

April 15th, 2020

Production of Dimethyl Ether (DME) for Transportation Fuel

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April 15th, 2020

Dear Prof. Vrana and Dr. Gopal,

Within this report is the process, financial, environmental, and safety analysis on the Production of Dimethyl Ether (DME) for transportation fuel. The report will address the feasibility of the total plant in relation to the goals set by Dr. Gopal's problem statement. The DME total plant will have the capacity to produce 309,675 metric tons of DME per year, paving the path towards a near zero particulate emission trucking industry. The DME total plant is designed to support a shipping region of 2,000 long-haul trucks and is one step towards a near zero particulate emission diesel vehicle future. The feasibility exemplified by the report shows that through proper design the plant will not only be able to cleanly support supply chains but will do so without any negative impacts on the surrounding environment.

The total plant, located in Beaumont, Texas, will receive its feed via a pipeline from a nearby methanol plant and produce 99.8% by weight pure DME, surpassing ISO standards. This pipeline allows for on-site storage of the product DME in a tank farm without the added cost of raw material storage. The plant has two byproducts, methanol and DME, which are dissolved into the bottoms water. The total plant will utilize a biotreatment facility to remove these chemicals and negate any potential harmful impacts on the surrounding Texas ecosystem.

The total plant utilizes reactive distillation to produce a product and bottoms stream each with minimal impurities. The column drives the product DME to the top, reacts the feed methanol, and draws the water to the bottom. Two columns will be built to accommodate the size of the project and to allow for 50% downturn in the off season for trucking. The plant will operate at 90% uptime in the full demand season. The product is mixed with mineral oil in a static mixer in order to meet the ISO standards for lubricity and viscosity while the bottoms is sent to biotreatment as mentioned before. The product is stored in a tank farm of spherical storage tanks where it will be sold for \$1.716 per gallon, less than the price of diesel, incentivizing companies to make the switch. The problem statement's scope stops at the tank farm and further fabrication for loading onto trucks will be required, either down the road or by the purchaser themselves.

The report concludes that with an investor's rate of return of 12.6% and a net present value of approximately \$12 million the plant will start making profits in 2033. The total DME plant represents a feasible and appealing alternative to diesel fuel that will pave the way towards a cleaner future in the long-haul trucking industry.

Sincerely,

Anita Yang

Carl Antrassian

Julian Kurtzman

Production of Dimethyl Ether (DME) for Transportation Fuel

Anita Yang Carl Antrassian Julian Kurtzman

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4 Abstract

Dimethyl Ether (DME) is a proposed alternative to diesel fuel that is being looked into by car and truck manufacturers worldwide. The current market, based almost completely in China, is primed for growth and a U.S. based DME total plant that is economical and environmentally feasible stands to pave the way for America's DME market, especially since states such as California have approved DME for use as vehicle fuel (Fuel Smarts). Conventionally, the DME is produced by feeding Methanol into a fixed-bed gas-phase reactor over a γ -alumina catalyst (Dimian et al). Using this process and normal operating conditions (250-400°C and up to 20 bar) operations can reach 70-80% Methanol conversion. The proposed process utilizes the innovative reactive distillation technology and Amberlyst 35 catalyst to achieve a 99.8% Methanol conversion and produce 35,418 kilograms of DME fuel per hour. The reactive distillation is executed at ~130°C (in the reactive stages) and 700 kPa (condenser pressure), and produces water as a byproduct, which exits as the bottoms stream. In order to create a process that is environmentally sustainable, the small amounts of Methanol and DME in the bottoms stream are removed using biotreatment and the water is then released into a nearby river. The product DME is mixed with mineral oil to meet ISO standards and is then stored in an on-site spherical tank farm. Diesel prices will be undercut by the DME product at \$1.716 a gallon in order to incentivise companies to make the switch to DME fuel.

The DME total plant, located in Beaumont, Texas, serves to provide the local long-haul trucking industry with a cleaner burning fuel for a plant life of 20 years. The DME total plant has an Internal Rate of Return (IRR) of 12.6%, a Net Present Value (NPV) in 2020 of approximately \$12 million, and will turn its first profit in 2033. The report addresses financial, economic, and process concerns to deliver recommendations for the construction that is safest for the environment, the investor, and the plant operator.

5 Introduction and Objective Time Chart

Dimethyl Ether (DME) is being pursued around the world as an alternative clean burning fuel to replace diesel because of its low emission and diesel-like performance. The production of DME from Methanol typically uses a fixed-bed gas-phase reactor followed by two distillation columns; in this report, an innovative approach of using reactive distillation is proposed for reducing capital and operating costs. Replacing diesel with DME is a conversion that has not yet been done in the U.S., but with proper economic motivation the switch can be accomplished. The current DME market exists largely in China, but there is promise of a potentially booming U.S. market in the coming years. With companies such as Volvo developing long-haul trucks that run on DME, and this report outlining a profitable, environmentally-friendly approach, it is only a matter of time before companies begin to make the switch to DME. The DME total plant report outlines safety, economic, process, and environmental considerations that result in a plan capable of bringing a DME-fueled long-haul trucking industry into fruition. Figure 5.1 below outlines the objective time table for the design process. The project began with an analysis of different catalysts and moved into a phase of Aspen simulations. Once a process was selected and deemed feasible the project moved into the design and fabrication steps. The project ended with a financial and economic analysis of the DME total plant's profitability and costs.

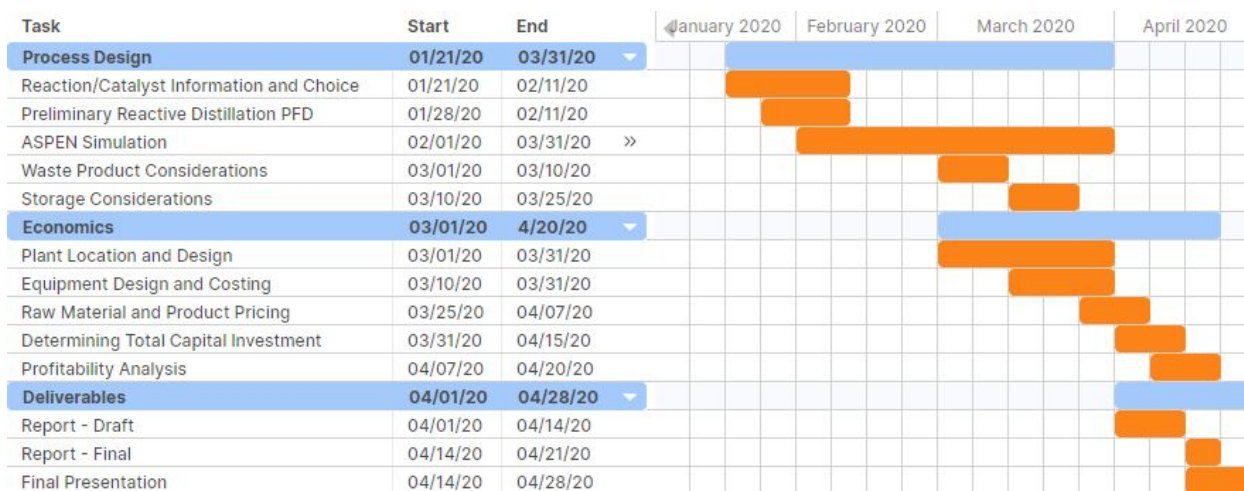


Figure 5.1. The objective time chart for the DME development process outlining the goals for different pieces of the report.

6 Innovation Map

N/A

7 Market and Competitive Analysis

The initial project proposal outlined that this Dimethyl Ether (DME) plant must be able to meet the demand of 2,000 trucks, using the provided assumptions, it was calculated that the rate of production must be 765,000 kg of DME / day (calculations are detailed in Section 28.1). The plant will be located in Beaumont, Texas, a crossroads between Texas and Louisiana. This choice of location serves to minimize transportation costs and allow ease of access to the large trucking market along the gulf coast.

The primary competitor in the US for DME is diesel. Diesel is the current go-to fuel for the trucking industry, but DME provides a greener alternative. DME is ultra low-emission and sulfur-free with comparable performance to diesel, removing the need for costly particulate filters. It boasts a higher cetane number than diesel, showing that it works efficiently in compression ignition engines. Unfortunately, DME has lower energy density than diesel, prompting the need for a larger gas tank. The fuel will also need to be pressurized, but not to the same degree as liquefied natural gas, and normal diesel engines would need to be replaced with engines specifically designed to use DME, requiring further capital investment on the part of shipping companies. However, the handling and infrastructure required for DME use are relatively simple and inexpensive making this fuel an attractive alternative. Additionally, to offset the required capital investments, DME will be priced below diesel, making it the better option in the long run. Over time, it is expected the price of and demand for DME will follow the fluctuations in the price of and demand for diesel.

In 2017, 42.7 billion gallons of diesel were consumed in the US, making up 24.0% of total highway fuel usage (Davis). The United States is a massive market for transportation fuel and with green initiatives becoming more commonplace, DME is beginning to make its way into the market

and is being seriously considered by automobile companies to replace diesel; corporations such as Volvo have begun development for DME compatible trucks. As of now, 85 % of DME is consumed in China. The size of the market in 2018 was \$3.9B, but this is expected to grow dramatically over the next few years; it is predicted to reach \$9.6B in 2025 at a CAGR of 12% (Global Market Insights). The time is now to transition into the world of Dimethyl Ether.

If/when global demand for DME balloons, the process described in this report would be relatively simple to scale. Provided enough Methanol feed, numerous copies of the designed column could be used to produce as much DME as necessary to fulfill demand.

8 Customer Requirements

The problem statements provide the necessary information to calculate the requirements that the plant should be designed to fulfill. The problem statement outlines requirements for the demand of the plant's production, the quality of the final product DME, pricing of the lubricant to be purchased, candidate catalysts for the reaction, and the pricing of the Methanol feed. In addition to this, there were requirements imposed on the location of the plant and pricing was provided for the transportation of Methanol if the designed plant required Methanol to be brought in by train. The plant was required to have a turn down of 50% in order to accommodate for offseason trucking traffic, and slight increases to accommodate unprecedented increases in demand. The statement also specified that the design should include a tank farm where the facilitation of truck loading will take place. The total plant should also include OSBL storage for raw material including the Methanol and the Amberlyst 35 catalyst.

The problem statement specifies that the product DME will be used as a transportation fuel, specifically as a diesel replacement. The plant needs to be capable of supporting a shipping region of 2,000 trucks performing at six miles per gallon of diesel, driving 12 hours per day, and traveling at an average speed of 60 miles per hour. Since the product DME will be a replacement to diesel fuel, this required an adjustment for DME's reported 5.3 miles per gallon fuel economy to calculate the required DME, and in turn the Methanol requirement for the plant. The calculation for the required rate of Methanol feed is detailed in Section 28.1 and was found to be 1537 kmol Methanol/hr.

The pricing of Methanol is obviously subject to change throughout the lifetime but prices can be assumed to be consistent with those listed on Methanex. The historical prices from Methanex were used to project the price of Methanol for the lifetime of the plant and it is assumed to be \$1.03 per

gallon (further detailed in Section 14.4). The problem statement also came with an associated cost for transporting the Methanol by train. Upon considering this cost, ($\$0.015 + \$0.0002/\text{mile}$) per gallon, it was decided that it would be easier and more financially reasonable to pipe in the Methanol, and to store the product DME in a tank farm for loading into trucks. In order to achieve this the plant will need to be located within close proximity of the feed Methanol plant.

While the problem statement did not place any restrictions on the location of the plant, it did specify that it needed to be located somewhere with adequate truck traffic that would be able to support the previously specified demand. This requirement coupled with the motivation to minimize the cost of Methanol transportation lead us to locate in Beaumont, Texas. Figure 8.1 below shows the average long-haul truck traffic on the National Highway System as of 2015. The Eastcoast, the Midwest, and the South are littered with heavily utilized trucking routes, and so any location along one of these routes would fit the specification of the trucking portion of the problem statement. Figure 8.2 shows the projected long-haul traffic truck traffic on the National Highway System in 2045. This helps show that the location decided upon will qualify and continue to work for the foreseeable future and lifetime of the DME plant (Bureau of Transportation Statistics). Since half of the United States qualifies as a possible location, the location of Methanol plants in the US was used to further narrow down the possible locations for the DME plant. Figure 8.3 below shows the placement of several Methanol plants located in the United States (U.S. Energy Information Administration). Most of these plants are located in Texas and Louisiana, specifically the southeast region of Texas. This area not only has several Methanol plants to choose from, but it also overlaps with a region that is already heavily traveled by long-haul trucks. In addition, the area's long-haul traffic is expected to increase,

allowing for expansion of the plant later in its lifetime. Beaumont, Texas is located in the epicenter of these Methanol plants and overlapped by several long-haul trucking routes.

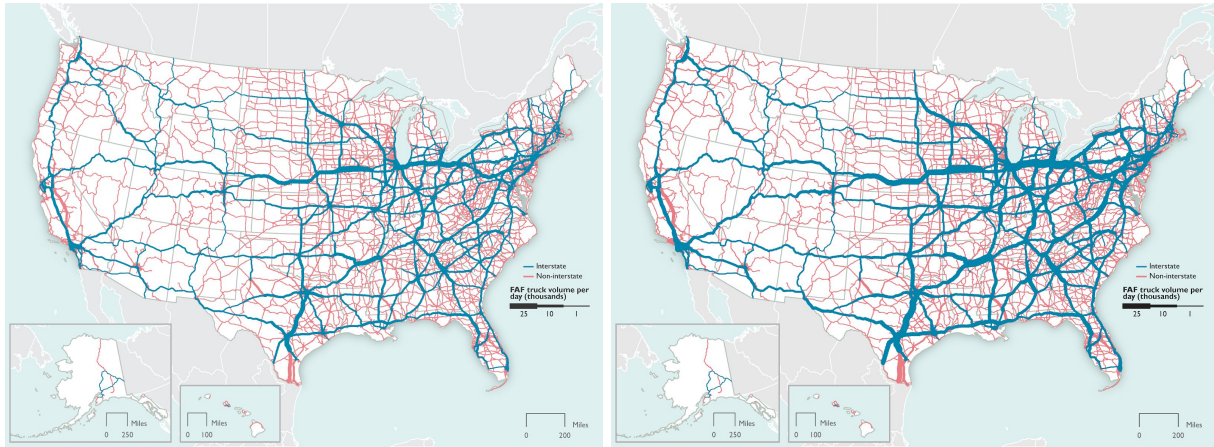


Figure 8.1-8.2. Figure 8.1 (left) shows the average long-haul truck traffic on the NHS as of 2015 while Figure 8.2 (right) shows the projected long-haul truck traffic on the NHS in 2045. This shows the possible locations for the placement of the DME plant along with verifying the location will work for the lifetime of the plant.



Figure 8.3. The active and in-service Methanol Plants located around the United States. Several plants are under construction and three are expected to come online in 2019-2020 increasing the availability and sources of the feed Methanol, potentially allowing a lower price.

While there are several plants located in Beaumont, Texas, the chosen plant must be capable of supporting the larger than normal customer demand of 431,693 metric tons of Methanol a year.

Natgasoline is one of the largest Methanol production facilities in the world and the largest in the

United States. The plant has a production capacity of 1.8 million metric tons a year, well enough to handle the load required for the feed stream of Methanol. Figure 8.4 below shows a map of the area south of Beaumont, Texas with the Natgasoline plant shown (Google Maps). In addition to the close proximity to the Natgasoline feed plant, the area is also conveniently close to the Neches River. This will be helpful in disposing of the 13,893 kg of water produced per hour after it passes through a biotreatment plant to remove the small amount of Methanol and DME coming out in the bottoms water. Beaumont, Texas fulfills the necessary requirement of being a high volume trucking area, has the needed feed Methanol plant nearby, and a river conveniently close.

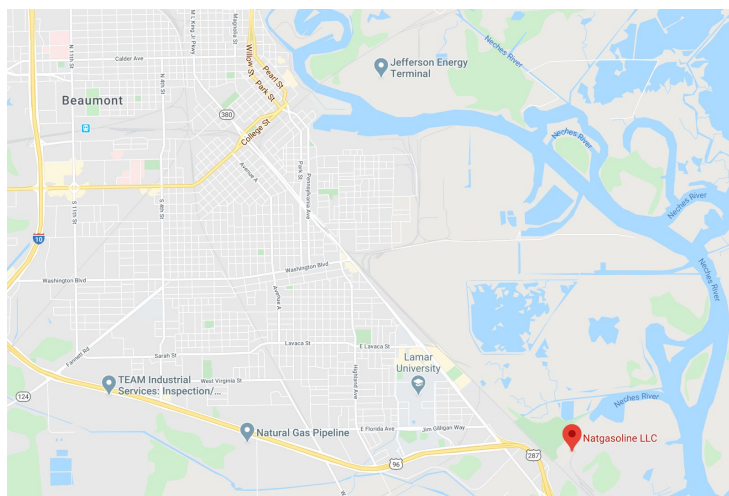


Figure 8.4. Map of the southern area of Beaumont, Texas, the proposed location of the DME plant. Natgasoline is shown in close proximity to the Neches River.

The produced DME must conform to the International Organization for Standardization (ISO) DME Fuel plant Gate Standard which pertains to the purity of the produced DME along with its lubricity (ref. ASTM D7901.144734). The standard addresses the amount of specific impurities allowed in the final DME along with the overall purity of the DME produced. Figure 8.5 below outlines these exact specifications.

Property	Test Method	Requirement
Dimethyl Ether, mass %, min. ^A	D2163	98.5
Methanol, mass %, max.	D2163	0.05
Water, mass %, max.	ISO 17197	0.03
Methyl Formate, mass %	D2163	report
Sulfur, mg / kg, max. ^B	D6667	3
Vapor Pressure, kPa (psig), at 37.8°C (100°F), max.	D1267 , D6897	758 (110)
Corrosion, Copper Strip, at 37.8°C (100°F), max.	D1838	No. 1
Residue	D2158	
Residue on evaporation of 100 mL, mL, max, Oil stain observation		0.05 pass
Lubricity	—	^C

Figure 8.5. Detailed requirements for Dimethyl Ether as transportation fuel by the ISO.

DME has a low viscosity and a poor lubricity and so to meet the standard set by the ISO a lubricant must be added to the final DME product to make it usable as a diesel fuel replacement. The potential wear on the inner mechanics of the diesel engines without the lubricant could be very destructive. The viscosity needs to be increased to allow for proper injection and passage. The ISO standard does not yet clarify how much or what kind of a lubricant needs to be added in, and so the problem statement specified 900 ppm to be assumed. Using this value of 900 ppm it was found that there was a requirement of about 0.96 cubic meter of lubricant per day. Upon collaboration with an industry consultant, mineral oil was suggested as the lubricant to be added. This lubricant also had a bulk cost provided by the problem statement of \$1.65/lb plus shipping. This cost was also provided by the problem statement which was the same as the cost of shipping the Methanol in by train: (\$0.015 + \$0.0002/mile) per gallon. Shell Lubricants is conveniently located in Houston and is a producer of mineral oil, which will help minimize the cost of shipping (Shell).

The motivation behind the problem was to find a way to produce a near zero particulate emission diesel replacement, and the process should reflect this by having as small a carbon footprint as possible. In addition to this, all safety and environmental aspects were considered to create a process

that is as clean as the solution it is creating. The waste stream (water with trace amounts of methanol and DME) is treated using biotreatment, producing clean water that can be released into the nearby river. The plant has a lifetime of 20 years, again specified by the problem statement, with a Minimum Acceptable Rate of Return (discounted rate) of 8%. The plant will operate 329 days a year and these off days will align with the downturn season.

9 Critical-to-quality Variables - Product Requirements

N/A

10 Product Concepts

N/A

11 Superior Product Concepts

N/A

12 Competitive Analysis

N/A

13 Preliminary Process Synthesis

13.1 Catalysts

Candidate catalysts for converting Methanol to DME are γ -alumina, various modified alumina (such as silica-alumina, phosphorous-alumina and fluorinated-alumina), hierarchical ZSM-5 (zeolite) and super-acid polymer resin (such as Amberlyst 35). Hierarchical ZSM-5 has comparatively low conversion of Methanol and is therefore not considered. Amongst the possible catalysts, the most commonly used is γ -alumina due to its low cost (\sim \$2/kg), thermal stability and high surface area. The conversion of Methanol with γ -alumina is strongly dependent on the operating temperature as seen in Figure 13.1.

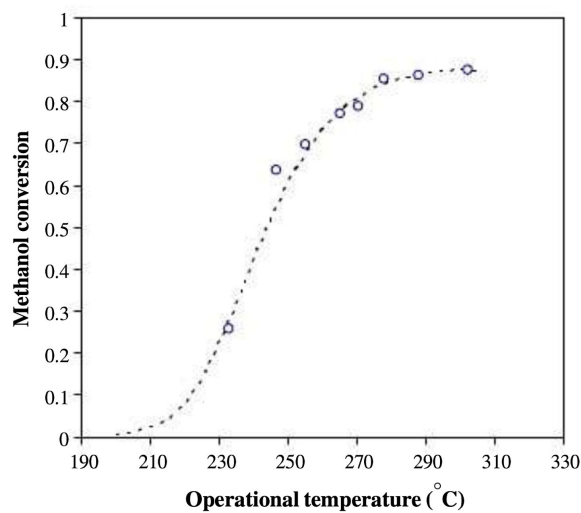


Figure 13.1. Experimental (circles) and calculated (line) conversion of Methanol using γ -alumina catalyst at different operational temperatures by Raouf et al. shows increasing conversion with higher temperature.

The Methanol conversion with various modified alumina catalysts also share similar dependency on the operational temperature. Modified alumina catalysts typically cost more than

γ -alumina but offer other advantages; for example, silica-alumina has been found to reduce hydrocarbon byproducts and coking (Yaripour et al.).

Super-acid polymer resin has a lower operational temperature. The Amberlyst 15, 35, 36 and 70 are some of the viable options for the reaction. Amongst the four, Amberlyst 35 and 36 are superior because of their high acidity which results in higher DME production. In comparison to Amberlyst 36, 35 has better catalytic and physical properties such as better thermal stability, less swelling and more crosslinks (Hosseininejad et al.); thus, Amberlyst 35 is preferred.

As Amberlyst's maximum operating temperature is 150 °C, the reaction must be conducted at a lower temperature range. The main advantage of using Amberlyst 35 as opposed to γ -alumina is its lower operating temperature; while γ -alumina have negligible conversion of Methanol at below 150 °C (seen in Figure 13.1), Amberlyst 35 is able to produce DME. This makes Amberlyst 35 an ideal candidate for use in units that require lower temperature such as reactive distillation.

13.2 Conventional Process

The conventional process for Methanol to DME conversion involves a pure Methanol fed into a fixed-bed gas-phase reactor containing γ -alumina catalyst. Typical operating conditions range from 250 to 400 °C with pressure up to 20 bar (Dimian et al.). Under these conditions, Methanol conversion is approximately 70 to 80%. The outlet stream is a mixture of water, DME and Methanol and is fed into the first distillation column (DC) which removes DME as the distillate and the bottoms mixture of water and Methanol is fed to a second DC. The Methanol that exits the second column as the distillate is recycled back to the reactor while the water exits from the bottom.

13.3 Dividing Wall Column

A dividing wall column (DWC) enables separation of ternary mixture, such as DME, water and Methanol mixture, to be done in a single column thus decreasing capital and operating cost significantly. A dividing wall column can be used in place of the two distillation columns in the conventional process.

13.4 Reactive Distillation

A reactive distillation (RD) column combines the reaction and separation steps in a single unit. In addition to reduced capital and operating cost, RD has the advantage of being able to push an equilibrium reaction to completion by continuously removing the products. RD can be used in various configurations for the Methanol to DME reaction. A single RD column may be sufficient to achieve > 98.5% purity in the distillate (DME) and bottoms (water) – essentially 100% conversion of Methanol. If conversion is not complete, a RD column followed by a DC is used to recover the Methanol. Another option for when conversion is not complete is to combine DWC and RD in a single unit, known as reactive dividing wall column (RDWC).

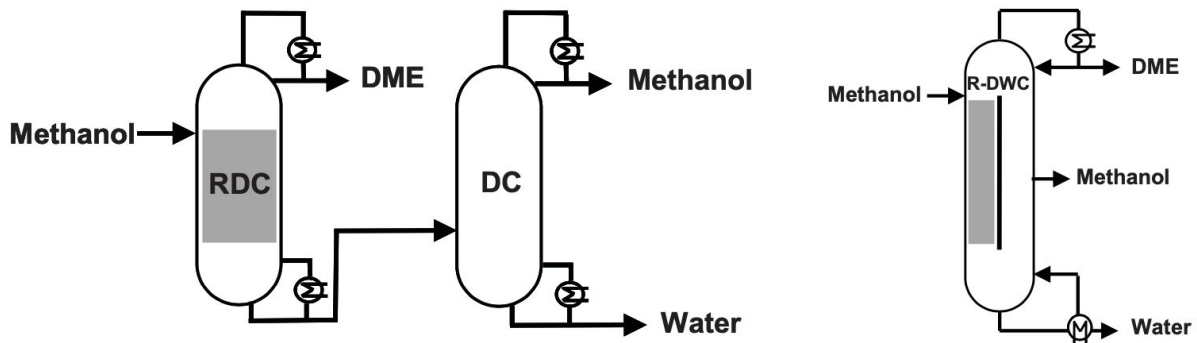


Figure 13.2. Reactive dividing wall column (RDWC) combines a reactive distillation column (RDC) and a distillation column (DC) into a single unit as proposed by Kiss et al.

For a reactive distillation, it is preferred to run the column at a lower temperature so that separation can occur; at higher temperature, excessive vaporization causes too much water to exit the distillate and thus lowering the purity of the distillate. Based on the discussion from Section 13.1, Amberlyst 35 is the most suitable catalyst.

13.5 Conclusion

Amongst all of the possible configurations, the ideal arrangement is a single RD column with complete conversion of Methanol. This configuration does not require an additional column nor requires a recycle stream for unreacted Methanol. In the case where conversion cannot reach completion, a RDWC column will be the preferred option. Both configurations only have one unit resulting in lower capital and operating cost.

14 Assembly of Database

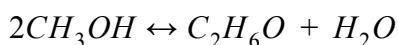
14.1 Thermophysical and Transport Properties

Methanol, the sole raw material for this process, is a liquid with a boiling point of 64.8°C and density of 0.792 kg/cum. At 25°C, the specific heat (C_p) is estimated to be about 80.3 J/mol-K (NIST) and the dynamic viscosity is 0.543 cP (Anton Paar).

The product, Dimethyl Ether, is a gas (boiling point of -24°C) at ambient pressure and thus requires pressurization and/or cooling to retain a liquid state. Figure 28.2 shows experimentally determined vapor pressures for Dimethyl Ether at a wide range of temperatures. The product will be stored at high pressure to prevent vaporization. As a liquid, Dimethyl Ether exhibits a density of 0.735 kg/cum. At 25°C, the specific heat (C_p) is about 65.6 J/mol-K (NIST) and the dynamic viscosity is 0.125 cP (Cousins and Laesecke).

14.2 Reaction Kinetics

Research on the kinetics of Amberlyst 35 has shown adsorption occurs on the surface of the catalyst and most agree that the mechanism follows either Langmuir-Hinshelwood or Eley-Rideal kinetic model, indicating that the surface reaction is the rate-determining step. The Methanol dehydration reaction only involves three components, Methanol as the reactant and DME and water as the products:



Both DME and water compete for the active sites of the catalyst thus inhibiting the dehydration reaction.

The kinetics equations, based on the Langmuir-Hinshelwood (Eq. 14.1) and Eley-Rideal (Eq. 14.2) models, both reflect the competitive chemisorption of water and DME with Methanol:

$$r_{DME} = \frac{k_s K_M^2 C_M^2}{(1 + K_W C_W + K_M C_M + K_D C_D)^2} \quad (14.1)$$

$$r_{DME} = \frac{k_s K_M C_M^2}{1 + K_W C_W + K_M C_M + K_D C_D} \quad (14.2)$$

In the above equations, k_s is the surface reaction rate constant, K_M , K_W and K_D , and C_M , C_W and C_D , are the adsorption equilibrium constants and concentration of Methanol, water and DME, respectively. As the adsorption equilibrium constants of the more polar components (Methanol and water) are much larger than the less polar component (DME), inhibition by DME is negligible compared to water and so the K_D term can be neglected (An et al.).

An et al. concluded that the Eley-Rideal model (Eq. 14.2) is most reflective of the reaction kinetics. This conclusion was reached by conducting several experiments with different concentrations of Methanol in water at 120°C and 820 kPa. On the other hand, Hosseinijad et al. found that the Langmuir-Hinshelwood mechanism is a better fit to experimental data by similarly conducting experiments with different concentrations of Methanol and water but at temperature 110 to 135°C and at 900 kPa. Because of the wider temperature used in Hosseinijad et al.'s study, which is reflective of the wide temperature profile of the reactive stages (Figure 16.4), the equation determined by Hosseinijad et al. will be used as the base kinetics model.

Dimian et al. further modified the kinetics equation from Hosseinijad et al. by introducing an equilibrium term, K_{eq} , so that the model can be used for when Methanol conversion approaches chemical equilibrium such as in a reactive distillation process. The resultant equation is:

$$r_{DME} = \frac{k_S}{(1 + \frac{K_W C_W}{K_M C_M})^2} \left(1 - \frac{1}{K_{eq}} \frac{C_D C_W}{C_M^2}\right) \quad (3)$$

The surface reaction rate constant (kmol/kg-s), the adsorption equilibrium constants and the equilibrium constant are dependent on the temperature (in Kelvin) as shown in equations (14.4), (14.5) and (14.6):

$$k_S = 6.12 \times 10^9 \exp\left(-\frac{11793}{T}\right) \quad (14.4)$$

$$\frac{K_W}{K_M} = \exp\left(-6.46 + \frac{2964.0}{T}\right) \quad (14.5)$$

$$K_{eq} = \exp\left(-2.6305 + \frac{2787}{T}\right) \quad (14.6)$$

The equation for the equilibrium constant, K_{eq} , was determined by Dimian et al. by regressing equilibrium values calculated from Aspen using the Gibbs free energies. In this proposed process, equations 14.3, 14.4, 14.5 and 14.6 are used for the reaction kinetics.

14.3 Safety

Methanol is a category 2 flammable liquid, category 3 toxic substance, and a category 1 health hazard. The permissible exposure limit (PEL) as set by the Occupational Safety and Health Administration (OSHA) is 200 ppm total weight average (TWA). A floating head storage tank is used to account for volatility and flammability concerns in our raw material. Furthermore, the concentration of Methanol in the bottoms stream is above the allowable limit as described in the Texas Surface Water Quality Standards after treatment. The most lenient limit listed is 30% of the LC_{50} value for the most sensitive species. Certain fish have LC_{50} values around 8 g/L, resulting in an upper concentration limit of 2.4 g/L. The bottoms stream exits the column at 5.01 g/L, so the stream will pass through biotreatment to remove the organic material.

