510690.0000
  LMTD CORRECTION FACTOR                                   1.00000
```

```
                             U-O-S BLOCK SECTION

BLOCK:  KR-3     MODEL: HEATX (CONTINUED)

  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                         2.8000
    COLD SIDE PRESSURE DROP        PSI                         0.7267

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT            BTU/HR-SQFT-R              59.7000

                       ***  OVERALL RESULTS  ***

  STREAMS:
                  --------------------------------------
                  |                                    |
  16        ----->|               HOT                  |-----> 19
  T=  3.8247D+02  |                                    |       T=  3.5176D+02
  P=  2.6737D+01  |                                    |       P=  2.3937D+01
  V=  1.0000D+00  |                                    |       V=  1.0000D+00
                  |                                    |
  18        <-----|               COLD                 |<----- 17
  T=  1.8582D+02  |                                    |       T=  1.8556D+02
  P=  1.5069D+02  |                                    |       P=  1.5142D+02
  V=  1.0000D+00  |                                    |       V=  0.0000D+00
                  --------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR               4510690.0000
    CALCULATED (REQUIRED) AREA     SQFT                     231.9113
```

ACTUAL EXCHANGER AREA	SQFT	231.9113
PER CENT OVER-DESIGN		0.0000
HEAT TRANSFER COEFFICIENT:		
AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	59.7000
UA (DIRTY)	BTU/HR-R	13845.1073
LOG-MEAN TEMPERATURE DIFFERENCE:		
LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	180.9982
NUMBER OF SHELLS IN SERIES		1
PRESSURE DROP:		
HOTSIDE, TOTAL	PSI	2.8000
COLDSIDE, TOTAL	PSI	0.7267

U-O-S BLOCK SECTION

HEATX COLD-TQCU KR-3 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -0.7267 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	151.4200	185.9604	0.9999
2.1479+05	151.4200	185.9604	0.9522
4.2959+05	151.4200	185.9604	0.9045
6.4438+05	151.4200	185.9604	0.8569
8.5918+05	151.4200	185.9604	0.8092
1.0740+06	151.4200	185.9604	0.7615
1.2888+06	151.4200	185.9604	0.7139
1.5036+06	151.4200	185.9604	0.6662
1.7184+06	151.4200	185.9604	0.6185
1.9332+06	151.4200	185.9604	0.5709
2.1479+06	151.4200	185.9604	0.5232

2.3627+06	151.4200	185.9604	0.4755
2.5775+06	151.4200	185.9604	0.4279
2.7923+06	151.4200	185.9604	0.3802
3.0071+06	151.4200	185.9604	0.3325
3.2219+06	151.4200	185.9604	0.2849
3.4367+06	151.4200	185.9604	0.2372
3.6515+06	151.4200	185.9604	0.1895
3.8663+06	151.4200	185.9604	0.1419
4.0811+06	151.4200	185.9604	9.4193-02
4.2959+06	151.4200	185.9604	4.6526-02
4.5056+06	151.4200	185.9604	BUB>0.0
4.5107+06	151.4200	185.5556	0.0

U-O-S BLOCK SECTION

HEATX HOT-TQCUR KR-3 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	26.7367	382.4664	1.0000
2.1479+05	26.7367	381.0230	1.0000
4.2959+05	26.7367	379.5777	1.0000
6.4438+05	26.7367	378.1306	1.0000
8.5918+05	26.7367	376.6816	1.0000
1.0740+06	26.7367	375.2308	1.0000
1.2888+06	26.7367	373.7781	1.0000
1.5036+06	26.7367	372.3235	1.0000
1.7184+06	26.7367	370.8671	1.0000
1.9332+06	26.7367	369.4087	1.0000
2.1479+06	26.7367	367.9484	1.0000

2.3627+06	26.7367	366.4862	1.0000
2.5775+06	26.7367	365.0220	1.0000
2.7923+06	26.7367	363.5559	1.0000
3.0071+06	26.7367	362.0879	1.0000
3.2219+06	26.7367	360.6179	1.0000
3.4367+06	26.7367	359.1459	1.0000
3.6515+06	26.7367	357.6719	1.0000
3.8663+06	26.7367	356.1959	1.0000
4.0811+06	26.7367	354.7179	1.0000
4.2959+06	26.7367	353.2378	1.0000
4.5056+06	26.7367	351.7912	1.0000
4.5107+06	26.7367	351.7558	1.0000

U-O-S BLOCK SECTION

```
BLOCK:  KR-4     MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:             20
  OUTLET STREAM:            24
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
  COLD SIDE:
  ----------
  INLET STREAM:             21
  OUTLET STREAM:            22
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                   ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           4728.75         4728.75         0.00000
      MASS(LB/HR   )           154629.         154629.         0.00000
      ENTHALPY(BTU/HR  )     -0.399521E+09   -0.399521E+09    0.298381E-15

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            2854.13      LB/HR
   PRODUCT STREAMS CO2E         2854.13      LB/HR
   NET STREAMS CO2E PRODUCTION  0.00000      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        0.00000      LB/HR
```

*** INPUT DATA ***

```
FLASH SPECS FOR HOT SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                       500
CONVERGENCE TOLERANCE                                          0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                       500
CONVERGENCE TOLERANCE                                          0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED EXCHANGER DUTY
  SPECIFIED VALUE                BTU/HR             3232360.0000
  LMTD CORRECTION FACTOR                                       1.00000
```

U-O-S BLOCK SECTION

BLOCK: KR-4   MODEL: HEATX (CONTINUED)

```
  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                          2.8000
    COLD SIDE PRESSURE DROP        PSI                          0.5450

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT            BTU/HR-SQFT-R               59.7000

                      ***  OVERALL RESULTS  ***

  STREAMS:
                --------------------------------------
                |                                    |
  20      ----->|                HOT                 |-----> 24
  T=  3.7762D+02 |                                    |       T=  3.5568D+02
  P=  1.8090D+01 |                                    |       P=  1.5290D+01
  V=  1.0000D+00 |                                    |       V=  1.0000D+00
                |                                    |
  22      <-----|                COLD                |<----- 21
  T=  1.8582D+02 |                                    |       T=  1.8556D+02
  P=  1.5088D+02 |                                    |       P=  1.5142D+02
  V=  1.0000D+00 |                                    |       V=  0.0000D+00
                --------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR                 3232360.0000
    CALCULATED (REQUIRED) AREA     SQFT                        166.4185
```

ACTUAL EXCHANGER AREA	SQFT	166.4185
PER CENT OVER-DESIGN		0.0000
HEAT TRANSFER COEFFICIENT:		
AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	59.7000
UA (DIRTY)	BTU/HR-R	9935.1855
LOG-MEAN TEMPERATURE DIFFERENCE:		
LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	180.7471
NUMBER OF SHELLS IN SERIES		1
PRESSURE DROP:		
HOTSIDE, TOTAL	PSI	2.8000
COLDSIDE, TOTAL	PSI	0.5450

U-O-S BLOCK SECTION

HEATX COLD-TQCU KR-4 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -0.5450 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY	PRES	TEMP	VFRAC
BTU/HR	PSIG	C	
0.0	151.4200	185.9604	0.9999
1.5392+05	151.4200	185.9604	0.9522
3.0784+05	151.4200	185.9604	0.9045
4.6177+05	151.4200	185.9604	0.8569
6.1569+05	151.4200	185.9604	0.8092
7.6961+05	151.4200	185.9604	0.7615
9.2353+05	151.4200	185.9604	0.7139
1.0775+06	151.4200	185.9604	0.6662
1.2314+06	151.4200	185.9604	0.6185
1.3853+06	151.4200	185.9604	0.5709
1.5392+06	151.4200	185.9604	0.5232

1.6931+06	151.4200	185.9604	0.4755
1.8471+06	151.4200	185.9604	0.4279
2.0010+06	151.4200	185.9604	0.3802
2.1549+06	151.4200	185.9604	0.3325
2.3088+06	151.4200	185.9604	0.2849
2.4628+06	151.4200	185.9604	0.2372
2.6167+06	151.4200	185.9604	0.1895
2.7706+06	151.4200	185.9604	0.1419
2.9245+06	151.4200	185.9604	9.4193-02
3.0784+06	151.4200	185.9604	4.6526-02
3.2287+06	151.4200	185.9604	BUB>0.0
3.2324+06	151.4200	185.5556	0.0

U-O-S BLOCK SECTION

HEATX HOT-TQCUR KR-4 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	18.0904	377.6200	1.0000
1.5392+05	18.0904	376.5849	1.0000
3.0784+05	18.0904	375.5488	1.0000
4.6177+05	18.0904	374.5118	1.0000
6.1569+05	18.0904	373.4738	1.0000
7.6961+05	18.0904	372.4349	1.0000
9.2353+05	18.0904	371.3950	1.0000
1.0775+06	18.0904	370.3542	1.0000
1.2314+06	18.0904	369.3124	1.0000
1.3853+06	18.0904	368.2696	1.0000
1.5392+06	18.0904	367.2259	1.0000

1.6931+06	18.0904	366.1812	1.0000
1.8471+06	18.0904	365.1355	1.0000
2.0010+06	18.0904	364.0889	1.0000
2.1549+06	18.0904	363.0413	1.0000
2.3088+06	18.0904	361.9926	1.0000
2.4628+06	18.0904	360.9430	1.0000
2.6167+06	18.0904	359.8924	1.0000
2.7706+06	18.0904	358.8408	1.0000
2.9245+06	18.0904	357.7881	1.0000
3.0784+06	18.0904	356.7345	1.0000
3.2287+06	18.0904	355.7051	1.0000
3.2324+06	18.0904	355.6799	1.0000

```
                             U-O-S BLOCK SECTION

BLOCK:  M-1      MODEL: MIXER
-----------------------------
  INLET STREAMS:         42          43          3           4
  OUTLET STREAM:         5
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           4461.42         4461.44       -0.461764E-05
      MASS(LB/HR   )           150856.         150857.       -0.437574E-05
      ENTHALPY(BTU/HR  )     -0.464260E+09   -0.464262E+09    0.454986E-05

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            109.905      LB/HR
   PRODUCT STREAMS CO2E         109.905      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         0.00000      LB/HR

                        ***  INPUT DATA  ***
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                  500
  CONVERGENCE TOLERANCE                                     0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES
```

U-O-S BLOCK SECTION

```
BLOCK:  M-2      MODEL: MIXER
-----------------------------
  INLET STREAMS:         10          14          18          22
  OUTLET STREAM:         23
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1346.29         1346.29         0.00000
      MASS(LB/HR   )            24253.8         24253.8         0.00000
      ENTHALPY(BTU/HR  )      -0.136789E+09   -0.136789E+09     0.00000

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

                        ***  INPUT DATA  ***
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                500
  CONVERGENCE TOLERANCE                                   0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES
```

U-O-S BLOCK SECTION

```
BLOCK:  M-3      MODEL: MIXER
-----------------------------
  INLET STREAMS:         35          34
  OUTLET STREAM:         36
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           107.024         107.024         0.00000
      MASS(LB/HR   )           1938.79         1938.79       -0.351828E-15
      ENTHALPY(BTU/HR  )     -0.374291E+07   -0.374291E+07    0.373235E-15

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            3064.98      LB/HR
   PRODUCT STREAMS CO2E         3064.98      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000     LB/HR
   UTILITIES CO2E PRODUCTION     0.00000     LB/HR
   TOTAL CO2E PRODUCTION         0.00000     LB/HR

                        ***  INPUT DATA  ***
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                   500
  CONVERGENCE TOLERANCE                                      0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES
```

U-O-S BLOCK SECTION

BLOCK: M-4 MODEL: MIXER

INLET STREAMS: 44 53
OUTLET STREAM: 45
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	1588.43	1588.43	0.00000
MASS(LB/HR)	57854.4	57854.4	0.00000
ENTHALPY(BTU/HR)	-0.200545E+09	-0.200545E+09	0.460682E-13

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

TWO PHASE FLASH
MAXIMUM NO. ITERATIONS 500
CONVERGENCE TOLERANCE 0.000100000
OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES

```
                             U-O-S BLOCK SECTION

BLOCK:  P-1      MODEL: PUMP
----------------------------
  INLET STREAM:          1
  OUTLET STREAM:         3
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1022.59         1022.59         0.00000
      MASS(LB/HR   )           32765.8         32765.8         0.00000
      ENTHALPY(BTU/HR  )     -0.104887E+09   -0.104873E+09   -0.130897E-03

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

                         ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIG                                    62.6058
   DRIVER EFFICIENCY                                         1.00000

   FLASH SPECIFICATIONS:
   LIQUID PHASE CALCULATION
   NO FLASH PERFORMED
```

```
MAXIMUM NUMBER OF ITERATIONS                                 500
TOLERANCE                                                     0.000100000

                       ***  RESULTS  ***
VOLUMETRIC FLOW RATE  CUFT/HR                               659.955
PRESSURE CHANGE  PSI                                         57.3017
NPSH AVAILABLE   FT-LBF/LB                                   51.6391
FLUID POWER  HP                                               2.75029
BRAKE POWER  HP                                               5.39585
ELECTRICITY  KW                                               4.02368
PUMP EFFICIENCY USED                                          0.50971
NET WORK REQUIRED  HP                                         5.39585
HEAD DEVELOPED FT-LBF/LB                                    166.197
```

U-O-S BLOCK SECTION

```
BLOCK:  P-2      MODEL: PUMP
----------------------------
  INLET STREAM:          2
  OUTLET STREAM:         4
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          542.771         542.771         0.00000
      MASS(LB/HR   )          25004.9         25004.9         0.00000
      ENTHALPY(BTU/HR  )    -0.648137E+08   -0.648024E+08   -0.173538E-03

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

                        ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIG                                  62.6058
   DRIVER EFFICIENCY                                       1.00000

   FLASH SPECIFICATIONS:
   LIQUID PHASE CALCULATION
   NO FLASH PERFORMED
```

MAXIMUM NUMBER OF ITERATIONS	500
TOLERANCE	0.000100000

*** RESULTS ***

VOLUMETRIC FLOW RATE CUFT/HR	500.167
PRESSURE CHANGE PSI	57.3017
NPSH AVAILABLE FT-LBF/LB	54.6621
FLUID POWER HP	2.08440
BRAKE POWER HP	4.42049
ELECTRICITY KW	3.29636
PUMP EFFICIENCY USED	0.47153
NET WORK REQUIRED HP	4.42049
HEAD DEVELOPED FT-LBF/LB	165.052

U-O-S BLOCK SECTION

```
BLOCK:  P-3      MODEL: PUMP
----------------------------
EDIT THIS OUTLET P AND OTHER FEED P'S WILL ADJUST ACCORDINGLY
  INLET STREAM:          32
  OUTLET STREAM:         43
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            2873.62         2873.62         0.00000
      MASS(LB/HR   )            92367.6         92367.6         0.00000
      ENTHALPY(BTU/HR  )      -0.292247E+09   -0.292213E+09   -0.113993E-03

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            106.261      LB/HR
   PRODUCT STREAMS CO2E         106.261      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         0.00000      LB/HR

                        ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIG                                  52.6058
   DRIVER EFFICIENCY                                       1.00000

   FLASH SPECIFICATIONS:
   LIQUID PHASE CALCULATION
```

```
NO FLASH PERFORMED
MAXIMUM NUMBER OF ITERATIONS                              500
TOLERANCE                                                   0.000100000