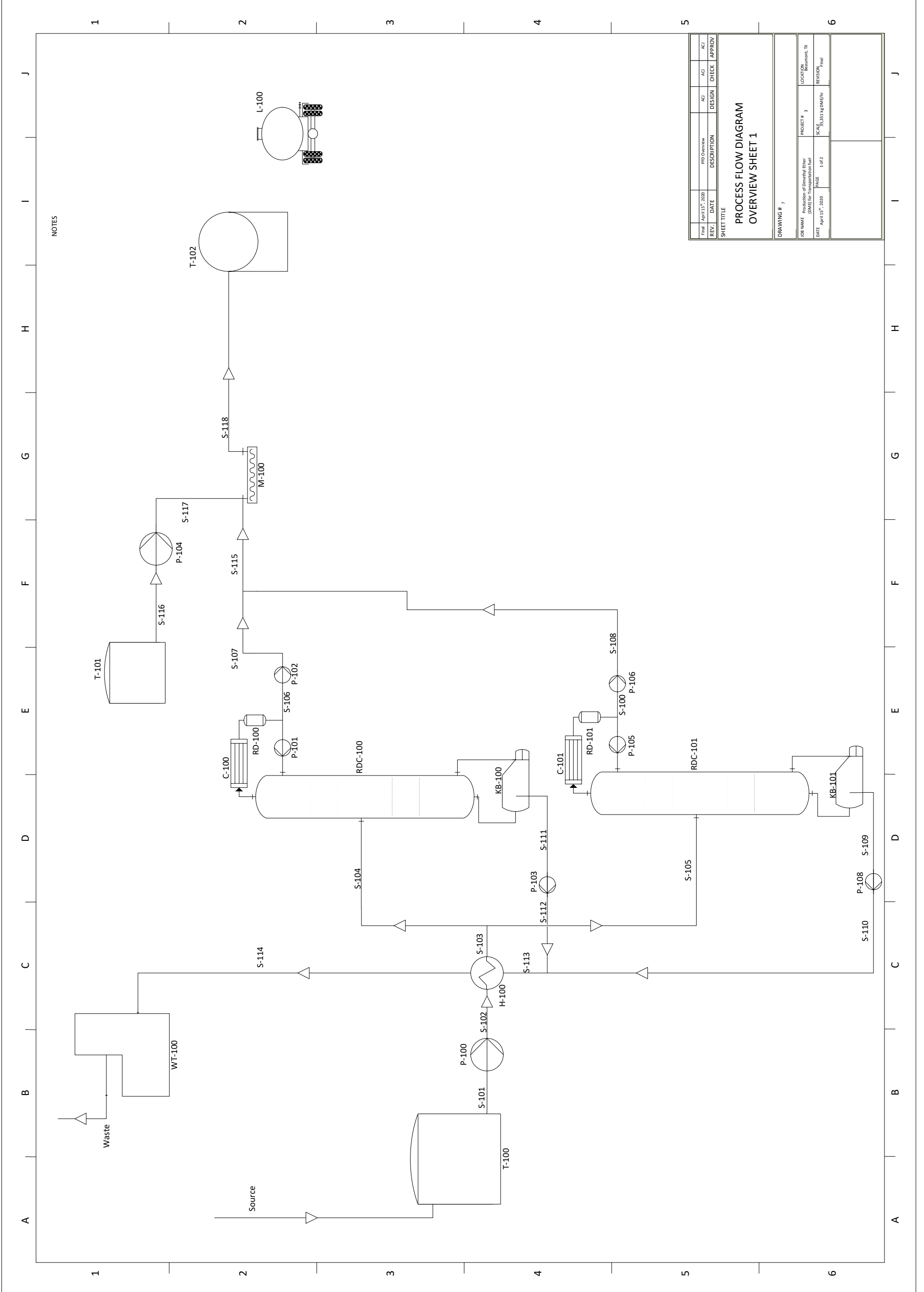
Dimethyl Ether is classified as a category 1 flammable gas. It is also noted in the SDS that under pressure, Dimethyl Ether contains gas and may explode if heated. Due to these concerns, the Dimethyl Ether will be produced in a column at 700 kPa and pumped into pressurized spherical tanks for storage at 1000 kPa. This will keep the product in liquid state up to temperatures of 42°C.

14.4 Prices

To prevent bias due to the COVID-19 pandemic, end-of-year 2019 data will be used to determine reasonable prices for the raw material and product. Using Methanex to price the Methanol, the price assumed for the raw material is \$1.03/gal (\$0.344/kg methanol). This will be sourced directly from Natgasoline through a pipeline, thus avoiding transportation costs. The lubricant (mineral oil) costs \$1.65/lb and will be purchased from Shell Lubricants and shipped in from Houston, resulting in an additional shipping cost of \$0.035/gal DME (total \$3.651/kg lubricant). The Dimethyl Ether product will be priced at \$1.716/gal (\$0.62/kg DME), slightly below the prevailing wholesale price of diesel at the end of 2019, \$1.943/gal (see 28.5 for explanation of DME pricing).

15 Process Flow Diagram and Material Balance

Below is the process flow diagram for the total DME plant and the material balance for the process.



NOTES

REV.	DATE	DESCRIPTION	DESIGN	CHECK	APPROV.
Final	April 15 th , 2020	FD Overview	ACJ	ACJ	ACJ

SHEET TITLE
**PROCESS FLOW DIAGRAM
OVERVIEW SHEET 1**

DRAWING # 7

JOB NAME	Production of Dimethyl Ether (DME) for Industrial Use	PROJECT #	3	LOCATION	Beaumont, TX
DATE	April 15 th , 2020	PAGE	1 of 2	SCALE	3/32" = 1'-0" (Final)
		REVISION			

Stream Identifier and Description

S-100 DME product stream
 S-101 Methanol from storage to pump
 S-102 Methanol from pump to heat exchanger
 S-103 Heated methanol feed stream to splitter
 S-104 Methanol feed to RDC-100
 S-105 Methanol feed to RDC-101
 S-106 DME product stream
 S-107 Pumped DME product stream
 S-108 DME product stream
 S-109 Bottoms water to pump
 S-110 Pumped bottoms water
 S-111 Bottoms water to pump
 S-112 Pumped bottoms water
 S-113 Combined bottoms water to heat exchanger
 S-114 Bottoms water to cooling tower
 S-115 Combined DME product stream to heat exchanger
 S-116 Lubricant to pump
 S-117 Pumped lubricant to DME stream
 S-118 Combined DME and lubricant stream to storage
 S-104-1-5 Split feed streams to column trays

Equipment Identifier and Description

T-100 On-site methanol storage
 P-100 Methanol feed centrifugal pump
 H-100 Methanol feed heat exchanger
 RDC-100 Reactive distillation column 1
 RDC-101 Reactive distillation column 2
 C-100 Condenser
 C-101 Condenser
 P-101 Centrifugal pump back to column
 P-102 Centrifugal pump to storage
 RD-100 Reflux drum back to column
 RD-101 Reflux drum back to column
 KB-100 Kettle reboiler
 KB-101 Kettle reboiler
 P-103 Bottoms centrifugal pump
 P-108 Bottoms centrifugal pump
 T-101 Lubricant storage tank
 M-100 Lubricant and DME static mixer
 P-104 Lubricant centrifugal pump to mixer
 P-105 Centrifugal pump back to column
 P-106 Centrifugal pump to storage
 T-102 Spherical storage tank of DME
 L-100 Loading station for tankers
 CT-100 Cooling tower for bottoms water
 WT-100 Water treatment facility

NOTES

Final	Apr 15 th , 2020	Legend	ACJ	ACJ	ACJ
REV.	DATE	DESCRIPTION	DESIGN	CHECK	APPROV.
SHEET TITLE					
PROCESS FLOW DIAGRAM OVERVIEW SHEET 3					
DRAWING # 7					
JOB NAME			PROJECT #		LOCATION
Production of Dimethyl Ether Plant for the Refinery			3		Beaumont, TX
DATE			PAGE		REVISION
Apr 15 th , 2020			2 of 2		Final

Table 15.1. Material balance block of the overall process flow diagram

Stream Number	101	102	103	104/105	106/100	107/108	109/111	110/112	113
Temperature (°C)	25.0	25.3	60.9	60.0	30.9	31.3	167	167	167
Pressure (kPa)	101	750	716	700	700	1100	737	737	737
Vapor fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass Flow (kg/hr)	49280	49280	49280	24639	17693	17693	6946	13893	13893
Molar Flow (kmol/hr)	1538	1538	1538	769	384	384	385	769.5	769.5
Component Mass Flow (kg/hr)									
Methanol	49280	49280	49280	24639	17.5	17.5	34.73	69.5	69.5
Water	-	-	-	-	0.147	0.147	6912	13823	13823
Dimethyl Ether	-	-	-	-	17675	17675	trace	trace	trace
Mineral Oil	-	-	-	-	-	-	-	-	-
Volume Flow (cum/hr)	62.2	62.2	65.8	356	27.4	27.4	8.25	16.5	14.9
Stream Number	114	115	116	117	118				
Temperature (°C)	84.9	31.3	25.0	25.0	31.3				
Pressure (kPa)	712	1100	101	1100	1000				
Vapor fraction	0.0	0.0	0.0	0.0	0.0				
Mass Flow (kg/hr)	13893	35386	31.9	31.9	35418				
Molar Flow (kmol/hr)	769.5	768	~0.07	~0.07	145.2				
Component Mass Flow (kg/hr)									
Methanol	69.5	35	-	-	35.1				
Water	13823	0.294	-	-	0.294				
Dimethyl Ether	trace	35350	-	-	35351				
Mineral Oil	-	-	31.9	31.9	31.9				
Volume Flow (cum/hr)	14.9	54.8	~0.04	~0.04	~55.2				

16 Process Description

16.1 Segment 1 – Feed

Segment 1 is shown in Figure 16.1 and includes the feed (Methanol) storage (T-100), pump (P-100) and heat exchanger (H-100). The Methanol will be sourced using a pipeline from a nearby Methanol plant and is then stored in a single floating-roof tank of continuous operation at ambient temperature and pressure (25°C and 101 kPa). The tank is designed to be 2,986 cum of carbon steel construction. This volume equates to two days worth of Methanol feed stored at the DME plant at all times. This is done so that in the case of an unexpected shutdown at the Methanol feed plant the DME plant can still operate for two days independently of their shutdown. In addition, if there is a problem with the actual pipeline from Natgasoline, the DME plant will again be able to operate for two days. This will hopefully be enough time for either scenario to be fixed without hindering the DME production.

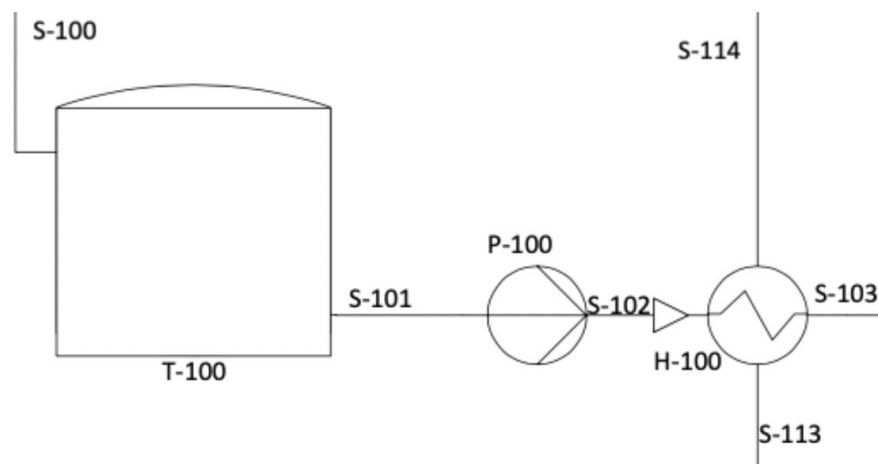


Figure 16.1. Segment 1 of the process flow diagram.

Stream (S-101) feeds the Methanol at a flow rate of 49,280 kg/hr into the pump (P-100) which increases the pressure to 750 kPa. The exiting stream (S-102) enters the feed heat exchanger (H-100) at

25°C and is heated to 61°C. As the bottom stream from the reactive distillation column is at 167°C with flow rate of 13,893 kg/hr, it is more than sufficient to be used as the heat source for the heat exchanger.

16.2 Segment 2 – Reactive Distillation

In Segment 2 of the process flow diagram, shown in Figure 16.2, the pressurized and heated Methanol stream (S-103) is split into two streams (S-104 and S-105) each with half the flow rate of S-103. Assuming a pressure drop of 50 kPa from piping, once S-104 and S-105 reaches the reactive distillation column, the pressure will be 700 kPa with temperatures of 61°C. S-104 and S-105 are each further split into 5 streams (S-104-[1-5] and S-105-[1-5]) which are fed into the columns (RDC-100 and RDC-101) at different tray locations. The feed streams were split into 5 smaller streams so as to prevent overloading on the first reactive stage. In other reactive distillation processes where the reaction occurs in the liquid phase, the feed stream typically enters above the first reactive stage so that the liquid feed is in contact with as much catalyst as possible before reaching the bottom of the column; this increases conversion of the reactant. Embodying the same idea, the 5 smaller streams are split such that the feed entering at a higher stage has higher flow rate. The flow rates of the feed entering above theoretical stage 6, 7, 8, 9 and 10 – corresponding to the 1st, 2nd, 3rd, 4th and 5th reactive trays from the top – are 304, 200, 100, 90, 75 kmol/hr, respectively.

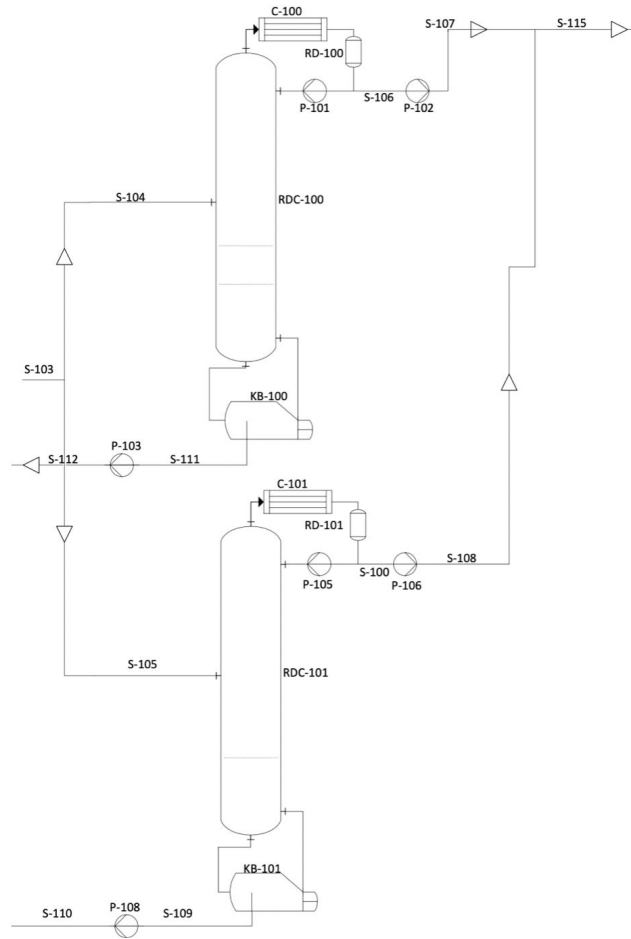


Figure 16.2. Segment 2 of the process flow diagram.

Note that the reactive distillation process for RDC-100 and RDC-101 are the same; that is, the feed streams (S-104 and S-105), the distillate streams (S-106 and S-100) and the bottom streams (S-111 and S-109) from both columns have the same properties and flow rates, and the columns (RDC-100 and RDC-101) are identical in every aspect. As the two processes are the same, for simplicity, discussion on the reactive distillation segment will be focused on one column but the exact comments are applicable for the other.

The reactive distillation process was simulated using Aspen Plus. Initially, the RadFrac block (a rigorous distillation calculation method) with Reac-Dist kinetics subroutine was used (as it is the only available kinetics subroutine for RadFrac). However, the Reac-Dist subroutine cannot account for adsorption which is required as adsorption on the catalyst is not negligible. This approach was therefore deemed not possible to model the reactive distillation process.

The RCSTR (a continuous stirred tank reactor model) block in Aspen, on the other hand, allows custom kinetics input that can include the adsorption terms. With the guidance of Professor Len Fabiano and Dave Kolesar a model was devised to represent each reactive stage as an RCSTR block. Since there is no reaction occurring in the rectifying and stripping sections, those sections were modelled as typical RadFrac distillation columns. Figure 16.3 shows the arrangements of the RCSTR and RadFrac blocks.

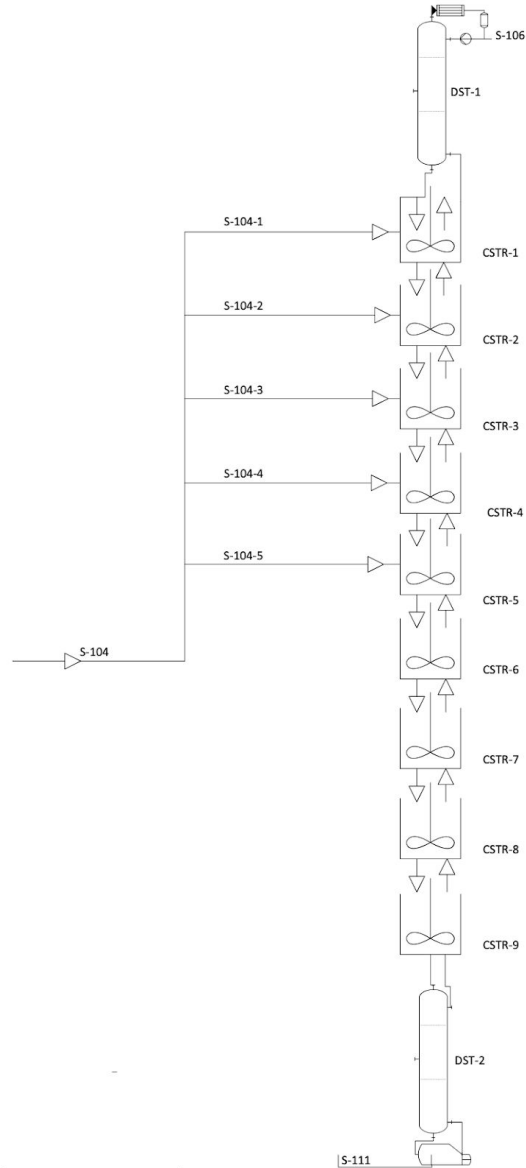


Figure 16.3. Simulation model of the reactive distillation column (RDC-100)

The condenser pressure was chosen to be 700 kPa because the temperature in the reactive stages must be kept below 150°C, the maximum operating temperature for Amberlyst 35; this is particularly necessary because the reaction is exothermic and changing the location of the reactive section (such as higher up the column where the temperature is lower), does not sufficiently decrease the temperature. Figure 16.4 Shows the temperature profile for each theoretical stage. The

temperature is kept as high as possible (below 150°C) in the reactive section to maximize conversion of Methanol (Hosseininejad et al.).

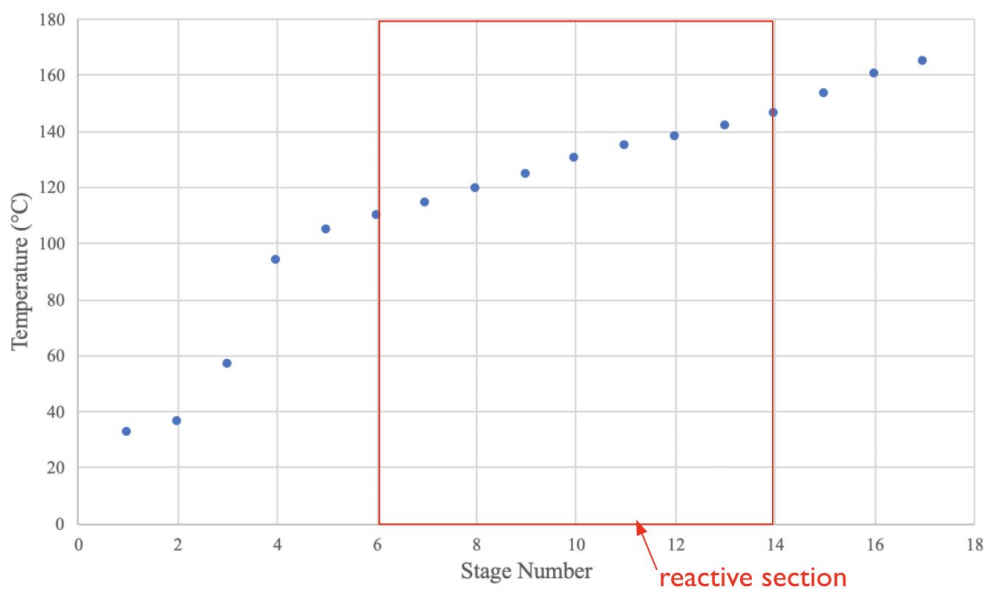


Figure 16.4. Temperature profile of each theoretical stage (excluding condenser and reboiler)

The number of reactive stages were adjusted based on how much unreacted Methanol there is in the last reactive tray (stage number 13) which can be seen in Figure 16.5 as the Methanol mass fraction. Increasing the number of reactive stages was deemed not necessary because the amount of water is larger than Methanol at lower stages (as shown in Figure 16.5) and as water competes with Methanol for the active sites of the catalyst, the amount of Methanol converted will be significantly impeded by water.

The catalyst load for each stage, tabulated in Table 16.1, is decreased for the lower stages because there is less Methanol to react with (indicated by the decrease of mass fraction of Methanol down the column in Figure 16.5), but for stages where the feed streams enter (stages 5 to 9), the load is maintained at 200 kg.

Table 16.1. Catalyst load and corresponding RCSTR block ID for each theoretical reactive stage in the reactive distillation column

Stage Number	CSTR ID	Catalyst Load (kg)
5	CSTR-1	200
6	CSTR-2	200
7	CSTR-3	200
8	CSTR-4	200
9	CSTR-5	200
10	CSTR-6	100
11	CSTR-7	50
12	CSTR-8	40
13	CSTR-9	30

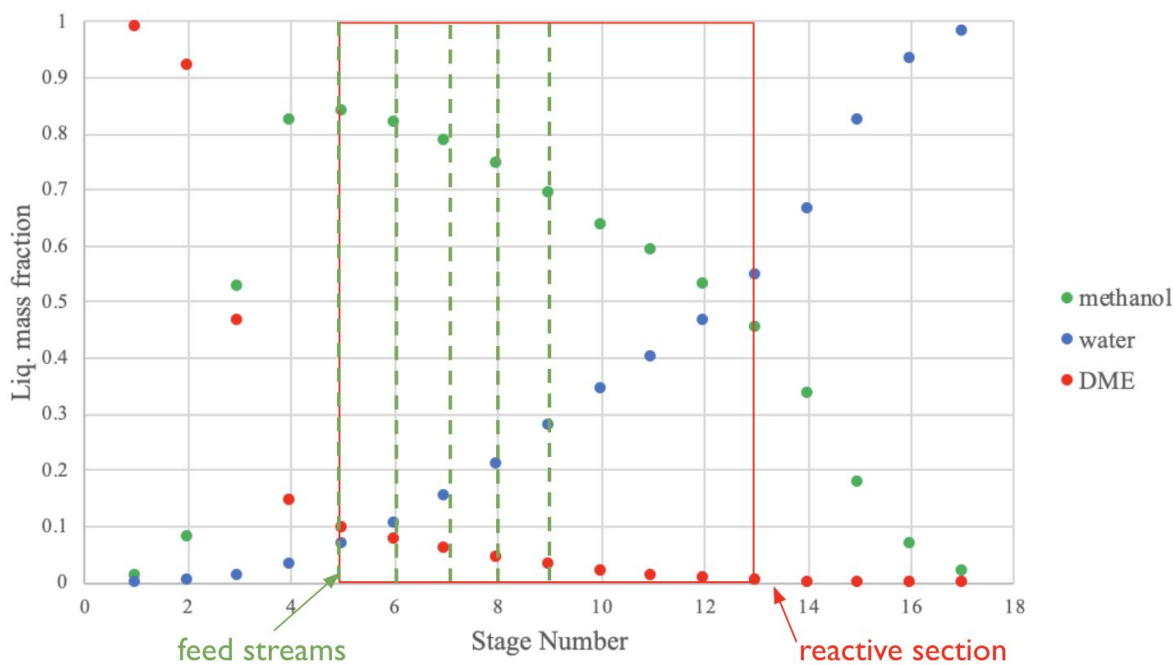


Figure 16.5. Liquid mass fraction of each component on each theoretical stage (excluding condenser and reboiler).

The rectifying section serves to separate DME from the DME, Methanol and water mixture so the light key is DME and the heavy key is Methanol. The stripping section, on the other hand, separates water from the DME, Methanol and water mixture so the light key is Methanol and the heavy key is water. The number of stages for the rectifying and stripping sections were adjusted so that the purity of DME in the distillate has purity of at least 98.5 mass % and the water in the bottom stream has at least 99 mass % purity. While the purity of the distillate is dictated by the ISO standard, a high purity of water in the bottoms is preferred to avoid the need to recycle or treat large quantities of Methanol. The number of stages for the rectifying section was determined to be 4 stages (excluding condenser) and for the stripping section, 4 stages (excluding reboiler) is also required. The simulated purity of the distillate is 99.9% and purity of the bottoms is 99.5%.

Sieved trays are used for each stage in the column and an additional modification was done for the reactive section to accommodate the catalyst. Figure 16.6 shows the proposed configuration of a reactive stage, designed with guidance of Professor Len Fabiano. The catalysts are caged and fitted next to the downcomer thus requiring a larger diameter than the rectifying and stripping sections. The diameters of the rectifying and stripping sections were determined using Aspen Plus; for the rectifying section, the diameter is 1.85 m and for the stripping section, it is 1.04 m. A larger diameter for the rectifying section is needed because there is more vapor at the top of the column and a smaller diameter would lead to weeping. Calculation on the reactive section diameter is shown in Section 28.2 and it was determined to be 2.4 m.

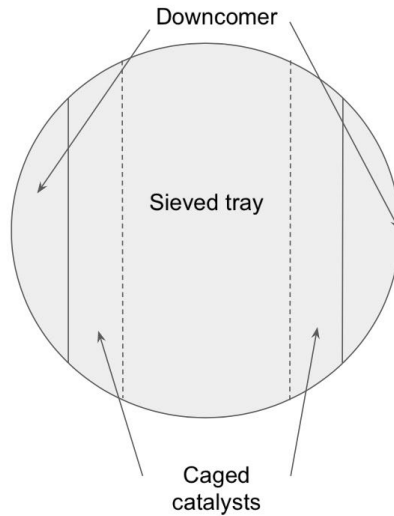


Figure 16.6. Proposed configuration of the reactive stages to accommodate the catalyst

The condenser (C-100/101), reboiler (KB-100/101), reflux accumulator (RD-100/101) and the reflux pump (P-101/105) are necessary equipment for the distillation column. The condenser uses chilled water at 4.4°C (40°F) and the reboiler uses steam at 1138 kPa (165 psig). The dimensions were determined using Aspen and are further detailed in Section 18.4.

The bottom pumps (P-103/108) are required to transport the bottom streams to the feed heat exchange (H-100). Using the assumption that piping pressure drop is 50 kPa, the bottom pumps only need to increase the pressure by 50 kPa. The bottom streams (S-110/112) are then combined (S-113) before entering the heat exchanger. The distillate pumps (P-102/106) are needed both to transport the product and to increase the pressure to storage condition, which is 1000 kPa. As there is pressure drop in piping and in the static mixer (both assumed to be 50 kPa), the pumps need to increase pressure to 1100 kPa. The two distillate streams (S-107/108) are then combined (S-115).

16.3 Segment 3 – Product

Segment 3 of the process flow diagram shown in Figure 16.7 largely deals with the storage of lubricant, mixing of lubricant with DME product stream and eventual storage of the DME and lubricant mixture. The equipment involved is a storage tank (T-101) for the mineral oil lubricant, pump for the lubricant (P-104), static mixer (M-100) to incorporate the lubricant into the DME product stream and storage tanks (T-102) for the finished product.

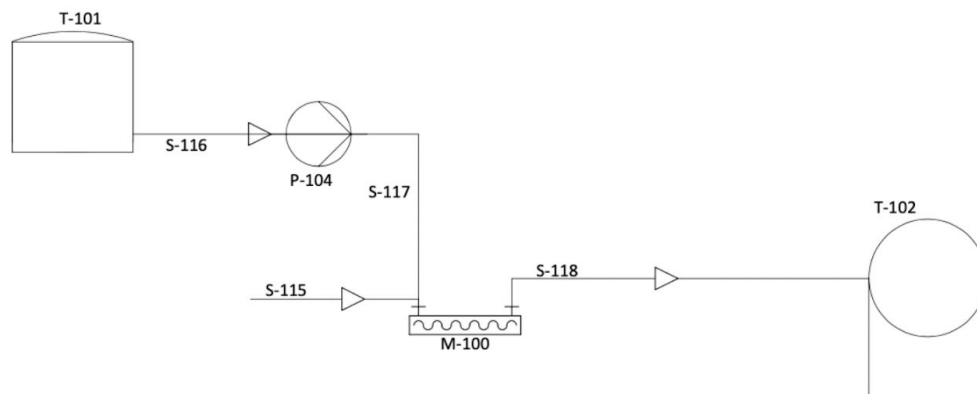


Figure 16.7. Segment 3 of the process flow diagram.

The lubricant storage serves as storage for the mineral oil needed to make the DME viable for a diesel replacement. The tank, 130.6 cubic meters in volume, will be of carbon steel cone-roof construction and hold the lubricant at ambient temperature and pressure (25°C and 101 kPa). The tank has a flow rate of 31.9 kg/hr to P-104, but the volume of the tank was calculated with more consideration towards how it would be delivered. The mineral oil will be shipped by rail from Houston in train cars of about 113.6 cubic meters, and so following specifications from Seider et al., the tank is designed to be 130.6 cubic meters. The pump (P-104) is used to both transport the lubricant from storage (S-116) into the mixer and to increase the lubricant pressure for storage condition which is 1000 kPa. Accounting for pressure drop in piping and in the mixer (both assumed

to be 50 kPa), the pump needs to increase pressure to 1100 kPa. The pressurized lubricant (S-117) and the pressurized DME product stream (S-115) are combined using the static mixer (M-100). The mixture (S-118) is then stored in pressurized storage at 1000 kPa. The tank farm (T-102) is the final design step included in the design of the DME plant as specified by the problem statement. From here, truck-loading spots (L-100) will be further fabricated to load the trucks from T-102. The DME storage will be two carbon steel constructed spherical tanks of 3,785.4 cum each. Each tank will have the capacity to store three days worth of final product DME, totaling six days worth of on-site storage in the tank farm for the product DME. The tanks will store the DME at the same conditions as the product stream feeding the tanks, S-118 (31.3°C and 1000 kPa). These conditions will ensure that the DME stays in liquid form, even when the tanks heat up some due the heat and sun. The tanks are spherical in design to accommodate the larger volume (1,000,000 gallons a piece) and higher pressure. The tanks will hold the DME at these conditions to prevent degradation and to prevent the temperature from rising.

16.4 Segment 4 – Waste

As the dehydration reaction produces only DME and water, there is no byproduct that can be monetized; the only waste stream produced is water with small quantities of Methanol and DME. In order to minimize environmental impacts, biotreatment is used to manage the Methanol and DME in the bottoms wastewater. The combined stream (S-114) leaving the DME plant has a flow rate that is 13,893 kg/hr with 99.5% by weight of that being water, 0.5% of that being Methanol, and a trace amount of DME. Although small amounts, these impurities still need to be removed before the wastewater is able to be released into the Neches River nearby. The DME plant's wastewater treatment

will utilize a secondary treatment that will remove the dissolved organic compounds by means of biological degradation (Seider et al.). The DME plant utilizes this biotreatment as a utility with an associated utility cost, \$0.33/kg of organic removed, to remove the Methanol and trace DME via an activated sludge. The exact process by which this will occur is beyond the scope of the problem statement and will most likely be handled by private or municipal treatment plants. If the location is off-site there may be some pretreatment that can be addressed if the private or municipal plant requires it, but due to the simple nature of the plant's wastewater this should not be necessary. This is a small price to pay for the enhanced stream and limited impact on the Texas ecosystem. Figure 16.8 below shows this segment of the process flow diagram. This process is regulated and governed by the U.S. Clean Water Act.

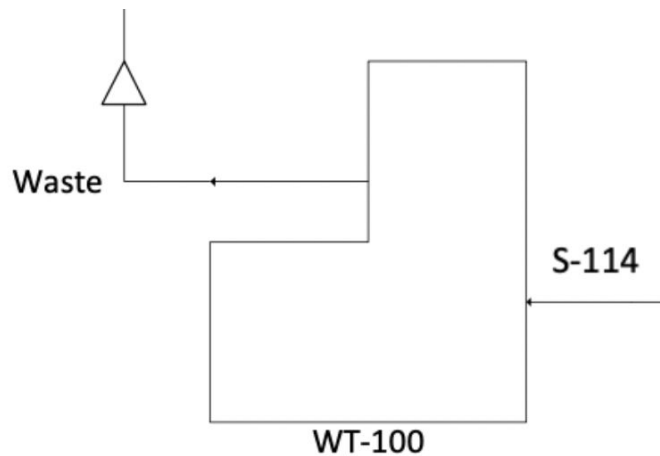


Figure 16.8. Segment Four of the Process Flow Diagram

17 Energy Balance and Utility Requirements

17.1 Energy Requirements

The heat exchanger, pumps, column condensers and column reboilers are the main contributors to the energy requirement of the plant. The heat duties and power requirement are broken down for each equipment in Table 17.1, which were determined using Aspen.

Table 17.1. Heat duties and power required for each equipment

Equipment ID	Requirement Description	Quantity (kW)
H-100	Feed heat exchanger heat duty	1454
KB-100/101	Column reboiler heat duty	6214 (per reboiler)
C-100/101	Column condenser heat duty	6957 (per condenser)
P-100	Feed pump power requirement	17.16
P-101/105	Reflux pump power requirement	18.6 (per pump)
P-102/106	Distillate pump power requirement	5.45 (per pump)
P-103/108	Bottom pump power requirement	0.292 (per pump)
P-104	Lubricant pump power requirement	0.0372

For each heat exchanger, the incoming and target temperatures are shown in Table 17.2 and indicates that temperature differences between the streams are not sufficiently large to network the heat exchangers. However, the waste stream (S-113) (i.e. the combined bottom streams from the columns) is at 167°C and can be used to heat the feed before it is transferred to a biotreatment facility.

Table 17.2. Incoming and target temperatures for each heat exchangers

Equipment ID	Description	Incoming Temp (°C)	Target Temp (°C)
H-100	Feed heat exchanger	25.3	60.9
KB-100/101	Column reboiler	167 (liquid)	167 (vapor)
C-100/101	Column condenser	30.9 (vapor)	30.9 (liquid)

17.2 Utility Demands

The energy requirement for the pumps are all fulfilled using electricity. As for the heat exchangers, the feed heat exchanger (H-100), as discussed in Section 17.1, does not require utility because the waste stream can be used as the heat source. The reboiler, however, requires steam at 1138 kPa (165 psig) and the quantity was determined from Aspen. For the condenser, chilled water at 4.44°C (40°F) is used (following guidelines from Seider et al.) and the quantity was also determined using Aspen. Table 17.3 summarizes the required utilities for each equipment. The wastewater treatment is also included because the waste stream (S-114) contains a small amount of Methanol that needs to be removed. The waste stream is 99.5 mass % water so it was deemed uneconomical to salvage the 0.5 mass % of Methanol.

Table 17.3. Utility requirements for each equipment. The wastewater treatment requirement is given as the quantity of Methanol to be removed per hour.

Utility	Equipment ID	Description	Quantity
Chilled water (4.44 °C / 40 °F)	C-100	Cool vapor stream to liquid (required heat duty of -6957 kW)	282,000 kg/hr
	C-101		282,000 kg/hr
Total (kg)			564,000 kg/hr
Low pressure steam (1138 kPa / 165 psig)	KB-100	Heat liquid stream to vapor (required heat duty of 6214 kW)	11.2 kg/hr
	KB-101		11.2 kg/hr
Total (kg)			22.4 kg/hr
Electricity	P-100	Increase pressure from 100 kPa to 750 kPa	17.2 kW
	P-101	Reflux pump	18.6 kW
	P-105		18.6 kW
	P-102	Increase pressure from 700 kPa to 1100 kPa	5.45 kW
	P-106		5.45 kW
	P-103	Increase pressure from 737 kPa to 787 kPa	0.292 kW
	P-108		0.292 kW
Total (kW)			65.9 kW
Wastewater Treatment	WT-100	Remove Methanol from bottoms	69.5 kg/hr
Total (kg)			69.5 kg/hr

18 Equipment List and Unit Descriptions

18.1 Pumps

Feed Pump

Unit ID: P-100	Outlet Temperature: 25.3°C
Type: Centrifugal pump	Pressure: 750 kPa
Material: Cast Iron	Work: 17.16 kW
Specification Sheet: Page 59	Bare module cost: \$54,300

The feed pump was designed using Aspen Plus for a pressure increase of 650 kPa with flow rate of 62.2 cum/hr; the head required for the pressure increase is 83.6 m. Following heuristics from Seider et al., a radial centrifugal pump with 1 stage, shaft rpm of 3600, Vertical Split Case (VSC) orientation and maximum motor hp of 75 is appropriate. As the feed stream contains 99.99% pure Methanol and is non-corrosive, cast iron was chosen as the material. The cost of the pump is calculated and detailed in Section 28.3.1. The calculated cost was found to corroborate with cost computed by Aspen Process Economic Analyzer (APEA).

Distillate Pumps

Unit ID: P-102 and P-106	Outlet Temperature: 31.0°C
Type: Centrifugal pump	Pressure: 1100 kPa
Material: Cast Iron	Work: 5.45 kW
Specification Sheet: Page 60	Bare Module Cost: \$43,200

The distillate pump is required to transport the distillate stream with flow rate of 457 cum/hr, to the mixer and eventually to storage. The pressure increase is 400 kPa so that it can be stored at 1000 kPa while accounting for piping and mixer pressure drop (assumed to be 50 kPa each). The head required for this pressure increase is 63.3 m. A radial centrifugal pump with 1 stage, shaft rpm of 3600, Vertical Split Case (VSC) orientation and maximum motor hp of 75 is chosen following guidelines (Seider et al.). The material of the pump is chosen as cast iron because the stream is non-corrosive so a higher grade material is not necessary. The bare module cost was computed using APEA.

Bottom Pumps

Unit ID: P-103 and P-108	Outlet Temperature: 166.6°C
Type: Centrifugal pump	Pressure: 787.4 kPa
Material: Stainless Steel	Work: 0.292 kW
Specification Sheet: Page 61	Bare Module Cost: \$46,800

The bottom pump is used to transport the bottom stream with flow rate of 137.5 cum/hr, to the feed heat exchanger and eventually to the biotreatment facility. To account for pressure drop caused by piping, the pressure increase is 50 kPa and head required is 6.05 m. A radial centrifugal pump with 1 stage, shaft rpm of 3600, Vertical Split Case (VSC) orientation and maximum motor hp of 75 is chosen. Stainless steel is chosen because the catalyst used in the reaction is acidic so the bottom stream is likely to contain traces of corrosive components.

Lubricant Pump

Unit ID: P-104	Outlet Temperature: 26.5°C
Type: Centrifugal pump	Pressure: 1100 kPa
Material: Cast Iron	Work: 0.0372 kW
Specification Sheet: Page 62	Bare Module Cost: \$41,500

The lubricant pump is used to transport the lubricant stream flowing at ~ 0.04 cum/hr to the mixer and eventually to storage. To account for pressure drop caused by piping and mixing (assumed to be 50 kPa each) and to eventually be stored at 1000 kPa, the required pressure increase is 1100 kPa and the head required is 126.5 m. A radial centrifugal pump with 1 stage, shaft rpm of 3600, Horizontal Split Case (HSC) orientation and maximum motor hp of 75 is chosen (Seider et al.). Cast iron is chosen because the lubricant is mineral oil and is non-corrosive so a higher grade is not necessary. APEA was used for the cost estimation.

18.2 Heat Exchangers

Feed Heat Exchanger

Unit ID: H-100	Inlet Hot Stream Temperature: 166.6°C
Type: Centrifugal pump	Outlet Hot Stream Temperature: 32.9°C
Material: Carbon Steel and Stainless Steel 316	Inlet Cold Stream Temperature: 25.3°C
Heat Duty: 1454 kW	Outlet Cold Stream Temperature: 60.9°C
Pressure: 799kPa	Area: 7.65m ²
Specification Sheet: Page 63	Bare Module Cost: \$90,600

The combined bottom stream (S-113) exiting the reactive distillation columns (RDC-100 and RDC-101) is utilized as the hot stream. The hot stream has a flow rate of 13,893 kg/hr which requires the heat exchanger area to be 7.65 m². The material of the heat exchanger is chosen to be stainless steel for the tube and carbon steel for the shell because while the cold stream contains non-corrosive material, the hot stream is likely to be slightly acidic due to the catalyst used in the reactive distillation columns. The heat exchanger has a log mean temperature difference (LMTD) of 81.04°C and heat transfer coefficient of 2344 W/m²°C. Using APEA, the bare module cost was estimated as \$90,600.

18.3 Mixer

Static Mixer

Unit ID: M-100

Temperature: 30.9°C

Material: Carbon Steel

Pressure: 1050 kPa

Specification Sheet: Page 64

Bare Module Cost: \$200,000

The static mixer is used to mix the lubricant with the DME stream before storage. The discharge flow rate is 915.2 cum/hr and as the required concentration of lubricant in the discharge stream is 900 ppm – a negligible amount, this flow rate is largely dominated by the DME stream. A pressure drop of 50 kPa in the static mixer is also assumed so that the DME and lubricant mixture can be stored at 1000 kPa and because neither the DME nor the lubricant stream contains corrosive components, carbon steel was chosen as the material for the mixer. The purchase cost is estimated as \$160,000 and the bare module factor as 1.25 from consultant advice.

18.4 Column

Reactive Distillation Column

Unit ID: RDC-100 and RDC-101	Pressure: 700 kPa
Type: Reactive Distillation Column	Height: 27.4 m
Material: Stainless Steel	Diameters: 1.85 m, 2.4 m, 1.0 m
Number of Theoretical Stages: 17	Condenser Temperature: 30.9°C
Number of Actual Stages: 38	Reboiler Temperature: 166.6°C
Specification Sheet: Page 65	Bare Module Cost: \$2,495,491

The reactive distillation column was simulated using Aspen Plus and consists of three sections: rectifying, reactive and stripping sections. The theoretical number of stages for the rectifying and stripping sections are 4 each (excluding reboiler and condenser), and for the reactive section, 9 stages; so in total 17 theoretical stages. The condenser pressure is 700 kPa and a pressure drop of 6.9 kPa at each stage was approximated to account for lower tray efficiencies, as advised by Professor Leonard Fabiano.

The tray efficiencies of the rectifying and stripping sections were estimated using the O'Connell correlation with data from Aspen Plus. As the reactive section was modelled as a series of continuous-stirred tank reactors (CSTRs), the efficiencies of the reactive stages were approximated as the average of the efficiencies of the rectifying and stripping sections (Section 28.2). The total number of actual trays required is 38 trays excluding reboiler and condenser and the feed streams which enter above stages 5, 6, 7, 8 and 9 in the theoretical trays, enter above stages 11, 13, 15, 17 and 19 in the actual trays. Assuming tray spacing of 0.61 m, 2.44 m for sump and 1.83 m for disengagement and nozzle (as advised by Professor Len Fabiano), the total height of the column is 27.4 m.

The reboiler, reflux accumulator and reflux pump were designed using Aspen. The reboiler is a kettle vaporizer and uses steam at 1138 kPa (165 psig) as the heat source. For a molar boil up ratio of 1.56, the required heat duty is 6214 kW. The material of the reboiler was chosen to be stainless steel to prevent corrosion because the liquid at the bottom is likely to contain traces of acidic components from the catalyst.

The reflux accumulator and pump were sized using Aspen. The reflux accumulator holds a volume of 11.4 m³ and has a diameter of 1.67 m. The reflux pump is designed to transport 107.5 cum/hr of the distillate back to the reactor. The material of the reflux accumulator is carbon steel and cast iron for the pump, as the distillate stream does not contain acidic components.

The total condenser was designed as a shell and tube heat exchanger on Aspen and using guidelines (Seider et al.), chilled water at 4.4°C (40°F) is used. From Aspen, with a molar reflux ratio of 2.56, the required heat duty to condense the vapor was found to be 6957 kW and the required heat exchanger area is 859 m². The log-mean-temperature-difference (LMTD) of the condenser is 9.54°F and the heat transfer coefficient is 850 W/m²°C. The estimated cost is calculated using APEA.

The tower cost is calculated following heuristics outlined in Seider et al. The tower is a stainless steel pressure vessel with three diameters. The bottom/stripping section has a 1.0 m diameter and is 7.3 m in height (including sump), the middle/reactive section has a 2.4 m diameter and is 12.2 m in height, and the top/rectifying section has a 1.85 m diameter and is 7.9 m in height. The thickness to withstand the internal pressure (t_w) was found normally based on equations laid out in Seider et al. However, the thickness to withstand wind load and earthquakes at the bottom of the column was conservatively estimated using the largest diameter (that of the middle section, 2.4 m). This extra thickness was then linearly scaled down all the way up the column. The average thickness of each section was then used

for the weight calculations. For weight and cost calculations each section was viewed as if it were an individual column with height equal to that of the entire column (27.4 m). Then, these 3 costs were averaged, weighted by the height of each section. This was done for both the vessel cost (C_V) and the platform and ladders cost (C_{PL}). The purchase cost was determined to be \$400,021 with a bare module factor of 4.16. This results in a final bare module cost of \$1,664,0991 for the tower. Calculations are detailed in section 28.3.3.

18.5 Storage

Methanol tank

Unit ID: T-100	Storage Temperature: 25.0°C
Type: Floating-roof	Pressure: 101 kPa
Material: Carbon Steel	Volume: 2,840 cum
Specification Sheet: Page 66	Bare module cost: \$1,963,993

The feed storage tank was designed to be able to store Methanol in the case of unforeseen closures on the feed pipeline from Natgasoline. The tank was designed to store Methanol at ambient temperature and pressure (25.0°C and 101 kPa) in one floating-roof tank. One tank is required to meet the 789,000 gallon (2986 cubic meter) requirement to store two days worth of Methanol for feed to the columns. The tank's flow rate will be continuous at 1,538 kmol/hr in and out of the tank. The feed stream contains Methanol with a 99.99% purity and is non-corrosive so carbon steel is the material of choice. The tank has a total bare module cost of \$1,963,993.

DME product tank

Unit ID: T-102	Storage Temperature: 31.3°C
Type: Spherical	Pressure: 1,000 kPa
Material: Carbon Steel	Volume: 3,785.4 cum
Specification Sheet: Page 67	Bare module cost: \$10,221,620

The DME storage tanks are the final step in the total plant design for the product. From here, tankers will be filled with the DME, but this was not included in the scope of the problem. Two tanks of 1,000,000 gallons a piece (3,785.4 cum) will be built in order for the plant to have enough capacity for six full days of product. This is done so that in the case of long weekends or holidays where trucks are unable to be filled the plant can remain at full production capacity without shutting down due to lack of storage. In addition, when the plant is at 50% downturn there will be an excess supply to account for unexpected surges in demand. Furthermore, in case the plant needs to unexpectedly shut down there will be almost a week's worth of DME to support the trucking traffic and not cause any disruption to supply chains dependent on the DME fuel. The tanks will be made to store the product DME at 31.3°C, the temperature of the distillate. The tank's pressure will be 1,000 kPa so that DME remains liquid even at slightly higher temperature. The spherical tank design was chosen to accommodate the large volume and higher pressure of the storage. The tanks have a flow rate of 17,709 kg/hr each with a feed that is 99.9% DME by mass and non-corrosive, and so carbon steel was selected as the build material. The two tanks combined have a total bare module cost of \$10,221,620.

Lubricant tank

Unit ID: T-101	Storage Temperature: 25.0°C
Type: Cone-roof	Pressure: 101 kPa
Material: Carbon Steel	Volume: 130.6 cum
Specification Sheet: Page 68	Bare module cost: \$238,658

In order for the product DME to be viable for use as a diesel replacement it requires mixing with a lubricant. This lubricant will be added and mixed into the product DME stream using the static mixer (M-100). While the required amount is only 900 ppm, or about 0.04 cubic meters per hour, the size of the tank was determined more on how the lubricant would be delivered. The mineral oil serving as the lubricant will be shipped in from Houston via train. The rail cars carrying the mineral oil will be about 113.5 cubic meters, and so following recommendations from Seider et al. this led to a storage tank of 130.6 cubic meters. The lubricant will be stored at ambient temperature and pressure: 25.0°C and 101 kPa. Only one tank (cone-roof) will be required to hold this volume and refilling will be done once approximately every four months. The contents will be mineral oil of presumably extremely high purity and will be non-corrosive, leading to a carbon steel construction. The single tank has a total bare module cost of \$238,658.

19 Specification Sheets

Below are the equipment specification sheets for the previously mentioned equipment.

SPECIFICATION SHEET
FEED PUMP

Identification:

Item No: P-100
No. Required: 1

Date: April 15, 2020
By: ACJ

Function: Pressurize ethanol feed

Operation: Continuous

Materials	Feed	Discharge
Temperature(°C):	25.0	25.3
Pressure (kPa):	100	750
Mass Flow (kg/hr):	49280	49280
Component Mass Flow (kg/hr)		
Methanol	49280	49280
Water	-	-
Dimethyl Ether	-	-
Molar Flow (kmol/hr):	1538	1538
Volume Flow (cum/hr)	62.15	62.18

Design Data:

Material: Cast Iron
No. Stages: 1
Shaft rpm: 3600
Type: Centrifugal Pump
Head: 83.6 m
Temperature: 25.3°C

Pressure: 750 kPa

Utilities: Electricity at 17.16 kW

Comments & Drawings: Refer to process flow diagrams

SPECIFICATION SHEET
DISTILLATE PUMP

Identification: Item No: P-102/106 Date: April 15, 2020
No. Required: 2 By: ACJ

Function: Pressurize distillate stream to transport to mixer and eventually storage

Operation: Continuous

Materials	Feed	Discharge
Temperature(°C):	30.9	31.3
Pressure (kPa):	699.8	1100
Mass Flow (kg/hr):	17694.3	17694.3
Component Mass Flow (kg/hr)		
Methanol	17.5	17.5
Water	0.147	0.147
Dimethyl Ether	17677	17677
Molar Flow (kmol/hr):	384.3	384.3
Volume Flow (cum/hr)	27.4	27.4

Design Data: Material: Cast Iron Pressure: 1100 kPa
No. Stages: 1
Shaft rpm: 3600
Type: Centrifugal Pump
Head: 63.3 m
Temperature: 31.0°C

Utilities: Electricity at 5.45 kW

Comments & Drawings: Refer to process flow diagrams

SPECIFICATION SHEET
BOTTOM PUMP

Identification:

Item No: P-103/108
No. Required: 2

Date: April 15, 2019
By: ACJ

Function: Pressurize bottom stream to transport to cooling tower

Operation: Continuous

Materials	Feed	Discharge
Temperature(°C):	166.6	166.6
Pressure (kPa):	737.4	787.4
Mass Flow (kg/hr):	6946	6946
Component Mass Flow (kg/hr)		
Methanol	34.73	34.73
Water	6912	6913
Dimethyl Ether	trace	trace
Molar Flow (kmol/hr):	384.7	384.7
Volume Flow (cum/hr)	137.5	137.5

Design Data:

Material: Stainless Steel
No. Stages: 1
Shaft rpm: 3600
Type: Centrifugal Pump
Head: 6.05 m
Temperature: 166.6°C

Pressure: 787.4 kPa

Utilities: Electricity at 0.292 kW

Comments & Drawings: Refer to process flow diagrams

SPECIFICATION SHEET
LUBRICANT PUMP

Identification: Item No: P-104 Date: April 15, 2019
No. Required: 1 By: ACJ

Function: Pressurize lubricant stream to transport to mixer and eventually storage

Operation: Continuous

Materials	Feed	Discharge
Temperature(°C):	25.0	26.5
Pressure (kPa):	101.3	1100
Mass Flow (kg/hr):	31.9	31.9
Component Mass Flow (kg/hr)		
Mineral Oil	31.9	31.9
Molar Flow (kmol/hr):	~ 0.07	~ 0.07
Volume Flow (cum/hr)	~ 0.04	~ 0.04

Design Data: Material: Cast Iron Pressure: 1100 kPa
No. Stages: 1
Shaft rpm: 3600
Type: Centrifugal Pump
Head: 126.5 m
Temperature: 26.5°C

Utilities: Electricity at 0.0372 kW

Comments & Drawings: Refer to process flow diagrams

SPECIFICATION SHEET
FEED HEAT EXCHANGER

Identification:

Item No: H-100
No. Required: 1

Date: April 15, 2020
By: ACJ

Function: Heat methanol feed stream for reactive distillation with bottom stream

Operation: Continuous

Materials	Cold In	Cold Out	Hot In	Hot Out
Temperature(°C)	25.3	60.9	166.6	84.9
Pressure (kPa)	750	716	737	712
Mass Flow (kg/hr)	49281	49281	13893	13893
Component Mass Flow (kg/hr)				
Methanol	49281	49281	69.5	69.5
Water	-	-	13823	13823
Dimethyl Ether	-	-	trace	trace
Molar Flow (kmol/hr)	1538	1538	769.5	769.5
Volume Flow (cum/hr)	62.2	65.8	16.5	14.9

Design Data:

Surface Area: 7.65 m²
Pressure: 799 kPa
LMTD: 81.04°C
Heat Duty: 1454 kW
Transfer Coefficients: 2344 W/m²°C
Type: BEM
Material: Carbon Steel (shell) / Stainless Steel 316 (tube)

Utilities: None

Comments & Drawings: Refer to process flow diagrams

SPECIFICATION SHEET
STATIC MIXER

Identification:

Item No: M-100
No. Required: 1

Date: April 15, 2020
By: ACJ

Function: Mixes lubricant and DME streams

Operation: Continuous

Materials	Feed 1	Feed 2	Discharge
Temperature(°C)	30.9	26.5	30.9
Pressure (kPa)	1100	1100	1050
Mass Flow (kg/hr)	35386	31.9	35418
Component Mass Flow (kg/hr)			
Methanol	35.1	-	35.1
Water	0.294	-	0.294
Dimethyl Ether	35351	-	35351
Mineral Oil	-	31.9	31.9
Molar Flow (kmol/hr)	145.1	~ 0.07	145.2
Volume Flow (cum/hr)	915.2	~ 0.04	915.2

Design Data:

Material: Carbon Steel

Pressure: 1050 kPa

Type: Static Mixer

Utilities: None

Comments& Drawings: Refer to process flow diagrams

SPECIFICATION SHEET
REACTIVE DISTILLATION COLUMN

Identification:

Item No: RDC-100/101
No. Required: 2

Date: April 15, 2020
By: ACJ

Function: Production and separation of dimethyl ether and water

Operation: Continuous

Materials	Feeds	Bottoms	Distillate
Temperature(°C)	60.0	166.6	30.9
Pressure (kPa)	700	737	700
Mass Flow (kg/hr)	24639	6946	17693
Component Mass Flow (kg/hr)			
Methanol	24639	34.73	17.55
Water	-	6912	0.1469
Dimethyl Ether	-	trace	17675
Molar Flow (kmol/hr)	769	384.7	384.2
Volume Flow (cum/hr)	356.1	8.25	27.43

Design Data:

Number of trays: 38
Feed Trays: 11, 13, 15, 17, 19
Tray Spacing: 0.30 m
Height: 27.4 m
Diameter (Top): 1.85 m
Diameter (Middle): 2.4 m
Diameter (Bottom): 1.0 m
Sump Height: 2.4 m
Disengagement Height: 1.8 m

Material: Stainless Steel 316
Pressure: 700 kPa
Molar reflux ratio: 2.56
Molar boil up ratio: 1.56

Utilities: Chilled water 4.4°C at 152.2 kg/hr and 165 psig steam at 11.2 kg/hr

Comments & Drawings: Refer to process flow diagrams

SPECIFICATION SHEET
METHANOL FEED STORAGE TANK

Identification:

Item No: T-100
No. Required: 1

Date: April 15, 2020
By: ACJ

Function: Store excess Methanol for feed to production process

Operation: Continuous

Materials	To Process
Temperature(°C)	25.0
Pressure (kPa)	101 kPa
Mass Flow (kg/hr) Component	49,280
Mass Flow (kg/hr)	
Methanol	49,280
Water	0.0
DME	0.0
Lubricant	0.0
Molar Flow (kmol/hr)	1,538
Volumetric Flow (cum/hr)	62.2

Design Data:

Amount Stored: 2 Days
Tank Type: Floating-roof
Volume: 2,986 cum
Temperature: 25.0°C
Pressure: 101 kPa
Material: Carbon Steel

Utilities: None

Comments & Drawings: Refer to process flow diagrams

SPECIFICATION SHEET
DME STORAGE TANK

Identification:

Item No: T-102
No. Required: 2

Date: April 15, 2020
By: ACJ

Function: Store DME product from production

Operation: Continuous

Materials	From Process
Temperature(°C)	31.3
Pressure (kPA)	1,000
Mass Flow (kg/hr) Component	17,709
Mass Flow (kg/hr)	
Methanol	17.55
Water	0.147
DME	17,675.5
Mineral Oil	16.0
Molar Flow (kmol/hr)	72.6
Volumetric Flow (cum/hr)	27.6

Design Data:

Amount Stored: 3 Days
Tank Type: Spherical
Volume: 3,785.4 cum
Temperature: 31.3°C
Pressure: 1,000 kPa
Material: Carbon Steel

Utilities: None

Comments & Drawings: Refer to process flow diagrams.

SPECIFICATION SHEET
LUBRICANT FEED STORAGE TANK

Identification: Item No: T-101 Date: April 15, 2020
No. Required: 1 By: ACJ

Function: Store excess lubricant for feed to production process

Operation: Continuous

Materials	To Process
Temperature(°C)	25.0
Pressure (kPa)	101
Mass Flow (kg/hr)	31.9
Component Mass Flow (kg/hr)	
Methanol	0.0
Water	0.0
DME	0.0
Lubricant	31.9
Molar Flow (kmol/hr)	0.07
Volumetric Flow (cum/hr)	0.04

Design Data: Amount Stored: 1 Day
Tank Type: Cone-roof
Volume: 130.6 cum
Temperature: 25.0°C
Pressure: 101 kPa
Material: Carbon Steel

Utilities: None

Comments & Drawings: Refer to process flow diagrams.

20 Equipment Cost Summary

The total capital investment (C_{TCI}) calculated is \$30,912,176 (discounted working capital); this is the cost for the design, construction and start-up of the plant. \$17,982,000 of the TCI is from the total bare module cost of the equipment. Figure 20.1 shows the breakdown of how much each type of equipment contributed to the cost. 69% of the cost (\$12,424,000) is from the Methanol, DME and lubricant storage tanks. While the sum of the cost for all the other equipment is only \$5,557,000, significantly less than cost of storage. Of the \$12,424,000 cost in storage, \$10,222,000 is for DME storage (T-102). It is therefore highly recommended to increase frequency of product transportation out of the plant to reduce the DME storage load; the proposed storage tanks for DME are designed to store about 6 days of produced DME.

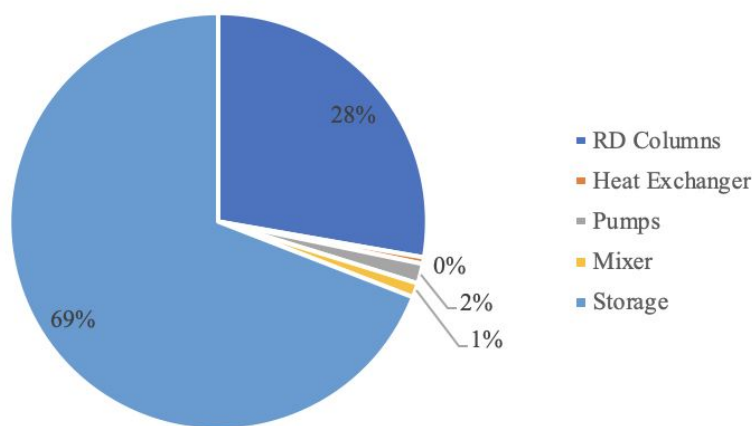


Figure 20.1. Breakdown of the contributions of each equipment to the total bare module cost. The reactive distillation (RD) columns include cost of condenser, reboiler, reflux accumulator and reflux pump.

The cost of each equipment is further broken down in Table 20.1. The cost of the towers (RDC-100/101) and storage tanks (T-100/101/102) were calculated following guidelines from Seider

et al. and the calculations are detailed in Section 28.2. The static mixer (M-100) costs were estimated following consultant advice. The costs of the remaining equipment (heat exchanger, condensers, reboilers and pump) were determined using Aspen Process Economic Analyzer (APEA).

Table 20.1. Estimated purchase cost and bare module cost for each equipment.

Equipment ID	Equipment Type	Purchase Cost (USD)	Bare Module Cost (USD)
RDC-100/101	Fabricated Equipment	400,022	1,664,091 (per column)
C-100/101	Fabricated Equipment	107,600	246,500 (per condenser)
RD-100/101	Fabricated Equipment	31,200	126,700 (per vessel)
P-101/105	Process Machinery	9,900	64,600 (per pump)
KB-100/101	Fabricated Equipment	222,400	393,600 (per reboiler)
P-102/106	Process Machinery	6,500	43,200 (per pump)
P-103/108	Process Machinery	6,000	46,800 (per pump)
P-100	Process Machinery	9,400	54,300
P-104	Process Machinery	16,000	41,500
H-100	Fabricated Equipment	11,000	90,600
M-100	Process Machinery	160,000	200,000
T-100	Methanol Storage	490,998	1,963,993
T-101	Lubricant Storage	59,664	238,658
T-102	DME Storage	5,110,810	10,221,620

21 Fixed-capital Investment Summary

All percentage estimates are based on heuristics found in Seider et al. regarding plant size and complexity. Based on the equipment list and costs found in Table 20.1 and the \$12,200 for the initial charge of catalyst, the total bare module cost (C_{TBM}) for the plant is \$17,793,851. The cost of site preparations and the cost of service facilities were estimated to be 5% of the total bare module cost. Adding these to C_{TBM} results in direct permanent investment (C_{DPI}), which equals \$19,573,236. To reach total depreciable capital (C_{TDC}), cost of contingencies and contractor fees is now included, estimated to be 18% of C_{DPI} . This means C_{TDC} equals \$23,096,419. The next step is to add cost of land, estimated to be 2% of C_{TDC} , and cost of plant startup, estimated to be 10% of C_{TDC} . This brings us to a total permanent investment (C_{TPI}) of \$25,867,989. Generally, this number would need to be adjusted by multiplying it by a site factor; however, we are located in the Gulf Coast region of the US which has a site factor of 1. The last step to estimating the total capital investment (C_{TCI}) is to add in working capital. The working capital calculations rely on several assumptions regarding accounts receivables, cash reserves, accounts payable, raw material inventory, and product inventory. The assumptions used here are that 30 days worth of accounts receivables, cash reserves, and accounts payable will always be maintained, that 4 days worth of product will always be in storage, and that 2 days worth of Methanol feed will always be on site. Based on overall input of Methanol and output of DME, as well as start-up over 3 years, the net present value of the working capital investment is \$5,044,187. Adding this to C_{TPI} brings us to a C_{TCI} of \$30,912,176 (the value used for ROI calculations includes undiscounted values for working capital, resulting in a total capital investment of \$31,627,799).

Table 21.1 Components of Capital Investment

Total bare-module investment, C_{TBM}	\$ 17,793,851				
Cost of site preparations, C_{site}	\$ 889,693				
Cost of service facilities, C_{serv}	\$ 889,693				
Total of direct permanent investment, C_{DPI}		\$ 19,573,236			
Cost of contingencies and contractor fees, C_{cont}		\$ 3,523,182			
Total depreciable capital, C_{TDC}			\$ 23,096,419		
Cost of land, C_{land}			\$ 461,928		
Cost of plant startup, $C_{startup}$			\$ 2,309,642		
Total permanent investment, C_{TPI}				\$ 25,867,989	
Working Capital (discounted), C_{wc}				\$ 5,044,187	
Total capital investment, C_{TCI}					\$ 30,912,176

22 Operating Costs

22.1 Variable Operating Costs

22.1.1 Raw Materials

The raw materials needed for the DME plant are: Methanol, lubricant (mineral oil), and Amberlyst 35 (reaction catalyst). The Methanol feed has been discussed previously and will be piped in continuously by Natgasoline to the Methanol storage tanks. The cost of this Methanol has been estimated using Methanex which provides a historical database of Methanol costs. Using price points from five previous months it has been estimated that the cost of the Methanol will be \$1.03/gal or \$0.344/kg plus shipping, consistent with the end of last year. In addition to this cost, due to the massive amount of Methanol being purchased, there is a chance that a discount could be negotiated. Also, since the Methanol will be provided throughout the year it allows for a consistent price through the year assuming the price is negotiated at the beginning of each year. In order to be thorough, no discounted rate was considered in this variable cost analysis. The lubricant has also been previously discussed and has a price of \$1.65/lb, plus shipping. The catalyst, Amberlyst 35, is the other raw material needed for the DME production. The cost of Amberlyst 35 has been found to be \$10/kg and has an approximate lifetime of two years, and will be replaced during scheduled maintenance (Dimian et al). Initially, the plant will require 1,220 kg of catalyst and so this is considered a capital cost and not a raw material in the profitability analysis. Table 22.1 below totals these raw material costs, totaling \$134,398,020 a year.

Table 22.1. Breakdown of Raw Material Costs

Raw Material	Required Ratio (per kg of DME produced)	Cost (USD/kg of DME produced)
Methanol	1.0 kg	0.344
Lubricant (Mineral oil)	9.0x10 ⁻⁴ kg	3.651
Total Weighted Average		0.481

22.1.2 Utility Costs

The required amount of utility per kg of DME produced and the corresponding cost are outlined in Table 22.2. The total cost of utility per kg of DME produced is \$0.00786 and to meet the production rate, the annual total cost of utility is \$2,194,454.

Table 22.2. Utility requirement and cost per kg of DME produced

Utility	Required Ratio (per kg of DME produced)	Cost (USD/kg of DME produced)
Chilled water	15.92 kg	0.0071
Low pressure steam (1138 kPa/ 165 psig)	0.000632 kg	0.0000097
Electricity	0.00186 kWh	0.00013
Wastewater treatment	0.00196 kg	0.00065
Total		0.00786

22.1.3 General Expenses

Using Chapter 17 of Seider et al., the costs for general expenses, along with the associated assumptions are outlined below in Table 22.3. The calculated total cost is \$19,893,573/year.