                       ***  RESULTS  ***
VOLUMETRIC FLOW RATE  CUFT/HR                          1,907.12
PRESSURE CHANGE  PSI                                      60.3017
NPSH AVAILABLE   FT-LBF/LB                                 0.0
FLUID POWER  HP                                            8.36381
BRAKE POWER  HP                                           13.0929
ELECTRICITY  KW                                            9.76339
PUMP EFFICIENCY USED                                       0.63880
NET WORK REQUIRED  HP                                     13.0929
HEAD DEVELOPED FT-LBF/LB                                 179.287
```

U-O-S BLOCK SECTION

BLOCK: P-4 MODEL: PUMP

INLET STREAM: 41
OUTLET STREAM: 42
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	22.4459	22.4459	0.00000
MASS(LB/HR)	717.714	717.714	0.00000
ENTHALPY(BTU/HR)	-0.237156E+07	-0.237102E+07	-0.227794E-03

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	3.64383	LB/HR
PRODUCT STREAMS CO2E	3.64383	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

*** INPUT DATA ***

OUTLET PRESSURE PSIG	62.6058
DRIVER EFFICIENCY	1.00000

FLASH SPECIFICATIONS:
LIQUID PHASE CALCULATION
NO FLASH PERFORMED

MAXIMUM NUMBER OF ITERATIONS	500
TOLERANCE	0.000100000

*** RESULTS ***

VOLUMETRIC FLOW RATE CUFT/HR	14.0800
PRESSURE CHANGE PSI	61.3017
NPSH AVAILABLE FT-LBF/LB	0.0
FLUID POWER HP	0.062773
BRAKE POWER HP	0.21232
ELECTRICITY KW	0.15832
PUMP EFFICIENCY USED	0.29566
NET WORK REQUIRED HP	0.21232
HEAD DEVELOPED FT-LBF/LB	173.175

U-O-S BLOCK SECTION

BLOCK: P-5 MODEL: PUMP

INLET STREAM: 33
OUTLET STREAM: 44
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	1544.34	1544.34	0.00000
MASS(LB/HR)	56551.2	56551.2	0.00000
ENTHALPY(BTU/HR)	-0.195100E+09	-0.195097E+09	-0.148935E-04

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

OUTLET PRESSURE PSIG	5.30405
DRIVER EFFICIENCY	1.00000

FLASH SPECIFICATIONS:
LIQUID PHASE CALCULATION
NO FLASH PERFORMED

```
MAXIMUM NUMBER OF ITERATIONS                                    500
TOLERANCE                                                        0.000100000

                       ***  RESULTS  ***
VOLUMETRIC FLOW RATE  CUFT/HR                                 1,119.21
PRESSURE CHANGE  PSI                                             8.10000
NPSH AVAILABLE   FT-LBF/LB                                      -0.58775
FLUID POWER  HP                                                  0.65932
BRAKE POWER  HP                                                  1.14199
ELECTRICITY  KW                                                  0.85158
PUMP EFFICIENCY USED                                             0.57734
NET WORK REQUIRED  HP                                            1.14199
HEAD DEVELOPED FT-LBF/LB                                        23.0844
NEGATIVE NPSH MAY BE DUE TO VAPOR IN THE FEED OR UNACCOUNTED SUCTION HEAD.
```

U-O-S BLOCK SECTION

```
BLOCK:  P-6      MODEL: PUMP
----------------------------
  INLET STREAM:          52
  OUTLET STREAM:         53
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           44.0925         44.0925         0.00000
      MASS(LB/HR   )           1303.22         1303.22        0.174470E-15
      ENTHALPY(BTU/HR  )      -0.544748E+07   -0.544742E+07   -0.116253E-04

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

                         ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIG                                  5.30405
   DRIVER EFFICIENCY                                      1.00000

   FLASH SPECIFICATIONS:
   LIQUID PHASE CALCULATION
   NO FLASH PERFORMED
```

```
MAXIMUM NUMBER OF ITERATIONS                             500
TOLERANCE                                                 0.000100000

                       ***  RESULTS  ***
VOLUMETRIC FLOW RATE  CUFT/HR                            25.2953
PRESSURE CHANGE  PSI                                      4.00000
NPSH AVAILABLE   FT-LBF/LB                               -0.57897
FLUID POWER  HP                                           0.0073586
BRAKE POWER  HP                                           0.024889
ELECTRICITY  KW                                           0.018560
PUMP EFFICIENCY USED                                      0.29566
NET WORK REQUIRED  HP                                     0.024889
HEAD DEVELOPED FT-LBF/LB                                 11.1800
NEGATIVE NPSH MAY BE DUE TO VAPOR IN THE FEED OR UNACCOUNTED SUCTION HEAD.
```

U-O-S BLOCK SECTION

```
BLOCK:  R-1      MODEL: RYIELD
------------------------------
  INLET STREAM:          7
  OUTLET STREAM:         8
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1


    ***********************************************************************
    *                                                                     *
    *     SPECIFIED YIELDS HAVE BEEN NORMALIZED TO MAINTAIN MASS BALANCE  *
    *                                                                     *
    ***********************************************************************


                    ***  MASS AND ENERGY BALANCE  ***
                            IN          OUT       GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)         4461.44      4485.82       24.3532     -0.538540E-05
  MASS(LB/HR   )         150857.      150858.                   -0.538540E-05
  ENTHALPY(BTU/HR  )   -0.357464E+09 -0.357463E+09              -0.355049E-05

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            109.905      LB/HR
   PRODUCT STREAMS CO2E         951.402      LB/HR
   NET STREAMS CO2E PRODUCTION  841.497      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        841.497      LB/HR
```

U-O-S BLOCK SECTION

BLOCK: R-1 MODEL: RYIELD (CONTINUED)

*** INPUT DATA ***

ONE PHASE PQ FLASH	SPECIFIED PHASE IS VAPOR	
PRESSURE DROP	PSI	5.84635
SPECIFIED HEAT DUTY	BTU/HR	0.0
MAXIMUM NO. ITERATIONS		500
CONVERGENCE TOLERANCE		0.000100000

MASS-YIELD

SUBSTREAM MIXED :

METHANOL	0.767	ETHANOL	0.117	IB-ALDEH	0.675E-03
PROPANOL	0.225E-02	ISBUT-OH	0.726E-01	2-ME1BOH	0.825E-03
H2	0.189E-03	CO2	0.549E-03	PROPANE	0.413E-04
C2H2	0.228E-03	ISOBU-01	0.943E-04	N-BUT-01	0.200E-03
TRANS-01	0.981E-04	CIS-2-01	0.431E-03	C2H4	0.700E-04
O2	0.350E-03	CH4	0.230E-03	CO	0.512E-03
WATER	0.370E-01				

*** RESULTS ***

OUTLET TEMPERATURE	C	393.77
OUTLET PRESSURE	PSIG	44.029
HEAT DUTY	BTU/HR	0.0000

U-O-S BLOCK SECTION

BLOCK: R-1 MODEL: RYIELD (CONTINUED)

ATOM BALANCE:

ATOM	MOLES IN	MOLES OUT	GENERATION	MASS IN	MASS OUT	GENERATION	ERROR/TOL
UNIT	LBMOL/HR	LBMOL/HR	LBMOL/HR	LB/HR	LB/HR	LB/HR	
C	5036.	5015.	-20.96	0.6049E+05	0.6024E+05	-251.8	41.80
H	0.1897E+05	0.1897E+05	0.1503	0.1912E+05	0.1912E+05	0.1515	0.7925E-01
O	4453.	4469.	15.78	0.7125E+05	0.7150E+05	252.4	35.43

U-O-S BLOCK SECTION

```
BLOCK:  R-2      MODEL: RYIELD
------------------------------
  INLET STREAM:           11
  OUTLET STREAM:          12
  PROPERTY OPTION SET:    NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:         HC-1


    ***********************************************************************
    *                                                                     *
    *     SPECIFIED YIELDS HAVE BEEN NORMALIZED TO MAINTAIN MASS BALANCE  *
    *                                                                     *
    ***********************************************************************


                    ***  MASS AND ENERGY BALANCE  ***
                             IN           OUT       GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)          4485.82       4499.80       13.9874       0.00000
  MASS(LB/HR   )          150858.       150858.                   -0.192923E-15
  ENTHALPY(BTU/HR  )   -0.364856E+09 -0.364856E+09                 0.163365E-15

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            951.402      LB/HR
   PRODUCT STREAMS CO2E         1744.22      LB/HR
   NET STREAMS CO2E PRODUCTION  792.816      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        792.816      LB/HR
```

U-O-S BLOCK SECTION

BLOCK: R-2   MODEL: RYIELD (CONTINUED)

```
                        ***  INPUT DATA  ***
  ONE    PHASE  PQ  FLASH   SPECIFIED PHASE IS  VAPOR
  PRESSURE DROP         PSI                                 5.84635
  SPECIFIED HEAT DUTY   BTU/HR                              0.0
  MAXIMUM NO. ITERATIONS                                  500
  CONVERGENCE TOLERANCE                                     0.000100000

   MASS-YIELD
    SUBSTREAM MIXED   :
    METHANOL  0.712        ETHANOL   0.750E-01    IB-ALDEH  0.124E-02
    PROPANOL  0.413E-02    ISBUT-OH  0.133        2-ME1BOH  0.151E-02
    H2        0.346E-03    CO2       0.101E-02    PROPANE   0.757E-04
    C2H2      0.417E-03    ISOBU-01  0.173E-03    N-BUT-01  0.366E-03
    TRANS-01  0.180E-03    CIS-2-01  0.790E-03    C2H4      0.128E-03
    O2        0.641E-03    CH4       0.422E-03    CO        0.939E-03
    WATER     0.679E-01

                         ***  RESULTS  ***
  OUTLET TEMPERATURE    C                                    386.50
  OUTLET PRESSURE       PSIG                                 35.383
  HEAT DUTY             BTU/HR                               0.0000
```

U-O-S BLOCK SECTION

BLOCK: R-2 MODEL: RYIELD (CONTINUED)

ATOM BALANCE:

ATOM	MOLES IN	MOLES OUT	GENERATION	MASS IN	MASS OUT	GENERATION	ERROR/TOL
UNIT	LBMOL/HR	LBMOL/HR	LBMOL/HR	LB/HR	LB/HR	LB/HR	
C	5015.	5015.	-.7393E-02	0.6024E+05	0.6024E+05	-.8879E-01	0.1474E-01
H	0.1897E+05	0.1897E+05	-.3021E-02	0.1912E+05	0.1912E+05	-.3045E-02	0.1593E-02
O	4469.	4469.	0.5740E-02	0.7150E+05	0.7150E+05	0.9184E-01	0.1284E-01

U-O-S BLOCK SECTION

BLOCK: R-3 MODEL: RYIELD

INLET STREAM: 15
OUTLET STREAM: 16
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

```
***********************************************************************
*                                                                     *
*     SPECIFIED YIELDS HAVE BEEN NORMALIZED TO MAINTAIN MASS BALANCE  *
*                                                                     *
***********************************************************************
```

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
TOTAL BALANCE				
MOLE(LBMOL/HR)	4499.80	4510.99	11.1896	0.403235E-15
MASS(LB/HR)	150858.	150858.		0.771690E-15
ENTHALPY(BTU/HR)	-0.370506E+09	-0.370506E+09		-0.804369E-15

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	1744.22	LB/HR
PRODUCT STREAMS CO2E	2378.46	LB/HR
NET STREAMS CO2E PRODUCTION	634.240	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	634.240	LB/HR

U-O-S BLOCK SECTION

BLOCK: R-3   MODEL: RYIELD (CONTINUED)

*** INPUT DATA ***

ONE PHASE PQ FLASH	SPECIFIED PHASE IS VAPOR	
PRESSURE DROP	PSI	5.84635
SPECIFIED HEAT DUTY	BTU/HR	0.0
MAXIMUM NO. ITERATIONS		500
CONVERGENCE TOLERANCE		0.000100000

MASS-YIELD

SUBSTREAM MIXED :

METHANOL	0.667	ETHANOL	0.417E-01	IB-ALDEH	0.169E-02
PROPANOL	0.563E-02	ISBUT-OH	0.181	2-ME1BOH	0.206E-02
H2	0.472E-03	CO2	0.137E-02	PROPANE	0.103E-03
C2H2	0.569E-03	ISOBU-01	0.236E-03	N-BUT-01	0.499E-03
TRANS-01	0.245E-03	CIS-2-01	0.108E-02	C2H4	0.175E-03
O2	0.874E-03	CH4	0.576E-03	CO	0.128E-02
WATER	0.926E-01				

*** RESULTS ***

OUTLET TEMPERATURE	C	382.47
OUTLET PRESSURE	PSIG	26.737
HEAT DUTY	BTU/HR	0.0000

U-O-S BLOCK SECTION

BLOCK: R-3 MODEL: RYIELD (CONTINUED)

ATOM BALANCE:

ATOM	MOLES IN	MOLES OUT	GENERATION	MASS IN	MASS OUT	GENERATION	ERROR/TOL
UNIT	LBMOL/HR	LBMOL/HR	LBMOL/HR	LB/HR	LB/HR	LB/HR	
C	5015.	5015.	-.5906E-02	0.6024E+05	0.6024E+05	-.7093E-01	0.1178E-01
H	0.1897E+05	0.1897E+05	-.2570E-02	0.1912E+05	0.1912E+05	-.2590E-02	0.1355E-02
O	4469.	4469.	0.4595E-02	0.7150E+05	0.7150E+05	0.7352E-01	0.1028E-01

U-O-S BLOCK SECTION

BLOCK: R-4   MODEL: RYIELD

INLET STREAM: 19
OUTLET STREAM: 20
PROPERTY OPTION SET: NRTL   RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

```
***********************************************************************
*                                                                     *
*     SPECIFIED YIELDS HAVE BEEN NORMALIZED TO MAINTAIN MASS BALANCE  *
*                                                                     *
***********************************************************************
```

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
TOTAL BALANCE				
MOLE(LBMOL/HR)	4510.99	4519.38	8.39210	-0.402486E-15
MASS(LB/HR)	150858.	150858.		-0.385845E-15
ENTHALPY(BTU/HR)	-0.375016E+09	-0.375016E+09		0.317878E-15

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	2378.46	LB/HR
PRODUCT STREAMS CO2E	2854.13	LB/HR
NET STREAMS CO2E PRODUCTION	475.671	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	475.671	LB/HR

U-O-S BLOCK SECTION

BLOCK: R-4   MODEL: RYIELD (CONTINUED)

*** INPUT DATA ***

ONE PHASE PQ FLASH SPECIFIED PHASE IS VAPOR		
PRESSURE DROP	PSI	5.84635
SPECIFIED HEAT DUTY	BTU/HR	0.0
MAXIMUM NO. ITERATIONS		500
CONVERGENCE TOLERANCE		0.000100000

MASS-YIELD

SUBSTREAM MIXED :

METHANOL	0.634	ETHANOL	0.167E-01	IB-ALDEH	0.203E-02
PROPANOL	0.675E-02	ISBUT-OH	0.218	2-ME1BOH	0.248E-02
H2	0.566E-03	CO2	0.165E-02	PROPANE	0.124E-03
C2H2	0.683E-03	ISOBU-01	0.283E-03	N-BUT-01	0.599E-03
TRANS-01	0.294E-03	CIS-2-01	0.129E-02	C2H4	0.210E-03
O2	0.105E-02	CH4	0.691E-03	CO	0.154E-02
WATER	0.111				

*** RESULTS ***

OUTLET TEMPERATURE	C	377.62
OUTLET PRESSURE	PSIG	18.090
HEAT DUTY	BTU/HR	0.0000

U-O-S BLOCK SECTION

BLOCK: R-4 MODEL: RYIELD (CONTINUED)

ATOM BALANCE:

ATOM	MOLES IN	MOLES OUT	GENERATION	MASS IN	MASS OUT	GENERATION	ERROR/TOL
UNIT	LBMOL/HR	LBMOL/HR	LBMOL/HR	LB/HR	LB/HR	LB/HR	
C	5015.	5015.	-.4424E-02	0.6024E+05	0.6024E+05	-.5314E-01	0.8822E-02
H	0.1897E+05	0.1897E+05	-.1838E-02	0.1912E+05	0.1912E+05	-.1853E-02	0.9690E-03
O	4469.	4469.	0.3437E-02	0.7150E+05	0.7150E+05	0.5499E-01	0.7691E-02

```
                             U-O-S BLOCK SECTION

BLOCK:  R-5      MODEL: RYIELD
------------------------------
  INLET STREAM:           24
  OUTLET STREAM:          25
  PROPERTY OPTION SET:    NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:         HC-1


    ***********************************************************************
    *                                                                     *
    *     SPECIFIED YIELDS HAVE BEEN NORMALIZED TO MAINTAIN MASS BALANCE  *
    *                                                                     *
    ***********************************************************************


                     ***  MASS AND ENERGY BALANCE  ***
                             IN          OUT       GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)         4519.38       4524.98       5.59461       0.00000
  MASS(LB/HR   )         150858.       150858.                    -0.578768E-15
  ENTHALPY(BTU/HR  )   -0.378249E+09 -0.378249E+09                 0.472742E-15