Table 22.3. Breakdown of General Expenses

General Expense	Sales Assumption	Cost (USD/year)
Selling/Transfer Expenses	3.0% of Sales	5,167,162
Direct Research	4.8% of Sales	8,267,459
Allocated Research	0.5% of Sales	861,194
Administrative Expense	2.0% of Sales	3,444,775
Management Incentive Compensation	1.25% of Sales	2,152,984
Total	11.55% of Sales	19,893,573

22.1.4 Summary of Variable Costs

Table 22.4 summarizes the raw material costs, utility costs, and the cost of general expenses. The total annual operating variable cost totals to \$156,486,047/year based on a production value of 35,418 kg of DME per hour.

Table 22.4. Summary of Annual Operating Variable Costs

Expense	Total Cost (USD/year)
Raw Materials	134,398,020
Utilities	2,194,454
General	19,893,573
Total	156,486,047

22.2 Fixed Operating Costs

22.2.1 Operations

As the designed process is relatively small, two engineers were deemed necessary and assuming a cost of \$200,000/year for each engineer, total engineer cost is \$400,000/year. An operator is needed for each reactive distillation column and due to the large production of the plant, following guidelines (Seider et al.), four daily operators per shift are needed at five shifts a day. Assuming each operator's wage is \$40/hr, the annual cost of direct wages and benefits is \$1,664,000/year. Other recommended assumptions from Seider et al. are shown in Table 22.5. The sum of all the calculated costs gives the total labor-related operation cost which is \$4,513,440/year.

Table 22.5. Assumptions and calculated costs for each component of operations costs

Fixed Operating Costs: Operations	Costing Details	Cost (USD/year)
Operators per Shift	4 (assuming 5 shifts)	-
Direct Wages and Benefits	\$40/hr	1,664,000
Direct Salaries and Benefits	15% of Direct Wages and Benefits	249,600
Operating Supplies and Services	6% of Direct Wages and Benefits	99,840
Technical Assistance to Manufacturing	\$60,000 per year, for each operator per shift	1,200,000
Control Laboratory	\$65,000 per year, for each operator per shift	1,300,000
	Total Cost	4,513,440

22.2.2 Maintenance

The annual maintenance costs are estimated as a percentage of total depreciable capital (C_{TDC}), as the amount of maintenance required will scale linearly with the amount of equipment on the plant. The recommended assumptions from Seider et al. and calculated costs for each component of maintenance can be found in Table 22.6. The calculated costs sum to give the total maintenance cost of \$2,390,479/year.

Table 22.6. Assumptions and calculated costs for each component of maintenance costs

Fixed Operating Costs: Maintenance	Costing Details	Cost (USD/year)
Wages and Benefits (MW&B)	4.5% of C_{TDC}	1,039,339
Salaries and Benefits	25% of MW&B	259,835
Materials and Services	100% of MW&B	1,039,339
Maintenance Overhead	5% of MW&B	51,967
Total Cost:		2,390,479

22.2.3 Operating Overhead

The maintenance and operations wages and benefits (MOWB) are the sum of the operation direct wages and benefits, the operation direct salaries and benefits, maintenance wages and benefits, and the maintenance salaries and benefits. These values are shown in Table 22.5 and 22.6 above. The calculated MOWB cost is \$3,212,774/year. This value is then used to estimate operating overhead using percentages found in Seider et al. which can be seen in Table 22.7.

Table 22.7. Assumptions and calculated costs for each component of operating overhead.

Fixed Operating Costs: Operating Overhead	Costing Details	Cost (USD/year)
General Plant Overhead	7.1% of MOWB	228,107
Mechanical Department Services	2.4% of MOWB	77,107
Employee Relations Department	5.9% of MOWB	189,554
Business Services	7.4% of MOWB	237,745
	Total Cost:	732,512

23 Other Considerations

23.1 Environmental Considerations

The motivation of the problem is to find a fuel that has a better environmental impact, and the process to create this fuel should be as clean as the fuel it produces. The reaction chosen for the production of DME produces a bottoms stream that is (by weight) 99.5% water, 0.5% Methanol, and a trace amount of DME. While these amounts are below the LC/LD50 values for Methanol and DME, the U.S. Clean Water Act of 1977 places a further restriction on the amounts of these chemicals that can be released into surface-water sources. Furthermore, the process designers wished to mitigate the impact on the Texas ecosystem where the plant is proposed to be built. This led to the decision to include a biotreatment facility to remove the Methanol and DME byproducts. This is included in the utility costs of Section 22.2.2. By removing the byproducts of the DME plant, the process is minimizing the environmental impact it will have on the surrounding ecosystem and the water can be released into the Neches River. The DME plant is designed to serve the needs of consumers, but this should not be done at the expense of the surrounding community. Biotreatment allows the plant to meet the demand it is built for, while respecting the surrounding land and communities.

23.2 Process Controllability

The decision to split the DME production process into two reactive distillation columns to meet the requirement of a turndown up to 50% (specified in the project proposal), was motivated by the process controllability. Consultant advised turndown of more than 40% for a column could result in problems such as flooding that would be very difficult to control and as a result purity of the distillate and bottom streams could be compromised. The consequence of not meeting the purity

requirement would mean another separation step (not available in the plant) would be required for the product to meet ISO standard; this would result in a significant financial loss for the plant.

Additionally, it is preferred to have another reactive distillation column than to overproduce and store the product to meet the production turndown requirement because the capital cost of the column is much lower than cost of storage. In the proposed plant, 69% of the total bare module cost is attributed to storage while only 28% for two reactive distillation columns.

23.3 Health and Safety Concerns and Considerations

The health and safety of the DME plant operators is of top priority. DME will react on contact with air to produce CO₂ and water, and so is non-toxic (An et al). Methanol is the key concern when it comes to health and safety exposures. While neither DME nor methanol are classified as Toxic and Hazardous Substances according to OSHA (Occupational Safety and Health Administration), exposure should still be limited as methanol could be toxic in some situations and is flammable. In order to protect against toxic concerns, appropriate personal protective equipment (PPE), will be required to be worn by all operators who are within the plant limits to protect against any potential exposures.

In addition to the measures taken by operators working day to day, the plant is also designed to be as safe as possible. Each of the towers are built to withstand an earthquake and most winds generated by a category 4 hurricane by being designed to withstand a wind load of 140 miles per hour acting uniformly over the entire column (Seider et al.). The column will also be equipped with leak detection due to the high pressure inside. Outside of actions from natural disasters, each of the tanks store flammable liquids and need to be protected from ignition. The Methanol is stored in a

floating-roof above ground tank to minimize Methanol vapor space within the tank, and all four tanks are grounded to avoid static discharge hazards. In addition, ignition control will be implemented by designation of a hazard zone with ignition control (Methanol Institute). This hazardous zone will be fenced, locked, and with appropriate signage surrounding the fenced vessels. All storage vessels' piping will be consistently labelled along with flow direction. Each tank will be bermed using appropriate materials consistent with the contents. In the case of a Methanol fire, infrared devices will be on-site for responders in case the flame is invisible in the bright Texas sunlight to allow for detection. All piping will be above ground in overhead pipe racks, and fire protection similar to gasoline tanks will be equipped to each storage vessel. In times of loading, unloading, or if the tank is ever empty the pressure in the DME spherical tank will need to be maintained. While the distillate pump, feeding at 1,100 kPA, and daytime temperatures will help hold this pressure, the tank should be designed to withstand a full vacuum. This will also help in cases of rapid cooldown such as a rainstorm (Professor Vrana). Leak detection and alcohol-compatible fire suppression foam will be outfitted for the Methanol tank. If possible, plant operators may want to consider storing fire response equipment on-site for rapid response similar to a nuclear power plant (Fire Engineering). Proper material of choice was considered for each individual piece of equipment to ensure maximum safety.

24 Profitability Analysis

The primary measure of success stipulated in the project proposal was a minimum internal rate of return (IRR) of 8%. This report describes a process with an estimated IRR of 12.57% and a net present value (NPV) of \$11,846,000 based on an 8% discount rate and a 20 year time horizon. Annual net earnings of \$3,087,402 requiring a total capital investment of \$31,627,799 (undiscounted working capital) produces a return on investment (ROI) of 9.76%.

24.1 Profitability Model

This plant is expected to take one year for design and one for construction, meaning production would begin in 2022. The entirety of the total permanent investment (\$24,867,989) is assumed to be paid upfront during construction. The operating factor is set at 0.9, corresponding to a 90% uptime as suggested by consultants. It is also assumed that production capacity will be 90% of design capacity, accounting for viability and safety concerns. As is industry standard, production will start at 50% capacity (45% of design capacity) in its first year and ramp up to full by year three. These initial years serve to keep assumptions conservative and are generally used to ensure plant safety and provide time for training and improvement (Lager).

For tax accounting purposes, the 5 year MACRS depreciation schedule will be used. This method, which rapidly depreciates the capital investment over the first 6 years following construction, will reduce tax liability up front. This temporary accounting difference has no effect on the total nominal taxes owed; however, due to the time value of money, saving on taxes in the early years of operation will have an overall positive effect on NPV.

As mentioned previously, a discount rate of 8% was assumed for this project. This assumption laid out in the project statement is backed up by cost of capital data provided by Professor Aswath Damodaram, showing discount rates below 8% for a majority of chemical companies. Table 24.3 shows the NPV for varying costs of capital, from 5% up to 15%.

There is also an assumption of steady pricings (no inflation) for raw materials and the product. A Methanol cost of \$1.03/gal (\$0.344/kg) is assumed based on methanex pricing from the end of 2019. The required lubricant is priced at \$1.65/lb, plus \$0.035/kg DME shipping costs (total \$3.651/kg). The DME product is assumed to sell at a price of \$1.72/gal (\$0.62/kg). This assumption is based on the wholesale price of diesel at the end of 2019 (\$1.943), with an adjustment based on fuel mileage. See section 28.5 for calculation.

24.2 Profitability Results

The most indicative measures of profitability are NPV, IRR, and ROI. This section will be delving into how each of these measures are determined and what their results say about the project at hand.

The first, net present value, represents the sum of all future cash flows discounted back to today. Table 24.1 shows how the cumulative NPV changes over the years of the project based on an 8% cost of capital. The last line in the table, representing the final year of the project, indicates that the overall NPV for this venture is \$11,846,000. This means that undertaking this project will result in a profit of \$11.8MM in today's dollars. The cumulative NPV first became positive in 2033, indicating that the break-even point in today's dollars lie sometime in that year, the 12th year of production.

While net present value represents how much profit this project will produce given a discount rate, the internal rate of return represents a minimum acceptable rate of return for this project. More specifically, it is the cost of capital that results in an NPV of \$0. The IRR for this project is 12.57%. This is above the minimum acceptable level of 8% laid out in the proposal, indicating the profitability of this design.

The final measure to be discussed is return on investment. This value states the net annual earnings as a percentage of the total capital investment (with undiscounted working capital). Generally, the third year of production is used for ROI analysis, accounting for full production and a specific level of depreciation. ROI represents investment efficiency, showing how much needs to be invested in order to achieve a specific annual return. As stated above, this project's ROI is 9.76%, meaning that \$100 invested will result in annual earnings of \$9.76. Table 24.2 outlines the calculation of ROI based on values from the third year of production.

Table 24.1. Cash Flows and Cumulative NPV by Year (8% Cost of Capital)

Year	Cash Flow (USD)	Cumulative NPV (USD)
2020	-	-
2021	(28,747,900)	(26,618,400)
2022	(1,155,000)	(27,608,600)
2023	2,211,700	(25,852,900)
2024	5,700,800	(21,662,700)
2025	5,292,800	(18,060,400)
2026	5,292,800	(14,725,100)
2027	4,986,900	(11,815,300)
2028	4,986,900	(9,286,300)
2029	4,986,900	(6,944,700)
2030	4,986,900	(4,776,600)
2031	4,986,900	(2,769,100)
2032	4,986,900	(910,200)
2033	4,986,900	810,900
2034	4,986,900	2,404,600
2035	4,986,900	3,880,200
2036	4,986,900	5,246,500
2037	4,986,900	6,511,600
2038	4,986,900	7,683,000
2039	4,986,900	8,767,600
2040	4,986,900	9,711,900
2041	10,440,700	11,846,000

Table 24.2. ROI Calculation (Third Year of Production)

Annual Sales (USD)	155,014,854
Annual Costs (USD)	(148,935,802)
Depreciation (USD)	(2,069,439)
Income Tax (USD)	(922,211)
Net Earnings (USD)	3,087,402
Total Capital Investment (USD)	31,627,799
ROI	9.76%

24.3 Sensitivity Analysis

It is very important to understand how profitability of a design will be affected by variations in certain inputs. For example, the company planning to invest in this plant might like to know how the IRR will change as the price of the DME product goes up or down. It is a good sign if a project can remain profitable even when the assumptions do not hold. To test how robust this design is, various inputs were altered and their effects on profitability were noted. The inputs considered were DME price, variable costs, fixed costs, and total permanent investment. Each of these were varied and their effects on IRR can be seen in the figures below. For the purposes of this proposal, an IRR greater than 8% would be considered profitable.

Table 24.3. Sensitivity of NPV to Variations in the Cost of Capital

	Cost of Capital										
	5%	6%	7%	8%	9%	10%	11%	12%	13%	14%	15%
NPV	\$ 24,811,000	\$ 19,857,000	\$ 15,569,000	\$ 11,846,000	\$ 8,604,000	\$ 5,773,000	\$ 3,294,000	\$ 1,117,000	\$ (799,000)	\$ (2,489,000)	\$ (3,984,000)

Table 24.4. Sensitivity of IRR to Variations in Variable Costs and Fixed Costs

	Variable Costs										
	\$ 140,837,442	\$ 143,967,163	\$ 147,096,884	\$ 150,226,605	\$ 153,356,326	\$ 156,486,047	\$ 159,615,768	\$ 162,745,489	\$ 165,875,210	\$ 169,004,931	\$ 172,134,652
Fixed Costs	\$ 4,049,180	\$ 4,859,016	\$ 5,668,852	\$ 6,478,688	\$ 7,288,524	\$ 8,098,360	\$ 8,908,196	\$ 9,718,032	\$ 10,527,868	\$ 11,337,704	\$ 12,147,540
	48.92%	47.13%	45.34%	43.56%	41.79%	40.03%	38.28%	36.53%	34.79%	33.06%	31.34%
	38.93%	37.11%	35.29%	33.49%	31.68%	29.89%	28.09%	26.30%	24.50%	22.71%	20.90%
	33.71%	31.87%	30.03%	28.19%	26.36%	24.52%	22.67%	20.82%	18.96%	17.08%	15.17%
	28.30%	26.42%	24.53%	22.64%	20.74%	18.82%	16.88%	14.92%	12.91%	10.85%	8.72%
	22.60%	20.65%	18.67%	16.68%	14.64%	12.57%	10.43%	8.20%	5.86%	3.35%	0.60%
	16.43%	14.35%	12.20%	9.97%	7.65%	5.18%	2.51%	-0.46%	-3.90%	-8.16%	-13.88%
	9.48%	7.04%	4.43%	1.58%	-1.65%	-5.50%	-10.44%	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	0.53%	-3.03%	-7.40%	-13.25%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR

Table 24.5. Sensitivity of IRR to Variations in Product Price and Total Permanent Investment

	Product (DME) Price (/kg)										
	\$ 0.558	\$ 0.570	\$ 0.583	\$ 0.595	\$ 0.608	\$ 0.620	\$ 0.632	\$ 0.645	\$ 0.657	\$ 0.670	\$ 0.682
Total Permanent Investment	\$ 12,933,995	\$ 15,520,793	\$ 18,107,592	\$ 20,694,391	\$ 23,281,190	\$ 25,867,989	\$ 28,454,788	\$ 31,041,587	\$ 33,628,386	\$ 36,215,185	\$ 38,801,984
	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	6.84%	3.02%	-0.36%	-3.45%	-6.34%	-9.14%	-11.94%	-14.84%	-17.74%	-20.64%	-23.54%
	24.11%	18.54%	14.01%	10.27%	7.10%	4.37%	1.95%	-0.23%	-2.20%	-4.05%	-5.89%
	38.70%	30.94%	24.82%	19.92%	15.91%	12.57%	9.73%	7.27%	5.11%	3.18%	1.43%
	52.20%	42.22%	34.43%	28.28%	23.33%	19.28%	15.90%	13.03%	10.55%	8.38%	6.45%
	64.48%	52.82%	43.39%	35.99%	30.09%	25.30%	21.34%	18.01%	15.18%	12.72%	10.57%
	77.20%	62.93%	51.90%	43.28%	36.43%	30.90%	26.35%	22.56%	19.35%	16.60%	14.21%
	88.95%	72.63%	60.06%	50.25%	42.48%	36.21%	31.09%	26.83%	23.24%	20.18%	17.54%
	100.29%	82.00%	67.93%	56.97%	48.29%	41.31%	35.61%	30.89%	26.93%	23.56%	20.66%

Table 24.3 shows how the NPV is highly dependent on the assumed cost of capital. The NPV goes up substantially by decreasing the discount rate, over doubling when the cost of capital is lowered to 5%. In contrast, the NPV turns negative when the cost of capital reaches 13%. This is logical since the IRR is 12.57%. This dependency on the cost of capital is due to the nature of the cash flows. As is often the case in projects of this nature, there are large negative cash flows at the start, followed by smaller annual cash flows from profit. The larger the cost of capital, the more reduced the effect of the profit cash flows in later years, leading to lower NPV. The rate of return demanded by the company implementing this project will greatly affect its perceived profitability.

Tables 24.4 shows how fluctuations in costs, both variable and fixed, affect the calculated IRR. The original variable costs of \$156,486,047 were varied $\pm 10\%$ and the original fixed costs of \$8,098,360 were varied $\pm 50\%$. As can be seen in the table, adjusting the variable costs just 2% at a time has a dramatic effect on IRR. Decreasing variable costs by 10% increases IRR from 12.57% all the way up to 40.03%, and increasing them by just 4% results in a negative value. The profitability of this venture is highly correlated to the price of methanol which represents a majority of the variable costs. This poses a major risk, as if the price rises too rapidly, this plan will quickly become unprofitable. That being said, profits would skyrocket given even small decreases in methanol prices. With regards to fixed costs, fluctuations will not go as noticed as these make up a much smaller portion of the overall expenses associated with the plant.

Table 24.5 shows the effects of product price and total permanent investment on IRR. Product price is varied $\pm 10\%$ and the investment is varied $\pm 50\%$. Obviously, profitability is going to be closely linked to the price of DME, as this directly determines the dollar amount of sales for the company. By increasing the price by a bit over six cents to \$0.682, the IRR jumps from 12.57% up to

41.31%. Just as the success of this plan is linked to the price of methanol, so too is it linked to the price of DME. Since it is assumed that the price for DME will be proportional to that of diesel, the price of diesel becomes a key factor in determining profitability, indirectly shown in the table above. If the price of DME drops just \$0.025, the IRR would then be negative, indicating the delicacy of the situation. Looking at total permanent investment, its effects on IRR are also quite substantial. If some of the upfront capital costs are avoided, the profitability could significantly increase.

24.4 Best Case Analysis

The previous analysis was done with conservative estimations and with assumptions that followed the plant being constructed from scratch. The analysis also accounts for companies paying to switch their trucks over to be DME compatible. It is recognized that these assumptions and the previous analysis allows for a safer approach to the profitability of the total DME plant. However, the report should also reflect what could be called a best case scenario for the development of the total DME plant. This “best case scenario” follows the same assumptions as the previous in depth analysis with a few key changes that drastically change the NPV, the IRR, and the TCI. With these assumptions, or even just a few, the plant’s profitability can be swung to be much more appealing.

The first, and perhaps most important assumption of this second analysis accounts for the \$12,000,000 spent on storage for the product, feed, and lubricant. This first assumption is centered around the idea of retrofitting or reallocating a plant’s portion of operations for the production of DME. A possible course for this case could take place at the same Natgasoline plant referenced earlier in this report. This location is already outfitted with enough storage to continue its normal operations while reallocating a portion of it’s storage for the product DME. The plant would continue to

produce methanol, while also producing DME. In summary, the plan would be to retrofit a pre-existing plant and save where possible. Accounting for the equipment costs of the rest of the total DME plant, only excluding the storage, the total capital investment falls to \$14,063,798. This is a much more manageable amount that would be more appealing to investors and other interested companies looking to tap into the growing U.S. market for DME.

The second assumption is centered around the retrofitting of trucks to be DME compatible and the cost associated with this. The recent pursuit of alternatively-fueled trucks has slowed down in the U.S. due to diesel prices lowering. Volvo had, however, designed and manufactured a limited line of DME fueled long-haul trucks designed for commercial production in 2015 (Lockridge). The second piece of this scenario hinges on these trucks being rolled out and widely purchased by companies for industrial use. This is important because the price would no longer have to be dropped to account for the cost of converting trucks to accommodate DME. Accounting for this increase in profit drives the NPV and IRR back up from the previously reported values. In addition, the price of these DME trucks will be comparable to normal diesel trucks (Volvo). Meaning that companies can purchase the DME trucks as their diesel trucks fall out of commission. This will steadily increase the demand for the DME, which works perfectly for the initial two years where production has not yet reached its capacity. Allowing for the DME to be sold at \$1.90 per gallon, the same price as diesel, the new IRR rises to 89% with an NPV of \$136,047,700.

This analysis is meant to be a little more liberal with the assumptions, but shows the profitability that could be accomplished by the DME plant. There could be more equipment costs associated with retrofitting certain aspects of the pre-existing plants storage, but these would be much smaller than the \$12 million associated with building new containments. In the end, retrofitting a

pre-existing plant and selling at diesel prices is not the primary analysis, but should be considered as a potential expansion option for existing companies whose plants could accommodate the storage.

25 Conclusion and Recommendations

An investigation was done on the production of DME as a sustainable transportation fuel using Methanol as the feed. The proposed process combines the reactive and separation steps of the production into a single main unit operation – the reactive distillation process – and can achieve mass purity of 99.9% DME in the distillate and mass purity of 99.5% water in the bottom stream, corresponding to 99.8% Methanol conversion. The high purity of DME and water means that additional separation steps are not necessary to recover unreacted Methanol or to meet the ISO standard, which requires 98.5% mass purity of DME. The innovative use of reactive distillation has shown to be preferable to the conventional DME production for lowering capital and operating cost; the conventional process typically involves a fixed-bed gas-phase reactor achieving Methanol conversion of 70 to 80% followed by two distillation columns in series to purify DME and recover Methanol.

The high purity of water in the bottom waste stream means that it can easily be treated using biotreatment to remove the small amount of Methanol and DME, so as to reduce the impact of the plant to the environment. In addition to these environmental and process concerns, extensive consideration was given to the safety of the plant operators and overall construction of the total plant.

The DME total plant assumes an uptime of 90% to produce 306,000 gallons of DME per day. The plant is profitable with an IRR of 12.57% and an NPV of \$11,846,000 in 2020. The plant has a total capital investment of \$30,912, 176 and a ROI of 9.76% in the third year of production. As cost of storage contributes to 69% of the total bare module cost, more frequent transportation of materials or an alternative arrangement with the customer that could alleviate storage cost is recommended.

In completion, the report provides a DME total plant that is innovative, safe, and feasible. It is recommended that the report be followed to ensure the safety of the plant's operators and any further actions that could be taken to protect the operators or the surrounding ecosystem be taken advantage of to the fullest.

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28 Appendix

28.1 Production Rate and Feed Requirement

The demand to be met is 2,000 trucks running at 6 miles/gal of diesel, 12 hours/day and traveling at an average speed of 60 mph. The calculated amount must be adjusted for the DME's fuel economy of 5.3 miles/gal and with slight excess to accommodate variations in truck traffic.

$$(2000 \text{ trucks} \cdot 12 \text{ hr/day} \cdot 50 \text{ miles/hr}) / (5.3 \text{ miles/gal}) = 271,698 \text{ gal/day}$$

Round up to 275,000 gal/day.

Liquid density of DME = 2.782 kg/gal

$$271,698 \text{ gal/day} \cdot 2.782 \text{ kg/gal} \approx 765,000 \text{ kg DME / day}$$

Molar mass of Methanol = 32.04 g/mol and DME = 46.069 g/mol

$$2 \cdot (765,000 \text{ kg DME/day}) / (46.069 \text{ kg/kmol}) = 33,211 \text{ kmol Methanol/day}$$

$$33,211 \text{ kmol Methanol/day} \cdot 32.04 \text{ kg/kmol} \approx 1,064,000 \text{ kg Methanol/day}$$

Assuming 90% uptime and converting to kmol/hour basis:

$$(33,211 \text{ kmol Methanol/day}) / (24 \text{ hrs/day} * 0.9 \text{ uptime}) = 1537 \text{ kmol Methanol/hr}$$

Thus, the Methanol required is 1537 kmol/hr.

28.2 Reactive Distillation Column

28.2.1 Reactive Section Diameter

The reactive section's diameter was initially estimated as the average of the rectifying and stripping sections' (1.85 m and 1.04 m, respectively), which is 1.45 m. The active area for a 1.45 m diameter column is 1.41m². The theoretical diameter for area of 1.41 m² is 1.34 m following this calculation:

$$D_{sieved\ tray} = 2 \cdot \left(\frac{1.41}{\pi}\right)^{1/2}$$

The downcomer width, estimated from Aspen, is 0.226 m and the caged catalyst width was approximated as 0.305 m (recommended by Professor Len Fabiano). The arrangement of the downcomer and the caged catalyst is shown in Figure 28.1. The stage diameter is therefore calculated as:

$$D_{reactive\ stage} = 1.34 + 2 \cdot (0.305 + 0.226) = 2.4\ m$$

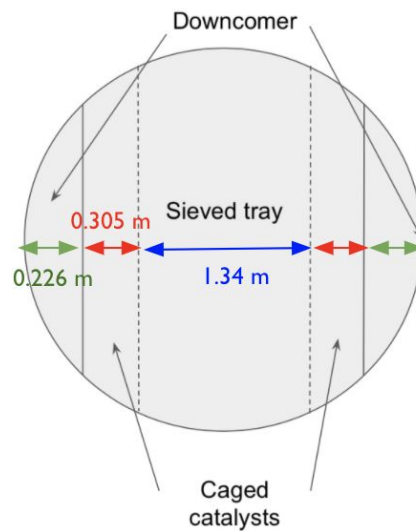


Figure 28.1. Proposed design for the reactive stages.

28.2.2 Tray Efficiency

The overall efficiency (E_O) of each trays in the rectifying section and in the stripping sections were calculated using the O'Connell correlation:

$$E_O = 0.492 \cdot (\alpha \cdot \mu)^{-0.245}$$

Where α is the relative volatility between the light and heavy keys – for the rectifying section, these are Dimethyl Ether and Methanol and for the stripping section, these are water and Methanol, and μ is the

viscosity of the liquid on the stage. Both α and μ were taken from running the Aspen simulation and as the reactive sections were simulated as a series of CSTRs, the necessary information were not available for the reactive stages. Their efficiencies were instead approximated as the average of the rectifying and stripping trays which is 0.463.

From the stage efficiency, the number of actual trays for each tray were calculated using the equation:

$$\text{Number of actual trays} = \frac{1}{E_o}$$

Table 28.2. Overall tray efficiency and number of actual trays of each stage in the rectifying, reactive and stripping sections.

Theoretical Stage	Efficiency	Number of Actual Trays
1	0.479	2.09
2	0.450	2.22
3	0.342	2.93
4	0.362	2.76
5	0.463	2.16
6	0.463	2.16
7	0.463	2.16
8	0.463	2.16
9	0.463	2.16
10	0.463	2.16
11	0.463	2.16
12	0.463	2.16
13	0.463	2.16
14	0.543	1.84
15	0.521	1.92
16	0.505	1.98
17	0.500	2.00

The sum of the number of actual trays for each stage rounded up to the closest integer gives the total number of actual trays, which is 38 stages excluding reboiler and condenser.

28.3 Equipment Cost Calculations

28.3.1 Pumps

As APEA did not account for the shaft speed and the number of stages on the types of pump, calculations were made based on equations from Seider et al.:

$$S = Q \cdot H^{0.5}$$

where S is the size factor, Q is flow rate in gallons per minute and H is the pump head in feet.

The flow rate and the pump head (Q and H) were estimated from Aspen. The graph that relates the size factor to purchase cost of a single stage, 3600 rpm radial centrifugal pump is provided by Seider et al. and is used for purchase cost estimation (this excludes the price of the motor).

To calculate price of the motor, another size factor, P_c is calculated using the following equation from Seider et al.:

$$P_c = (Q \cdot H \cdot \rho) / (33000 \cdot \eta_p \cdot \eta_m)$$

ρ is the liquid density in pounds per gallon provided by ASPEN, while η_p and η_m are calculated using the following equations:

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

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

For Q in range 50 to 5000 gpm and the pump brake horsepower, P_B , in the range 1 to 1,500 Hp.

Calculation for P-100:

The size factor is calculated as:

$$S = 273.6 \cdot 274.3^{0.5} = 4531.4$$

From the graph, the purchase cost of a pump, excluding motor, is approximately \$5,600 using cast iron casing material.

To calculate cost of motor:

$$\eta_p = -0.316 + 0.24015(\ln 273.6) - 0.01199 (\ln 273.6)^2 = 0.941$$

$$\eta_m = 0.80 + 0.0319(\ln 23.0) - 0.00182 (\ln 23.0)^2 = 0.882$$

$$P_c = (273.6 \cdot 274.3 \cdot 6.61)/(33000 \cdot 0.941 \cdot 0.882) = 18.11$$

From the graph, the purchase cost of the motor is approximately \$4,000.

Thus the sum purchase cost of pump and motor is \$9,600 which conforms with equipment cost calculated from APEA, \$9,400.

28.3.2 Storage Calculations

Using a volumetric flow rate from aspen, such as the data on the Material Balance Sheet (page XXX), and a storage goal, the number of tanks and storage volume can be found.

Stream S-101: Volumetric Flow rate = 62.2 cum of feed Methanol per hour

Methanol storage goal: 2 Days

$$62.2 \frac{\text{cum}}{\text{hr}} \times 24 \frac{\text{hr}}{\text{day}} \times 2 \text{ days} = 2,985.6 \text{ cum} \approx 790,000 \text{ gal}$$

Following the rule that it is generally cheaper to build one tank than two and as long as the calculated volume falls within the bounds of the equations used to calculate storage costs in Seider et al., one tank was chosen.

Build material is carbon steel since Methanol is non corrosive.

Ambient conditions were chosen due to Methanols specific qualities, other cases required different conditions.

Equipment Costing Sheet was provided and used for lubricant and Methanol tanks. DME tank purchase cost was calculated using Table 16.32 of Seider et al.:

$$C_p = 53 \times V^{0.78} = 53 \times 1,000,000^{0.78} = \$2,536,739$$

Two tanks and a $F_{\text{BM}} = 2$ leads to a $C_{\text{BM}} = \$10,221,620$ for both tanks.

28.3.3 Tower Calculations

The cost for the tower was estimated using equations and heuristics from Seider et al:

$$P_d = \exp[0.60608 + 0.91615(\ln P_o) + 0.0015655(\ln P_o)^2]$$

where P_o is the operating pressure in psig and P_d is the design pressure in psig. The wall thickness is then calculated:

$$t_p = \frac{P_d D_i}{2SE - 1.2P_d}$$

where t_p is the wall thickness to withstand the internal pressure in inches, D_i is internal diameter in inches, S is the maximum allowable stress in psi, and E is the fractional weld efficiency. If t_p is less than

the minimum wall thickness for the corresponding internal diameter, use $t_p = t_{\min}$. A factor is then added to the wall thickness to account for wind load or earthquakes at the bottom of the column.

$$t_w = \frac{0.22(D_o+18)L^2}{SD_o^2}$$

where D_o is the outside diameter ($D_i + t_p$) in inches, L is the length in inches, and t_w is the necessary thickness to withstand the wind load or earthquake at the bottom of the column in inches. The thickness at the bottom of the column is equal to the sum of t_p and t_w . This added thickness decreases proportionally up the column, so at the top $t = t_p$. The vessel thickness, t_v , is the average wall thickness, calculated by averaging t_p and $(t_p + t_w)$. The weight of the column, in pounds, is then calculated:

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

where t_s is the shell thickness (equal to t_v in this case) in inches and ρ is the density of the material in pounds per cubic inch. The vessel cost, C_V , and the cost for platforms and ladders, C_{PL} (use ft), are then calculated:

$$C_V = \exp[10.5449 - 0.4672(\ln W) + 0.05482(\ln W)^2]$$

$$C_{PL} = 341(D_i)^{0.63316}(L)^{0.80161}$$

The purchase cost is then found:

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

The cost for the installed trays, C_T , is found separately using the following equation:

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

where N_T is the number of trays, F_{NT} is a factor corresponding to the number of trays, F_{TT} is a factor corresponding to the type of tray ($F_{TT}=1$ for sieve trays), F_{TM} is the material of construction factor, and C_{BT} is the base cost.

If $N_T > 20$, $F_{NT} = 1$, otherwise

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

For 316 stainless steel, F_{TM} , is found using the following equation (D_i in ft):

$$F_{TM} = 1.401 + .0724D_i$$

$$C_{BT} = 468 \exp(0.1482D_i)$$

To get the bare module cost today, the following equation is used:

$$C_{BM} = C_{P_b} \frac{I}{I_b} F_{BM}$$

where C_{P_b} and I_b are the calculated purchase cost and corresponding price index, I is the price index of interest, and F_{BM} is the bare module factor.

Calculation for RDC-100:

The design pressure is calculated as:

$$P_d = \exp[0.60608 + 0.91615(\ln 101.5) + 0.0015655(\ln 101.5)^2] = 130.6$$

As this is a triple diameter column, each section is now approached separately. The data for each section is listed below.

	Top	Middle	Bottom
L (ft)	26	40	24
D_i (in)	72.8	94.5	39.4

To find the overall C_v , the C_v was calculated for each section as if it were a full 90 ft column and a weighted average was taken. The same is done for C_{PL} . As 316 stainless steel is used,

S=20,000 psi, E=1, $F_M = 2.1$, and $\rho=0.289 \text{ lb/in}^3$ are used. The following calculation corresponds to the bottom section.

$$t_p = \frac{(130.6)(39.4)}{2(20000)(1)-1.2(130.6)} = 0.129$$

The minimum thickness for this internal diameter is 0.25 in. Since the calculated $t_p < 0.25$, t_p is set equal to 0.25 in.

To remain conservative in cost estimates, the calculated t_w for the base of the column is based on the largest of the three column diameters. This additional thickness is then scaled down proportionally up the column (added thickness at height x ft up the column is equal to $t_w * (1-x/90)$). To determine the weight for each section, the average thickness for that section is used and is based on this formula.

$$t_w = \frac{0.22(95.2)+18(90)^2}{(20000)(95.2)^2} = 0.16$$

The $D_o=95.2$ in is based on the middle section, where $D_i = 94.5$ and $t_p=0.375$.

Based on this t_w , the thickness at the bottom of the column is $0.25+0.16=0.41$ and the thickness at the top of the bottom section is $0.25+0.16*(1-24/90)=0.37$. This means $t_v=0.39$ for the bottom section.

$$W = \pi(39.4 + 0.39)(90 * 12 + 0.8(39.4))(0.39)(0.289) = 15601$$

$$C_V = \exp[10.5449 - 0.4672(\ln 15601) + 0.05482(\ln W 15601)^2] = 69175$$

$$C_{PL} = 341(39.4/12)^{0.63316}(90)^{0.80161} = 26668$$

These calculations were done for all three sections of the column to produce the following:

	Top	Middle	Bottom
C_V	104552	138744	69175
C_{PL}	39369	45423	26668

$$C_{V,total} = \frac{L_1 C_{V1} + L_2 C_{V2} + L_3 C_{V3}}{L_1 + L_2 + L_3} = \frac{26*104552 + 40*138744 + 24*69175}{90} = 110315$$

A similar average was done for C_{PL} , resulting in $C_{PL,total} = 39117$

$$C_P = (2.1)(110315) + (39117) = 270778$$

The cost of the trays was also calculated by section. The top section has 10 trays, the middle has 20, and the bottom has 8. Each section uses sieve trays ($F_{TT}=1$). The following calculations correspond to the bottom section ($N_T=8$).

$$F_{NT} = \frac{2.25}{1.0414^8} = 1.63$$

$$F_{TM} = 1.401 + .0724(39.4/12) = 1.64$$

$$C_{BT} = 468 \exp(0.1482(39.4/12)) = 761$$

$$C_T = (8)(1.63)(1)(1.64)(761) = 16225$$

	Top	Middle	Bottom
C_T	31756	59261	16225

The total tray cost is the sum of the costs for the three sections, so $C_{T,total} = 107243$.

The total purchase cost is $C_P + C_T = 378021$. The bare module factor, F_{BM} , is 4.16 for towers.

$$C_{BM} = (378021) \frac{600}{567} (4.16) = 1664091$$

28.4 Vapor Pressure of Dimethyl Ether

If we assume the DME storage tank will never exceed a maximum temperature of 38°C, 1000 kPa will be enough to retain the liquid state of the product, since the vapor pressure is below 1000 kPa at 313 K (40°C).

<i>T/K</i>	<i>P/kPa</i>	<i>T/K</i>	<i>P/kPa</i>	<i>T/K</i>	<i>P/kPa</i>
213.076	16.46	278.166	316.12	333.165	1449.22
218.110	22.24	283.160	372.90	338.166	1621.53
223.152	29.61	288.134	436.69	343.163	1809.11
228.058	38.64	293.165	509.01	348.160	2012.44
233.092	49.96	298.084	588.17	353.162	2232.34
238.110	63.84	298.784	600.51	358.159	2468.87
243.070	80.36	303.151	679.68	363.157	2723.27
248.123	100.43	303.782	691.56	368.136	2996.38
253.125	124.09	308.127	778.92	373.136	3291.17
258.135	152.40	313.166	889.98	378.151	3608.63
263.132	184.96	318.164	1011.55	383.150	3948.62
268.130	222.70	323.165	1144.73	388.162	4313.91
273.167	266.50	328.161	1290.23	393.163	4706.18

Figure 28.4. Experimental Vapor Pressure of Dimethyl Ether (Wu and Yin)

28.5 Dimethyl Ether Pricing

The assumed price for the product is based on the prevailing wholesale price of diesel at the end of 2019, \$1.943/gallon. With each truck traveling at a speed of 60 miles/hour for 12 hours each day, the total distance traveled is 720 miles per truck. Given the gas mileage of 6 miles/gallon of diesel, the necessary fuel is 120 gallons of diesel. For DME, which has mileage of 5.3 miles/gallon, 135.85 gallons are required. For companies to be indifferent between the two prices, this equation must hold:

$$\$1.943/gal * (60 \text{ mi/hr} * 12 \text{ hr/day} / 6 \text{ mi/gal}) = x * (60 \text{ mi/hr} * 12 \text{ hr/day} / 5.3 \text{ mi/gal})$$

$$\$1.943/gal * 120 \text{ gal} = x * 135.85 \text{ gal}$$

This results in a price for DME of \$1.716/gallon. This is a reasonable estimate if the costs of a truck that uses matches that of one that uses diesel. However, given the lack of a market in the US at present, the price of DME might need to be lowered initially to incentivize companies to make the transition to DME now. It is important to look at the sensitivity analysis regarding DME price found in Section 24.3 to see its effects on NPV.

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Methanol, Lab Grade, 4L

SECTION 1 : Identification of the substance/mixture and of the supplier

Product name : Methanol, Lab Grade, 4L

Manufacturer/Supplier Trade name:

Manufacturer/Supplier Article number: S25426A

Recommended uses of the product and uses restrictions on use:

Manufacturer Details:

AquaPhoenix Scientific
9 Barnhart Drive, Hanover, PA 17331

Supplier Details:

Fisher Science Education
15 Jet View Drive, Rochester, NY 14624

Emergency telephone number:

Fisher Science Education Emergency Telephone No.: 800-535-5053

SECTION 2 : Hazards identification

Classification of the substance or mixture:



Flammable

Flammable liquids, category 2



Toxic

Acute toxicity (oral, dermal, inhalation), category 3



Health hazard

Specific target organ toxicity following single exposure, category 1

AcTox Dermal. 3

Flammable liq. 2

AcTox Oral. 3

AcTox Inhaln. 3

Stot SE. 1

Signal word :Danger

Hazard statements:

Highly flammable liquid and vapour

Toxic if swallowed

Toxic in contact with skin

Toxic if inhaled

Causes damage to organs

Precautionary statements:

If medical advice is needed, have product container or label at hand

Keep out of reach of children

Read label before use

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Wear protective gloves/protective clothing/eye protection/face protection
Wash skin thoroughly after handling
Do not eat, drink or smoke when using this product
Avoid breathing dust/fume/gas/mist/vapours/spray
Keep away from heat/sparks/open flames/hot surfaces. No smoking
Do not breathe dust/fume/gas/mist/vapours/spray
Specific treatment (see supplemental first aid instructions on this label)
IF ON SKIN: Wash with soap and water
Call a POISON CENTER or doctor/physician if you feel unwell
Specific measures (see supplemental first aid instructions on this label)
Take off contaminated clothing and wash before reuse
Wash contaminated clothing before reuse
IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
IF exposed: Call a POISON CENTER or doctor/physician
IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Store locked up
Store in a well ventilated place. Keep cool
Dispose of contents and container as instructed in Section 13

Other Non-GHS Classification:

WHMIS



NFPA/HMIS



NFPA SCALE (0-4)

Health	2
Flammability	3
Physical Hazard	0
Personal Protection	X

HMIS RATINGS (0-4)

SECTION 3 : Composition/information on ingredients

Ingredients:

CAS 67-56-1

Methanol

>90 %

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Percentages are by weight

SECTION 4 : First aid measures

Description of first aid measures

After inhalation: Move exposed individual to fresh air. Loosen clothing as necessary and position individual in a comfortable position. Get medical assistance. If breathing is difficult, give oxygen

After skin contact: Wash affected area with soap and water. Rinse/flush exposed skin gently using water for 15-20 minutes. Seek medical attention if irritation persists or if concerned.

After eye contact: Protect unexposed eye. Rinse or flush eye gently with water for at least 15-20 minutes, lifting upper and lower lids. Seek medical attention if irritation persists or if concerned

After swallowing: Rinse mouth thoroughly. Do not induce vomiting. Have exposed individual drink sips of water. Dilute mouth with water or milk after rinsing. Get medical assistance.

Most important symptoms and effects, both acute and delayed:

Poison. Toxic by ingestion, absorption through skin and inhalation, potentially causing irreversible effects. Irritating to eyes, skin, and respiratory tract. Irritation- all routes of exposure. Shortness of breath. Nausea. Headache. May be fatal or cause blindness if swallowed. Cannot be made non-poisonous. May cause gastrointestinal irritation, vomiting, and diarrhea. Central nervous system disorders. Skin disorders, preexisting eye disorders, gastrointestinal tract; Toxic: danger of very serious irreversible effects by inhalation, ingestion or absorption through skin. Experiments have shown reproductive toxicity effects on laboratory animals. May cause adverse kidney and liver effects

Indication of any immediate medical attention and special treatment needed:

If seeking medical attention, provide SDS document to physician. Physician should treat symptomatically.

SECTION 5 : Firefighting measures

Extinguishing media

Suitable extinguishing agents: Dry chemical, foam, dry sand, or Carbon Dioxide. Water spray can keep containers cool.

For safety reasons unsuitable extinguishing agents: Water may be ineffective.

Special hazards arising from the substance or mixture:

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

Advice for firefighters:

Protective equipment: Wear protective eyewear, gloves, and clothing. Refer to Section 8.

Additional information (precautions): Remove all sources of ignition. Avoid contact with skin, eyes, and clothing. Ensure adequate ventilation. Take precautions against static discharge.

SECTION 6 : Accidental release measures

Personal precautions, protective equipment and emergency procedures:

Use spark-proof tools and explosion-proof equipment. Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapor and mists below the applicable workplace exposure limits (Occupational Exposure Limits-OELs) indicated above. Ensure adequate ventilation.

Environmental precautions:

Prevent from reaching drains, sewer or waterway. Should not be released into environment.

Methods and material for containment and cleaning up:

If necessary use trained response staff or contractor. Remove all sources of ignition. Contain spillage and then

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collect. Do not flush to sewer. Absorb with a noncombustible absorbent material such as sand or earth and containerize for disposal. Ventilate area of leak or spill. Use spark-proof tools and explosion-proof equipment. Follow proper disposal methods. Refer to Section 13.

Reference to other sections:

SECTION 7 : Handling and storage

Precautions for safe handling:

Use in a chemical fume hood. Wash hands before breaks and immediately after handling the product. Avoid contact with skin, eyes, and clothing. Take precautions against static discharge.

Conditions for safe storage, including any incompatibilities:

Store in a cool location. Provide ventilation for containers. Avoid storage near extreme heat, ignition sources or open flame. Keep container tightly sealed. Store with like hazards. Protect from freezing and physical damage.

SECTION 8 : Exposure controls/personal protection



Control Parameters:

67-56-1, Methanol, ACGIH: 250 ppm STEL; 200 ppm TWA
67-56-1, Methanol, NIOSH: 250 ppm STEL; 325 mg/m³ STEL
67-56-1, Methanol, NIOSH: 200 ppm TWA; 260 mg/m³ TWA

Appropriate Engineering controls: Emergency eye wash fountains and safety showers should be available in the immediate vicinity of use or handling. Ensure that dust-handling systems (exhaust ducts, dust collectors, vessels, and processing equipment) are designed to prevent the escape of dust into the work area.

Respiratory protection: Use in a chemical fume hood. If exposure limit is exceeded, a full-face respirator with organic cartridge may be worn.

Protection of skin: Select glove material impermeable and resistant to the substance. Select glove material based on rates of diffusion and degradation.

Eye protection: Safety glasses with side shields or goggles.

General hygienic measures: Wash hands before breaks and at the end of work. Avoid contact with the eyes and skin. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Perform routine housekeeping.

SECTION 9 : Physical and chemical properties

Appearance (physical state,color):	Clear colorless liquid	Explosion limit lower: Explosion limit upper:	6 31
Odor:	Alcohol	Vapor pressure:	128 hPa @ 20°C
Odor threshold:	Not Available	Vapor density:	1.11
pH-value:	Not Available	Relative density:	0.79
Melting/Freezing point:	-98°C	Solubilities:	Miscible at 20 °C

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Boiling point/Boiling range:	64.7°C @ 760mmHg	Partition coefficient (n-octanol/water):	Not Available
Flash point (closed cup):	12°C	Auto/Self-ignition temperature:	455°C
Evaporation rate:	5.2	Decomposition temperature:	Not Available
Flammability (solid,gaseous):	Flammable	Viscosity:	a. Kinematic:Not Available b. Dynamic: Not Available
Density: Not Available			

SECTION 10 : Stability and reactivity

Reactivity:Vapours may form explosive mixture with air.

Chemical stability:Stable under normal conditions.

Possible hazardous reactions:None under normal processing.

Conditions to avoid:Excess heat, Incompatible Materials, flames, or sparks.

Incompatible materials: Oxidizing agents, reducing agents, alkali metals, acids, sodium, potassium, metals as powders, acid chlorides, acid anhydrides, powdered magnesium, and aluminum.

Hazardous decomposition products:carbon monoxide, formaldehyde.

SECTION 11 : Toxicological information

Acute Toxicity:		
Dermal:	(rabbit)	LD-50 15800 mg/kg
Oral:	(rat)	LD-50 5628 mg/kg
Inhalation:	(rat)	LC-50 130,7 mg/l
Chronic Toxicity: No additional information.		
Corrosion Irritation:		
Ocular:		Irritating to eyes
Dermal:		Irritating to skin
Sensitization: No additional information.		
Single Target Organ (STOT):		Classified as causing damage to organs: Eyes, skin, optic nerve, gastrointestinal tract, central nervous system, respiratory system, liver, spleen, kidney, blood
Numerical Measures: No additional information.		
Carcinogenicity:		Teratogenicity : has occurred in experimental animals.
Mutagenicity:		Mutagenetic effects have occurred in experimental animals.

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Reproductive Toxicity:

Developmental Effects (Immediate/Delayed) have occurred in experimental animals

SECTION 12 : Ecological information

Ecotoxicity

Freshwater Fish: 96 Hr LC50 Pimephales promelas: 28200 mg/L

Freshwater Fish: 96 Hr LC50 Oncorhynchus mykiss: 19500 - 20700 mg/L

Freshwater Fish: 96 Hr LC50 Pimephales promelas: >100 mg/L

Freshwater Fish: 96 Hr LC50 Oncorhynchus mykiss: 18 - 20 mL/L

Freshwater Fish: 96 Hr LC50 Lepomis macrochirus: 13500 - 17600 mg/L

Persistence and degradability: Not persistent.

Bioaccumulative potential: Not Bioaccumulative.

Mobility in soil: Aqueous solution has high mobility in soil.

Other adverse effects:

SECTION 13 : Disposal considerations

Waste disposal recommendations:

Methanol RCRA waste code U154. Do not allow product to reach sewage system or open water. It is the responsibility of the waste generator to properly characterize all waste materials according to applicable regulatory entities (US 40CFR262.11). Absorb with a noncombustible absorbent material such as sand or earth and containerize for disposal. Provide ventilation. Have fire extinguishing agent available in case of fire. Eliminate all sources of ignition. Use spark-proof tools and explosion-proof equipment. 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. Ensure complete and accurate classification.

SECTION 14 : Transport information

UN-Number

UN1230

UN proper shipping name

Methanol

Transport hazard class(es)



Class:

3 Flammable liquids



Class:

6.1 Toxic substances

Packing group: II

Environmental hazard:

Transport in bulk:

Special precautions for user:

SECTION 15 : Regulatory information

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United States (USA)

SARA Section 311/312 (Specific toxic chemical listings):

Acute, Chronic, Fire

SARA Section 313 (Specific toxic chemical listings):

67-56-1 Methanol

RCRA (hazardous waste code):

67-56-1 Methanol RCRA waste code U154

TSCA (Toxic Substances Control Act):

All ingredients are listed.

CERCLA (Comprehensive Environmental Response, Compensation, and Liability Act):

67-56-1 Methanol 5000 lbs

Proposition 65 (California):

Chemicals known to cause cancer:

None of the ingredients is listed

Chemicals known to cause reproductive toxicity for females:

None of the ingredients is listed

Chemicals known to cause reproductive toxicity for males:

None of the ingredients is listed

Chemicals known to cause developmental toxicity:

67-56-1 Methanol

Canada

Canadian Domestic Substances List (DSL):

All ingredients are listed.

Canadian NPRI Ingredient Disclosure list (limit 0.1%):

None of the ingredients is listed

Canadian NPRI Ingredient Disclosure list (limit 1%):

67-56-1 Methanol

SECTION 16 : Other information

This product has been classified in accordance with hazard criteria of the Controlled Products Regulations and the SDS contains all the information required by the Controlled Products Regulations. Note: The responsibility to provide a safe workplace remains with the user. The user should consider the health hazards and safety information contained herein as a guide and should take those precautions required in an individual operation to instruct employees and develop work practice procedures for a safe work environment. The information contained herein is, to the best of our knowledge and belief, accurate. However, since the conditions of handling and use are beyond our control, we make no guarantee of results, and assume no liability for damages incurred by the use of this material. It is the responsibility of the user to comply with all applicable laws and regulations applicable to this material.

GHS Full Text Phrases:

Abbreviations and acronyms:

IMDG: International Maritime Code for Dangerous Goods

PNEC: Predicted No-Effect Concentration (REACH)

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Methanol, Lab Grade, 4L

CFR: Code of Federal Regulations (USA)

SARA: Superfund Amendments and Reauthorization Act (USA)

RCRA: Resource Conservation and Recovery Act (USA)

TSCA: Toxic Substances Control Act (USA)

NPRI: National Pollutant Release Inventory (Canada)

DOT: US Department of Transportation

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

ACGIH: American Conference of Governmental Industrial Hygienists

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMIS: Hazardous Materials Identification System (USA)

WHMIS: Workplace Hazardous Materials Information System (Canada)

DNEL: Derived No-Effect Level (REACH)

Effective date : 01.08.2015

Last updated : 03.27.2015

AMBERLYST™ 35DRY Polymeric Catalyst

Industrial-grade, Strongly Acidic Catalyst

Description

AMBERLYST™ 35DRY Polymeric Catalyst is a bead-form, strongly acidic resin developed particularly for heterogeneous acid catalysis of a wide variety of organic reactions. It is also useful in non-aqueous ion exchange systems for the removal of cationic impurities.

The macroporous pore structure of AMBERLYST™ 35DRY permits ready access of liquid or gaseous reactants to the hydrogen ion sites located throughout the bead, thus facilitating successful performance even in non-swelling organic media.

The minimal water content of AMBERLYST™ 35DRY makes it excellent for use in non-aqueous systems where the presence of water will have a negative effect on catalytic activity. Its exceptional thermal resistance coupled with very high dry weight capacity make it the catalyst of choice for phenol alkylation, esterification, etherification, condensation, and hydrolysis.

Applications

- Esterification (acetates, acrylates, fatty acid esters)
- Etherification (MTBE, ETBE, TAME)
- Phenol alkylation
- Condensation
- Hydrolysis
- Non-aqueous ion exchange systems

Typical Properties

Physical Properties

Copolymer	Styrene-divinylbenzene
Matrix	Macroporous
Type	Strong acid cation
Functional Group	Sulfonic acid
Physical Form	Gray to black, opaque, spherical beads

Nitrogen BET

Surface Area	50 m ² /g
Total Pore Volume	0.35 cc/g
Average Pore Diameter	300 Å

Chemical Properties

Ionic Form as Shipped	H ⁺
Concentration of Acid Sites †	≥ 5.00 eq/kg
Catalyst Volatiles	≤ 3.0%

Particle Size §

< 300 µm	≤ 0.3%
> 850 µm	≤ 10.0%

Swelling (in solvent)

Phenol	27%
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Density

Shipping Weight	560 g/L
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† Dry Weight Capacity ≥ 5.00 eq/kg

§ For additional particle size information, please refer to the [Particle Size Distribution Cross Reference Chart](#) (Form No. 177-01775).

Suggested Operating Conditions

Maximum Operating Temperature	150°C (300°F) in non-aqueous media
Bed Depth, min.	600 mm (2.0 ft)
Pressure Drop, max.	1 bar (15 psig) across the bed
Flowrates	
Linear Hourly Space Velocity (LHSV)	0.5 – 5 h ⁻¹

SECTION: 1. Product and company identification

1.1. Product identifier

Product form : Substance
 Substance name : Dimethyl Ether
 CAS-No. : 115-10-6
 Formula : C₂H₆O

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

Use of the substance/mixture : Industrial use; Use as directed.

1.3. Details of the supplier of the safety data sheet

Praxair, Inc.
 10 Riverview Drive
 Danbury, CT 06810-6268 - USA
 T 1-800-772-9247 (1-800-PRAXAIR) - F 1-716-879-2146
www.praxair.com

1.4. Emergency telephone number

Emergency number : Onsite Emergency: 1-800-645-4633

CHEMTREC, 24hr/day 7days/week
 — Within USA: 1-800-424-9300, Outside USA: 001-703-527-3887
 (collect calls accepted, Contract 17729)

SECTION 2: Hazard identification

2.1. Classification of the substance or mixture

GHS US classification

Flam. Gas 1 H220
 Press. Gas (Liq.) H280
 STOT SE 3 H336

2.2. Label elements

GHS US labeling

Hazard pictograms (GHS US) :



Signal word (GHS US) :

Danger

Hazard statements (GHS US) :

H220 - EXTREMELY FLAMMABLE GAS
 H280 - CONTAINS GAS UNDER PRESSURE; MAY EXPLODE IF HEATED
 H336 - MAY CAUSE DROWSINESS OR DIZZINESS
 OSHA-H01 - MAY DISPLACE OXYGEN AND CAUSE RAPID SUFFOCATION.
 CGA-HG04 - MAY FORM EXPLOSIVE MIXTURES WITH AIR
 CGA-HG01 - MAY CAUSE FROSTBITE.

Precautionary statements (GHS US) :

P202 - Do not handle until all safety precautions have been read and understood.
 P210 - Keep away from Heat, Open flames, Sparks, Hot surfaces. - No smoking
 P261 - Avoid breathing gas
 P262 - Do not get in eyes, on skin, or on clothing.
 P264 - Wash hands thoroughly after handling
 P271+P403 - Use and store only outdoors or in a well-ventilated place.
 P280 - Wear protective gloves, protective clothing, eye protection, face protection.
 P304 - IF INHALED:
 P340 - Remove person to fresh air and keep comfortable for breathing.
 P312 - Call a poison center/doctor if you feel unwell

Dimethyl Ether

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- P302 - IF ON SKIN:
- P336 - Thaw frosted parts with lukewarm water. Do not rub affected area.
- P315 - Get immediate medical advice/attention.
- P377 - LEAKING GAS FIRE: Do not extinguish, unless leak can be stopped safely.
- P381 - Eliminate all ignition sources if safe to do so.
- CGA-PG05 - Use a back flow preventive device in the piping.
- CGA-PG06 - Close valve after each use and when empty.
- CGA-PG11 - Never put cylinders into unventilated areas of passenger vehicles.
- CGA-PG02 - Protect from sunlight when ambient temperature exceeds 52°C (125°F).

2.3. Other hazards

Other hazards not contributing to the classification : Contact with liquid may cause cold burns/frostbite.

2.4. Unknown acute toxicity (GHS US)

No data available

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%
Dimethyl Ether (Main constituent)	(CAS-No.) 115-10-6	100

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

- First-aid measures after inhalation : Remove to fresh air and keep at rest in a position comfortable for breathing. If not breathing, give artificial respiration. If breathing is difficult, trained personnel should give oxygen. Call a physician.
- First-aid measures after skin contact : The liquid may cause frostbite. For exposure to liquid, immediately warm frostbite area with warm water not to exceed 105°F (41°C). Water temperature should be tolerable to normal skin. Maintain skin warming for at least 15 minutes or until normal coloring and sensation have returned to the affected area. In case of massive exposure, remove clothing while showering with warm water. Seek medical evaluation and treatment as soon as possible.
- First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Hold the eyelids open and away from the eyeballs to ensure that all surfaces are flushed thoroughly. Contact an ophthalmologist immediately..
- First-aid measures after ingestion : Ingestion is not considered a potential route of exposure.

4.2. Most important symptoms and effects, both acute and delayed

No additional information available

4.3. Indication of any immediate medical attention and special treatment needed

None. Obtain medical assistance.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Carbon dioxide, Dry chemical, Water spray or fog.

5.2. Special hazards arising from the substance or mixture

- Fire hazard : EXTREMELY FLAMMABLE GAS. If venting or leaking gas catches fire, do not extinguish flames. Flammable vapors may spread from leak, creating an explosive reignition hazard. Vapors can be ignited by pilot lights, other flames, smoking, sparks, heaters, electrical equipment, static discharge, or other ignition sources at locations distant from product handling point. Explosive atmospheres may linger. Before entering an area, especially a confined area, check the atmosphere with an appropriate device.
- Explosion hazard : EXTREMELY FLAMMABLE GAS. Forms explosive mixtures with air and oxidizing agents.
- Reactivity : No reactivity hazard other than the effects described in sub-sections below.

5.3. Advice for firefighters

- Firefighting instructions : Evacuate all personnel from the danger area. Use self-contained breathing apparatus (SCBA) and protective clothing. Immediately cool containers with water from maximum distance. Stop flow of gas if safe to do so, while continuing cooling water spray. Remove ignition sources if safe to do so. Remove containers from area of fire if safe to do so. On-site fire brigades must comply with OSHA 29 CFR 1910.156 and applicable standards under 29 CFR 1910 Subpart L—Fire Protection.
- Protection during firefighting : Compressed gas: asphyxiant. Suffocation hazard by lack of oxygen.
- Special protective equipment for fire fighters : Standard protective clothing and equipment (Self Contained Breathing Apparatus) for fire fighters.
- Specific methods : Use fire control measures appropriate for the surrounding fire. Exposure to fire and heat radiation may cause gas containers to rupture. Cool endangered containers with water spray jet from a protected position. Prevent water used in emergency cases from entering sewers and drainage systems.
- Stop flow of product if safe to do so.
- Use water spray or fog to knock down fire fumes if possible.
- Do not extinguish a leaking gas flame unless absolutely necessary. Spontaneous/explosive re-ignition may occur. Extinguish any other fire.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

- General measures : **Danger: Flammable, liquefied gas.** FORMS EXPLOSIVE MIXTURES WITH AIR. Immediately evacuate all personnel from danger area. Use self-contained breathing apparatus where needed. Remove all sources of ignition if safe to do so. Reduce vapors with fog or fine water spray, taking care not to spread liquid with water. Shut off flow if safe to do so. Ventilate area or move container to a well-ventilated area. Flammable vapors may spread from leak and could explode if reignited by sparks or flames. Explosive atmospheres may linger. Before entering area, especially confined areas, check atmosphere with an appropriate device. Prevent from entering sewers, basements and workpits, or any place where its accumulation can be dangerous.

6.1.1. For non-emergency personnel

No additional information available

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Try to stop release. Reduce vapor with fog or fine water spray. Prevent waste from contaminating the surrounding environment. Prevent soil and water pollution. Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.

6.3. Methods and material for containment and cleaning up

No additional information available

6.4. Reference to other sections

See also sections 8 and 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

- Precautions for safe handling : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Use only non-sparking tools. Use only explosion-proof equipment.
- All piped systems and associated equipment must be grounded.
- Leak-check system with soapy water; never use a flame.
- Wear leather safety gloves and safety shoes when handling cylinders. Protect cylinders from physical damage; do not drag, roll, slide or drop. While moving cylinder, always keep in place removable valve cover. Never attempt to lift a cylinder by its cap; the cap is intended solely to protect the valve. When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders. Never insert an object (e.g, wrench, screwdriver, pry bar) into cap openings; doing so may damage the valve and cause a leak. Use an adjustable strap wrench to remove over-tight or rusted caps. Open the valve slowly. If the valve is hard to open, discontinue use and contact your supplier. Close the container valve after each use; keep closed even when empty. Never apply flame or localized heat directly to any part of the container. High temperatures may damage the container and could cause the pressure relief device to activate prematurely, venting the container contents. For other precautions in using this product, see section 16.

7.2. Conditions for safe storage, including any incompatibilities

- Storage conditions : Store only where temperature will not exceed 125°F (52°C). Post "No Smoking/No Open Flames" signs in storage and use areas. There must be no sources of ignition. Separate packages and protect against potential fire and/or explosion damage following appropriate codes and requirements (e.g, NFPA 30, NFPA 55, NFPA 70, and/or NFPA 221 in the U.S.) or according to requirements determined by the Authority Having Jurisdiction (AHJ). Always secure containers upright to keep them from falling or being knocked over. Install valve protection cap, if provided, firmly in place by hand when the container is not in use. Store full and empty containers separately. Use a first-in, first-out inventory system to prevent storing full containers for long periods. For other precautions in using this product, see section 16.

OTHER PRECAUTIONS FOR HANDLING, STORAGE, AND USE: When handling product under pressure, use piping and equipment adequately designed to withstand the pressures to be encountered. Never work on a pressurized system. Use a back flow preventive device in the piping. Gases can cause rapid suffocation because of oxygen deficiency; store and use with adequate ventilation. If a leak occurs, close the container valve and blow down the system in a safe and environmentally correct manner in compliance with all international, federal/national, state/provincial, and local laws; then repair the leak. Never place a container where it may become part of an electrical circuit.

7.3. Specific end use(s)

None.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Dimethyl Ether (115-10-6)	
ACGIH	Not established
USA OSHA	Not established

8.2. Exposure controls

- Appropriate engineering controls : Use an explosion-proof local exhaust system. Local exhaust and general ventilation must be adequate to meet exposure standards. **MECHANICAL (GENERAL): Inadequate - Use only in a closed system.** Use explosion proof equipment and lighting.
- Hand protection : Wear working gloves when handling gas containers.
- Eye protection : Wear safety glasses with side shields. Wear safety glasses with side shields or goggles when transfilling or breaking transfer connections.