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            2854.13      LB/HR
   PRODUCT STREAMS CO2E         3171.24      LB/HR
   NET STREAMS CO2E PRODUCTION   317.111      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         317.111      LB/HR
```

U-O-S BLOCK SECTION

BLOCK: R-5 MODEL: RYIELD (CONTINUED)

*** INPUT DATA ***

ONE PHASE PQ FLASH	SPECIFIED PHASE IS VAPOR	
PRESSURE DROP	PSI	5.84635
SPECIFIED HEAT DUTY	BTU/HR	0.0
MAXIMUM NO. ITERATIONS		500
CONVERGENCE TOLERANCE		0.000100000

MASS-YIELD

SUBSTREAM MIXED :

METHANOL	0.612	IB-ALDEH	0.225E-02	PROPANOL	0.750E-02
ISBUT-OH	0.242	2-ME1BOH	0.275E-02	H2	0.629E-03
CO2	0.183E-02	PROPANE	0.138E-03	C2H2	0.758E-03
ISOBU-01	0.314E-03	N-BUT-01	0.665E-03	TRANS-01	0.327E-03
CIS-2-01	0.144E-02	C2H4	0.233E-03	O2	0.117E-02
CH4	0.768E-03	CO	0.171E-02	WATER	0.123

*** RESULTS ***

OUTLET TEMPERATURE	C	372.88
OUTLET PRESSURE	PSIG	9.4440
HEAT DUTY	BTU/HR	0.0000

U-O-S BLOCK SECTION

BLOCK: R-5 MODEL: RYIELD (CONTINUED)

ATOM BALANCE:

ATOM	MOLES IN	MOLES OUT	GENERATION	MASS IN	MASS OUT	GENERATION	ERROR/TOL
UNIT	LBMOL/HR	LBMOL/HR	LBMOL/HR	LB/HR	LB/HR	LB/HR	
C	5015.	5015.	-.2963E-02	0.6024E+05	0.6024E+05	-.3558E-01	0.5907E-02
H	0.1897E+05	0.1897E+05	-.1329E-02	0.1912E+05	0.1912E+05	-.1340E-02	0.7008E-03
O	4469.	4469.	0.2308E-02	0.7150E+05	0.7150E+05	0.3692E-01	0.5164E-02

```
                             U-O-S BLOCK SECTION

BLOCK:  R-6      MODEL: RSTOIC
------------------------------
  INLET STREAM:          54
  OUTLET STREAM:         55
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                             IN          OUT       GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)         984.666      1500.10      515.434      0.151572E-15
  MASS(LB/HR   )         46468.4      46468.4                    0.00000
  ENTHALPY(BTU/HR  )   -0.993411E+08 -0.993411E+08             -0.150000E-15

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

                        ***  INPUT DATA  ***
  STOICHIOMETRY MATRIX:

   REACTION #   1:
    SUBSTREAM MIXED   :
    ISBUT-OH  -1.00    WATER      1.00    IBUTENE    1.00
```

```
 REACTION #   2:
  SUBSTREAM MIXED   :
  PROPANOL  -1.00    WATER      1.00    PROPENE    1.00

 REACTION #   3:
  SUBSTREAM MIXED   :
  2-ME1BOH  -1.00    WATER      1.00    2ME1BENE   1.00


REACTION CONVERSION SPECS: NUMBER=    3
  REACTION #   1:
  SUBSTREAM:MIXED    KEY COMP:ISBUT-OH CONV FRAC:  1.000
  REACTION #   2:
  SUBSTREAM:MIXED    KEY COMP:PROPANOL CONV FRAC:  1.000
  REACTION #   3:
  SUBSTREAM:MIXED    KEY COMP:2-ME1BOH CONV FRAC:  1.000
```

```
                             U-O-S BLOCK SECTION

BLOCK:  R-6      MODEL: RSTOIC (CONTINUED)
  TWO    PHASE  PQ  FLASH
  PRESSURE DROP         PSI                                  5.00000
  SPECIFIED HEAT DUTY   BTU/HR                               0.0
  MAXIMUM NO. ITERATIONS                                   500
  CONVERGENCE TOLERANCE                                      0.000100000
  SIMULTANEOUS REACTIONS
  GENERATE COMBUSTION REACTIONS FOR FEED SPECIES           NO

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    C                                     198.03
  OUTLET PRESSURE       PSIG                                  8.3041
  VAPOR FRACTION                                              1.0000



  REACTION EXTENTS:

     REACTION          REACTION
     NUMBER            EXTENT
                       LBMOL/HR
     1                  491.97
     2                  18.759
     3                  4.7064

  V-L PHASE EQUILIBRIUM :

     COMP              F(I)          X(I)          Y(I)          K(I)
```

METHANOL	0.31956E-03	0.56804E-04	0.31956E-03	78.108
WATER	0.65608	0.97074	0.65608	9.3871
IBUTENE	0.32796	0.28123E-01	0.32796	54.574
PROPENE	0.12505E-01	0.36905E-03	0.12505E-01	124.68
2ME1BENE	0.31374E-02	0.70905E-03	0.31374E-02	23.840

U-O-S BLOCK SECTION

```
BLOCK:  ST-1     MODEL: HEATX
-----------------------------
HOT STREAM OUTLET T = 110 C
  HOT SIDE:
  ---------
  INLET STREAM:              25
  OUTLET STREAM:             26
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
  COLD SIDE:
  ----------
  INLET STREAM:              5
  OUTLET STREAM:             6
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                   ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           8986.42         8986.42         0.00000
      MASS(LB/HR   )           301714.         301714.         0.00000
      ENTHALPY(BTU/HR  )     -0.842511E+09   -0.842511E+09     0.00000

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            3281.14      LB/HR
   PRODUCT STREAMS CO2E         3281.14      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
```

```
 TOTAL CO2E PRODUCTION         0.00000      LB/HR

                       ***  INPUT DATA  ***

FLASH SPECS FOR HOT SIDE:
ONE    PHASE      FLASH   SPECIFIED PHASE IS  VAPOR
MAXIMUM NO. ITERATIONS                                        500
CONVERGENCE TOLERANCE                                           0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                        500
CONVERGENCE TOLERANCE                                           0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED HOT OUTLET TEMP
  SPECIFIED VALUE                C                            110.0000
  LMTD CORRECTION FACTOR                                        1.00000
```

U-O-S BLOCK SECTION

BLOCK: ST-1   MODEL: HEATX (CONTINUED)

```
  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                         1.9300
    COLD SIDE PRESSURE DROP        PSI                         0.7300

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT            BTU/HR-SQFT-R              29.4700

                       ***  OVERALL RESULTS  ***

  STREAMS:
                --------------------------------------
                |                                    |
  25      ----->|               HOT                  |-----> 26
  T=  3.7288D+02  |                                    |       T=  1.1000D+02
  P=  9.4440D+00  |                                    |       P=  7.5140D+00
  V=  1.0000D+00  |                                    |       V=  1.0000D+00
                |                                    |
  6       <-----|               COLD                 |<----- 5
  T=  1.0951D+02  |                                    |       T=  3.6269D+01
  P=  5.1876D+01  |                                    |       P=  5.2606D+01
  V=  2.7209D-01  |                                    |       V=  0.0000D+00
                --------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR              34038226.8365
    CALCULATED (REQUIRED) AREA     SQFT                    4307.8748
```

ACTUAL EXCHANGER AREA	SQFT	4307.8748
PER CENT OVER-DESIGN		0.0000
HEAT TRANSFER COEFFICIENT:		
AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	29.4700
UA (DIRTY)	BTU/HR-R	126953.0700
LOG-MEAN TEMPERATURE DIFFERENCE:		
LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	148.9537
NUMBER OF SHELLS IN SERIES		1
PRESSURE DROP:		
HOTSIDE, TOTAL	PSI	1.9300
COLDSIDE, TOTAL	PSI	0.7300

U-O-S BLOCK SECTION

HEATX COLD-TQCU ST-1   TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -0.7300   PSI
PROPERTY OPTION SET: NRTL   RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	52.6058	109.8726	0.2708
1.6209+06	52.6058	109.8517	0.2448
3.2417+06	52.6058	109.8288	0.2188
4.8626+06	52.6058	109.8034	0.1929
6.4835+06	52.6058	109.7742	0.1670
8.1043+06	52.6058	109.7397	0.1410
9.7252+06	52.6058	109.6969	0.1151
1.1346+07	52.6058	109.6401	8.9255-02
1.2967+07	52.6058	109.5571	6.3486-02
1.4588+07	52.6058	109.4140	3.7942-02
1.6209+07	52.6058	109.0648	1.3213-02

1.7239+07	52.6058	108.2419	BUB>0.0
1.7830+07	52.6058	106.0653	0.0
1.9450+07	52.6058	99.9831	0.0
2.1071+07	52.6058	93.7369	0.0
2.2692+07	52.6058	87.3138	0.0
2.4313+07	52.6058	80.7033	0.0
2.5934+07	52.6058	73.8933	0.0
2.7555+07	52.6058	66.8697	0.0
2.9176+07	52.6058	59.6159	0.0
3.0796+07	52.6058	52.1131	0.0
3.2417+07	52.6058	44.3394	0.0
3.4038+07	52.6058	36.2692	0.0

U-O-S BLOCK SECTION

HEATX HOT-TQCUR ST-1   TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0   PSI
PROPERTY OPTION SET: NRTL   RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	9.4440	372.8795	1.0000
1.6209+06	9.4440	361.9102	1.0000
3.2417+06	9.4440	350.8321	1.0000
4.8626+06	9.4440	339.6404	1.0000
6.4835+06	9.4440	328.3297	1.0000
8.1043+06	9.4440	316.8946	1.0000
9.7252+06	9.4440	305.3288	1.0000
1.1346+07	9.4440	293.6260	1.0000
1.2967+07	9.4440	281.7789	1.0000
1.4588+07	9.4440	269.7800	1.0000
1.6209+07	9.4440	257.6208	1.0000

1.7239+07	9.4440	249.8050	1.0000
1.7830+07	9.4440	245.2924	1.0000
1.9450+07	9.4440	232.7847	1.0000
2.1071+07	9.4440	220.0869	1.0000
2.2692+07	9.4440	207.1874	1.0000
2.4313+07	9.4440	194.0731	1.0000
2.5934+07	9.4440	180.7300	1.0000
2.7555+07	9.4440	167.1428	1.0000
2.9176+07	9.4440	153.2948	1.0000
3.0796+07	9.4440	139.1681	1.0000
3.2417+07	9.4440	124.7433	1.0000
3.4038+07	9.4440	110.0000	1.0000

U-O-S BLOCK SECTION

```
BLOCK:  ST-2     MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:             26
  OUTLET STREAM:            29
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
  COLD SIDE:
  ----------
  INLET STREAM:             27
  OUTLET STREAM:            28
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           372100.         372100.         0.00000
      MASS(LB/HR   )          0.677282E+07    0.677282E+07     0.00000
      ENTHALPY(BTU/HR  )     -0.454920E+11   -0.454920E+11     0.00000

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            3171.24      LB/HR
   PRODUCT STREAMS CO2E         3171.24      LB/HR
   NET STREAMS CO2E PRODUCTION  0.00000      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        0.00000      LB/HR
```

```
                       ***  INPUT DATA  ***

FLASH SPECS FOR HOT SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                    500
CONVERGENCE TOLERANCE                                       0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                    500
CONVERGENCE TOLERANCE                                       0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED HOT OUTLET TEMP
  SPECIFIED VALUE                C                         40.0000
  LMTD CORRECTION FACTOR                                    1.00000
```

U-O-S BLOCK SECTION

BLOCK: ST-2   MODEL: HEATX (CONTINUED)

```
  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                          1.4100
    COLD SIDE PRESSURE DROP        PSI                          5.0500

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT            BTU/HR-SQFT-R              103.5700

                       ***  OVERALL RESULTS  ***

  STREAMS:
                --------------------------------------
                |                                    |
  26      ----->|               HOT                  |-----> 29
  T=  1.1000D+02  |                                    |       T=  4.0000D+01
  P=  7.5140D+00  |                                    |       P=  6.1040D+00
  V=  1.0000D+00  |                                    |       V=  2.0212D-02
                |                                    |
  28      <-----|               COLD                 |<----- 27
  T=  3.9441D+01  |                                    |       T=  3.2222D+01
  P=  2.2541D+00  |                                    |       P=  7.3041D+00
  V=  0.0000D+00  |                                    |       V=  0.0000D+00
                --------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR             85534874.7505
    CALCULATED (REQUIRED) AREA     SQFT                  16115.7175
```

ACTUAL EXCHANGER AREA	SQFT	16115.7175
PER CENT OVER-DESIGN		0.0000
HEAT TRANSFER COEFFICIENT:		
AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	103.5700
UA (DIRTY)	BTU/HR-R	1669104.8649
LOG-MEAN TEMPERATURE DIFFERENCE:		
LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	28.4700
NUMBER OF SHELLS IN SERIES		1
PRESSURE DROP:		
HOTSIDE, TOTAL	PSI	1.4100
COLDSIDE, TOTAL	PSI	5.0500

U-O-S BLOCK SECTION

HEATX COLD-TQCU ST-2 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -5.0500 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY	PRES	TEMP	VFRAC
BTU/HR	PSIG	C	
0.0	7.3041	39.4407	0.0
2.0085+06	7.3041	39.2718	0.0
4.0731+06	7.3041	39.0982	0.0
8.1462+06	7.3041	38.7555	0.0
1.2219+07	7.3041	38.4127	0.0
1.6292+07	7.3041	38.0698	0.0
2.0365+07	7.3041	37.7268	0.0
2.4439+07	7.3041	37.3837	0.0
2.8512+07	7.3041	37.0404	0.0
3.2585+07	7.3041	36.6970	0.0
3.6658+07	7.3041	36.3535	0.0

4.0731+07	7.3041	36.0099	0.0
4.4804+07	7.3041	35.6662	0.0
4.8877+07	7.3041	35.3223	0.0
5.2950+07	7.3041	34.9783	0.0
5.7023+07	7.3041	34.6342	0.0
6.1096+07	7.3041	34.2900	0.0
6.5169+07	7.3041	33.9457	0.0
6.9243+07	7.3041	33.6012	0.0
7.3316+07	7.3041	33.2566	0.0
7.7389+07	7.3041	32.9120	0.0
8.1462+07	7.3041	32.5671	0.0
8.5535+07	7.3041	32.2222	0.0

U-O-S BLOCK SECTION

HEATX HOT-TQCUR ST-2 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	7.5140	110.0000	1.0000
2.0085+06	7.5140	91.2569	DEW>1.0000
4.0731+06	7.5140	90.7930	0.9682
8.1462+06	7.5140	89.9284	0.9063
1.2219+07	7.5140	89.1144	0.8452
1.6292+07	7.5140	88.3378	0.7847
2.0365+07	7.5140	87.5906	0.7249
2.4439+07	7.5140	86.8678	0.6655
2.8512+07	7.5140	86.1658	0.6065
3.2585+07	7.5140	85.4808	0.5478
3.6658+07	7.5140	84.8076	0.4894

4.0731+07	7.5140	84.1373	0.4313
4.4804+07	7.5140	83.4555	0.3734
4.8877+07	7.5140	82.7375	0.3160
5.2950+07	7.5140	81.9383	0.2592
5.7023+07	7.5140	80.9684	0.2034
6.1096+07	7.5140	79.6304	0.1496
6.5169+07	7.5140	77.4443	0.1004
6.9243+07	7.5140	73.3706	6.1634-02
7.3316+07	7.5140	66.5394	3.8683-02
7.7389+07	7.5140	57.9130	2.7825-02
8.1462+07	7.5140	48.8643	2.2608-02
8.5535+07	7.5140	40.0509	1.9831-02

U-O-S BLOCK SECTION

```
BLOCK:  ST-3     MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:              36
  OUTLET STREAM:             39
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
  COLD SIDE:
  ----------
  INLET STREAM:              37
  OUTLET STREAM:             38
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                   ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          3003.93         3003.93         0.00000
      MASS(LB/HR   )          54127.4         54127.4         0.00000
      ENTHALPY(BTU/HR  )    -0.361798E+09   -0.361798E+09    0.164745E-15