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Respiratory protection	: When workplace conditions warrant respirator use, follow a respiratory protection program that meets OSHA 29 CFR 1910.134, ANSI Z88.2, or MSHA 30 CFR 72.710 (where applicable). Use an air-supplied or air-purifying cartridge if the action level is exceeded. Ensure that the respirator has the appropriate protection factor for the exposure level. If cartridge type respirators are used, the cartridge must be appropriate for the chemical exposure. For emergencies or instances with unknown exposure levels, use a self-contained breathing apparatus (SCBA).
Thermal hazard protection	: Wear cold insulating gloves when transfilling or breaking transfer connections. None necessary.
Environmental exposure controls	: Refer to local regulations for restriction of emissions to the atmosphere. See section 13 for specific methods for waste gas treatment. Refer to local regulations for restriction of emissions to the atmosphere.
Other information	: Consider the use of flame resistant anti-static safety clothing. Wear safety shoes while handling containers.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Gas
Molecular mass	: 46 g/mol
Color	: Colorless.
Odor	: Ethereal. Poor warning properties at low concentrations.
Odor threshold	: No data available
pH	: Not applicable.
Relative evaporation rate (butyl acetate=1)	: No data available
Relative evaporation rate (ether=1)	: Not applicable.
Melting point	: -141.5 °C
Freezing point	: No data available
Boiling point	: -24.8 °C
Flash point	: Not applicable.
Critical temperature	: 126.9 °C
Auto-ignition temperature	: 350 °C
Decomposition temperature	: No data available
Flammability (solid, gas)	: 3.4 - 18
Vapor pressure	: 510 kPa
Critical pressure	: 5370 kPa
Relative vapor density at 20 °C	: No data available
Relative density	: 0.73
Density	: 668.3 kg/m ³ (at 20 °C)
Relative gas density	: 1.6
Solubility	: Water: No data available
Log Pow	: 0.1
Log Kow	: Not applicable.
Viscosity, kinematic	: Not applicable.
Viscosity, dynamic	: Not applicable.
Explosive properties	: Not applicable.
Oxidizing properties	: None.
Explosion limits	: No data available

9.2. Other information

Gas group	: Press. Gas (Liq.)
Additional information	: Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level.

SECTION 10: Stability and reactivity

10.1. Reactivity

No reactivity hazard other than the effects described in sub-sections below.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

May occur. The presence of oxygen or prolonged standing in or exposure to direct sunlight may lead to formation of unstable peroxides, which may explode spontaneously or when heated.

10.4. Conditions to avoid

High temperature. direct sunlight.

10.5. Incompatible materials

Oxidizing agents. Halogens. Acids. carbon monoxide. Aluminum hydride. Lithium aluminium hydride.

10.6. Hazardous decomposition products

Thermal decomposition may produce : Carbon monoxide. Carbon dioxide.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

Dimethyl Ether (f)115-10-6	
LC50 inhalation rat (ppm)	163754 ppm/1h
ATE US (vapors)	308.5 mg/l/4h
ATE US (dust, mist)	308.5 mg/l/4h

Skin corrosion/irritation : Not classified

pH: Not applicable.

Serious eye damage/irritation : Not classified

pH: Not applicable.

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

Reproductive toxicity : Not classified

Specific target organ toxicity – single exposure : MAY CAUSE DROWSINESS OR DIZZINESS.

Specific target organ toxicity – repeated exposure : Not classified

Aspiration hazard : Not classified

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : No ecological damage caused by this product.

12.2. Persistence and degradability

Dimethyl Ether (115-10-6)	
Persistence and degradability	Not readily biodegradable.

12.3. Bioaccumulative potential

Dimethyl Ether (115-10-6)	
Log Pow	0.1
Log Kow	Not applicable.
Bioaccumulative potential	Not expected to bioaccumulate due to the low log Kow (log Kow < 4). Refer to section 9.

Dimethyl Ether

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12.4. Mobility in soil

Dimethyl Ether (115-10-6)	
Mobility in soil	No data available.
Ecology - soil	Because of its high volatility, the product is unlikely to cause ground or water pollution.

12.5. Other adverse effects

Other adverse effects : May cause pH changes in aqueous ecological systems.
 Effect on ozone layer : None.
 Global warming potential [CO2=1] : 1
 Effect on the global warming : No known effects from this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product/Packaging disposal recommendations : Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.

SECTION 14: Transport information

In accordance with DOT
 Transport document description : UN1033 Dimethyl ether, 2.1
 UN-No.(DOT) : UN1033
 Proper Shipping Name (DOT) : Dimethyl ether
 Class (DOT) : 2.1 - Class 2.1 - Flammable gas 49 CFR 173.115
 Hazard labels (DOT) : 2.1 - Flammable gas



DOT Special Provisions (49 CFR 172.102) : T50 - When portable tank instruction T50 is referenced in Column (7) of the 172.101 Table, the applicable liquefied compressed gases are authorized to be transported in portable tanks in accordance with the requirements of 173.313 of this subchapter.

Additional information

Emergency Response Guide (ERG) Number : 115
 Other information : No supplementary information available.
 Special transport precautions : Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers:
 - Ensure there is adequate ventilation. - Ensure that containers are firmly secured. - Ensure cylinder valve is closed and not leaking. - Ensure valve outlet cap nut or plug (where provided) is correctly fitted. - Ensure valve protection device (where provided) is correctly fitted.

Transport by sea

UN-No. (IMDG) : 1033
 Proper Shipping Name (IMDG) : Dimethyl Ether
 Class (IMDG) : 2 - Gases
 Division (IMDG) : 2.1 - Flammable gases
 MFAG-No : 115

Air transport

UN-No. (IATA) : 1033
 Proper Shipping Name (IATA) : Dimethyl ether
 Class (IATA) : 2

Dimethyl Ether

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Civil Aeronautics Law

: Gases under pressure/Gases flammable under pressure

SECTION 15: Regulatory information

15.1. US Federal regulations

Dimethyl Ether (115-10-6)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

SARA Section 311/312 Hazard Classes

Immediate (acute) health hazard
Delayed (chronic) health hazard
Sudden release of pressure hazard
Fire hazard

15.2. International regulations

CANADA

Dimethyl Ether (115-10-6)

Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

Dimethyl Ether (115-10-6)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

15.2.2. National regulations

Dimethyl Ether (115-10-6)

Listed on the AICS (Australian Inventory of Chemical Substances)
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)
Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory
Listed on the Japanese ISHL (Industrial Safety and Health Law)
Listed on the Korean ECL (Existing Chemicals List)
Listed on NZIoC (New Zealand Inventory of Chemicals)
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)
Listed on INSQ (Mexican National Inventory of Chemical Substances)
Listed on the TCSI (Taiwan Chemical Substance Inventory)

15.3. US State regulations

Dimethyl Ether(115-10-6)

U.S. - California - Proposition 65 - Carcinogens List

No

U.S. - California - Proposition 65 - Developmental Toxicity

No

U.S. - California - Proposition 65 - Reproductive Toxicity - Female

No

U.S. - California - Proposition 65 - Reproductive Toxicity - Male

No

State or local regulations

U.S. - Massachusetts - Right To Know List
U.S. - New Jersey - Right to Know Hazardous Substance List
U.S. - Pennsylvania - RTK (Right to Know) List

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SECTION 16: Other information

Other information

: When you mix two or more chemicals, you can create additional, unexpected hazards. Obtain and evaluate the safety information for each component before you produce the mixture. Consult an industrial hygienist or other trained person when you evaluate the end product. Before using any plastics, confirm their compatibility with this product.

Praxair asks users of this product to study this SDS and become aware of the product hazards and safety information. To promote safe use of this product, a user should (1) notify employees, agents, and contractors of the information in this SDS and of any other known product hazards and safety information, (2) furnish this information to each purchaser of the product, and (3) ask each purchaser to notify its employees and customers of the product hazards and safety information.

The opinions expressed herein are those of qualified experts within Praxair, Inc. We believe that the information contained herein is current as of the date of this Safety Data Sheet. Since the use of this information and the conditions of use are not within the control of Praxair, Inc, it is the user's obligation to determine the conditions of safe use of the product.

Praxair SDSs are furnished on sale or delivery by Praxair or the independent distributors and suppliers who package and sell our products. To obtain current SDSs for these products, contact your Praxair sales representative, local distributor, or supplier, or download from www.praxair.com. If you have questions regarding Praxair SDSs, would like the document number and date of the latest SDS, or would like the names of the Praxair suppliers in your area, phone or write the Praxair Call Center (Phone: 1-800-PRAXAIR/1-800-772-9247; Address: Praxair Call Center, Praxair, Inc, P.O. Box 44, Tonawanda, NY 14151-0044).

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Revision date

: 01/17/2019

NFPA health hazard

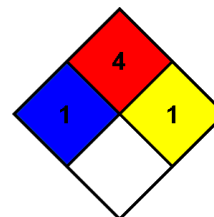
: 1 - Materials that, under emergency conditions, can cause significant irritation.

NFPA fire hazard

: 4 - Materials that rapidly or completely vaporize at atmospheric pressure and normal ambient temperature or that are readily dispersed in air and burn readily.

NFPA reactivity

: 1 - Materials that in themselves are normally stable but can become unstable at elevated temperatures and pressures.



SDS US (GHS HazCom 2012) - Praxair

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.

SAFETY DATA SHEET

Revision Date 07/31/2015

1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifiers**

Product name : ViaTrap (Mineral Oil)
 Product Number : 225-9598, 225-9598A, 225-9599
 Brand : SKC Inc.
 CAS-No. : 8042-47-5

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

Identified uses : To be used with SKC BioSampler

1.3 Details of the supplier of the safety data sheet

Company : SKC, Inc.
 863 Valley View Rd.
 Eighty Four, PA 15330
 USA
 Telephone : 724-941-9701; 800-752-8472 (Mon - Fri, 8:30 a.m. - 5:00 p.m. EST)
 Fax : 724-941-1369 (Mon-Fri, 8:30 a.m. - 5:00 p.m. EST)

1.4 Emergency telephone number

Emergency Phone # : CHEMTREC at 800-424-9300 (U.S./Canada); 703-741-5970 (Global)

2. HAZARDS IDENTIFICATION**2.1 Classification of the substance or mixture**

Not a hazardous substance or mixture.

2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none**3. COMPOSITION/INFORMATION ON INGREDIENTS****3.1 Substances**

CAS-No. : 8042-47-5
 EC-No. : 232-455-8

Hazardous components

Component	Classification	Concentration
Mineral oil		
		<= 100 %

4. FIRST AID MEASURES**4.1 Description of first aid measures****If inhaled**

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

In case of skin contact

Wash off with soap and plenty of water.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

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

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES**5.1 Extinguishing media****Suitable extinguishing media**

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES**6.1 Personal precautions, protective equipment and emergency procedures**

Avoid breathing vapours, mist or gas.
For personal protection see section 8.

6.2 Environmental precautions

No special environmental precautions required.

6.3 Methods and materials for containment and cleaning up

Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE**7.1 Precautions for safe handling**

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.
Storage class (TRGS 510): Combustible liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Mineral oil	8042-47-5	TWA	5.0 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	5.0 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	5.0 mg/m ³	USA. NIOSH Recommended Exposure Limits
		ST	10.0 mg/m ³	USA. NIOSH Recommended Exposure Limits
		TWA	5.0 mg/m ³	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Not classifiable as a human carcinogen		

8.2 Exposure controls

Appropriate engineering controls

General industrial hygiene practice.

Personal protective equipment

Eye/face protection

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

Skin protection

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

Full contact

Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 480 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact

Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 30 min
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

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

Respiratory protection

Respiratory protection not required. For nuisance exposures use type OV/AG (US) or type ABEK (EU EN 14387) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

No special environmental precautions required.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance	Form: viscous liquid Colour: colourless
b) Odour	odourless
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: ca. -14.99 °C (5.02 °F) at ca. 1,013 hPa (760 mmHg)
f) Initial boiling point and boiling range	218 - 800 °C (424 - 1,472 °F) at ca. 1,013 hPa (760 mmHg)
g) Flash point	> 112 °C (> 234 °F) - closed cup - ISO 2719
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapour pressure	<= 0.0001 hPa (<= 0.0001 mmHg) at ca. 20 °C (68 °F) - OECD Test Guideline 104
l) Vapour density	No data available
m) Relative density	0.84 g/mL at 25 °C (77 °F) -
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Auto-ignition temperature	325 - 355 °C (617 - 671 °F) at 1,013.25 hPa (760.00 mmHg)
q) Decomposition temperature	No data available
r) Viscosity	> 20.5 mm ² /s at 40 °C (104 °F) -
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - No data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - > 5,000 mg/kg
(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - > 5 mg/l
(OECD Test Guideline 403)

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Skin - Rabbit
Result: No skin irritation
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitisation

Buehler Test - Guinea pig
Did not cause sensitisation on laboratory animals.
(OECD Test Guideline 406)

Germ cell mutagenicity

in vitro assay
S. typhimurium
Result: negative

Carcinogenicity

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

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

Repeated dose toxicity - Rat - female - Oral - No observed adverse effect level - 1,600 mg/kg - Lowest observed adverse effect level - 160 mg/kg
RTECS: PY8047000

Aspiration may lead to: lipid pneumonia, Effects due to ingestion may include: laxative effect, Gastrointestinal disturbance, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish static test LC50 - Oncorhynchus mykiss (rainbow trout) - > 100 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates static test LC50 - Daphnia magna (Water flea) - > 100 mg/l - 48 h (OECD Test Guideline 202)

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

15. REGULATORY INFORMATION

SARA 302 Components

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

SARA 313 Components

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

SARA 311/312 Hazards

No SARA Hazards

Massachusetts Right To Know Components

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

Pennsylvania Right To Know Components

Mineral oil

CAS-No.
8042-47-5

Revision Date

New Jersey Right To Know Components

Mineral oil

CAS-No.
8042-47-5

Revision Date

California Prop. 65 Components

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

16. OTHER INFORMATION**HMIS Rating**

Health hazard: 0

Chronic Health Hazard:

Flammability: 1

Physical Hazard 0

NFPA Rating

Health hazard: 0

Fire Hazard: 1

Reactivity Hazard: 0

Disclaimer

For approved uses only. Not for drug, household, or other uses.

The above information is believed to be correct but does not purport to be all-inclusive and shall be used only as a guide. SKC Inc. shall not be held liable for any damage resulting from handling or from contact with the above product.

Latest Change(s): Updated SDS to bring into compliance with the GHS

Last Update: July 2015

CSTR-5V CSTR-6L CSTR-6V CSTR-7L CSTR-7V..... 37
 CSTR-8L CSTR-8V CSTR-9L CSTR-9V CWIN..... 38
 DMEIN DST-1L DST-2V S-104-1 S-104-2..... 39
 S-104-3 S-104-4 S-104-5 S-106 S-111..... 40
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RUN CONTROL SECTION

RUN CONTROL INFORMATION

THIS COPY OF ASPEN PLUS LICENSED TO UNIVERSITY OF PENNSYLVAN

TYPE OF RUN: EDIT

INPUT FILE NAME: _0435pdr.inm

INPUT PROBLEM DATA FILE NAME : _0435pdr

OUTPUT PROBLEM DATA FILE NAME: _5818gaz

LOCATED IN:

PDF SIZE USED FOR INPUT TRANSLATION:

NUMBER OF FILE RECORDS (PSIZE) = 0
 NUMBER OF IN-CORE RECORDS = 256
 PSIZE NEEDED FOR SIMULATION = 1

CALLING PROGRAM NAME: apmain

LOCATED IN: C:\Program Files\AspenTech\Aspen Plus V11.0\Engine\XeQ

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

DESCRIPTION

Specialty Chemicals Simulation with English Units : F, psi,
 lb/hr, lbmol/hr, Btu/hr, gal/hr. Property Method: NRTL Flow basis
 for input: Mass Stream report composition: Mass flow

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FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
S-104-1	----	CSTR-1	S-104-2	----	CSTR-2
S-104-3	----	CSTR-3	S-104-4	----	CSTR-4
S-104-5	----	CSTR-5	CSTR-9V	CSTR-9	CSTR-8
CSTR-9L	CSTR-9	DST-2	CSTR-1V	CSTR-1	DST-1
CSTR-1L	CSTR-1	CSTR-2	CSTR-2V	CSTR-2	CSTR-1
CSTR-2L	CSTR-2	CSTR-3	CSTR-3V	CSTR-3	CSTR-2
CSTR-3L	CSTR-3	CSTR-4	CSTR-4V	CSTR-4	CSTR-3
CSTR-4L	CSTR-4	CSTR-5	CSTR-5V	CSTR-5	CSTR-4
CSTR-5L	CSTR-5	CSTR-6	DST-2V	DST-2	CSTR-9
S-111	DST-2	----	S-106	DST-1	----
DST-1L	DST-1	CSTR-1	CSTR-6V	CSTR-6	CSTR-5
CSTR-6L	CSTR-6	CSTR-7	CSTR-7V	CSTR-7	CSTR-6
CSTR-7L	CSTR-7	CSTR-8	CSTR-8V	CSTR-8	CSTR-7
CSTR-8L	CSTR-8	CSTR-9			

FLWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
CSTR-9	DST-2V CSTR-8L	CSTR-9V CSTR-9L
CSTR-1	CSTR-2V DST-1L S-104-1	CSTR-1V CSTR-1L
CSTR-2	CSTR-1L CSTR-3V S-104-2	CSTR-2V CSTR-2L
CSTR-3	CSTR-2L CSTR-4V S-104-3	CSTR-3V CSTR-3L
CSTR-4	CSTR-3L CSTR-5V S-104-4	CSTR-4V CSTR-4L
CSTR-5	CSTR-4L CSTR-6V S-104-5	CSTR-5V CSTR-5L
DST-2	CSTR-9L	DST-2V S-111
DST-1	CSTR-1V	S-106 DST-1L
CSTR-6	CSTR-7V CSTR-5L	CSTR-6V CSTR-6L
CSTR-7	CSTR-6L CSTR-8V	CSTR-7V CSTR-7L
CSTR-8	CSTR-7L CSTR-9V	CSTR-8V CSTR-8L

CONVERGENCE STATUS SUMMARY

TEAR STREAM SUMMARY

STREAM ID	VARIABLE ID	MAXIMUM ERR/TOL	MAX. ERR. RELATIVE	ABSOLUTE ERROR	STAT	CONV BLOCK
CSTR-1L	METHANOLMOLEFLOW	0.20499	0.20499E-05	0.38297E-06	#	\$OLVER01
CSTR-9L	METHANOLMOLEFLOW	0.45320	0.45320E-05	0.41182E-06	#	\$OLVER01
CSTR-2L	METHANOLMOLEFLOW	0.22286	0.22286E-05	0.48327E-06	#	\$OLVER01
CSTR-3L	METHANOLMOLEFLOW	0.26591	0.26591E-05	0.56619E-06	#	\$OLVER01
CSTR-4L	METHANOLMOLEFLOW	0.43283	0.43283E-05	0.87334E-06	#	\$OLVER01
CSTR-5L	METHANOLMOLEFLOW	0.76309	0.76309E-05	0.13934E-05	#	\$OLVER01
DST-1L	METHANOLMOLEFLOW	0.26647	0.26647E-05	0.31381E-06	#	\$OLVER01
CSTR-6L	METHANOLMOLEFLOW	0.87229	0.87229E-05	0.13518E-05	#	\$OLVER01
CSTR-7L	METHANOLMOLEFLOW	0.99971	0.99971E-05	0.13502E-05	#	\$OLVER01
CSTR-8L	METHANOLMOLEFLOW	0.93362	0.93362E-05	0.10690E-05	#	\$OLVER01
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FLWSHEET SECTION

CONVERGENCE STATUS SUMMARY (CONTINUED)

= CONVERGED
* = NOT CONVERGED

CONVERGENCE BLOCK: \$OLVER01

Tear Stream : CSTR-1L CSTR-9L CSTR-2L CSTR-3L CSTR-4L
Tolerance used: 0.100D-04 0.100D-04 0.100D-04 0.100D-04 0.100D-04
Trace molefrac: 0.100D-06 0.100D-06 0.100D-06 0.100D-06 0.100D-06

Tear Stream : CSTR-5L DST-1L CSTR-6L CSTR-7L CSTR-8L
Tolerance used: 0.100D-04 0.100D-04 0.100D-04 0.100D-04 0.100D-04
Trace molefrac: 0.100D-06 0.100D-06 0.100D-06 0.100D-06 0.100D-06

MAXIT= 500 WAIT 2 ITERATIONS BEFORE ACCELERATING
ACCELERATE EVERY 3 ITERATIONS
QMAX = 1.0 QMIN = 0.0
METHOD: WEGSTEIN STATUS: CONVERGED
TOTAL NUMBER OF ITERATIONS: 178
NUMBER OF ITERATIONS ON LAST OUTER LOOP: 0

*** FINAL VALUES ***

VAR#	TEAR STREAM	VAR	STREAM	SUBSTREA	COMPONEN	UNIT	VALUE	PREV
1	TOTAL MOLEFLOW		CSTR-1L	MIXED		KMOL/HR	822.8797	

822.8781	0.1967					
2	TOTAL MOLEFLOW	CSTR-9L	MIXED		KMOL/HR	1030.0702
1030.0661	0.4023					
3	TOTAL MOLEFLOW	CSTR-2L	MIXED		KMOL/HR	1008.7712
1008.7691	0.2093					
4	TOTAL MOLEFLOW	CSTR-3L	MIXED		KMOL/HR	1071.9866
1071.9840	0.2393					
5	TOTAL MOLEFLOW	CSTR-4L	MIXED		KMOL/HR	1119.5980
1119.5938	0.3723					
6	TOTAL MOLEFLOW	CSTR-5L	MIXED		KMOL/HR	1146.4442
1146.4369	0.6387					
7	TOTAL MOLEFLOW	DST-1L	MIXED		KMOL/HR	504.4385
504.4372	0.2625					
8	TOTAL MOLEFLOW	CSTR-6L	MIXED		KMOL/HR	1105.4868
1105.4791	0.6913					
9	TOTAL MOLEFLOW	CSTR-7L	MIXED		KMOL/HR	1078.9059
1078.8973	0.7999					
10	TOTAL MOLEFLOW	CSTR-8L	MIXED		KMOL/HR	1053.9456
1053.9372	0.7977					
11	MOLE-FLOW	CSTR-1L	MIXED	METHANOL	KMOL/HR	672.5686
672.5672	0.2050					
12	MOLE-FLOW	CSTR-1L	MIXED	WATER	KMOL/HR	97.7811
97.7810	0.1388					
13	MOLE-FLOW	CSTR-1L	MIXED	DME	KMOL/HR	52.5300
52.5299	0.1984					
14	PRESSURE	CSTR-1L	MIXED		BAR	7.2533
7.2533	0.0					
15	MASS ENTHALPY	CSTR-1L	MIXED		KCAL/KG	-1779.9239
-1779.9239	4.5788-03					
16	MOLE-FLOW	CSTR-9L	MIXED	METHANOL	KMOL/HR	327.1311
327.1296	0.4532					
17	MOLE-FLOW	CSTR-9L	MIXED	WATER	KMOL/HR	702.0997
702.0970	0.3794					
18	MOLE-FLOW	CSTR-9L	MIXED	DME	KMOL/HR	0.8394
0.8394	-0.2797					
19	PRESSURE	CSTR-9L	MIXED		BAR	7.3305
7.3305	0.0					
20	MASS ENTHALPY	CSTR-9L	MIXED		KCAL/KG	-2759.0970
-2759.0974	1.2501-02					
21	MOLE-FLOW	CSTR-2L	MIXED	METHANOL	KMOL/HR	780.6573
780.6556	0.2229					
22	MOLE-FLOW	CSTR-2L	MIXED	WATER	KMOL/HR	178.0753
178.0751	0.1496					
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FLWSHEET SECTION

CONVERGENCE BLOCK: \$SOLVER01 (CONTINUED)						
23	MOLE-FLOW	CSTR-2L	MIXED	DME	KMOL/HR	50.0386
50.0385	0.2106					
24	PRESSURE	CSTR-2L	MIXED		BAR	7.2629
7.2629	0.0					
25	MASS ENTHALPY	CSTR-2L	MIXED		KCAL/KG	-1861.0009
-1861.0011	7.1145-03					
26	MOLE-FLOW	CSTR-3L	MIXED	METHANOL	KMOL/HR	766.5336
766.5316	0.2659					
27	MOLE-FLOW	CSTR-3L	MIXED	WATER	KMOL/HR	264.9584
264.9579	0.1626					
28	MOLE-FLOW	CSTR-3L	MIXED	DME	KMOL/HR	40.4946
40.4945	0.2390					
29	PRESSURE	CSTR-3L	MIXED		BAR	7.2726
7.2726	0.0					
30	MASS ENTHALPY	CSTR-3L	MIXED		KCAL/KG	-1962.5086
-1962.5089	1.3075-02					
31	MOLE-FLOW	CSTR-4L	MIXED	METHANOL	KMOL/HR	726.3918
726.3886	0.4328					
32	MOLE-FLOW	CSTR-4L	MIXED	WATER	KMOL/HR	362.6807
362.6798	0.2519					
33	MOLE-FLOW	CSTR-4L	MIXED	DME	KMOL/HR	30.5255
30.5254	0.3613					
34	PRESSURE	CSTR-4L	MIXED		BAR	7.2822

7.2822	0.0						
35	MASS ENTHALPY	CSTR-4L	MIXED		KCAL/KG		-2079.7302
-2079.7308	2.7510-02						
36	MOLE-FLOW	CSTR-5L	MIXED	METHANOL	KMOL/HR		657.3875
657.3825	0.7631						
37	MOLE-FLOW	CSTR-5L	MIXED	WATER	KMOL/HR		468.6222
468.6200	0.4669						
38	MOLE-FLOW	CSTR-5L	MIXED	DME	KMOL/HR		20.4346
20.4345	0.5788						
39	PRESSURE	CSTR-5L	MIXED		BAR		7.2919
7.2919	0.0						
40	MASS ENTHALPY	CSTR-5L	MIXED		KCAL/KG		-2218.5497
-2218.5509	5.0884-02						
41	MOLE-FLOW	DST-1L	MIXED	METHANOL	KMOL/HR		423.9577
423.9566	0.2665						
42	MOLE-FLOW	DST-1L	MIXED	WATER	KMOL/HR		28.4650
28.4649	0.2038						
43	MOLE-FLOW	DST-1L	MIXED	DME	KMOL/HR		52.0158
52.0157	0.2620						
44	PRESSURE	DST-1L	MIXED		BAR		7.2215
7.2215	4.0096-04						
45	MASS ENTHALPY	DST-1L	MIXED		KCAL/KG		-1679.6295
-1679.6295	2.1183-03						
46	MOLE-FLOW	CSTR-6L	MIXED	METHANOL	KMOL/HR		557.9028
557.8979	0.8723						
47	MOLE-FLOW	CSTR-6L	MIXED	WATER	KMOL/HR		536.9392
536.9365	0.5079						
48	MOLE-FLOW	CSTR-6L	MIXED	DME	KMOL/HR		10.6448
10.6447	0.4544						
49	PRESSURE	CSTR-6L	MIXED		BAR		7.3015
7.3015	0.0						
50	MASS ENTHALPY	CSTR-6L	MIXED		KCAL/KG		-2357.4523
-2357.4539	6.6016-02						
51	MOLE-FLOW	CSTR-7L	MIXED	METHANOL	KMOL/HR		486.2209
486.2160	0.9997						
52	MOLE-FLOW	CSTR-7L	MIXED	WATER	KMOL/HR		587.4123
587.4085	0.6397						
53	MOLE-FLOW	CSTR-7L	MIXED	DME	KMOL/HR		5.2728
5.2727	0.2243						
54	PRESSURE	CSTR-7L	MIXED		BAR		7.3112
7.3112	0.0						
55	MASS ENTHALPY	CSTR-7L	MIXED		KCAL/KG		-2470.7784
-2470.7800	6.5939-02						
56	MOLE-FLOW	CSTR-8L	MIXED	METHANOL	KMOL/HR		412.2037
412.1999	0.9336						
57	MOLE-FLOW	CSTR-8L	MIXED	WATER	KMOL/HR		639.2264
639.2219	0.7131						
58	MOLE-FLOW	CSTR-8L	MIXED	DME	KMOL/HR		2.5155
2.5155	5.0165-02						
59	PRESSURE	CSTR-8L	MIXED		BAR		7.3209
7.3209	0.0						
60	MASS ENTHALPY	CSTR-8L	MIXED		KCAL/KG		-2596.1459
-2596.1470	3.9797-02						

*** ITERATION HISTORY ***

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FLWSHEET SECTION

CONVERGENCE BLOCK: \$SOLVER01 (CONTINUED)

TEAR STREAMS AND TEAR VARIABLES:

ITERATION ELEMENT	MAX-ERR/TOL	VAR#	STREAM ID	VAR DESCRIPTION	SUBSTREA	COMPONEN	ATTRIBUT
1	34.67	51	CSTR-7L	MOLE-FLO	MIXED	METHANOL	
2	16.85	56	CSTR-8L	MOLE-FLO	MIXED	METHANOL	
3	-17.17	58	CSTR-8L	MOLE-FLO	MIXED	DME	
4	-19.90	58	CSTR-8L	MOLE-FLO	MIXED	DME	

5	-9.270	18	CSTR-9L	MOLE-FLO	MIXED	DME
6	-5.755	53	CSTR-7L	MOLE-FLO	MIXED	DME
7	-4.702	58	CSTR-8L	MOLE-FLO	MIXED	DME
8	-3.932	58	CSTR-8L	MOLE-FLO	MIXED	DME
9	-3.060	18	CSTR-9L	MOLE-FLO	MIXED	DME
10	1.926	51	CSTR-7L	MOLE-FLO	MIXED	METHANOL
11	1.738	46	CSTR-6L	MOLE-FLO	MIXED	METHANOL
12	2.689	46	CSTR-6L	MOLE-FLO	MIXED	METHANOL
13	1.818	51	CSTR-7L	MOLE-FLO	MIXED	METHANOL
14	1.313	56	CSTR-8L	MOLE-FLO	MIXED	METHANOL
15	1.181	51	CSTR-7L	MOLE-FLO	MIXED	METHANOL
16	1.587	36	CSTR-5L	MOLE-FLO	MIXED	METHANOL
17	1.444	46	CSTR-6L	MOLE-FLO	MIXED	METHANOL
18	1.226	51	CSTR-7L	MOLE-FLO	MIXED	METHANOL
19	0.9997	51	CSTR-7L	MOLE-FLO	MIXED	METHANOL

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:

\$SOLVER01 DST-2 CSTR-9 CSTR-8 CSTR-7 CSTR-6 CSTR-5 CSTR-4 CSTR-3 CSTR-2
 | CSTR-1 DST-1
 (RETURN \$SOLVER01)

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***				
	IN	OUT	GENERATION	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/HR)				
METHANOL	769.000	1.63151	-767.339	0.383702E-04
WATER	0.00000	383.652	383.669	0.461319E-04
DME	0.00000	383.669	383.669	0.189891E-05
TOTAL BALANCE				
MOLE (KMOL/HR)	769.000	768.952	0.199840E-12	0.623327E-04
MASS (KG/HR)	24640.4	24639.1		0.526723E-04
ENTHALPY (GCAL/HR)	-43.1617	-43.8077		0.147464E-01
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FLOWSHEET SECTION

OVERALL FLOWSHEET BALANCE (CONTINUED)

*** CO2 EQUIVALENT SUMMARY ***				
FEED STREAMS CO2E	0.00000	KG/HR		
PRODUCT STREAMS CO2E	17675.3	KG/HR		
NET STREAMS CO2E PRODUCTION	17675.3	KG/HR		
UTILITIES CO2E PRODUCTION	0.00000	KG/HR		
TOTAL CO2E PRODUCTION	17675.3	KG/HR		
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PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME	
METHANOL	C	CH4O	METHANOL	
WATER	C	H2O	WATER	
DME	C	C2H6O-1	DIMETHYL-ETHER	
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REACTION SECTION

REACTION: BOOK TYPE: GENERAL

Unit operations referencing this reaction model:

Reactor Name	Block Type	Reactor Name	Block Type
--------------	------------	--------------	------------

1	RCSTR	2	RCSTR
3	RCSTR	4	RCSTR
5	RCSTR	6	RCSTR
7	RCSTR	8	RCSTR
9	RCSTR	CSTR-5	RCSTR
CSTR-7	RCSTR	CSTR-3	RCSTR
CSTR-4	RCSTR	CSTR-6	RCSTR
CSTR-9	RCSTR		

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U-O-S BLOCK SECTION

BLOCK: CSTR-1 MODEL: RCSTR

 INLET STREAMS: CSTR-2V DST-1L S-104-1
 OUTLET STREAMS: CSTR-1V CSTR-1L
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
TOTAL BALANCE				
MOLE (KMOL/HR)	1711.54	1711.54	-0.249800E-13	0.945714E-06
MASS (KG/HR)	59918.7	59918.6		0.858193E-06
ENTHALPY (GCAL/HR)	-86.1119	-86.1122		0.313110E-05

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	20205.7	KG/HR
PRODUCT STREAMS CO2E	22491.6	KG/HR
NET STREAMS CO2E PRODUCTION	2285.84	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	2285.84	KG/HR

*** INPUT DATA ***

REACTOR TYPE: DUTY SPEC TWO PHASE REACTOR

REACTOR VOLUME	CUM	2.1000
LIQUID PHASE VOLUME	CUM	1.0000
REACTOR PRESSURE	BAR	7.2533
REACTOR HEAT DUTY	GCAL/HR	0.0000

REACTION PARAGRAPH ID: BOOK TYPE: GENERAL

GLOBAL BASES:
 KBASIS MOLE-GAMMA
 CBASIS MOLARITY
 SBASIS GLOBAL

STOICHIOMETRY:

REACTION NUMBER: 1
 SUBSTREAM: MIXED
 METHANOL -2.0000 WATER 1.0000 DME 1.0000

REAC-DATA ENTRIES:

REACTION NO	TYPE	PHASE	DELT C	BASIS
1	KINETIC	L	0.0000	MOLARITY

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U-O-S BLOCK SECTION

BLOCK: CSTR-1 MODEL: RCSTR (CONTINUED)

*** RESULTS ***

REACTOR TEMPERATURE C 104.79

RESIDENCE TIME	HR	0.50883E-03
VAPOR PHASE VOLUME FRACTION		0.40476
LIQUID PHASE VOLUME FRACTION		0.47619
VAPOR PHASE VOLUME	CUM	0.85000
LIQUID PHASE VOLUME	CUM	1.0000
VAPOR PHASE RESIDENCE TIME	HR	0.23622E-03
LIQUID PHASE RESIDENCE TIME	HR	0.26724E-01

BLOCK: CSTR-2 MODEL: RCSTR

 INLET STREAMS: CSTR-1L CSTR-3V S-104-2
 OUTLET STREAMS: CSTR-2V CSTR-2L
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***
 IN OUT GENERATION RELATIVE DIFF.
 TOTAL BALANCE
 MOLE (KMOL/HR) 1911.88 1911.87 0.149880E-12 0.110444E-05
 MASS (KG/HR) 64211.5 64211.5 0.101851E-05
 ENTHALPY (GCAL/HR) -98.1602 -98.1573 -0.300528E-04

*** CO2 EQUIVALENT SUMMARY ***
 FEED STREAMS CO2E 17581.7 KG/HR
 PRODUCT STREAMS CO2E 20114.6 KG/HR
 NET STREAMS CO2E PRODUCTION 2532.98 KG/HR
 UTILITIES CO2E PRODUCTION 0.00000 KG/HR
 TOTAL CO2E PRODUCTION 2532.98 KG/HR

*** INPUT DATA ***

REACTOR TYPE: DUTY SPEC TWO PHASE REACTOR

REACTOR VOLUME	CUM	2.1000
LIQUID PHASE VOLUME	CUM	1.0000
REACTOR PRESSURE	BAR	7.2629
REACTOR HEAT DUTY	GCAL/HR	0.0000

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

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U-O-S BLOCK SECTION

BLOCK: CSTR-2 MODEL: RCSTR (CONTINUED)

STOICHIOMETRY:

REACTION NUMBER:	1				
SUBSTREAM: MIXED					
METHANOL	-2.0000	WATER	1.0000	DME	1.0000

REAC-DATA ENTRIES:

REACTION NO	TYPE	PHASE	DELT C	BASIS
1	KINETIC	L	0.0000	MOLARITY

*** RESULTS ***

REACTOR TEMPERATURE	C	109.58
RESIDENCE TIME	HR	0.49346E-03
VAPOR PHASE VOLUME FRACTION		0.40476
LIQUID PHASE VOLUME FRACTION		0.47619
VAPOR PHASE VOLUME	CUM	0.85000

LIQUID PHASE VOLUME	CUM	1.0000
VAPOR PHASE RESIDENCE TIME	HR	0.22943E-03
LIQUID PHASE RESIDENCE TIME	HR	0.22589E-01

BLOCK: CSTR-3 MODEL: RCSTR

 INLET STREAMS: CSTR-2L CSTR-4V S-104-3
 OUTLET STREAMS: CSTR-3V CSTR-3L
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		***	***
TOTAL BALANCE	IN	OUT	GENERATION	RELATIVE DIFF.
MOLE (KMOL/HR)	1960.99	1960.98	-0.499600E-13	0.130841E-05
MASS (KG/HR)	63271.3	63271.2		0.122533E-05
ENTHALPY (GCAL/HR)	-102.363	-102.364		0.124439E-04

*** CO2 EQUIVALENT SUMMARY ***				
FEED STREAMS CO2E	14365.0	KG/HR		
PRODUCT STREAMS CO2E	17027.2	KG/HR		
NET STREAMS CO2E PRODUCTION	2662.23	KG/HR		
UTILITIES CO2E PRODUCTION	0.00000	KG/HR		
TOTAL CO2E PRODUCTION	2662.23	KG/HR		

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U-O-S BLOCK SECTION

BLOCK: CSTR-3 MODEL: RCSTR (CONTINUED)

*** INPUT DATA ***

REACTOR TYPE: DUTY SPEC TWO PHASE REACTOR

REACTOR VOLUME	CUM	2.1000
LIQUID PHASE VOLUME	CUM	1.0000
REACTOR PRESSURE	BAR	7.2726
REACTOR HEAT DUTY	GCAL/HR	0.0000

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

STOICHIOMETRY:

REACTION NUMBER:	1				
SUBSTREAM: MIXED					
METHANOL	-2.0000	WATER	1.0000	DME	1.0000

REAC-DATA ENTRIES:

REACTION NO	TYPE	PHASE	DELT C	BASIS
1	KINETIC	L	0.0000	MOLARITY

*** RESULTS ***

REACTOR TEMPERATURE	C	114.21
RESIDENCE TIME	HR	0.49491E-03
VAPOR PHASE VOLUME FRACTION		0.40476
LIQUID PHASE VOLUME FRACTION		0.47619
VAPOR PHASE VOLUME	CUM	0.85000
LIQUID PHASE VOLUME	CUM	1.0000
VAPOR PHASE RESIDENCE TIME	HR	0.23016E-03
LIQUID PHASE RESIDENCE TIME	HR	0.22232E-01

BLOCK: CSTR-4 MODEL: RCSTR

INLET STREAMS: CSTR-3L CSTR-5V S-104-4
OUTLET STREAMS: CSTR-4V CSTR-4L
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***
IN OUT GENERATION RELATIVE DIFF.
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U-O-S BLOCK SECTION

BLOCK: CSTR-4 MODEL: RCSTR (CONTINUED)

TOTAL BALANCE
MOLE (KMOL/HR) 1971.81 1971.81 0.149880E-12 0.211367E-05
MASS (KG/HR) 60755.1 60755.0 0.201265E-05
ENTHALPY (GCAL/HR) -104.854 -104.858 0.434136E-04

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E 10602.2 KG/HR
PRODUCT STREAMS CO2E 13466.0 KG/HR
NET STREAMS CO2E PRODUCTION 2863.83 KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION 2863.83 KG/HR

*** INPUT DATA ***

REACTOR TYPE: DUTY SPEC TWO PHASE REACTOR

REACTOR VOLUME CUM 2.1000
LIQUID PHASE VOLUME CUM 1.0000
REACTOR PRESSURE BAR 7.2822
REACTOR HEAT DUTY GCAL/HR 0.0000

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

STOICHIOMETRY:

REACTION NUMBER: 1
SUBSTREAM: MIXED
METHANOL -2.0000 WATER 1.0000 DME 1.0000

REAC-DATA ENTRIES:

REACTION NO	TYPE	PHASE	DELT C	BASIS
1	KINETIC	L	0.0000	MOLARITY

*** RESULTS ***

REACTOR TEMPERATURE C 119.11
RESIDENCE TIME HR 0.50931E-03
VAPOR PHASE VOLUME FRACTION 0.40476
LIQUID PHASE VOLUME FRACTION 0.47619
VAPOR PHASE VOLUME CUM 0.85000
LIQUID PHASE VOLUME CUM 1.0000
VAPOR PHASE RESIDENCE TIME HR 0.23692E-03
LIQUID PHASE RESIDENCE TIME HR 0.22398E-01

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U-O-S BLOCK SECTION

BLOCK: CSTR-5 MODEL: RCSTR

INLET STREAMS: CSTR-4L CSTR-6V S-104-5
OUTLET STREAMS: CSTR-5V CSTR-5L
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***
IN OUT GENERATION RELATIVE DIFF.
TOTAL BALANCE
MOLE (KMOL/HR) 1956.27 1956.27 -0.249800E-13 0.374317E-05
MASS (KG/HR) 57119.0 57118.8 0.359954E-05
ENTHALPY (GCAL/HR) -106.119 -106.121 0.186739E-04

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E 6518.84 KG/HR
PRODUCT STREAMS CO2E 9678.06 KG/HR
NET STREAMS CO2E PRODUCTION 3159.22 KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION 3159.22 KG/HR

*** INPUT DATA ***

REACTOR TYPE: DUTY SPEC TWO PHASE REACTOR

REACTOR VOLUME CUM 2.1000
LIQUID PHASE VOLUME CUM 1.0000
REACTOR PRESSURE BAR 7.2919
REACTOR HEAT DUTY GCAL/HR 0.0000

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

STOICHIOMETRY:

REACTION NUMBER: 1
SUBSTREAM: MIXED
METHANOL -2.0000 WATER 1.0000 DME 1.0000

REAC-DATA ENTRIES:

REACTION NO	TYPE	PHASE	DELT C	BASIS
1	KINETIC	L	0.0000	MOLARITY

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U-O-S BLOCK SECTION

BLOCK: CSTR-5 MODEL: RCSTR (CONTINUED)

*** RESULTS ***

REACTOR TEMPERATURE C 124.60
RESIDENCE TIME HR 0.52805E-03
VAPOR PHASE VOLUME FRACTION 0.40476
LIQUID PHASE VOLUME FRACTION 0.47619
VAPOR PHASE VOLUME CUM 0.85000
LIQUID PHASE VOLUME CUM 1.0000
VAPOR PHASE RESIDENCE TIME HR 0.24564E-03
LIQUID PHASE RESIDENCE TIME HR 0.23210E-01

BLOCK: CSTR-6 MODEL: RCSTR

INLET STREAMS: CSTR-7V CSTR-5L
OUTLET STREAMS: CSTR-6V CSTR-6L

PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		GENERATION	RELATIVE DIFF.
TOTAL BALANCE	IN	OUT		
MOLE (KMOL/HR)	1867.17	1867.16	-0.124900E-13	0.409268E-05
MASS (KG/HR)	51540.7	51540.5		0.402180E-05
ENTHALPY (GCAL/HR)	-103.095	-103.093		-0.224538E-04

*** CO2 EQUIVALENT SUMMARY ***		
FEED STREAMS CO2E	3725.05	KG/HR
PRODUCT STREAMS CO2E	5602.95	KG/HR
NET STREAMS CO2E PRODUCTION	1877.91	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	1877.91	KG/HR

*** INPUT DATA ***

REACTOR TYPE: DUTY SPEC TWO PHASE REACTOR

REACTOR VOLUME	CUM	2.1000
LIQUID PHASE VOLUME	CUM	1.0000
REACTOR PRESSURE	BAR	7.3015
REACTOR HEAT DUTY	GCAL/HR	0.0000

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

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U-O-S BLOCK SECTION

BLOCK: CSTR-6 MODEL: RCSTR (CONTINUED)
STOICHIOMETRY:

REACTION NUMBER:	1				
SUBSTREAM:	MIXED				
METHANOL	-2.0000	WATER	1.0000	DME	1.0000

REAC-DATA ENTRIES:

REACTION NO	TYPE	PHASE	DELT C	BASIS
1	KINETIC	L	0.0000	MOLARITY

*** RESULTS ***

REACTOR TEMPERATURE	C	130.50
RESIDENCE TIME	HR	0.59038E-03
VAPOR PHASE VOLUME FRACTION		0.46429
LIQUID PHASE VOLUME FRACTION		0.47619
VAPOR PHASE VOLUME	CUM	0.97500
LIQUID PHASE VOLUME	CUM	1.0000
VAPOR PHASE RESIDENCE TIME	HR	0.29491E-03
LIQUID PHASE RESIDENCE TIME	HR	0.25473E-01

BLOCK: CSTR-7 MODEL: RCSTR

INLET STREAMS:	CSTR-6L	CSTR-8V
OUTLET STREAMS:	CSTR-7V	CSTR-7L
PROPERTY OPTION SET:	NRTL-RK RENON (NRTL) / REDLICH-KWONG	

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	GENERATION RELATIVE DIFF.

TOTAL BALANCE
MOLE (KMOL/HR) 1799.64 1799.63 0.936751E-13 0.479544E-05
MASS (KG/HR) 47497.9 47497.7 0.471570E-05
ENTHALPY (GCAL/HR) -100.790 -100.786 -0.419128E-04

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 2004.92 KG/HR
PRODUCT STREAMS CO2E 3026.56 KG/HR
NET STREAMS CO2E PRODUCTION 1021.64 KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION 1021.64 KG/HR

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U-O-S BLOCK SECTION

BLOCK: CSTR-7 MODEL: RCSTR (CONTINUED)

*** INPUT DATA ***

REACTOR TYPE: DUTY SPEC TWO PHASE REACTOR

REACTOR VOLUME CUM 2.1000
LIQUID PHASE VOLUME CUM 1.0000
REACTOR PRESSURE BAR 7.3112
REACTOR HEAT DUTY GCAL/HR 0.0000

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

STOICHIOMETRY:

REACTION NUMBER: 1
SUBSTREAM: MIXED
METHANOL -2.0000 WATER 1.0000 DME 1.0000

REAC-DATA ENTRIES:

REACTION NO	TYPE	PHASE	DELT C	BASIS
1	KINETIC	L	0.0000	MOLARITY

*** RESULTS ***

REACTOR TEMPERATURE C 134.70
RESIDENCE TIME HR 0.63696E-03
VAPOR PHASE VOLUME FRACTION 0.49405
LIQUID PHASE VOLUME FRACTION 0.47619
VAPOR PHASE VOLUME CUM 1.0375
LIQUID PHASE VOLUME CUM 1.0000
VAPOR PHASE RESIDENCE TIME HR 0.32810E-03
LIQUID PHASE RESIDENCE TIME HR 0.27331E-01

BLOCK: CSTR-8 MODEL: RCSTR

INLET STREAMS: CSTR-7L CSTR-9V
OUTLET STREAMS: CSTR-8V CSTR-8L
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

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U-O-S BLOCK SECTION

BLOCK: CSTR-8 MODEL: RCSTR (CONTINUED)

TOTAL BALANCE				
MOLE (KMOL/HR)	1748.10	1748.09	-0.156125E-13	0.480966E-05
MASS (KG/HR)	44297.8	44297.6		0.463871E-05
ENTHALPY (GCAL/HR)	-99.1776	-99.1745		-0.307836E-04

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	853.419	KG/HR
PRODUCT STREAMS CO2E	1630.41	KG/HR
NET STREAMS CO2E PRODUCTION	776.992	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	776.992	KG/HR

*** INPUT DATA ***

REACTOR TYPE: DUTY SPEC TWO PHASE REACTOR

REACTOR VOLUME	CUM	2.1000
LIQUID PHASE VOLUME	CUM	1.0000
REACTOR PRESSURE	BAR	7.3209
REACTOR HEAT DUTY	GCAL/HR	0.0000

REACTION PARAGRAPH ID: BOOK TYPE: GENERAL

GLOBAL BASES:

KBASIS	MOLE-GAMMA
CBASIS	MOLARITY
SBASIS	GLOBAL

STOICHIOMETRY:

REACTION NUMBER:	1				
SUBSTREAM: MIXED					
METHANOL	-2.0000	WATER	1.0000	DME	1.0000

REAC-DATA ENTRIES:

REACTION NO	TYPE	PHASE	DELT C	BASIS
1	KINETIC	L	0.0000	MOLARITY

*** RESULTS ***

REACTOR TEMPERATURE	C	138.04
RESIDENCE TIME	HR	0.66007E-03
VAPOR PHASE VOLUME FRACTION		0.50000
LIQUID PHASE VOLUME FRACTION		0.47619
VAPOR PHASE VOLUME	CUM	1.0500
LIQUID PHASE VOLUME	CUM	1.0000
VAPOR PHASE RESIDENCE TIME	HR	0.34182E-03
LIQUID PHASE RESIDENCE TIME	HR	0.29469E-01

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U-O-S BLOCK SECTION

BLOCK: CSTR-9 MODEL: RCSTR

INLET STREAMS:	DST-2V	CSTR-8L
OUTLET STREAMS:	CSTR-9V	CSTR-9L
PROPERTY OPTION SET:	NRTL-RK	RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
TOTAL BALANCE				
MOLE (KMOL/HR)	1699.28	1699.27	-0.173299E-12	0.243860E-05
MASS (KG/HR)	41062.3	41062.2		0.232287E-05
ENTHALPY (GCAL/HR)	-97.8611	-97.8633		0.224945E-04

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	154.556	KG/HR
PRODUCT STREAMS CO2E	649.181	KG/HR
NET STREAMS CO2E PRODUCTION	494.625	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	494.625	KG/HR

*** INPUT DATA ***

REACTOR TYPE: DUTY SPEC TWO PHASE REACTOR

REACTOR VOLUME	CUM	2.1000
LIQUID PHASE VOLUME	CUM	1.0000
REACTOR PRESSURE	BAR	7.3305
REACTOR HEAT DUTY	GCAL/HR	0.0000

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

STOICHIOMETRY:

REACTION NUMBER:	1				
SUBSTREAM: MIXED					
METHANOL	-2.0000	WATER	1.0000	DME	1.0000

REAC-DATA ENTRIES:

REACTION NO	TYPE	PHASE	DELT C	BASIS
1	KINETIC	L	0.0000	MOLARITY

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U-O-S BLOCK SECTION

BLOCK: CSTR-9 MODEL: RCSTR (CONTINUED)

*** RESULTS ***

REACTOR TEMPERATURE	C	141.65
RESIDENCE TIME	HR	0.68273E-03
VAPOR PHASE VOLUME FRACTION		0.50595
LIQUID PHASE VOLUME FRACTION		0.47619
VAPOR PHASE VOLUME	CUM	1.0625
LIQUID PHASE VOLUME	CUM	1.0000
VAPOR PHASE RESIDENCE TIME	HR	0.35536E-03
LIQUID PHASE RESIDENCE TIME	HR	0.32250E-01

BLOCK: DST-1 MODEL: RADFRAC

 INLETS - CSTR-1V STAGE 5
 OUTLETS - S-106 STAGE 1
 DST-1L STAGE 5

PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

TOTAL BALANCE	IN	OUT	RELATIVE DIFF.
MOLE (KMOL/HR)	888.663	888.662	0.148991E-05
MASS (KG/HR)	34186.6	34186.5	0.127233E-05
ENTHALPY (GCAL/HR)	-40.3111	-46.3059	0.129461

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	20071.6	KG/HR
PRODUCT STREAMS CO2E	20071.6	KG/HR

NET STREAMS CO2E PRODUCTION -0.619800E-02 KG/HR
 UTILITIES CO2E PRODUCTION 0.00000 KG/HR
 TOTAL CO2E PRODUCTION -0.619800E-02 KG/HR
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U-O-S BLOCK SECTION

BLOCK: DST-1 MODEL: RADFRAC (CONTINUED)

 **** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	5
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	BROYDEN
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.100000-05
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
REBOILER DUTY GCAL/HR	0.0
MASS REFLUX RATIO	3.00000

**** PROFILES ****

P-SPEC	STAGE	1	PRES, BAR	6.99818
--------	-------	---	-----------	---------

 **** RESULTS ****

*** COMPONENT SPLIT FRACTIONS ***

		OUTLET STREAMS	
		S-106	DST-1L
COMPONENT:			
METHANOL	.12900E-02	.99871	
WATER	.28632E-03	.99971	
DME	.88061	.11939	

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U-O-S BLOCK SECTION

BLOCK: DST-1 MODEL: RADFRAC (CONTINUED)

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	C	30.9255
BOTTOM STAGE TEMPERATURE	C	93.6124
TOP STAGE LIQUID FLOW	KMOL/HR	984.825
BOTTOM STAGE LIQUID FLOW	KMOL/HR	504.439
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOILUP VAPOR FLOW	KMOL/HR	920.538
MOLAR REFLUX RATIO		2.56315
CONDENSER DUTY (W/O SUBCOOL)	GCAL/HR	-5.99489

REBOILER DUTY GCAL/HR 0.0

**** MANIPULATED VARIABLES ****

	BOUNDS		CALCULATED
	LOWER	UPPER	VALUE
MASS REFLUX RATIO	1.0000	5.0000	2.5632

**** DESIGN SPECIFICATIONS ****

NO	SPEC-TYPE	QUALIFIERS	UNIT	SPECIFIED VALUE	CALCULATED VALUE
1	MASS-FRAC	STREAMS: S-106 COMPS: DME		0.99900	0.99900

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

DEW POINT	0.12862E-06	STAGE=	4
BUBBLE POINT	0.72473E-07	STAGE=	4
COMPONENT MASS BALANCE	0.74861E-08	STAGE=	4 COMP=WATER
ENERGY BALANCE	0.12049E-07	STAGE=	5

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U-O-S BLOCK SECTION

BLOCK: DST-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 BAR	ENTHALPY KCAL/MOL		HEAT DUTY GCAL/HR
			LIQUID	VAPOR	
1	30.926	6.9982	-48.416	-44.053	-5.9948
2	32.474	7.2050	-48.488	-44.038	
3	36.010	7.2112	-49.253	-44.017	
4	56.544	7.2168	-53.188	-43.955	
5	93.612	7.2215	-54.919	-44.684	

STAGE	FLOW RATE KMOL/HR		FEED RATE KMOL/HR			PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	1369.	0.000				384.2245	
2	962.8	1369.					
3	808.0	1347.					
4	536.3	1192.					
5	504.4	920.5		888.6630		504.4372	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE KG/HR		FEED RATE KG/HR			PRODUCT RATE KG/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.6304E+05	0.000				.17693+05	
2	0.4415E+05	0.6304E+05					
3	0.3592E+05	0.6185E+05					
4	0.1986E+05	0.5361E+05					
5	0.1649E+05	0.3755E+05		.34187+05		.16494+05	

STAGE	**** MOLE-X-PROFILE ****		
	METHANOL	WATER	DME
1	0.14252E-02	0.21218E-04	0.99855
2	0.14415E-01	0.20385E-03	0.98538
3	0.11142	0.17999E-02	0.88678
4	0.60658	0.19188E-01	0.37423
5	0.84045	0.56429E-01	0.10312

U-O-S BLOCK SECTION

BLOCK: DST-1 MODEL: RADFRAC (CONTINUED)

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

STAGE	METHANOL	WATER	DME
1	0.13758E-03	0.22193E-05	0.99986
2	0.14252E-02	0.21218E-04	0.99855
3	0.10710E-01	0.15176E-03	0.98914
4	0.75970E-01	0.12267E-02	0.92280
5	0.35399	0.11188E-01	0.63482

**** K-VALUES ****

STAGE	METHANOL	WATER	DME
1	0.96535E-01	0.10459	1.0013
2	0.98868E-01	0.10408	1.0134
3	0.96123E-01	0.84312E-01	1.1154
4	0.12524	0.63931E-01	2.4659
5	0.42119	0.19826	6.1563

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

STAGE	METHANOL	WATER	DME
1	0.99170E-03	0.83009E-05	0.99900
2	0.10072E-01	0.80077E-04	0.98985
3	0.80307E-01	0.72941E-03	0.91896
4	0.52498	0.93368E-02	0.46568
5	0.82362	0.31091E-01	0.14529

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

STAGE	METHANOL	WATER	DME
1	0.95695E-04	0.86788E-06	0.99990
2	0.99170E-03	0.83009E-05	0.99900
3	0.74741E-02	0.59544E-04	0.99247
4	0.54131E-01	0.49143E-03	0.94538
5	0.27808	0.49412E-02	0.71698

U-O-S BLOCK SECTION

BLOCK: DST-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	30.926	32.474
2	32.474	36.010
3	36.010	56.544

4	56.544	93.612
5	93.612	104.75

STAGE	MASS FLOW KG/HR		VOLUME FLOW CUM/HR		MOLECULAR WEIGHT	
	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	63043.	63043.	97.732	4314.2	46.048	46.048
2	44155.	61848.	68.537	4306.1	45.861	45.915
3	35919.	53612.	55.104	4135.9	44.456	44.969
4	19856.	37549.	28.512	3620.3	37.022	40.790
5	16494.	34187.	23.879	3614.8	32.697	38.470

STAGE	DENSITY KG/CUM		VISCOSITY CP		SURFACE TENSION DYNE/CM	
	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	645.05	14.613	0.10721	0.98132E-02	10.946	10.946
2	644.25	14.363	0.10858	0.99265E-02	10.883	10.883
3	651.85	12.963	0.12384	0.10593E-01	11.571	11.571
4	696.40	10.372	0.22520	0.11935E-01	15.960	15.960
5	690.73	9.4573	0.23824	0.12409E-01	17.273	17.273

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U-O-S BLOCK SECTION

BLOCK: DST-1 MODEL: RADFRAC (CONTINUED)

STAGE	MARANGONI INDEX DYNE/CM	FLOW PARAM	QR CUM/HR	REDUCED F-FACTOR (GM-L) **.5/MIN
1		0.15051	656.82	0.27486E+06
2	-.62330E-01	0.10660	650.24	0.27199E+06
3	0.68807	0.94479E-01	589.13	0.24818E+06
4	4.3882	0.64533E-01	445.14	0.19432E+06
5	1.3138	0.56454E-01	425.91	0.18528E+06

 ***** TRAY RATING CALCULATIONS *****

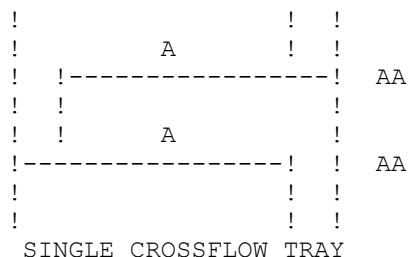
 *** SECTION 1 ***

STARTING STAGE NUMBER	2
ENDING STAGE NUMBER	5
FLOODING CALCULATION METHOD	GLITSCH6
PEAK CAPACITY FACTOR	1.00000
SYSTEM FOAMING FACTOR	1.00000
OVERALL TRAY EFFICIENCY	1.00000

TRAY SPECIFICATIONS

DOWNCOMER ARRANGEMENT

CONVENTIONAL



NUMBER OF PASSES 1
 DIAMETER METER 2.00000
 TRAY SPACING METER 0.60960
 DECK THICKNESS METER 0.0034036
 TRAY TYPE SIEVE
 HOLE AREA/ACTIVE AREA 0.100000
 HOLE DIAMETER METER 0.012700
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U-O-S BLOCK SECTION

BLOCK: DST-1 MODEL: RADFRAC (CONTINUED)

DOWNCOMER DIMENSIONS

 WEIR HEIGHT METER 0.050800
 DC CLEARANCE METER 0.038100
 TOP DC WIDTH METER 0.28918
 BOTTOM DC WIDTH METER 0.28918

***** RATING RESULTS *****

DIAMETER METER 2.00000
 STAGE-MAX FLOODING FACTOR 2
 FLOODING FACTOR 0.62154
 STAGE-MAX DC BACKUP/(TSPC+WHT) 2
 DC BACKUP METER 0.23513
 DC BACKUP/(TSPC+WHT) 0.35605
 STAGE-MAX DC VELOCITY 2
 DC VELOCITY M/SEC 0.067954
 STAGE-MAX WEIRLOADING 2 (PANEL A)
 WEIR LOADING SQCM/SEC 135.334
 SECTION PRESSURE DROP BAR 0.021014
 MAX APPROACH TO SYSTEM LIMIT 0.43624
 STAGE-MAX SYSTEM LIMIT 2

**** RATING PROFILES ****

STAGE	FLOODING FACTOR	DC VELOCITY M/SEC	DC BACKUP METER	DC BACKUP/(TSPC+WHT)	PRES. DROP BAR
2	0.6215	0.6795E-01	0.2351	0.3560	0.6177E-02
3	0.5508	0.5464E-01	0.2080	0.3150	0.5625E-02
4	0.3941	0.2827E-01	0.1635	0.2476	0.4720E-02
5	0.3712	0.2368E-01	0.1575	0.2385	0.4492E-02

**** ADDITIONAL RATING PROFILES ****

STAGE	HEIGHT OVER WEIR METER	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.1189	0.6010	0.2300	43.62
3	0.9408E-01	0.6018	0.2455	38.79
4	0.5048E-01	0.6049	0.2935	27.11
5	0.4344E-01	0.6047	0.3038	25.29

BLOCK: DST-2 MODEL: RADFRAC

 INLETS - CSTR-9L STAGE 1
 OUTLETS - DST-2V STAGE 1
 S-111 STAGE 5

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U-O-S BLOCK SECTION

BLOCK: DST-2 MODEL: RADFRAC (CONTINUED)

PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

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*** MASS AND ENERGY BALANCE ***
                                IN          OUT          RELATIVE DIFF.
TOTAL BALANCE
MOLE (KMOL/HR )                1030.07      1030.07          0.00000
MASS (KG/HR )                  23169.1      23169.1         -0.785093E-15
ENTHALPY (GCAL/HR )            -63.9258     -58.5792         -0.836368E-01

```

```

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E                38.6716      KG/HR
PRODUCT STREAMS CO2E              38.6716      KG/HR
NET STREAMS CO2E PRODUCTION        0.00000      KG/HR
UTILITIES CO2E PRODUCTION          0.00000      KG/HR
TOTAL CO2E PRODUCTION              0.00000      KG/HR

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

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**** INPUT PARAMETERS ****

```

NUMBER OF STAGES                    5
ALGORITHM OPTION                    STANDARD
ABSORBER OPTION                     NO
INITIALIZATION OPTION               STANDARD
HYDRAULIC PARAMETER CALCULATIONS   NO
INSIDE LOOP CONVERGENCE METHOD       BROYDEN
DESIGN SPECIFICATION METHOD          NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS 25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS 10
MAXIMUM NUMBER OF FLASH ITERATIONS  30
FLASH TOLERANCE                     0.100000-05
OUTSIDE LOOP CONVERGENCE TOLERANCE  0.000100000
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U-O-S BLOCK SECTION

BLOCK: DST-2 MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

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MOLAR VAPOR DIST / TOTAL DIST      1.00000
CONDENSER DUTY (W/O SUBCOOL) GCAL/HR 0.0
MASS BOILUP RATIO                   7.80000

```

**** PROFILES ****

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P-SPEC          STAGE 1 PRES, BAR      7.34016

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

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*** COMPONENT SPLIT FRACTIONS ***

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                                OUTLET STREAMS
                                -----
                                DST-2V      S-111
COMPONENT:
METHANOL      .99669      .33134E-02
WATER         .45357      .54643
DME           1.0000      .22563E-08

```

*** SUMMARY OF KEY RESULTS ***

```

TOP STAGE TEMPERATURE      C          146.371
BOTTOM STAGE TEMPERATURE   C          166.571
TOP STAGE LIQUID FLOW      KMOL/HR     1,007.87

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BOTTOM STAGE LIQUID FLOW	KMOL/HR	384.728
TOP STAGE VAPOR FLOW	KMOL/HR	645.339
BOILUP VAPOR FLOW	KMOL/HR	601.998
MOLAR BOILUP RATIO		1.56474
CONDENSER DUTY (W/O SUBCOOL)	GCAL/HR	0.0
REBOILER DUTY	GCAL/HR	5.34655

**** MANIPULATED VARIABLES ****

	BOUNDS		CALCULATED
	LOWER	UPPER	VALUE
MASS BOILUP RATIO	1.0000	10.000	1.5813

**** DESIGN SPECIFICATIONS ****

NO	SPEC-TYPE	QUALIFIERS	UNIT	SPECIFIED VALUE	CALCULATED VALUE
1	MASS-FRAC	STREAMS: S-111 COMPS: WATER		0.99500	0.99500

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U-O-S BLOCK SECTION

BLOCK: DST-2 MODEL: RADFRAC (CONTINUED)

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

DEW POINT	0.30554E-07	STAGE= 5
BUBBLE POINT	0.30410E-07	STAGE= 5
COMPONENT MASS BALANCE	0.73452E-09	STAGE= 5 COMP=METHANOL
ENERGY BALANCE	0.14549E-07	STAGE= 2

**** PROFILES ****

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

STAGE	TEMPERATURE C	PRESSURE BAR	ENTHALPY KCAL/MOL		HEAT DUTY GCAL/HR
			LIQUID	VAPOR	
1	146.37	7.3402	-63.202	-51.716	
2	153.16	7.3496	-64.470	-53.195	
3	160.54	7.3581	-65.197	-54.944	
4	164.92	7.3664	-65.445	-56.077	
5	166.57	7.3745	-65.514	-56.519	5.3465

STAGE	FLOW RATE KMOL/HR		FEED RATE KMOL/HR			PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	1008.	645.3	1030.0661				645.3385
2	988.1	623.1					
3	984.4	603.3					
4	986.7	599.6					
5	384.7	602.0					384.7275