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             3064.98      LB/HR
   PRODUCT STREAMS CO2E          3064.98      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         0.00000      LB/HR
```

```
                       ***  INPUT DATA  ***

FLASH SPECS FOR HOT SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                         500
CONVERGENCE TOLERANCE                                            0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                         500
CONVERGENCE TOLERANCE                                            0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED HOT OUTLET TEMP
  SPECIFIED VALUE                C                              10.0000
  LMTD CORRECTION FACTOR                                         1.00000
```

U-O-S BLOCK SECTION

BLOCK: ST-3   MODEL: HEATX (CONTINUED)

```
  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                         1.1200
    COLD SIDE PRESSURE DROP        PSI                         0.5800

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT            BTU/HR-SQFT-R              99.1300

                      ***  OVERALL RESULTS  ***

  STREAMS:
                --------------------------------------
                |                                    |
  36      ----->|                HOT                 |-----> 39
  T=  5.5456D+01  |                                    |       T=  1.0000D+01
  P=  5.3041D+00  |                                    |       P=  4.1841D+00
  V=  1.0000D+00  |                                    |       V=  7.8233D-01
                |                                    |
  38      <-----|                COLD                |<----- 37
  T=  7.2617D+00  |                                    |       T=  2.0000D+00
  P=  2.7241D+00  |                                    |       P=  3.3041D+00
  V=  0.0000D+00  |                                    |       V=  0.0000D+00
                --------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR                  478886.7328
    CALCULATED (REQUIRED) AREA     SQFT                       119.9083
```

ACTUAL EXCHANGER AREA	SQFT	119.9083
PER CENT OVER-DESIGN		0.0000
HEAT TRANSFER COEFFICIENT:		
AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	99.1300
UA (DIRTY)	BTU/HR-R	11886.5089
LOG-MEAN TEMPERATURE DIFFERENCE:		
LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	22.3824
NUMBER OF SHELLS IN SERIES		1
PRESSURE DROP:		
HOTSIDE, TOTAL	PSI	1.1200
COLDSIDE, TOTAL	PSI	0.5800

U-O-S BLOCK SECTION

HEATX COLD-TQCU ST-3 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -0.5800 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY	PRES	TEMP	VFRAC
BTU/HR	PSIG	C	
0.0	3.3041	7.2617	0.0
1.8588+04	3.3041	7.0578	0.0
2.2804+04	3.3041	7.0115	0.0
4.5608+04	3.3041	6.7613	0.0
6.8412+04	3.3041	6.5111	0.0
9.1217+04	3.3041	6.2608	0.0
1.1402+05	3.3041	6.0105	0.0
1.3682+05	3.3041	5.7602	0.0
1.5963+05	3.3041	5.5098	0.0
1.8243+05	3.3041	5.2593	0.0
2.0524+05	3.3041	5.0088	0.0

2.2804+05	3.3041	4.7583	0.0
2.5085+05	3.3041	4.5078	0.0
2.7365+05	3.3041	4.2572	0.0
2.9645+05	3.3041	4.0065	0.0
3.1926+05	3.3041	3.7558	0.0
3.4206+05	3.3041	3.5051	0.0
3.6487+05	3.3041	3.2544	0.0
3.8767+05	3.3041	3.0036	0.0
4.1047+05	3.3041	2.7527	0.0
4.3328+05	3.3041	2.5019	0.0
4.5608+05	3.3041	2.2510	0.0
4.7889+05	3.3041	2.0000	0.0

U-O-S BLOCK SECTION

HEATX HOT-TQCUR ST-3 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	5.3041	55.4561	1.0000
1.8588+04	5.3041	44.1650	DEW>1.0000
2.2804+04	5.3041	43.9680	0.9978
4.5608+04	5.3041	42.9068	0.9861
6.8412+04	5.3041	41.8413	0.9744
9.1217+04	5.3041	40.7609	0.9627
1.1402+05	5.3041	39.6575	0.9509
1.3682+05	5.3041	38.5232	0.9393
1.5963+05	5.3041	37.3502	0.9276
1.8243+05	5.3041	36.1308	0.9160
2.0524+05	5.3041	34.8569	0.9045

2.2804+05	5.3041	33.5192	0.8931
2.5085+05	5.3041	32.1079	0.8818
2.7365+05	5.3041	30.6124	0.8707
2.9645+05	5.3041	29.0204	0.8597
3.1926+05	5.3041	27.3182	0.8488
3.4206+05	5.3041	25.4899	0.8382
3.6487+05	5.3041	23.5171	0.8279
3.8767+05	5.3041	21.3784	0.8178
4.1047+05	5.3041	19.0491	0.8081
4.3328+05	5.3041	16.5007	0.7987
4.5608+05	5.3041	13.7002	0.7898
4.7889+05	5.3041	10.6117	0.7814

U-O-S BLOCK SECTION

```
BLOCK:  ST-5     MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:              45
  OUTLET STREAM:             48
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
  COLD SIDE:
  ----------
  INLET STREAM:              46
  OUTLET STREAM:             47
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                   ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          25160.0         25160.0         0.00000
      MASS(LB/HR   )          482504.         482504.         0.00000
      ENTHALPY(BTU/HR  )    -0.309138E+10   -0.309138E+10     0.00000

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

```
                     ***  INPUT DATA  ***

FLASH SPECS FOR HOT SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                   500
CONVERGENCE TOLERANCE                                      0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                   500
CONVERGENCE TOLERANCE                                      0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED HOT OUTLET TEMP
  SPECIFIED VALUE                C                        40.0000
  LMTD CORRECTION FACTOR                                   1.00000
```

U-O-S BLOCK SECTION

BLOCK: ST-5   MODEL: HEATX (CONTINUED)

```
  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                          1.6200
    COLD SIDE PRESSURE DROP        PSI                          1.3400

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT            BTU/HR-SQFT-R              115.6200

                       ***  OVERALL RESULTS  ***

  STREAMS:
                ---------------------------------------
                |                                     |
  45       ----->|               HOT                   |-----> 48
  T=  8.3626D+01 |                                     |       T=  4.0000D+01
  P=  5.3041D+00 |                                     |       P=  3.6841D+00
  V=  0.0000D+00 |                                     |       V=  0.0000D+00
                |                                     |
  47       <-----|               COLD                  |<----- 46
  T=  3.7620D+01 |                                     |       T=  3.2222D+01
  P=  1.9641D+00 |                                     |       P=  3.3041D+00
  V=  0.0000D+00 |                                     |       V=  0.0000D+00
                ---------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR                 4097518.6801
    CALCULATED (REQUIRED) AREA     SQFT                       915.4613
```

ACTUAL EXCHANGER AREA	SQFT	915.4613
PER CENT OVER-DESIGN		0.0000
HEAT TRANSFER COEFFICIENT:		
AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	115.6200
UA (DIRTY)	BTU/HR-R	105845.6401
LOG-MEAN TEMPERATURE DIFFERENCE:		
LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	21.5068
NUMBER OF SHELLS IN SERIES		1
PRESSURE DROP:		
HOTSIDE, TOTAL	PSI	1.6200
COLDSIDE, TOTAL	PSI	1.3400

U-O-S BLOCK SECTION

HEATX COLD-TQCU ST-5 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -1.3400 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	3.3041	37.6196	0.0
1.9512+05	3.3041	37.3632	0.0
3.9024+05	3.3041	37.1068	0.0
5.8536+05	3.3041	36.8503	0.0
7.8048+05	3.3041	36.5938	0.0
9.7560+05	3.3041	36.3372	0.0
1.1707+06	3.3041	36.0805	0.0
1.3658+06	3.3041	35.8237	0.0
1.5610+06	3.3041	35.5669	0.0
1.7561+06	3.3041	35.3100	0.0
1.9512+06	3.3041	35.0531	0.0

2.1463+06	3.3041	34.7960	0.0
2.3414+06	3.3041	34.5389	0.0
2.5366+06	3.3041	34.2818	0.0
2.7317+06	3.3041	34.0246	0.0
2.9268+06	3.3041	33.7673	0.0
3.1219+06	3.3041	33.5099	0.0
3.3170+06	3.3041	33.2525	0.0
3.5122+06	3.3041	32.9951	0.0
3.7073+06	3.3041	32.7375	0.0
3.9024+06	3.3041	32.4799	0.0
4.0975+06	3.3041	32.2222	0.0

HEATX HOT-TQCUR ST-5 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	5.3041	83.6259	0.0
1.9512+05	5.3041	81.6031	0.0
3.9024+05	5.3041	79.5745	0.0
5.8536+05	5.3041	77.5402	0.0
7.8048+05	5.3041	75.5001	0.0
9.7560+05	5.3041	73.4545	0.0
1.1707+06	5.3041	71.4032	0.0
1.3658+06	5.3041	69.3465	0.0
1.5610+06	5.3041	67.2842	0.0
1.7561+06	5.3041	65.2165	0.0
1.9512+06	5.3041	63.1434	0.0

2.1463+06	5.3041	61.0650	0.0
2.3414+06	5.3041	58.9814	0.0
2.5366+06	5.3041	56.8925	0.0
2.7317+06	5.3041	54.7984	0.0
2.9268+06	5.3041	52.6992	0.0
3.1219+06	5.3041	50.5950	0.0
3.3170+06	5.3041	48.4858	0.0
3.5122+06	5.3041	46.3716	0.0
3.7073+06	5.3041	44.2525	0.0
3.9024+06	5.3041	42.1287	0.0
4.0975+06	5.3041	40.0000	0.0

U-O-S BLOCK SECTION

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BLOCK:  ST-7     MODEL: HEATX
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  HOT SIDE:
  ---------
  INLET STREAM:              55
  OUTLET STREAM:             58
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1
  COLD SIDE:
  ----------
  INLET STREAM:              56
  OUTLET STREAM:             57
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
  HENRY-COMPS ID:        HC-1

                    ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          29297.3         29297.3         0.00000
      MASS(LB/HR   )          547243.         547243.         0.00000
      ENTHALPY(BTU/HR  )    -0.350841E+10   -0.350841E+10   -0.135913E-15

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

FLASH SPECS FOR HOT SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                 500
CONVERGENCE TOLERANCE                                    0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                 500
CONVERGENCE TOLERANCE                                    0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED HOT OUTLET TEMP
  SPECIFIED VALUE                C                        90.0000
  LMTD CORRECTION FACTOR                                   1.00000
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U-O-S BLOCK SECTION

BLOCK: ST-7   MODEL: HEATX (CONTINUED)

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  PRESSURE SPECIFICATION:
    HOT  SIDE PRESSURE DROP        PSI                         1.5000
    COLD SIDE PRESSURE DROP        PSI                         1.8600

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
    OVERALL COEFFICIENT            BTU/HR-SQFT-R             238.6700

                       ***  OVERALL RESULTS  ***

  STREAMS:
                  --------------------------------------
                  |                                    |
  55        ----->|               HOT                  |-----> 58
  T=  1.9803D+02  |                                    |       T=  9.0000D+01
  P=  8.3041D+00  |                                    |       P=  6.8041D+00
  V=  1.0000D+00  |                                    |       V=  5.8079D-01
                  |                                    |
  57        <-----|               COLD                 |<----- 56
  T=  4.8888D+01  |                                    |       T=  3.2222D+01
  P=  7.4441D+00  |                                    |       P=  9.3041D+00
  V=  0.0000D+00  |                                    |       V=  0.0000D+00
                  --------------------------------------

  DUTY AND AREA:
    CALCULATED HEAT DUTY           BTU/HR               15009239.6198
    CALCULATED (REQUIRED) AREA     SQFT                      362.6265
```

ACTUAL EXCHANGER AREA	SQFT	362.6265
PER CENT OVER-DESIGN		0.0000
HEAT TRANSFER COEFFICIENT:		
AVERAGE COEFFICIENT (DIRTY)	BTU/HR-SQFT-R	238.6700
UA (DIRTY)	BTU/HR-R	86548.0684
LOG-MEAN TEMPERATURE DIFFERENCE:		
LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	96.3449
NUMBER OF SHELLS IN SERIES		1
PRESSURE DROP:		
HOTSIDE, TOTAL	PSI	1.5000
COLDSIDE, TOTAL	PSI	1.8600

U-O-S BLOCK SECTION

HEATX COLD-TQCU ST-7 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -1.8600 PSI
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	9.3041	48.8877	0.0
7.1473+05	9.3041	48.1010	0.0
1.4295+06	9.3041	47.3136	0.0
2.1442+06	9.3041	46.5254	0.0
2.8589+06	9.3041	45.7366	0.0
3.5736+06	9.3041	44.9470	0.0
3.8326+06	9.3041	44.6608	0.0
4.2884+06	9.3041	44.1568	0.0
5.0031+06	9.3041	43.3658	0.0
5.7178+06	9.3041	42.5742	0.0
6.4325+06	9.3041	41.7818	0.0

7.1473+06	9.3041	40.9888	0.0
7.8620+06	9.3041	40.1951	0.0
8.5767+06	9.3041	39.4008	0.0
9.2914+06	9.3041	38.6058	0.0
1.0006+07	9.3041	37.8101	0.0
1.0721+07	9.3041	37.0137	0.0
1.1436+07	9.3041	36.2168	0.0
1.2150+07	9.3041	35.4191	0.0
1.2865+07	9.3041	34.6208	0.0
1.3580+07	9.3041	33.8219	0.0
1.4295+07	9.3041	33.0224	0.0
1.5009+07	9.3041	32.2222	0.0

U-O-S BLOCK SECTION

HEATX HOT-TQCUR ST-7   TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0   PSI
PROPERTY OPTION SET: NRTL   RENON (NRTL) / IDEAL GAS
HENRY-COMPS ID: HC-1

DUTY BTU/HR	PRES PSIG	TEMP C	VFRAC
0.0	8.3041	198.0273	1.0000
7.1473+05	8.3041	180.8961	1.0000
1.4295+06	8.3041	163.4087	1.0000
2.1442+06	8.3041	145.5352	1.0000
2.8589+06	8.3041	127.2432	1.0000
3.5736+06	8.3041	108.4984	1.0000
3.8326+06	8.3041	101.5891	DEW>1.0000
4.2884+06	8.3041	101.3650	0.9826
5.0031+06	8.3041	100.9958	0.9553
5.7178+06	8.3041	100.6031	0.9280
6.4325+06	8.3041	100.1845	0.9008

7.1473+06	8.3041	99.7376	0.8736
7.8620+06	8.3041	99.2594	0.8464
8.5767+06	8.3041	98.7466	0.8192
9.2914+06	8.3041	98.1956	0.7921
1.0006+07	8.3041	97.6019	0.7650
1.0721+07	8.3041	96.9607	0.7380
1.1436+07	8.3041	96.2662	0.7110
1.2150+07	8.3041	95.5120	0.6840
1.2865+07	8.3041	94.6905	0.6571
1.3580+07	8.3041	93.7927	0.6303
1.4295+07	8.3041	92.8084	0.6035
1.5009+07	8.3041	91.7255	0.5768

STREAM SECTION

1 2 3 4 5

STREAM ID	1	2	3	4	5
FROM :	----	----	P-1	P-2	M-1
TO :	P-1	P-2	M-1	M-1	ST-1
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
METHANOL	1022.5850	0.0	1022.5850	0.0	3899.2375
ETHANOL	0.0	542.7710	0.0	542.7710	542.7710
IB-ALDEH	0.0	0.0	0.0	0.0	4.6859
PROPANOL	0.0	0.0	0.0	0.0	7.0594-02
ISBUT-OH	0.0	0.0	0.0	0.0	0.4361
2-ME1BOH	0.0	0.0	0.0	0.0	1.1286-03
H2	0.0	0.0	0.0	0.0	8.8154-03
CO2	0.0	0.0	0.0	0.0	0.4992
PROPANE	0.0	0.0	0.0	0.0	0.3613
C2H2	0.0	0.0	0.0	0.0	1.4733
ISOBU-01	0.0	0.0	0.0	0.0	0.7398
N-BUT-01	0.0	0.0	0.0	0.0	1.0957
TRANS-01	0.0	0.0	0.0	0.0	0.8245
CIS-2-01	0.0	0.0	0.0	0.0	3.6437
C2H4	0.0	0.0	0.0	0.0	0.3164
O2	0.0	0.0	0.0	0.0	5.5991-03
CH4	0.0	0.0	0.0	0.0	0.2192
CO	0.0	0.0	0.0	0.0	7.7824-03

WATER	0.0	0.0	0.0	0.0	5.0403
COMPONENTS: LB/HR					
METHANOL	3.2766+04	0.0	3.2766+04	0.0	1.2494+05
ETHANOL	0.0	2.5005+04	0.0	2.5005+04	2.5005+04
IB-ALDEH	0.0	0.0	0.0	0.0	337.8894
PROPANOL	0.0	0.0	0.0	0.0	4.2424
ISBUT-OH	0.0	0.0	0.0	0.0	32.3239
2-ME1BOH	0.0	0.0	0.0	0.0	9.9485-02
H2	0.0	0.0	0.0	0.0	1.7771-02
CO2	0.0	0.0	0.0	0.0	21.9719
PROPANE	0.0	0.0	0.0	0.0	15.9309
C2H2	0.0	0.0	0.0	0.0	38.3622
ISOBU-01	0.0	0.0	0.0	0.0	42.9995
N-BUT-01	0.0	0.0	0.0	0.0	63.6841
TRANS-01	0.0	0.0	0.0	0.0	46.2612
CIS-2-01	0.0	0.0	0.0	0.0	204.4387
C2H4	0.0	0.0	0.0	0.0	8.8758
O2	0.0	0.0	0.0	0.0	0.1792
CH4	0.0	0.0	0.0	0.0	3.5173
CO	0.0	0.0	0.0	0.0	0.2180
WATER	0.0	0.0	0.0	0.0	90.8028
COMPONENTS: MASS FRAC					
METHANOL	1.0000	0.0	1.0000	0.0	0.8282
ETHANOL	0.0	1.0000	0.0	1.0000	0.1658
IB-ALDEH	0.0	0.0	0.0	0.0	2.2398-03
PROPANOL	0.0	0.0	0.0	0.0	2.8122-05
ISBUT-OH	0.0	0.0	0.0	0.0	2.1427-04
2-ME1BOH	0.0	0.0	0.0	0.0	6.5947-07

STREAM SECTION

1 2 3 4 5 (CONTINUED)

STREAM ID	1	2	3	4	5
H2	0.0	0.0	0.0	0.0	1.1780-07
CO2	0.0	0.0	0.0	0.0	1.4565-04
PROPANE	0.0	0.0	0.0	0.0	1.0560-04
C2H2	0.0	0.0	0.0	0.0	2.5430-04
ISOBU-01	0.0	0.0	0.0	0.0	2.8504-04
N-BUT-01	0.0	0.0	0.0	0.0	4.2215-04
TRANS-01	0.0	0.0	0.0	0.0	3.0666-04
CIS-2-01	0.0	0.0	0.0	0.0	1.3552-03
C2H4	0.0	0.0	0.0	0.0	5.8836-05
O2	0.0	0.0	0.0	0.0	1.1876-06
CH4	0.0	0.0	0.0	0.0	2.3316-05
CO	0.0	0.0	0.0	0.0	1.4450-06
WATER	0.0	0.0	0.0	0.0	6.0191-04
TOTAL FLOW:					
LBMOL/HR	1022.5850	542.7710	1022.5850	542.7710	4461.4379
LB/HR	3.2766+04	2.5005+04	3.2766+04	2.5005+04	1.5086+05
CUFT/HR	659.9545	500.1674	660.2985	500.4559	3091.8920
STATE VARIABLES:					
TEMP C	23.0000	23.0000	23.3496	23.4013	36.2692
PRES PSIG	5.3041	5.3041	62.6058	62.6058	52.6058
VFRAC	0.0	0.0	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					

BTU/LBMOL	-1.0257+05	-1.1941+05	-1.0256+05	-1.1939+05	-1.0406+05
BTU/LB	-3201.1152	-2592.0344	-3200.6961	-2591.5845	-3077.5055
BTU/HR	-1.0489+08	-6.4814+07	-1.0487+08	-6.4802+07	-4.6426+08
ENTROPY:					
BTU/LBMOL-R	-57.5190	-82.9817	-57.4951	-82.9431	-59.1435
BTU/LB-R	-1.7951	-1.8012	-1.7944	-1.8004	-1.7491
DENSITY:					
LBMOL/CUFT	1.5495	1.0852	1.5487	1.0846	1.4429
LB/CUFT	49.6486	49.9931	49.6228	49.9643	48.7911
AVG MW	32.0422	46.0690	32.0422	46.0690	33.8135

STREAM SECTION

6 7 8 9 10

STREAM ID	6	7	8	9	10
FROM :	ST-1	FH-1	R-1	----	KR-1
TO :	FH-1	R-1	KR-1	KR-1	M-2
CONV. MAX. REL. ERR:	0.0	0.0	-8.9360-06	0.0	0.0
SUBSTREAM: MIXED					
PHASE:	MIXED	VAPOR	VAPOR	LIQUID	VAPOR
COMPONENTS: LBMOL/HR					
METHANOL	3899.2375	3899.2375	3610.6646	0.0	0.0
ETHANOL	542.7710	542.7710	382.2696	0.0	0.0
IB-ALDEH	4.6859	4.6859	1.4123	0.0	0.0
PROPANOL	7.0594-02	7.0594-02	5.6492	0.0	0.0
ISBUT-OH	0.4361	0.4361	147.7271	0.0	0.0
2-ME1BOH	1.1286-03	1.1286-03	1.4123	0.0	0.0
H2	8.8154-03	8.8154-03	14.1233	0.0	0.0
CO2	0.4992	0.4992	1.8831	0.0	0.0
PROPANE	0.3613	0.3613	0.1412	0.0	0.0
C2H2	1.4733	1.4733	1.3181	0.0	0.0
ISOBU-01	0.7398	0.7398	0.2448	0.0	0.0
N-BUT-01	1.0957	1.0957	0.5178	0.0	0.0
TRANS-01	0.8245	0.8245	0.2636	0.0	0.0
CIS-2-01	3.6437	3.6437	1.1581	0.0	0.0
C2H4	0.3164	0.3164	0.3766	0.0	0.0
O2	5.5991-03	5.5991-03	1.6477	0.0	0.0

CH4	0.2192	0.2192	2.1655	0.0	0.0
CO	7.7824-03	7.7824-03	2.7587	0.0	0.0
WATER	5.0403	5.0403	310.0815	478.8370	478.8370
COMPONENTS: LB/HR					
METHANOL	1.2494+05	1.2494+05	1.1569+05	0.0	0.0
ETHANOL	2.5005+04	2.5005+04	1.7611+04	0.0	0.0
IB-ALDEH	337.8894	337.8894	101.8369	0.0	0.0
PROPANOL	4.2424	4.2424	339.4953	0.0	0.0
ISBUT-OH	32.3239	32.3239	1.0950+04	0.0	0.0
2-ME1BOH	9.9485-02	9.9485-02	124.4942	0.0	0.0
H2	1.7771-02	1.7771-02	28.4708	0.0	0.0
CO2	21.9719	21.9719	82.8744	0.0	0.0
PROPANE	15.9309	15.9309	6.2277	0.0	0.0
C2H2	38.3622	38.3622	34.3217	0.0	0.0
ISOBU-01	42.9995	42.9995	14.2285	0.0	0.0
N-BUT-01	63.6841	63.6841	30.0988	0.0	0.0
TRANS-01	46.2612	46.2612	14.7916	0.0	0.0
CIS-2-01	204.4387	204.4387	64.9772	0.0	0.0
C2H4	8.8758	8.8758	10.5654	0.0	0.0
O2	0.1792	0.1792	52.7249	0.0	0.0
CH4	3.5173	3.5173	34.7411	0.0	0.0
CO	0.2180	0.2180	77.2728	0.0	0.0
WATER	90.8028	90.8028	5586.2057	8626.3827	8626.3827
COMPONENTS: MASS FRAC					
METHANOL	0.8282	0.8282	0.7669	0.0	0.0
ETHANOL	0.1658	0.1658	0.1167	0.0	0.0
IB-ALDEH	2.2398-03	2.2398-03	6.7505-04	0.0	0.0
PROPANOL	2.8122-05	2.8122-05	2.2504-03	0.0	0.0

STREAM SECTION

6 7 8 9 10 (CONTINUED)

STREAM ID	6	7	8	9	10
ISBUT-OH	2.1427-04	2.1427-04	7.2585-02	0.0	0.0
2-ME1BOH	6.5947-07	6.5947-07	8.2524-04	0.0	0.0
H2	1.1780-07	1.1780-07	1.8873-04	0.0	0.0
CO2	1.4565-04	1.4565-04	5.4936-04	0.0	0.0
PROPANE	1.0560-04	1.0560-04	4.1282-05	0.0	0.0
C2H2	2.5430-04	2.5430-04	2.2751-04	0.0	0.0
ISOBU-01	2.8504-04	2.8504-04	9.4318-05	0.0	0.0
N-BUT-01	4.2215-04	4.2215-04	1.9952-04	0.0	0.0
TRANS-01	3.0666-04	3.0666-04	9.8050-05	0.0	0.0
CIS-2-01	1.3552-03	1.3552-03	4.3072-04	0.0	0.0
C2H4	5.8836-05	5.8836-05	7.0036-05	0.0	0.0
O2	1.1876-06	1.1876-06	3.4950-04	0.0	0.0
CH4	2.3316-05	2.3316-05	2.3029-04	0.0	0.0
CO	1.4450-06	1.4450-06	5.1222-04	0.0	0.0
WATER	6.0191-04	6.0191-04	3.7030-02	1.0000	1.0000
TOTAL FLOW:					
LBMOL/HR	4461.4379	4461.4379	4485.8153	478.8370	478.8370
LB/HR	1.5086+05	1.5086+05	1.5086+05	8626.3827	8626.3827
CUFT/HR	1.3736+05	8.0765+05	9.8405+05	168.3461	2.5724+04
STATE VARIABLES:					
TEMP C	109.5105	332.0000	393.7659	185.5556	185.8170
PRES PSIG	51.8758	49.8758	44.0294	151.4200	150.3300
VFRAC	0.2721	1.0000	1.0000	0.0	1.0000
LFRAC	0.7279	0.0	0.0	1.0000	0.0

SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-9.6432+04	-8.0123+04	-7.9687+04	-1.1704+05	-1.0160+05
BTU/LB	-2851.8728	-2369.5618	-2369.5406	-6496.9159	-5639.9159
BTU/HR	-4.3022+08	-3.5746+08	-3.5746+08	-5.6045+07	-4.8652+07
ENTROPY:					
BTU/LBMOL-R	-47.8176	-26.0406	-23.3973	-30.5980	-11.9041
BTU/LB-R	-1.4142	-0.7701	-0.6957	-1.6984	-0.6608
DENSITY:					
LBMOL/CUFT	3.2480-02	5.5240-03	4.5585-03	2.8444	1.8614-02
LB/CUFT	1.0983	0.1868	0.1533	51.2420	0.3353
AVG MW	33.8135	33.8135	33.6299	18.0153	18.0153

STREAM SECTION

11 12 13 14 15

STREAM ID	11	12	13	14	15
FROM :	KR-1	R-2	----	KR-2	KR-2
TO :	R-2	KR-2	KR-2	M-2	R-3
SUBSTREAM: MIXED					
PHASE:	VAPOR	VAPOR	LIQUID	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
METHANOL	3610.6646	3350.4561	0.0	0.0	3350.4561
ETHANOL	382.2696	245.7419	0.0	0.0	245.7419
IB-ALDEH	1.4123	2.5892	0.0	0.0	2.5892
PROPANOL	5.6492	10.3568	0.0	0.0	10.3568
ISBUT-OH	147.7271	270.8297	0.0	0.0	270.8297
2-ME1BOH	1.4123	2.5892	0.0	0.0	2.5892
H2	14.1233	25.8924	0.0	0.0	25.8924
CO2	1.8831	3.4523	0.0	0.0	3.4523
PROPANE	0.1412	0.2589	0.0	0.0	0.2589
C2H2	1.3181	2.4166	0.0	0.0	2.4166
ISOBU-01	0.2448	0.4488	0.0	0.0	0.4488
N-BUT-01	0.5178	0.9494	0.0	0.0	0.9494
TRANS-01	0.2636	0.4833	0.0	0.0	0.4833
CIS-2-01	1.1581	2.1231	0.0	0.0	2.1231
C2H4	0.3766	0.6905	0.0	0.0	0.6905
O2	1.6477	3.0208	0.0	0.0	3.0208
CH4	2.1655	3.9701	0.0	0.0	3.9701
CO	2.7587	5.0576	0.0	0.0	5.0576

WATER	310.0815	568.4761	365.9295	365.9295	568.4761
COMPONENTS: LB/HR					
METHANOL	1.1569+05	1.0736+05	0.0	0.0	1.0736+05
ETHANOL	1.7611+04	1.1321+04	0.0	0.0	1.1321+04
IB-ALDEH	101.8369	186.6987	0.0	0.0	186.6987
PROPANOL	339.4953	622.4007	0.0	0.0	622.4007
ISBUT-OH	1.0950+04	2.0075+04	0.0	0.0	2.0075+04
2-ME1BOH	124.4942	228.2366	0.0	0.0	228.2366
H2	28.4708	52.1960	0.0	0.0	52.1960
CO2	82.8744	151.9347	0.0	0.0	151.9347
PROPANE	6.2277	11.4174	0.0	0.0	11.4174
C2H2	34.3217	62.9223	0.0	0.0	62.9223
ISOBU-01	14.2285	26.0853	0.0	0.0	26.0853
N-BUT-01	30.0988	55.1805	0.0	0.0	55.1805
TRANS-01	14.7916	27.1176	0.0	0.0	27.1176
CIS-2-01	64.9772	119.1234	0.0	0.0	119.1234
C2H4	10.5654	19.3698	0.0	0.0	19.3698
O2	52.7249	96.6611	0.0	0.0	96.6611
CH4	34.7411	63.6913	0.0	0.0	63.6913
CO	77.2728	141.6650	0.0	0.0	141.6650
WATER	5586.2057	1.0241+04	6592.3221	6592.3221	1.0241+04
COMPONENTS: MASS FRAC					
METHANOL	0.7669	0.7116	0.0	0.0	0.7116
ETHANOL	0.1167	7.5045-02	0.0	0.0	7.5045-02
IB-ALDEH	6.7505-04	1.2376-03	0.0	0.0	1.2376-03
PROPANOL	2.2504-03	4.1258-03	0.0	0.0	4.1258-03
ISBUT-OH	7.2585-02	0.1331	0.0	0.0	0.1331
2-ME1BOH	8.2524-04	1.5129-03	0.0	0.0	1.5129-03

STREAM SECTION

11 12 13 14 15 (CONTINUED)

STREAM ID	11	12	13	14	15
H2	1.8873-04	3.4600-04	0.0	0.0	3.4600-04
CO2	5.4936-04	1.0071-03	0.0	0.0	1.0071-03
PROPANE	4.1282-05	7.5683-05	0.0	0.0	7.5683-05
C2H2	2.2751-04	4.1710-04	0.0	0.0	4.1710-04
ISOBU-01	9.4318-05	1.7291-04	0.0	0.0	1.7291-04
N-BUT-01	1.9952-04	3.6578-04	0.0	0.0	3.6578-04
TRANS-01	9.8050-05	1.7976-04	0.0	0.0	1.7976-04
CIS-2-01	4.3072-04	7.8964-04	0.0	0.0	7.8964-04
C2H4	7.0036-05	1.2840-04	0.0	0.0	1.2840-04
O2	3.4950-04	6.4074-04	0.0	0.0	6.4074-04
CH4	2.3029-04	4.2220-04	0.0	0.0	4.2220-04
CO	5.1222-04	9.3906-04	0.0	0.0	9.3906-04
WATER	3.7030-02	6.7887-02	1.0000	1.0000	6.7887-02
TOTAL FLOW:					
LBMOL/HR	4485.8153	4499.8027	365.9295	365.9295	4499.8027
LB/HR	1.5086+05	1.5086+05	6592.3221	6592.3221	1.5086+05
CUFT/HR	9.5463+05	1.1449+06	128.6509	1.9637+04	1.1417+06
STATE VARIABLES:					
TEMP C	342.9838	386.4972	185.5556	185.8170	347.8557
PRES PSIG	41.2294	35.3831	151.4200	150.5117	32.5831
VFRAC	1.0000	1.0000	0.0	1.0000	1.0000
LFRAC	0.0	0.0	1.0000	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					

BTU/LBMOL	-8.1335+04	-8.1083+04	-1.1704+05	-1.0160+05	-8.2338+04
BTU/LB	-2418.5458	-2418.5458	-6496.9159	-5639.9159	-2455.9959
BTU/HR	-3.6486+08	-3.6486+08	-4.2830+07	-3.7180+07	-3.7051+08
ENTROPY:					
BTU/LBMOL-R	-24.7271	-22.9310	-30.5980	-11.9063	-23.9062
BTU/LB-R	-0.7353	-0.6840	-1.6984	-0.6609	-0.7131
DENSITY:					
LBMOL/CUFT	4.6990-03	3.9302-03	2.8444	1.8635-02	3.9413-03
LB/CUFT	0.1580	0.1318	51.2420	0.3357	0.1321
AVG MW	33.6299	33.5254	18.0153	18.0153	33.5254

STREAM SECTION

16 17 18 19 20

STREAM ID	16	17	18	19	20
FROM :	R-3	----	KR-3	KR-3	R-4
TO :	KR-3	KR-3	M-2	R-4	KR-4
SUBSTREAM: MIXED					
PHASE:	VAPOR	LIQUID	VAPOR	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
METHANOL	3142.2938	0.0	0.0	3142.2938	2986.1746
ETHANOL	136.5220	0.0	0.0	136.5220	54.6084
IB-ALDEH	3.5307	0.0	0.0	3.5307	4.2368
PROPANOL	14.1228	0.0	0.0	14.1228	16.9472
ISBUT-OH	369.3098	0.0	0.0	369.3098	443.1686
2-ME1BOH	3.5307	0.0	0.0	3.5307	4.2368
H2	35.3074	0.0	0.0	35.3074	42.3686
CO2	4.7076	0.0	0.0	4.7076	5.6491
PROPANE	0.3531	0.0	0.0	0.3531	0.4237
C2H2	3.2953	0.0	0.0	3.2953	3.9543
ISOBU-01	0.6120	0.0	0.0	0.6120	0.7344
N-BUT-01	1.2946	0.0	0.0	1.2946	1.5535
TRANS-01	0.6591	0.0	0.0	0.6591	0.7909
CIS-2-01	2.8951	0.0	0.0	2.8951	3.4742
C2H4	0.9415	0.0	0.0	0.9415	1.1298
O2	4.1192	0.0	0.0	4.1192	4.9430
CH4	5.4137	0.0	0.0	5.4137	6.4964
CO	6.8966	0.0	0.0	6.8966	8.2759

WATER	775.1874	292.1603	292.1603	775.1874	930.2182
COMPONENTS: LB/HR					
METHANOL	1.0069+05	0.0	0.0	1.0069+05	9.5683+04
ETHANOL	6289.4359	0.0	0.0	6289.4359	2515.7564
IB-ALDEH	254.5868	0.0	0.0	254.5868	305.5019
PROPANOL	848.7202	0.0	0.0	848.7202	1018.4569
ISBUT-OH	2.7374+04	0.0	0.0	2.7374+04	3.2849+04
2-ME1BOH	311.2286	0.0	0.0	311.2286	373.4718
H2	71.1755	0.0	0.0	71.1755	85.4101
CO2	207.1816	0.0	0.0	207.1816	248.6163
PROPANE	15.5690	0.0	0.0	15.5690	18.6828
C2H2	85.8023	0.0	0.0	85.8023	102.9621
ISOBU-01	35.5705	0.0	0.0	35.5705	42.6844
N-BUT-01	75.2454	0.0	0.0	75.2454	90.2938
TRANS-01	36.9781	0.0	0.0	36.9781	44.3735
CIS-2-01	162.4395	0.0	0.0	162.4395	194.9261
C2H4	26.4130	0.0	0.0	26.4130	31.6953
O2	131.8095	0.0	0.0	131.8095	158.1703
CH4	86.8510	0.0	0.0	86.8510	104.2205
CO	193.1777	0.0	0.0	193.1777	231.8117
WATER	1.3965+04	5263.3489	5263.3489	1.3965+04	1.6758+04
COMPONENTS: MASS FRAC					
METHANOL	0.6674	0.0	0.0	0.6674	0.6343
ETHANOL	4.1691-02	0.0	0.0	4.1691-02	1.6676-02
IB-ALDEH	1.6876-03	0.0	0.0	1.6876-03	2.0251-03
PROPANOL	5.6260-03	0.0	0.0	5.6260-03	6.7511-03
ISBUT-OH	0.1815	0.0	0.0	0.1815	0.2177
2-ME1BOH	2.0631-03	0.0	0.0	2.0631-03	2.4757-03

STREAM SECTION

16 17 18 19 20 (CONTINUED)

STREAM ID	16	17	18	19	20
H2	4.7181-04	0.0	0.0	4.7181-04	5.6616-04
CO2	1.3734-03	0.0	0.0	1.3734-03	1.6480-03
PROPANE	1.0320-04	0.0	0.0	1.0320-04	1.2384-04
C2H2	5.6876-04	0.0	0.0	5.6876-04	6.8251-04
ISOBU-01	2.3579-04	0.0	0.0	2.3579-04	2.8294-04
N-BUT-01	4.9878-04	0.0	0.0	4.9878-04	5.9854-04
TRANS-01	2.4512-04	0.0	0.0	2.4512-04	2.9414-04
CIS-2-01	1.0768-03	0.0	0.0	1.0768-03	1.2921-03
C2H4	1.7509-04	0.0	0.0	1.7509-04	2.1010-04
O2	8.7374-04	0.0	0.0	8.7374-04	1.0485-03
CH4	5.7572-04	0.0	0.0	5.7572-04	6.9085-04
CO	1.2805-03	0.0	0.0	1.2805-03	1.5366-03
WATER	9.2572-02	1.0000	1.0000	9.2572-02	0.1111
TOTAL FLOW:					
LBMOL/HR	4510.9923	292.1603	292.1603	4510.9923	4519.3844
LB/HR	1.5086+05	5263.3489	5263.3489	1.5086+05	1.5086+05
CUFT/HR	1.3788+06	102.7156	1.5661+04	1.4095+06	1.7328+06
STATE VARIABLES:					
TEMP C	382.4665	185.5556	185.8170	351.7558	377.6200
PRES PSIG	26.7367	151.4200	150.6933	23.9367	18.0904
VFRAC	1.0000	0.0	1.0000	1.0000	1.0000
LFRAC	0.0	1.0000	0.0	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					

BTU/LBMOL	-8.2134+04	-1.1704+05	-1.0160+05	-8.3134+04	-8.2979+04
BTU/LB	-2455.9959	-6496.9159	-5639.9159	-2485.8962	-2485.8962
BTU/HR	-3.7051+08	-3.4196+07	-2.9685+07	-3.7502+08	-3.7502+08
ENTROPY:					
BTU/LBMOL-R	-22.4812	-30.5980	-11.9085	-23.2099	-22.0692
BTU/LB-R	-0.6722	-1.6984	-0.6610	-0.6940	-0.6611
DENSITY:					
LBMOL/CUFT	3.2716-03	2.8444	1.8655-02	3.2004-03	2.6082-03
LB/CUFT	0.1094	51.2420	0.3361	0.1070	8.7061-02
AVG MW	33.4422	18.0153	18.0153	33.4422	33.3801

STREAM SECTION

21 22 23 24 25

STREAM ID	21	22	23	24	25
FROM :	----	KR-4	M-2	KR-4	R-5
TO :	KR-4	M-2	----	R-5	ST-1
SUBSTREAM: MIXED					
PHASE:	LIQUID	VAPOR	VAPOR	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
METHANOL	0.0	0.0	0.0	2986.1746	2882.0963
ETHANOL	0.0	0.0	0.0	54.6084	0.0
IB-ALDEH	0.0	0.0	0.0	4.2368	4.7075
PROPANOL	0.0	0.0	0.0	16.9472	18.8301
ISBUT-OH	0.0	0.0	0.0	443.1686	492.4072
2-ME1BOH	0.0	0.0	0.0	4.2368	4.7075
H2	0.0	0.0	0.0	42.3686	47.0760
CO2	0.0	0.0	0.0	5.6491	6.2768
PROPANE	0.0	0.0	0.0	0.4237	0.4708
C2H2	0.0	0.0	0.0	3.9543	4.3937
ISOBU-01	0.0	0.0	0.0	0.7344	0.8160
N-BUT-01	0.0	0.0	0.0	1.5535	1.7261
TRANS-01	0.0	0.0	0.0	0.7909	0.8787
CIS-2-01	0.0	0.0	0.0	3.4742	3.8602
C2H4	0.0	0.0	0.0	1.1298	1.2553
O2	0.0	0.0	0.0	4.9430	5.4922
CH4	0.0	0.0	0.0	6.4964	7.2182
CO	0.0	0.0	0.0	8.2759	9.1954

WATER	209.3620	209.3620	1346.2888	930.2182	1033.5710
COMPONENTS: LB/HR					
METHANOL	0.0	0.0	0.0	9.5683+04	9.2349+04
ETHANOL	0.0	0.0	0.0	2515.7564	0.0
IB-ALDEH	0.0	0.0	0.0	305.5019	339.4450
PROPANOL	0.0	0.0	0.0	1018.4569	1131.6134
ISBUT-OH	0.0	0.0	0.0	3.2849+04	3.6499+04
2-ME1BOH	0.0	0.0	0.0	373.4718	414.9666
H2	0.0	0.0	0.0	85.4101	94.8996
CO2	0.0	0.0	0.0	248.6163	276.2390
PROPANE	0.0	0.0	0.0	18.6828	20.7585
C2H2	0.0	0.0	0.0	102.9621	114.4016
ISOBU-01	0.0	0.0	0.0	42.6844	47.4268
N-BUT-01	0.0	0.0	0.0	90.2938	100.3259
TRANS-01	0.0	0.0	0.0	44.3735	49.3035
CIS-2-01	0.0	0.0	0.0	194.9261	216.5835
C2H4	0.0	0.0	0.0	31.6953	35.2169
O2	0.0	0.0	0.0	158.1703	175.7439
CH4	0.0	0.0	0.0	104.2205	115.8000
CO	0.0	0.0	0.0	231.8117	257.5673
WATER	3771.7153	3771.7153	2.4254+04	1.6758+04	1.8620+04
COMPONENTS: MASS FRAC					
METHANOL	0.0	0.0	0.0	0.6343	0.6122
ETHANOL	0.0	0.0	0.0	1.6676-02	0.0
IB-ALDEH	0.0	0.0	0.0	2.0251-03	2.2501-03
PROPANOL	0.0	0.0	0.0	6.7511-03	7.5012-03
ISBUT-OH	0.0	0.0	0.0	0.2177	0.2419
2-ME1BOH	0.0	0.0	0.0	2.4757-03	2.7507-03

STREAM SECTION

21 22 23 24 25 (CONTINUED)

STREAM ID	21	22	23	24	25
H2	0.0	0.0	0.0	5.6616-04	6.2907-04
CO2	0.0	0.0	0.0	1.6480-03	1.8311-03
PROPANE	0.0	0.0	0.0	1.2384-04	1.3760-04
C2H2	0.0	0.0	0.0	6.8251-04	7.5834-04
ISOBU-01	0.0	0.0	0.0	2.8294-04	3.1438-04
N-BUT-01	0.0	0.0	0.0	5.9854-04	6.6504-04
TRANS-01	0.0	0.0	0.0	2.9414-04	3.2682-04
CIS-2-01	0.0	0.0	0.0	1.2921-03	1.4357-03
C2H4	0.0	0.0	0.0	2.1010-04	2.3344-04
O2	0.0	0.0	0.0	1.0485-03	1.1650-03
CH4	0.0	0.0	0.0	6.9085-04	7.6761-04
CO	0.0	0.0	0.0	1.5366-03	1.7074-03
WATER	1.0000	1.0000	1.0000	0.1111	0.1234
TOTAL FLOW:					
LBMOL/HR	209.3620	209.3620	1346.2888	4519.3844	4524.9790
LB/HR	3771.7153	3771.7153	2.4254+04	1.5086+05	1.5086+05
CUFT/HR	73.6060	1.1210+04	7.2326+04	1.8307+06	2.3392+06
STATE VARIABLES:					
TEMP C	185.5556	185.8170	185.8170	355.6799	372.8795
PRES PSIG	151.4200	150.8750	150.3300	15.2904	9.4440
VFRAC	0.0	1.0000	1.0000	1.0000	1.0000
LFRAC	1.0000	0.0	0.0	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					

BTU/LBMOL	-1.1704+05	-1.0160+05	-1.0160+05	-8.3695+04	-8.3591+04
BTU/LB	-6496.9159	-5639.9159	-5639.9159	-2507.3228	-2507.3228
BTU/HR	-2.4505+07	-2.1272+07	-1.3679+08	-3.7825+08	-3.7825+08
ENTROPY:					
BTU/LBMOL-R	-30.5980	-11.9106	-11.9041	-22.5130	-21.5886
BTU/LB-R	-1.6984	-0.6611	-0.6608	-0.6744	-0.6475
DENSITY:					
LBMOL/CUFT	2.8444	1.8676-02	1.8614-02	2.4687-03	1.9344-03
LB/CUFT	51.2420	0.3364	0.3353	8.2404-02	6.4492-02
AVG MW	18.0153	18.0153	18.0153	33.3801	33.3388

STREAM SECTION

26 27 28 29 30

STREAM ID	26	27	28	29	30
FROM :	ST-1	----	ST-2	ST-2	FD-1
TO :	ST-2	ST-2	----	FD-1	DC-1
CONV. MAX. REL. ERR:	-1.1943-07	0.0	0.0	0.0	0.0
SUBSTREAM: MIXED					
PHASE:	VAPOR	LIQUID	LIQUID	MIXED	LIQUID
COMPONENTS: LBMOL/HR					
METHANOL	2882.0963	0.0	0.0	2882.0963	2866.8989
IB-ALDEH	4.7075	0.0	0.0	4.7075	4.6585
PROPANOL	18.8301	0.0	0.0	18.8301	18.8092
ISBUT-OH	492.4072	0.0	0.0	492.4072	491.9773
2-ME1BOH	4.7075	0.0	0.0	4.7075	4.7064
H2	47.0760	0.0	0.0	47.0760	0.4271
CO2	6.2768	0.0	0.0	6.2768	1.4602
PROPANE	0.4708	0.0	0.0	0.4708	0.4048
C2H2	4.3937	0.0	0.0	4.3937	2.4345
ISOBU-01	0.8160	0.0	0.0	0.8160	0.7676
N-BUT-01	1.7261	0.0	0.0	1.7261	1.4650
TRANS-01	0.8787	0.0	0.0	0.8787	0.8420
CIS-2-01	3.8602	0.0	0.0	3.8602	3.7110
C2H4	1.2553	0.0	0.0	1.2553	0.6001
O2	5.4922	0.0	0.0	5.4922	0.1335
CH4	7.2182	0.0	0.0	7.2182	1.1626

CO	9.1954	0.0	0.0	9.1954	0.2011
WATER	1033.5710	3.6757+05	3.6757+05	1033.5710	1031.7360
COMPONENTS: LB/HR					
METHANOL	9.2349+04	0.0	0.0	9.2349+04	9.1862+04
IB-ALDEH	339.4450	0.0	0.0	339.4450	335.9129
PROPANOL	1131.6134	0.0	0.0	1131.6134	1130.3554
ISBUT-OH	3.6499+04	0.0	0.0	3.6499+04	3.6467+04
2-ME1BOH	414.9666	0.0	0.0	414.9666	414.8667
H2	94.8996	0.0	0.0	94.8996	0.8610
CO2	276.2390	0.0	0.0	276.2390	64.2630
PROPANE	20.7585	0.0	0.0	20.7585	17.8522
C2H2	114.4016	0.0	0.0	114.4016	63.3904
ISOBU-01	47.4268	0.0	0.0	47.4268	44.6127
N-BUT-01	100.3259	0.0	0.0	100.3259	85.1498
TRANS-01	49.3035	0.0	0.0	49.3035	47.2446
CIS-2-01	216.5835	0.0	0.0	216.5835	208.2137
C2H4	35.2169	0.0	0.0	35.2169	16.8337
O2	175.7439	0.0	0.0	175.7439	4.2733
CH4	115.8000	0.0	0.0	115.8000	18.6513
CO	257.5673	0.0	0.0	257.5673	5.6316
WATER	1.8620+04	6.6220+06	6.6220+06	1.8620+04	1.8587+04
COMPONENTS: MASS FRAC					
METHANOL	0.6122	0.0	0.0	0.6122	0.6150
IB-ALDEH	2.2501-03	0.0	0.0	2.2501-03	2.2488-03
PROPANOL	7.5012-03	0.0	0.0	7.5012-03	7.5673-03
ISBUT-OH	0.2419	0.0	0.0	0.2419	0.2441
2-ME1BOH	2.7507-03	0.0	0.0	2.7507-03	2.7774-03
H2	6.2907-04	0.0	0.0	6.2907-04	5.7638-06

STREAM SECTION

26 27 28 29 30 (CONTINUED)

STREAM ID	26	27	28	29	30
CO2	1.8311-03	0.0	0.0	1.8311-03	4.3022-04
PROPANE	1.3760-04	0.0	0.0	1.3760-04	1.1951-04
C2H2	7.5834-04	0.0	0.0	7.5834-04	4.2437-04
ISOBU-01	3.1438-04	0.0	0.0	3.1438-04	2.9867-04
N-BUT-01	6.6504-04	0.0	0.0	6.6504-04	5.7005-04
TRANS-01	3.2682-04	0.0	0.0	3.2682-04	3.1628-04
CIS-2-01	1.4357-03	0.0	0.0	1.4357-03	1.3939-03
C2H4	2.3344-04	0.0	0.0	2.3344-04	1.1270-04
O2	1.1650-03	0.0	0.0	1.1650-03	2.8608-05
CH4	7.6761-04	0.0	0.0	7.6761-04	1.2486-04
CO	1.7074-03	0.0	0.0	1.7074-03	3.7701-05
WATER	0.1234	1.0000	1.0000	0.1234	0.1244
TOTAL FLOW:					
LBMOL/HR	4524.9790	3.6757+05	3.6757+05	4524.9790	4432.3958
LB/HR	1.5086+05	6.6220+06	6.6220+06	1.5086+05	1.4937+05
CUFT/HR	1.5079+06	1.0747+05	1.0825+05	2.9573+04	2974.9531
STATE VARIABLES:					
TEMP C	110.0000	32.2222	39.4407	40.0000	40.0000
PRES PSIG	7.5140	7.3041	2.2541	6.1040	5.3041
VFRAC	1.0000	0.0	0.0	2.0212-02	0.0
LFRAC	0.0	1.0000	1.0000	0.9798	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-9.1114+04	-1.2264+05	-1.2241+05	-1.1002+05	-1.1168+05

BTU/LB	-2732.9543	-6807.5962	-6794.6794	-3299.9453	-3313.9315
BTU/HR	-4.1229+08	-4.5080+10	-4.4994+10	-4.9782+08	-4.9501+08
ENTROPY:					
BTU/LBMOL-R	-29.6166	-38.5412	-38.1244	-59.2633	-60.4473
BTU/LB-R	-0.8884	-2.1394	-2.1162	-1.7776	-1.7937
DENSITY:					
LBMOL/CUFT	3.0009-03	3.4201	3.3957	0.1530	1.4899
LB/CUFT	0.1000	61.6141	61.1742	5.1012	50.2104
AVG MW	33.3388	18.0153	18.0153	33.3388	33.7004

STREAM SECTION

31 32 33 34 35

STREAM ID	31	32	33	34	35
FROM :	DC-1	DC-1	DC-1	FD-1	B-1
TO :	B-1	P-3	P-5	M-3	M-3
SUBSTREAM: MIXED					
PHASE:	VAPOR	LIQUID	LIQUID	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
METHANOL	9.8440	2856.5706	0.4843	15.1978	9.8440
IB-ALDEH	1.9416-02	4.6391	4.7352-15	4.8985-02	1.9416-02
PROPANOL	3.5066-05	5.0325-02	18.7588	2.0935-02	3.5066-05
ISBUT-OH	3.3954-06	7.4566-03	491.9698	0.4300	3.3954-06
2-ME1BOH	8.0079-15	5.9638-11	4.7064	1.1343-03	8.0079-15
H2	0.4202	6.8681-03	0.0	46.6489	0.4202
CO2	0.9761	0.4841	0.0	4.8166	0.9761
PROPANE	4.9078-02	0.3558	3.6359-23	6.5908-02	4.9078-02
C2H2	0.9886	1.4459	5.6273-33	1.9591	0.9886
ISOBU-01	3.8782-02	0.7288	5.1937-17	4.8416-02	3.8782-02
N-BUT-01	0.3862	1.0787	2.3729-16	0.2611	0.3862
TRANS-01	2.9774-02	0.8123	6.3883-15	3.6696-02	2.9774-02
CIS-2-01	0.1213	3.5897	8.4569-14	0.1492	0.1213
C2H4	0.2895	0.3105	7.9672-35	0.6553	0.2895
O2	0.1286	4.9450-03	0.0	5.3587	0.1286
CH4	0.9508	0.2118	0.0	6.0556	0.9508
CO	0.1940	7.0753-03	0.0	8.9944	0.1940
WATER	3.7503-03	3.3115	1028.4208	1.8351	3.7503-03

COMPONENTS: LB/HR					
METHANOL	315.4237	9.1531+04	15.5192	486.9691	315.4237
IB-ALDEH	1.4000	334.5129	3.4144-13	3.5321	1.4000
PROPANOL	2.1073-03	3.0243	1127.3290	1.2581	2.1073-03
ISBUT-OH	2.5167-04	0.5527	3.6466+04	31.8737	2.5167-04
2-ME1BOH	7.0590-13	5.2570-09	414.8667	9.9990-02	7.0590-13
H2	0.8471	1.3845-02	0.0	94.0386	0.8471
CO2	42.9598	21.3032	0.0	211.9760	42.9598
PROPANE	2.1642	15.6880	1.6033-21	2.9063	2.1642
C2H2	25.7418	37.6485	1.4652-31	51.0113	25.7418
ISOBU-01	2.2541	42.3586	3.0188-15	2.8141	2.2541
N-BUT-01	22.4498	62.7000	1.3792-14	15.1762	22.4498
TRANS-01	1.6706	45.5740	3.5843-13	2.0589	1.6706
CIS-2-01	6.8055	201.4081	4.7450-12	8.3699	6.8055
C2H4	8.1228	8.7109	2.2351-33	18.3832	8.1228
O2	4.1150	0.1582	0.0	171.4707	4.1150
CH4	15.2530	3.3983	0.0	97.1487	15.2530
CO	5.4334	0.1982	0.0	251.9358	5.4334
WATER	6.7562-02	59.6570	1.8527+04	33.0598	6.7562-02
COMPONENTS: MASS FRAC					
METHANOL	0.6937	0.9909	2.7443-04	0.3281	0.6937
IB-ALDEH	3.0789-03	3.6215-03	6.0378-18	2.3800-03	3.0789-03
PROPANOL	4.6344-06	3.2742-05	1.9935-02	8.4773-04	4.6344-06
ISBUT-OH	5.5348-07	5.9837-06	0.6448	2.1477-02	5.5348-07
2-ME1BOH	1.5524-15	5.6914-14	7.3361-03	6.7375-05	1.5524-15
H2	1.8630-03	1.4989-07	0.0	6.3365-02	1.8630-03
CO2	9.4477-02	2.3063-04	0.0	0.1428	9.4477-02
PROPANE	4.7595-03	1.6984-04	2.8351-26	1.9583-03	4.7595-03

STREAM SECTION

31 32 33 34 35 (CONTINUED)

STREAM ID	31	32	33	34	35
C2H2	5.6611-02	4.0759-04	0.0	3.4372-02	5.6611-02
ISOBU-01	4.9573-03	4.5859-04	5.3381-20	1.8962-03	4.9573-03
N-BUT-01	4.9372-02	6.7881-04	2.4388-19	1.0226-02	4.9372-02
TRANS-01	3.6739-03	4.9340-04	6.3382-18	1.3873-03	3.6739-03
CIS-2-01	1.4967-02	2.1805-03	8.3906-17	5.6398-03	1.4967-02
C2H4	1.7864-02	9.4306-05	0.0	1.2387-02	1.7864-02
O2	9.0498-03	1.7131-06	0.0	0.1155	9.0498-03
CH4	3.3544-02	3.6791-05	0.0	6.5460-02	3.3544-02
CO	1.1949-02	2.1456-06	0.0	0.1698	1.1949-02
WATER	1.4858-04	6.4587-04	0.3276	2.2276-02	1.4858-04
TOTAL FLOW:					
LBMOL/HR	14.4403	2873.6154	1544.3401	92.5837	14.4403
LB/HR	454.7107	9.2368+04	5.6551+04	1484.0825	454.7107
CUFT/HR	1.2422+04	1907.1165	1123.3310	2.8002+04	5543.0103
STATE VARIABLES:					
TEMP C	38.5929	38.5929	84.9594	40.0000	124.2895
PRES PSIG	-7.6959	-7.6959	-2.7959	5.3041	5.3041
VFRAC	1.0000	0.0	0.0	1.0000	1.0000
LFRAC	0.0	1.0000	1.0000	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-6.7588+04	-1.0170+05	-1.2633+05	-3.0164+04	-6.5802+04
BTU/LB	-2146.3956	-3163.9533	-3449.9729	-1881.7775	-2089.6700
BTU/HR	-9.7599+05	-2.9225+08	-1.9510+08	-2.7927+06	-9.5020+05

ENTROPY:					
BTU/LBMOL-R	-20.3420	-56.4066	-64.7556	-2.2079	-19.6221
BTU/LB-R	-0.6460	-1.7548	-1.7684	-0.1377	-0.6231
DENSITY:					
LBMOL/CUFT	1.1624-03	1.5068	1.3748	3.3063-03	2.6051-03
LB/CUFT	3.6604-02	48.4331	50.3424	5.3000-02	8.2033-02
AVG MW	31.4891	32.1433	36.6183	16.0296	31.4891

STREAM SECTION

36 37 38 39 40

STREAM ID	36	37	38	39	40
FROM :	M-3	----	ST-3	ST-3	FD-2
TO :	ST-3	ST-3	----	FD-2	----
SUBSTREAM: MIXED					
PHASE:	VAPOR	LIQUID	LIQUID	MIXED	VAPOR
COMPONENTS: LBMOL/HR					
METHANOL	25.0418	0.0	0.0	25.0418	4.9805
IB-ALDEH	6.8401-02	0.0	0.0	6.8401-02	2.1575-02
PROPANOL	2.0970-02	0.0	0.0	2.0970-02	7.0040-04
ISBUT-OH	0.4300	0.0	0.0	0.4300	1.3867-03
2-ME1BOH	1.1343-03	0.0	0.0	1.1343-03	5.7289-06
H2	47.0691	0.0	0.0	47.0691	47.0672
CO2	5.7927	0.0	0.0	5.7927	5.7775
PROPANE	0.1150	0.0	0.0	0.1150	0.1095
C2H2	2.9477	0.0	0.0	2.9477	2.9203
ISOBU-01	8.7198-02	0.0	0.0	8.7198-02	7.6170-02
N-BUT-01	0.6473	0.0	0.0	0.6473	0.6304
TRANS-01	6.6470-02	0.0	0.0	6.6470-02	5.4223-02
CIS-2-01	0.2705	0.0	0.0	0.2705	0.2165
C2H4	0.9448	0.0	0.0	0.9448	0.9390
O2	5.4873	0.0	0.0	5.4873	5.4866
CH4	7.0064	0.0	0.0	7.0064	6.9990
CO	9.1883	0.0	0.0	9.1883	9.1876
WATER	1.8388	2896.9077	2896.9077	1.8388	0.1100

COMPONENTS: LB/HR					
METHANOL	802.3928	0.0	0.0	802.3928	159.5857
IB-ALDEH	4.9322	0.0	0.0	4.9322	1.5557
PROPANOL	1.2602	0.0	0.0	1.2602	4.2091-02
ISBUT-OH	31.8739	0.0	0.0	31.8739	0.1028
2-ME1BOH	9.9990-02	0.0	0.0	9.9990-02	5.0500-04
H2	94.8857	0.0	0.0	94.8857	94.8818
CO2	254.9358	0.0	0.0	254.9358	254.2671
PROPANE	5.0705	0.0	0.0	5.0705	4.8277
C2H2	76.7531	0.0	0.0	76.7531	76.0395
ISOBU-01	5.0682	0.0	0.0	5.0682	4.4272
N-BUT-01	37.6259	0.0	0.0	37.6259	36.6419
TRANS-01	3.7295	0.0	0.0	3.7295	3.0423
CIS-2-01	15.1754	0.0	0.0	15.1754	12.1448
C2H4	26.5061	0.0	0.0	26.5061	26.3412
O2	175.5857	0.0	0.0	175.5857	175.5648
CH4	112.4017	0.0	0.0	112.4017	112.2827
CO	257.3692	0.0	0.0	257.3692	257.3493
WATER	33.1274	5.2189+04	5.2189+04	33.1274	1.9816
COMPONENTS: MASS FRAC					
METHANOL	0.4139	0.0	0.0	0.4139	0.1307
IB-ALDEH	2.5439-03	0.0	0.0	2.5439-03	1.2740-03
PROPANOL	6.4999-04	0.0	0.0	6.4999-04	3.4471-05
ISBUT-OH	1.6440-02	0.0	0.0	1.6440-02	8.4178-05
2-ME1BOH	5.1573-05	0.0	0.0	5.1573-05	4.1357-07
H2	4.8941-02	0.0	0.0	4.8941-02	7.7703-02
CO2	0.1315	0.0	0.0	0.1315	0.2082
PROPANE	2.6153-03	0.0	0.0	2.6153-03	3.9536-03

STREAM SECTION

36 37 38 39 40 (CONTINUED)

STREAM ID	36	37	38	39	40
C2H2	3.9588-02	0.0	0.0	3.9588-02	6.2272-02
ISOBU-01	2.6141-03	0.0	0.0	2.6141-03	3.6257-03
N-BUT-01	1.9407-02	0.0	0.0	1.9407-02	3.0008-02
TRANS-01	1.9236-03	0.0	0.0	1.9236-03	2.4915-03
CIS-2-01	7.8272-03	0.0	0.0	7.8272-03	9.9460-03
C2H4	1.3671-02	0.0	0.0	1.3671-02	2.1572-02
O2	9.0564-02	0.0	0.0	9.0564-02	0.1438
CH4	5.7975-02	0.0	0.0	5.7975-02	9.1954-02
CO	0.1327	0.0	0.0	0.1327	0.2108
WATER	1.7087-02	1.0000	1.0000	1.7087-02	1.6228-03
TOTAL FLOW:					
LBMOL/HR	107.0240	2896.9077	2896.9077	107.0240	84.5781
LB/HR	1938.7933	5.2189+04	5.2189+04	1938.7933	1221.0788
CUFT/HR	3.3967+04	822.9150	826.9602	2.4270+04	2.8912+04
STATE VARIABLES:					
TEMP C	55.4561	2.0000	7.2617	10.0000	10.0000
PRES PSIG	5.3041	3.3041	2.7241	4.1841	1.3041
VFRAC	1.0000	0.0	0.0	0.7823	1.0000
LFRAC	0.0	1.0000	1.0000	0.2177	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-3.4973+04	-1.2360+05	-1.2343+05	-3.9447+04	-2.1713+04
BTU/LB	-1930.5352	-6860.7982	-6851.6221	-2177.5376	-1503.9764
BTU/HR	-3.7429+06	-3.5806+08	-3.5758+08	-4.2218+06	-1.8365+06

ENTROPY:					
BTU/LBMOL-R	-4.2797	-40.3665	-40.0385	-12.3448	0.7626
BTU/LB-R	-0.2362	-2.2407	-2.2225	-0.6814	5.2823-02
DENSITY:					
LBMOL/CUFT	3.1508-03	3.5203	3.5031	4.4097-03	2.9253-03
LB/CUFT	5.7079-02	63.4192	63.1090	7.9883-02	4.2234-02
AVG MW	18.1155	18.0153	18.0153	18.1155	14.4373

STREAM SECTION

41 42 43 44 45

STREAM ID	41	42	43	44	45
FROM :	FD-2	P-4	P-3	P-5	M-4
TO :	P-4	M-1	M-1	M-4	ST-5
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
METHANOL	20.0613	20.0613	2856.5706	0.4843	0.6450
IB-ALDEH	4.6826-02	4.6826-02	4.6391	4.7352-15	4.7352-15
PROPANOL	2.0269-02	2.0269-02	5.0325-02	18.7588	19.9191
ISBUT-OH	0.4286	0.4286	7.4566-03	491.9698	500.0795
2-ME1BOH	1.1286-03	1.1286-03	5.9638-11	4.7064	4.7462
H2	1.9474-03	1.9474-03	6.8681-03	0.0	0.0
CO2	1.5194-02	1.5194-02	0.4841	0.0	0.0
PROPANE	5.5067-03	5.5067-03	0.3558	3.6359-23	3.6359-23
C2H2	2.7407-02	2.7407-02	1.4459	5.6273-33	5.6273-33
ISOBU-01	1.1028-02	1.1028-02	0.7288	5.1937-17	5.1937-17
N-BUT-01	1.6930-02	1.6930-02	1.0787	2.3729-16	2.3729-16
TRANS-01	1.2247-02	1.2247-02	0.8123	6.3883-15	6.3883-15
CIS-2-01	5.4013-02	5.4013-02	3.5897	8.4569-14	8.4569-14
C2H4	5.8782-03	5.8782-03	0.3105	7.9672-35	7.9672-35
O2	6.5407-04	6.5407-04	4.9450-03	0.0	0.0
CH4	7.4180-03	7.4180-03	0.2118	0.0	0.0
CO	7.0718-04	7.0718-04	7.0753-03	0.0	0.0
WATER	1.7289	1.7289	3.3115	1028.4208	1063.0428

COMPONENTS: LB/HR					
METHANOL	642.8070	642.8070	9.1531+04	15.5192	20.6672
IB-ALDEH	3.3765	3.3765	334.5129	3.4144-13	3.4144-13
PROPANOL	1.2181	1.2181	3.0243	1127.3290	1197.0557
ISBUT-OH	31.7712	31.7712	0.5527	3.6466+04	3.7067+04
2-ME1BOH	9.9485-02	9.9485-02	5.2570-09	414.8667	418.3748
H2	3.9256-03	3.9256-03	1.3845-02	0.0	0.0
CO2	0.6687	0.6687	21.3032	0.0	0.0
PROPANE	0.2428	0.2428	15.6880	1.6033-21	1.6033-21
C2H2	0.7136	0.7136	37.6485	1.4652-31	1.4652-31
ISOBU-01	0.6410	0.6410	42.3586	3.0188-15	3.0188-15
N-BUT-01	0.9841	0.9841	62.7000	1.3792-14	1.3792-14
TRANS-01	0.6871	0.6871	45.5740	3.5843-13	3.5843-13
CIS-2-01	3.0306	3.0306	201.4081	4.7450-12	4.7450-12
C2H4	0.1649	0.1649	8.7109	2.2351-33	2.2351-33
O2	2.0929-02	2.0929-02	0.1582	0.0	0.0
CH4	0.1190	0.1190	3.3983	0.0	0.0
CO	1.9809-02	1.9809-02	0.1982	0.0	0.0
WATER	31.1458	31.1458	59.6570	1.8527+04	1.9151+04
COMPONENTS: MASS FRAC					
METHANOL	0.8956	0.8956	0.9909	2.7443-04	3.5723-04
IB-ALDEH	4.7045-03	4.7045-03	3.6215-03	6.0378-18	5.9018-18
PROPANOL	1.6972-03	1.6972-03	3.2742-05	1.9935-02	2.0691-02
ISBUT-OH	4.4267-02	4.4267-02	5.9837-06	0.6448	0.6407
2-ME1BOH	1.3861-04	1.3861-04	5.6914-14	7.3361-03	7.2315-03
H2	5.4697-06	5.4697-06	1.4989-07	0.0	0.0
CO2	9.3171-04	9.3171-04	2.3063-04	0.0	0.0
PROPANE	3.3833-04	3.3833-04	1.6984-04	2.8351-26	2.7712-26

STREAM SECTION

41 42 43 44 45 (CONTINUED)

STREAM ID	41	42	43	44	45
C2H2	9.9431-04	9.9431-04	4.0759-04	0.0	0.0
ISOBU-01	8.9310-04	8.9310-04	4.5859-04	5.3381-20	5.2179-20
N-BUT-01	1.3711-03	1.3711-03	6.7881-04	2.4388-19	2.3839-19
TRANS-01	9.5740-04	9.5740-04	4.9340-04	6.3382-18	6.1954-18
CIS-2-01	4.2225-03	4.2225-03	2.1805-03	8.3906-17	8.2016-17
C2H4	2.2977-04	2.2977-04	9.4306-05	0.0	0.0
O2	2.9161-05	2.9161-05	1.7131-06	0.0	0.0
CH4	1.6581-04	1.6581-04	3.6791-05	0.0	0.0
CO	2.7599-05	2.7599-05	2.1456-06	0.0	0.0
WATER	4.3396-02	4.3396-02	6.4587-04	0.3276	0.3310
TOTAL FLOW:					
LBMOL/HR	22.4459	22.4459	2873.6154	1544.3401	1588.4326
LB/HR	717.7145	717.7145	9.2368+04	5.6551+04	5.7854+04
CUFT/HR	14.0800	14.0873	1907.9470	1119.2665	1144.5405
STATE VARIABLES:					
TEMP C	10.0000	10.3660	38.8691	83.4905	83.6258
PRES PSIG	1.3041	62.6058	52.6058	5.3041	5.3041
VFRAC	0.0	0.0	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.0566+05	-1.0563+05	-1.0169+05	-1.2633+05	-1.2625+05
BTU/LB	-3304.3180	-3303.5653	-3163.5926	-3449.9215	-3466.3663
BTU/HR	-2.3716+06	-2.3710+06	-2.9221+08	-1.9510+08	-2.0054+08

ENTROPY:					
BTU/LBMOL-R	-59.2991	-59.2532	-56.3869	-64.7774	-64.4430
BTU/LB-R	-1.8545	-1.8531	-1.7542	-1.7690	-1.7693
DENSITY:					
LBMOL/CUFT	1.5942	1.5933	1.5061	1.3798	1.3878
LB/CUFT	50.9740	50.9476	48.4120	50.5252	50.5481
AVG MW	31.9753	31.9753	32.1433	36.6183	36.4223

STREAM SECTION

46 47 48 49 50

STREAM ID	46	47	48	49	50
FROM :	----	ST-5	ST-5	DEC-1	DEC-1
TO :	ST-5	----	DEC-1	DC-2	FH-2
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
METHANOL	0.0	0.0	0.6450	0.1656	0.4794
PROPANOL	0.0	0.0	19.9191	1.1604	18.7587
ISBUT-OH	0.0	0.0	500.0795	8.1101	491.9694
2-ME1BOH	0.0	0.0	4.7462	3.9798-02	4.7064
WATER	2.3572+04	2.3572+04	1063.0428	594.2907	468.7521
COMPONENTS: LB/HR					
METHANOL	0.0	0.0	20.6672	5.3073	15.3599
PROPANOL	0.0	0.0	1197.0557	69.7359	1127.3197
ISBUT-OH	0.0	0.0	3.7067+04	601.1433	3.6466+04
2-ME1BOH	0.0	0.0	418.3748	3.5081	414.8667
WATER	4.2465+05	4.2465+05	1.9151+04	1.0706+04	8444.6996
COMPONENTS: MASS FRAC					
METHANOL	0.0	0.0	3.5723-04	4.6612-04	3.3055-04
PROPANOL	0.0	0.0	2.0691-02	6.1247-03	2.4260-02
ISBUT-OH	0.0	0.0	0.6407	5.2797-02	0.7848
2-ME1BOH	0.0	0.0	7.2315-03	3.0811-04	8.9279-03
WATER	1.0000	1.0000	0.3310	0.9403	0.1817
TOTAL FLOW:					

LBMOL/HR	2.3572+04	2.3572+04	1588.4326	603.7667	984.6659
LB/HR	4.2465+05	4.2465+05	5.7854+04	1.1386+04	4.6468+04
CUFT/HR	6892.0800	6929.0317	1076.2199	188.5636	891.5753
STATE VARIABLES:					
TEMP C	32.2222	37.6196	40.0000	40.0000	40.0000
PRES PSIG	3.3041	1.9641	3.6841	3.3041	3.3041
VFRAC	0.0	0.0	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.2264+05	-1.2247+05	-1.2883+05	-1.2262+05	-1.3276+05
BTU/LB	-6807.5962	-6797.9470	-3537.1910	-6502.0365	-2813.2131
BTU/HR	-2.8908+09	-2.8867+09	-2.0464+08	-7.4032+07	-1.3073+08
ENTROPY:					
BTU/LBMOL-R	-38.5412	-38.2290	-68.6686	-39.3598	-86.7734
BTU/LB-R	-2.1394	-2.1220	-1.8853	-2.0871	-1.8387
DENSITY:					
LBMOL/CUFT	3.4201	3.4019	1.4759	3.2019	1.1044
LB/CUFT	61.6141	61.2855	53.7571	60.3829	52.1194
AVG MW	18.0153	18.0153	36.4223	18.8583	47.1920

STREAM SECTION

51 52 53 54 55

STREAM ID	51	52	53	54	55
FROM :	DC-2	DC-2	P-6	FH-2	R-6
TO :	----	P-6	M-4	R-6	ST-7
CONV. MAX. REL. ERR:	0.0	-1.6222-06	0.0	0.0	0.0
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
METHANOL	4.9697-03	0.1607	0.1607	0.4794	0.4794
PROPANOL	1.5471-04	1.1603	1.1603	18.7587	0.0
ISBUT-OH	3.9964-04	8.1097	8.1097	491.9694	0.0
2-ME1BOH	1.9854-09	3.9798-02	3.9798-02	4.7064	0.0
WATER	559.6687	34.6220	34.6220	468.7521	984.1865
IBUTENE	0.0	0.0	0.0	0.0	491.9694
PROPENE	0.0	0.0	0.0	0.0	18.7587
2ME1BENE	0.0	0.0	0.0	0.0	4.7064
COMPONENTS: LB/HR					
METHANOL	0.1592	5.1480	5.1480	15.3599	15.3599
PROPANOL	9.2973-03	69.7267	69.7267	1127.3197	0.0
ISBUT-OH	2.9622-02	601.1139	601.1139	3.6466+04	0.0
2-ME1BOH	1.7501-07	3.5081	3.5081	414.8667	0.0
WATER	1.0083+04	623.7256	623.7256	8444.6996	1.7730+04
IBUTENE	0.0	0.0	0.0	0.0	2.7603+04
PROPENE	0.0	0.0	0.0	0.0	789.3770

2ME1BENE	0.0	0.0	0.0	0.0	330.0797
COMPONENTS: MASS FRAC					
METHANOL	1.5793-05	3.9502-03	3.9502-03	3.3055-04	3.3055-04
PROPANOL	9.2209-07	5.3503-02	5.3503-02	2.4260-02	0.0
ISBUT-OH	2.9379-06	0.4613	0.4613	0.7848	0.0
2-ME1BOH	1.7357-11	2.6919-03	2.6919-03	8.9279-03	0.0
WATER	1.0000	0.4786	0.4786	0.1817	0.3816
IBUTENE	0.0	0.0	0.0	0.0	0.5940
PROPENE	0.0	0.0	0.0	0.0	1.6987-02
2ME1BENE	0.0	0.0	0.0	0.0	7.1033-03
TOTAL FLOW:					
LBMOL/HR	559.6742	44.0925	44.0925	984.6659	1500.1004
LB/HR	1.0083+04	1303.2223	1303.2223	4.6468+04	4.6468+04
CUFT/HR	176.9758	25.3734	25.2963	4.0632+05	5.9362+05
STATE VARIABLES:					
TEMP C	105.3325	92.2267	89.9872	325.0000	198.0273
PRES PSIG	3.0141	1.3041	5.3041	13.3041	8.3041
VFRAC	0.0	0.0	0.0	1.0000	1.0000
LFRAC	1.0000	1.0000	1.0000	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.2018+05	-1.2355+05	-1.2355+05	-1.0089+05	-6.6223+04
BTU/LB	-6670.9177	-4180.0118	-4179.9632	-2137.8198	-2137.8198
BTU/HR	-6.7261+07	-5.4475+06	-5.4474+06	-9.9341+07	-9.9341+07
ENTROPY:					
BTU/LBMOL-R	-34.5734	-52.7368	-52.7642	-42.8329	-20.5142
BTU/LB-R	-1.9191	-1.7843	-1.7852	-0.9076	-0.6622

STREAM SECTION

51 52 53 54 55 (CONTINUED)

STREAM ID	51	52	53	54	55
DENSITY:					
LBMOL/CUFT	3.1624	1.7377	1.7430	2.4234-03	2.5271-03
LB/CUFT	56.9727	51.3617	51.5183	0.1144	7.8280-02
AVG MW	18.0155	29.5566	29.5566	47.1920	30.9769

STREAM SECTION

56 57 58

STREAM ID	56	57	58
FROM :	----	ST-7	ST-7
TO :	ST-7	----	----
SUBSTREAM: MIXED			
PHASE:	LIQUID	LIQUID	MIXED
COMPONENTS: LBMOL/HR			
METHANOL	0.0	0.0	0.4794
WATER	2.7797+04	2.7797+04	984.1865
IBUTENE	0.0	0.0	491.9694
PROPENE	0.0	0.0	18.7587
2ME1BENE	0.0	0.0	4.7064
COMPONENTS: LB/HR			
METHANOL	0.0	0.0	15.3599
WATER	5.0077+05	5.0077+05	1.7730+04
IBUTENE	0.0	0.0	2.7603+04
PROPENE	0.0	0.0	789.3770
2ME1BENE	0.0	0.0	330.0797
COMPONENTS: MASS FRAC			
METHANOL	0.0	0.0	3.3055-04
WATER	1.0000	1.0000	0.3816
IBUTENE	0.0	0.0	0.5940
PROPENE	0.0	0.0	1.6987-02
2ME1BENE	0.0	0.0	7.1033-03
TOTAL FLOW:			

LBMOL/HR	2.7797+04	2.7797+04	1500.1004
LB/HR	5.0077+05	5.0077+05	4.6468+04
CUFT/HR	8127.5968	8264.5596	2.8450+05
STATE VARIABLES:			
TEMP C	32.2222	48.8877	90.0000
PRES PSIG	9.3041	7.4441	6.8041
VFRAC	0.0	0.0	0.5808
LFRAC	1.0000	1.0000	0.4192
SFRAC	0.0	0.0	0.0
ENTHALPY:			
BTU/LBMOL	-1.2264+05	-1.2210+05	-7.6228+04
BTU/LB	-6807.5962	-6777.6242	-2460.8187
BTU/HR	-3.4091+09	-3.3941+09	-1.1435+08
ENTROPY:			
BTU/LBMOL-R	-38.5412	-37.5887	-34.9587
BTU/LB-R	-2.1394	-2.0865	-1.1285
DENSITY:			
LBMOL/CUFT	3.4201	3.3634	5.2728-03
LB/CUFT	61.6141	60.5930	0.1633
AVG MW	18.0153	18.0153	30.9769

PROBLEM STATUS SECTION

BLOCK STATUS

```
****************************************************************************
*                                                                          *
* Calculations were completed with warnings                                *
*                                                                          *
* The following Unit Operation blocks were                                 *
* completed with warnings:                                                 *
*   R-1       R-2       R-3       R-4       R-5                            *
*                                                                          *
* All streams were flashed normally                                        *
*                                                                          *
* All Convergence blocks were completed normally                           *
*                                                                          *
* All Calculator blocks were completed normally                            *
*                                                                          *
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