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE KG/HR		FEED RATE KG/HR			PRODUCT RATE KG/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.2127E+05	0.1622E+05	.23169+05				.16223+05
2	0.1930E+05	0.1432E+05					
3	0.1826E+05	0.1236E+05					
4	0.1793E+05	0.1132E+05					
5	6946.	0.1098E+05					6946.1785

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U-O-S BLOCK SECTION

BLOCK: DST-2 MODEL: RADFRAC (CONTINUED)

```

**** MOLE-X-PROFILE ****
STAGE  METHANOL  WATER  DME
1      0.22016  0.77980  0.38656E-04
2      0.10843  0.89157  0.11289E-05
3      0.38259E-01  0.96174  0.21679E-07
4      0.11123E-01  0.98888  0.33938E-09
5      0.28174E-02  0.99718  0.49230E-11

```

```

**** MOLE-Y-PROFILE ****
STAGE  METHANOL  WATER  DME
1      0.50523  0.49347  0.13008E-02
2      0.35434  0.64559  0.62522E-04
3      0.17577  0.82423  0.18487E-05
4      0.60999E-01  0.93900  0.35586E-07
5      0.16431E-01  0.98357  0.55312E-09

```

```

**** K-VALUES ****
STAGE  METHANOL  WATER  DME
1      2.2949  0.63281  33.650
2      3.2680  0.72411  55.386
3      4.5942  0.85702  85.273
4      5.4839  0.94956  104.86
5      5.8322  0.98635  112.36

```

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**** MASS-X-PROFILE ****
STAGE  METHANOL  WATER  DME
1      0.33426  0.66566  0.84382E-04
2      0.17784  0.82216  0.26620E-05
3      0.66080E-01  0.93392  0.53835E-07
4      0.19614E-01  0.98039  0.86041E-09
5      0.50000E-02  0.99500  0.12562E-10

```

```

**** MASS-Y-PROFILE ****
STAGE  METHANOL  WATER  DME
1      0.64398  0.35364  0.23838E-02
2      0.49392  0.50595  0.12530E-03
3      0.27499  0.72500  0.41583E-05
4      0.10357  0.89643  0.86875E-07
5      0.28856E-01  0.97114  0.13966E-08

```

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U-O-S BLOCK SECTION

BLOCK: DST-2 MODEL: RADFRAC (CONTINUED)

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*****
***** HYDRAULIC PARAMETERS *****
*****

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*** DEFINITIONS ***

```

MARANGONI INDEX = SIGMA - SIGMATO
FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
QR = QV*SQRT(RHOV/(RHOL-RHOV))
F FACTOR = QV*SQRT(RHOV)

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WHERE:

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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	146.37	153.16
2	153.16	160.54
3	160.54	164.92
4	164.92	166.57
5	166.57	166.57

STAGE	MASS FLOW KG/HR		VOLUME FLOW CUM/HR		MOLECULAR WEIGHT	
	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	21271.	14325.	27.563	2876.9	21.105	22.987
2	19303.	12357.	23.941	2844.2	19.536	20.481
3	18262.	11315.	21.991	2859.8	18.552	18.871
4	17930.	10984.	21.356	2881.6	18.171	18.246
5	6946.2	0.0000	8.2473	0.0000	18.055	

STAGE	DENSITY KG/CUM		VISCOSITY CP		SURFACE TENSION DYNE/CM	
	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	
1	771.71	4.9791	0.18410	0.14865E-01	40.641	
2	806.27	4.3446	0.17564	0.15122E-01	43.604	
3	830.43	3.9567	0.16718	0.15206E-01	44.750	
4	839.59	3.8118	0.16254	0.15219E-01	44.846	
5	842.24		0.16087		44.804	

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U-O-S BLOCK SECTION

BLOCK: DST-2 MODEL: RADFRAC (CONTINUED)

STAGE	MARANGONI INDEX DYNE/CM	FLOW PARAM	QR CUM/HR	REDUCED F-FACTOR (GM-L) **.5/MIN
1		0.11928	231.84	0.10699E+06
2	2.9631	0.11467	209.35	98807.
3	1.1459	0.11140	197.87	94810.
4	0.95252E-01	0.10999	194.60	93765.
5	-.41855E-01		0.0000	0.0000

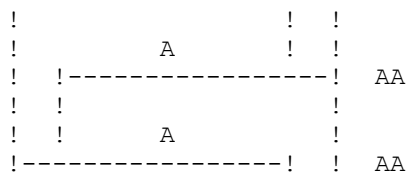
 ***** TRAY RATING CALCULATIONS *****

 *** SECTION 1 ***

STARTING STAGE NUMBER 1
 ENDING STAGE NUMBER 4
 FLOODING CALCULATION METHOD GLITSCH6
 PEAK CAPACITY FACTOR 1.00000
 SYSTEM FOAMING FACTOR 1.00000
 OVERALL TRAY EFFICIENCY 1.00000

TRAY SPECIFICATIONS

DOWNCOMER ARRANGEMENT CONVENTIONAL



! !
! !
SINGLE CROSSFLOW TRAY

NUMBER OF PASSES		1
DIAMETER	METER	1.00000
TRAY SPACING	METER	0.60960
DECK THICKNESS	METER	0.0034036
TRAY TYPE		SIEVE
HOLE AREA/ACTIVE AREA		0.100000
HOLE DIAMETER	METER	0.012700
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		PAGE 34

U-O-S BLOCK SECTION

BLOCK: DST-2 MODEL: RADFRAC (CONTINUED)

DOWNCOMER DIMENSIONS

WEIR HEIGHT	METER	0.050800
DC CLEARANCE	METER	0.038100
TOP DC WIDTH	METER	0.12950
BOTTOM DC WIDTH	METER	0.12950

***** RATING RESULTS *****

DIAMETER	METER	1.00000
STAGE-MAX FLOODING FACTOR		1
FLOODING FACTOR		0.78407
STAGE-MAX DC BACKUP/(TSPC+WHT)		1
DC BACKUP	METER	0.26663
DC BACKUP/(TSPC+WHT)		0.40373
STAGE-MAX DC VELOCITY		1
DC VELOCITY	M/SEC	0.12833
STAGE-MAX WEIRLOADING		1 (PANEL A)
WEIR LOADING	SQCM/SEC	114.020
SECTION PRESSURE DROP	BAR	0.034344
MAX APPROACH TO SYSTEM LIMIT		0.44275
STAGE-MAX SYSTEM LIMIT		1

**** RATING PROFILES ****

STAGE	FLOODING FACTOR	DC VELOCITY M/SEC	DC BACKUP METER	DC BACKUP/ (TSPC+WHT)	PRES. DROP BAR
1	0.7841	0.1283	0.2666	0.4037	0.9402E-02
2	0.7042	0.1115	0.2371	0.3590	0.8580E-02
3	0.6632	0.1024	0.2231	0.3378	0.8224E-02
4	0.6512	0.9943E-01	0.2190	0.3316	0.8137E-02

**** ADDITIONAL RATING PROFILES ****

STAGE	HEIGHT OVER WEIR METER	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
1	0.1634	0.6072	0.1797	44.27
2	0.1451	0.6076	0.1865	39.50
3	0.1351	0.6078	0.1905	37.24
4	0.1320	0.6079	0.1917	36.66

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STREAM SECTION

CIN CSTR-1L CSTR-1V CSTR-2L CSTR-2V

STREAM ID	CIN	CSTR-1L	CSTR-1V	CSTR-2L	CSTR-2V
-----------	-----	---------	---------	---------	---------

FROM :	----	CSTR-1	CSTR-1	CSTR-2	CSTR-2
TO :	----	CSTR-2	DST-1	CSTR-3	CSTR-1
CONV. MAX. REL. ERR:	0.0	2.0499-06	0.0	2.2286-06	0.0
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	VAPOR	LIQUID	VAPOR
COMPONENTS: KMOL/HR					
METHANOL	1.1893-02	672.5672	424.5053	780.6556	468.3530
WATER	1.7722-04	97.7810	28.4731	178.0751	48.1715
DME	8.3325	52.5299	435.6846	50.0385	386.5810
COMPONENTS: KG/HR					
METHANOL	0.3811	2.1551+04	1.3602+04	2.5014+04	1.5007+04
WATER	3.1927-03	1761.5519	512.9513	3208.0724	867.8230
DME	383.8707	2419.9999	2.0072+04	2305.2246	1.7809+04
TOTAL FLOW:					
KMOL/HR	8.3446	822.8781	888.6630	1008.7691	903.1055
KG/HR	384.2550	2.5732+04	3.4187+04	3.0527+04	3.3684+04
CUM/HR	0.5957	37.4199	3598.3391	44.2702	3704.7948
STATE VARIABLES:					
TEMP C	30.9000	104.7900	104.7900	109.5824	109.5824
PRES BAR	7.0000	7.2533	7.2533	7.2629	7.2629
VFRAC	0.0	0.0	1.0000	0.0	1.0000
LFRAC	1.0000	1.0000	0.0	1.0000	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
KCAL/MOL	-48.4171	-55.6597	-45.3615	-56.3173	-45.7822
KCAL/KG	-1051.4389	-1779.9239	-1179.1494	-1861.0011	-1227.4618
GCAL/HR	-0.4040	-45.8011	-40.3111	-56.8111	-41.3462
ENTROPY:					
CAL/MOL-K	-75.2899	-49.4718	-42.3630	-47.7664	-40.1209
CAL/GM-K	-1.6350	-1.5820	-1.1012	-1.5784	-1.0757
DENSITY:					
KMOL/CUM	14.0091	21.9904	0.2470	22.7866	0.2438
KG/CUM	645.0957	687.6573	9.5007	689.5654	9.0921
AVG MW	46.0485	31.2708	38.4697	30.2618	37.2983
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STREAM SECTION

CSTR-3L CSTR-3V CSTR-4L CSTR-4V CSTR-5L

STREAM ID	CSTR-3L	CSTR-3V	CSTR-4L	CSTR-4V	CSTR-5L
FROM :	CSTR-3	CSTR-3	CSTR-4	CSTR-4	CSTR-5
TO :	CSTR-4	CSTR-2	CSTR-5	CSTR-3	CSTR-6
CONV. MAX. REL. ERR:	2.6591-06	0.0	4.3283-06	0.0	7.6309-06
SUBSTREAM: MIXED					
PHASE:	LIQUID	VAPOR	LIQUID	VAPOR	LIQUID
COMPONENTS: KMOL/HR					
METHANOL	766.5316	486.4076	726.3886	487.8615	657.3825
WATER	264.9579	73.4836	362.6798	102.5790	468.6200
DME	40.4945	329.1075	30.5254	261.7757	20.4345
COMPONENTS: KG/HR					
METHANOL	2.4561+04	1.5586+04	2.3275+04	1.5632+04	2.1064+04
WATER	4773.2916	1323.8274	6533.7779	1847.9890	8442.3205
DME	1865.5426	1.5162+04	1406.2742	1.2060+04	941.3958
TOTAL FLOW:					
KMOL/HR	1071.9840	888.9987	1119.5938	852.2162	1146.4369
KG/HR	3.1200+04	3.2071+04	3.1215+04	2.9540+04	3.0448+04
CUM/HR	44.9804	3693.0628	44.6457	3587.6913	43.0845
STATE VARIABLES:					
TEMP C	114.2066	114.2066	119.1143	119.1143	124.6030
PRES BAR	7.2726	7.2726	7.2822	7.2822	7.2919
VFRAC	0.0	1.0000	0.0	1.0000	0.0
LFRAC	1.0000	0.0	1.0000	0.0	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
KCAL/MOL	-57.1189	-46.2697	-57.9845	-46.8651	-58.9214

KCAL/KG	-1962.5089	-1282.5815	-2079.7308	-1352.0439	-2218.5509
GCAL/HR	-61.2306	-41.1337	-64.9190	-39.9392	-67.5497
ENTROPY:					
CAL/MOL-K	-45.9292	-37.8557	-44.0574	-35.3237	-42.0732
CAL/GM-K	-1.5780	-1.0493	-1.5802	-1.0191	-1.5842
DENSITY:					
KMOL/CUM	23.8322	0.2407	25.0773	0.2375	26.6090
KG/CUM	693.6384	8.6841	699.1739	8.2337	706.6962
AVG MW	29.1051	36.0755	27.8807	34.6624	26.5585
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STREAM SECTION

CSTR-5V CSTR-6L CSTR-6V CSTR-7L CSTR-7V

STREAM ID	CSTR-5V	CSTR-6L	CSTR-6V	CSTR-7L	CSTR-7V
FROM :	CSTR-5	CSTR-6	CSTR-6	CSTR-7	CSTR-7
TO :	CSTR-4	CSTR-7	CSTR-5	CSTR-8	CSTR-6
CONV. MAX. REL. ERR:	0.0	8.7229-06	0.0	9.9971-06	0.0
SUBSTREAM: MIXED					
PHASE:	VAPOR	LIQUID	VAPOR	LIQUID	VAPOR
COMPONENTS: KMOL/HR					
METHANOL	482.0495	557.8979	475.2001	486.2160	457.2463
WATER	138.1378	536.9365	175.5043	587.4085	203.0606
DME	189.6428	10.6447	110.9761	5.2727	60.4235
COMPONENTS: KG/HR					
METHANOL	1.5446+04	1.7876+04	1.5226+04	1.5579+04	1.4651+04
WATER	2488.5919	9673.0611	3161.7599	1.0582+04	3658.1939
DME	8736.6609	490.3915	5112.5622	242.9101	2783.6505
TOTAL FLOW:					
KMOL/HR	809.8301	1105.4791	761.6805	1078.8973	720.7304
KG/HR	2.6671+04	2.8040+04	2.3501+04	2.6405+04	2.1093+04
CUM/HR	3460.3778	39.2569	3306.0430	36.5888	3162.1824
STATE VARIABLES:					
TEMP C	124.6030	130.4954	130.4954	134.7005	134.7005
PRES BAR	7.2919	7.3015	7.3015	7.3112	7.3112
VFRAC	1.0000	0.0	1.0000	0.0	1.0000
LFRAC	0.0	1.0000	0.0	1.0000	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
KCAL/MOL	-47.6293	-59.7952	-48.5648	-60.4692	-49.3191
KCAL/KG	-1446.1938	-2357.4539	-1574.0269	-2470.7800	-1685.1917
GCAL/HR	-38.5717	-66.1023	-36.9908	-65.2401	-35.5458
ENTROPY:					
CAL/MOL-K	-32.3377	-40.3946	-28.8963	-39.2086	-26.3873
CAL/GM-K	-0.9819	-1.5926	-0.9366	-1.6021	-0.9016
DENSITY:					
KMOL/CUM	0.2340	28.1602	0.2304	29.4871	0.2279
KG/CUM	7.7076	714.2627	7.1084	721.6604	6.6704
AVG MW	32.9343	25.3643	30.8538	24.4737	29.2662
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STREAM SECTION

CSTR-8L CSTR-8V CSTR-9L CSTR-9V CWIN

STREAM ID	CSTR-8L	CSTR-8V	CSTR-9L	CSTR-9V	CWIN
FROM :	CSTR-8	CSTR-8	CSTR-9	CSTR-9	----
TO :	CSTR-9	CSTR-7	DST-2	CSTR-8	----
CONV. MAX. REL. ERR:	9.3362-06	0.0	4.5320-06	0.0	0.0
SUBSTREAM: MIXED					
PHASE:	LIQUID	VAPOR	LIQUID	VAPOR	LIQUID
COMPONENTS: KMOL/HR					
METHANOL	412.1999	429.9220	327.1296	389.6413	0.0
WATER	639.2219	231.3601	702.0970	266.3122	11.1017

DME	2.5155	32.8752	0.8394	13.2520	0.0
COMPONENTS: KG/HR					
METHANOL	1.3208+04	1.3776+04	1.0482+04	1.2485+04	0.0
WATER	1.1516+04	4168.0163	1.2648+04	4797.6882	200.0000
DME	115.8844	1514.5269	38.6716	610.5089	0.0
TOTAL FLOW:					
KMOL/HR	1053.9372	694.1572	1030.0661	669.2055	11.1017
KG/HR	2.4839+04	1.9458+04	2.3169+04	1.7893+04	200.0000
CUM/HR	33.9340	3071.8123	31.0074	2989.9495	0.2002
STATE VARIABLES:					
TEMP C	138.0396	138.0396	141.6496	141.6496	20.0000
PRES BAR	7.3209	7.3209	7.3305	7.3305	1.0133
VFRAC	0.0	1.0000	0.0	1.0000	0.0
LFRAC	1.0000	0.0	1.0000	0.0	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
KCAL/MOL	-61.1866	-49.9710	-62.0599	-50.7131	-68.3507
KCAL/KG	-2596.1470	-1782.6827	-2759.0974	-1896.6759	-3794.0415
GCAL/HR	-64.4868	-34.6877	-63.9258	-33.9375	-0.7588
ENTROPY:					
CAL/MOL-K	-38.0713	-24.5004	-36.7835	-22.5813	-39.2641
CAL/GM-K	-1.6154	-0.8740	-1.6353	-0.8445	-2.1795
DENSITY:					
KMOL/CUM	31.0585	0.2260	33.2200	0.2238	55.4400
KG/CUM	731.9931	6.3344	747.2115	5.9844	998.7672
AVG MW	23.5682	28.0314	22.4928	26.7379	18.0153
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STREAM SECTION

DMEIN DST-1L DST-2V S-104-1 S-104-2

STREAM ID	DMEIN	DST-1L	DST-2V	S-104-1	S-104-2
FROM :	----	DST-1	DST-2	----	----
TO :	----	CSTR-1	CSTR-9	CSTR-1	CSTR-2

CONV. MAX. REL. ERR:	0.0	2.6647-06	0.0	0.0	0.0
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
METHANOL	0.5476	423.9566	326.0457	304.0000	200.0000
WATER	8.1607-03	28.4649	318.4534	0.0	0.0
DME	383.6992	52.0157	0.8394	0.0	0.0
COMPONENTS: KG/HR					
METHANOL	17.5473	1.3584+04	1.0447+04	9740.8166	6408.4320
WATER	0.1470	512.8034	5737.0271	0.0	0.0
DME	1.7677+04	2396.3123	38.6716	0.0	0.0
TOTAL FLOW:					
KMOL/HR	384.2550	504.4372	645.3385	304.0000	200.0000
KG/HR	1.7694+04	1.6494+04	1.6223+04	9740.8166	6408.4320
CUM/HR	27.4290	23.8787	2921.5637	12.9906	8.5465
STATE VARIABLES:					
TEMP C	30.9000	93.6124	146.3713	60.0000	60.0000
PRES BAR	7.0000	7.2215	7.3402	7.0000	7.0000
VFRAC	0.0	0.0	1.0000	0.0	0.0
LFRAC	1.0000	1.0000	0.0	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
KCAL/MOL	-48.4171	-54.9189	-51.7159	-56.1271	-56.1271
KCAL/KG	-1051.4389	-1679.6295	-2057.2316	-1751.6627	-1751.6627
GCAL/HR	-18.6045	-27.7031	-33.3743	-17.0626	-11.2254
ENTROPY:					
CAL/MOL-K	-75.2899	-52.1946	-20.2845	-54.9237	-54.9237
CAL/GM-K	-1.6350	-1.5963	-0.8069	-1.7141	-1.7141
DENSITY:					
KMOL/CUM	14.0091	21.1250	0.2209	23.4015	23.4015
KG/CUM	645.0957	690.7254	5.5528	749.8353	749.8353
AVG MW	46.0485	32.6970	25.1386	32.0422	32.0422
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STREAM SECTION

S-104-3 S-104-4 S-104-5 S-106 S-111

STREAM ID	S-104-3	S-104-4	S-104-5	S-106	S-111
FROM :	----	----	----	DST-1	DST-2
TO :	CSTR-3	CSTR-4	CSTR-5	----	----
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
METHANOL	100.0000	90.0000	75.0000	0.5476	1.0839
WATER	0.0	0.0	0.0	8.1524-03	383.6436
DME	0.0	0.0	0.0	383.6688	1.8940-09
COMPONENTS: KG/HR					
METHANOL	3204.2160	2883.7944	2403.1620	17.5461	34.7309
WATER	0.0	0.0	0.0	0.1469	6911.4476
DME	0.0	0.0	0.0	1.7675+04	8.7255-08
TOTAL FLOW:					
KMOL/HR	100.0000	90.0000	75.0000	384.2245	384.7276
KG/HR	3204.2160	2883.7944	2403.1620	1.7693+04	6946.1785
CUM/HR	4.2732	3.8459	3.2049	27.4287	8.2473
STATE VARIABLES:					
TEMP C	60.0000	60.0000	60.0000	30.9255	166.5705
PRES BAR	7.0000	7.0000	7.0000	6.9982	7.3745
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:					
KCAL/MOL	-56.1271	-56.1271	-56.1271	-48.4164	-65.5137
KCAL/KG	-1751.6627	-1751.6627	-1751.6627	-1051.4231	-3628.6052
GCAL/HR	-5.6127	-5.0514	-4.2095	-18.6028	-25.2049
ENTROPY:					
CAL/MOL-K	-54.9237	-54.9237	-54.9237	-75.2876	-31.6507
CAL/GM-K	-1.7141	-1.7141	-1.7141	-1.6350	-1.7530
DENSITY:					
KMOL/CUM	23.4015	23.4015	23.4015	14.0081	46.6489
KG/CUM	749.8353	749.8353	749.8353	645.0534	842.2356
AVG MW	32.0422	32.0422	32.0422	46.0485	18.0548
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STREAM SECTION

SFEED

STREAM ID	SFEED
FROM :	----
TO :	----

SUBSTREAM: MIXED	
PHASE:	LIQUID
COMPONENTS: KMOL/HR	
METHANOL	769.0000
WATER	0.0
DME	0.0
COMPONENTS: KG/HR	
METHANOL	2.4640+04
WATER	0.0
DME	0.0
TOTAL FLOW:	
KMOL/HR	769.0000
KG/HR	2.4640+04
CUM/HR	36.9565
STATE VARIABLES:	
TEMP C	120.0000
PRES BAR	9.0000
VFRAC	0.0
LFRAC	1.0000

SFRAC 0.0
 ENTHALPY:
 KCAL/MOL -54.4394
 KCAL/KG -1698.9918
 GCAL/HR -41.8639
 ENTROPY:
 CAL/MOL-K -50.4934
 CAL/GM-K -1.5758
 DENSITY:
 KMOL/CUM 20.8083
 KG/CUM 666.7416
 AVG MW 32.0422

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PHYSICAL PROPERTY TABLES SECTION

FLASH CURVE TABLE: BINRY-1

PROPERTIES ALONG A FLASH CURVE FOR THE MIXTURE: (KMOL/HR)
 METHANOL 1.000 , WATER 1.000 ,

STATE SPECIFICATIONS:
 VAPOR FRACTION: 0.000

VARIED VARIABLE(S): PRES MOLEFRAC

PROPERTY SET(S): \$PS-TXY

3 PHASE PV FLASHES WERE PERFORMED.

PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG
 ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/06/2020 PAGE 43

PHYSICAL PROPERTY TABLES SECTION

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

! PRES	! MOLEFRAC	! TEMP	! KVL	! KVL	! GAMMA
! BAR	! METHANOL	! TOTAL	! TOTAL	! TOTAL	! LIQUID 1
! C	! METHANOL	! WATER	! METHANOL	! WATER	! METHANOL
! 1.0133	! 0.0	! 100.0178	! 7.5328	! 1.0000	! 2.2311
! 1.0133	! 2.0000-02	! 96.7179	! 6.4317	! 0.8891	! 2.1073
! 1.0133	! 4.0000-02	! 94.0381	! 5.6182	! 0.8076	! 2.0014
! 1.0133	! 6.0000-02	! 91.8039	! 4.9928	! 0.7451	! 1.9094
! 1.0133	! 8.0000-02	! 89.9022	! 4.4969	! 0.6959	! 1.8284
! 1.0133	! 0.1000	! 88.2563	! 4.0942	! 0.6562	! 1.7565
! 1.0133	! 0.1200	! 86.8117	! 3.7606	! 0.6236	! 1.6921
! 1.0133	! 0.1400	! 85.5286	! 3.4799	! 0.5963	! 1.6341
! 1.0133	! 0.1600	! 84.3773	! 3.2404	! 0.5733	! 1.5816
! 1.0133	! 0.1800	! 83.3347	! 3.0337	! 0.5536	! 1.5338
! 1.0133	! 0.2000	! 82.3829	! 2.8535	! 0.5366	! 1.4902
! 1.0133	! 0.2200	! 81.5078	! 2.6951	! 0.5219	! 1.4504
! 1.0133	! 0.2400	! 80.6979	! 2.5548	! 0.5090	! 1.4138
! 1.0133	! 0.2600	! 79.9439	! 2.4297	! 0.4977	! 1.3802
! 1.0133	! 0.2800	! 79.2380	! 2.3175	! 0.4876	! 1.3492
! 1.0133	! 0.3000	! 78.5739	! 2.2162	! 0.4788	! 1.3206
! 1.0133	! 0.3200	! 77.9463	! 2.1245	! 0.4708	! 1.2942
! 1.0133	! 0.3400	! 77.3507	! 2.0410	! 0.4637	! 1.2697
! 1.0133	! 0.3600	! 76.7832	! 1.9647	! 0.4574	! 1.2471
! 1.0133	! 0.3800	! 76.2406	! 1.8946	! 0.4517	! 1.2261
! 1.0133	! 0.4000	! 75.7201	! 1.8302	! 0.4465	! 1.2066

!	1.0133	!	0.4200	!	75.2193	!	1.7707	!	0.4419	!	1.1886	!
!	1.0133	!	0.4400	!	74.7361	!	1.7157	!	0.4377	!	1.1718	!
!	1.0133	!	0.4600	!	74.2688	!	1.6646	!	0.4339	!	1.1562	!
!	1.0133	!	0.4800	!	73.8156	!	1.6170	!	0.4304	!	1.1418	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	0.5000	!	73.3753	!	1.5727	!	0.4273	!	1.1284	!
!	1.0133	!	0.5200	!	72.9466	!	1.5312	!	0.4245	!	1.1160	!
!	1.0133	!	0.5400	!	72.5284	!	1.4924	!	0.4219	!	1.1044	!
!	1.0133	!	0.5600	!	72.1199	!	1.4560	!	0.4196	!	1.0937	!
!	1.0133	!	0.5800	!	71.7202	!	1.4218	!	0.4175	!	1.0838	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	0.6000	!	71.3285	!	1.3896	!	0.4156	!	1.0747	!
!	1.0133	!	0.6200	!	70.9442	!	1.3592	!	0.4139	!	1.0662	!
!	1.0133	!	0.6400	!	70.5668	!	1.3305	!	0.4124	!	1.0585	!
!	1.0133	!	0.6600	!	70.1956	!	1.3034	!	0.4110	!	1.0513	!
!	1.0133	!	0.6800	!	69.8303	!	1.2777	!	0.4098	!	1.0447	!

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PHYSICAL PROPERTY TABLES SECTION

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

!	PRES	!	MOLEFRAC	!	TEMP	!	KVL	!	KVL	!	GAMMA	!
!		!		!	TOTAL	!	TOTAL	!	TOTAL	!	LIQUID 1	!
!		!	METHANOL	!		!	METHANOL	!	WATER	!	METHANOL	!
!	BAR	!		!	C	!		!		!		!
=====		=====		=====		=====		=====		=====		=====
!	1.0133	!	0.7000	!	69.4704	!	1.2534	!	0.4087	!	1.0387	!
!	1.0133	!	0.7200	!	69.1155	!	1.2303	!	0.4077	!	1.0332	!
!	1.0133	!	0.7400	!	68.7653	!	1.2084	!	0.4069	!	1.0282	!
!	1.0133	!	0.7600	!	68.4195	!	1.1875	!	0.4062	!	1.0237	!
!	1.0133	!	0.7800	!	68.0778	!	1.1677	!	0.4056	!	1.0196	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	0.8000	!	67.7400	!	1.1487	!	0.4050	!	1.0160	!
!	1.0133	!	0.8200	!	67.4059	!	1.1307	!	0.4046	!	1.0128	!
!	1.0133	!	0.8400	!	67.0752	!	1.1135	!	0.4043	!	1.0100	!
!	1.0133	!	0.8600	!	66.7478	!	1.0970	!	0.4040	!	1.0076	!
!	1.0133	!	0.8800	!	66.4235	!	1.0813	!	0.4039	!	1.0055	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	0.9000	!	66.1021	!	1.0662	!	0.4038	!	1.0038	!
!	1.0133	!	0.9200	!	65.7835	!	1.0518	!	0.4038	!	1.0024	!
!	1.0133	!	0.9400	!	65.4676	!	1.0381	!	0.4038	!	1.0013	!
!	1.0133	!	0.9600	!	65.1542	!	1.0248	!	0.4040	!	1.0006	!
!	1.0133	!	0.9800	!	64.8433	!	1.0122	!	0.4042	!	1.0001	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	1.0000	!	64.5348	!	1.0000	!	0.4044	!	1.0000	!

!	PRES	!	MOLEFRAC	!	GAMMA	!	GAMMA	!	GAMMA	!	KVL2	!
!		!		!	LIQUID 1	!	LIQUID 2	!	LIQUID 2	!	TOTAL	!
!		!	METHANOL	!	WATER	!	METHANOL	!	WATER	!	METHANOL	!
!	BAR	!		!		!		!		!		!
=====		=====		=====		=====		=====		=====		=====
!	1.0133	!	0.0	!	1.0000	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	2.0000-02	!	1.0005	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	4.0000-02	!	1.0019	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	6.0000-02	!	1.0042	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	8.0000-02	!	1.0072	!	MISSING	!	MISSING	!	MISSING	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	0.1000	!	1.0110	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	0.1200	!	1.0154	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	0.1400	!	1.0204	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	0.1600	!	1.0260	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	0.1800	!	1.0322	!	MISSING	!	MISSING	!	MISSING	!

PHYSICAL PROPERTY TABLES SECTION

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES	MOLEFRAC	GAMMA	GAMMA	GAMMA	KVL2
		LIQUID 1	LIQUID 2	LIQUID 2	TOTAL
	METHANOL	WATER	METHANOL	WATER	METHANOL
BAR					
1.0133	0.2000	1.0389	MISSING	MISSING	MISSING
1.0133	0.2200	1.0461	MISSING	MISSING	MISSING
1.0133	0.2400	1.0539	MISSING	MISSING	MISSING
1.0133	0.2600	1.0621	MISSING	MISSING	MISSING
1.0133	0.2800	1.0708	MISSING	MISSING	MISSING
1.0133	0.3000	1.0800	MISSING	MISSING	MISSING
1.0133	0.3200	1.0896	MISSING	MISSING	MISSING
1.0133	0.3400	1.0997	MISSING	MISSING	MISSING
1.0133	0.3600	1.1102	MISSING	MISSING	MISSING
1.0133	0.3800	1.1211	MISSING	MISSING	MISSING
1.0133	0.4000	1.1325	MISSING	MISSING	MISSING
1.0133	0.4200	1.1442	MISSING	MISSING	MISSING
1.0133	0.4400	1.1564	MISSING	MISSING	MISSING
1.0133	0.4600	1.1690	MISSING	MISSING	MISSING
1.0133	0.4800	1.1819	MISSING	MISSING	MISSING
1.0133	0.5000	1.1953	MISSING	MISSING	MISSING
1.0133	0.5200	1.2091	MISSING	MISSING	MISSING
1.0133	0.5400	1.2232	MISSING	MISSING	MISSING
1.0133	0.5600	1.2377	MISSING	MISSING	MISSING
1.0133	0.5800	1.2527	MISSING	MISSING	MISSING
1.0133	0.6000	1.2680	MISSING	MISSING	MISSING
1.0133	0.6200	1.2837	MISSING	MISSING	MISSING
1.0133	0.6400	1.2998	MISSING	MISSING	MISSING
1.0133	0.6600	1.3163	MISSING	MISSING	MISSING
1.0133	0.6800	1.3331	MISSING	MISSING	MISSING
1.0133	0.7000	1.3504	MISSING	MISSING	MISSING
1.0133	0.7200	1.3681	MISSING	MISSING	MISSING
1.0133	0.7400	1.3862	MISSING	MISSING	MISSING
1.0133	0.7600	1.4046	MISSING	MISSING	MISSING
1.0133	0.7800	1.4235	MISSING	MISSING	MISSING
1.0133	0.8000	1.4428	MISSING	MISSING	MISSING
1.0133	0.8200	1.4626	MISSING	MISSING	MISSING
1.0133	0.8400	1.4827	MISSING	MISSING	MISSING
1.0133	0.8600	1.5033	MISSING	MISSING	MISSING
1.0133	0.8800	1.5243	MISSING	MISSING	MISSING

PHYSICAL PROPERTY TABLES SECTION

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES	MOLEFRAC	GAMMA	GAMMA	GAMMA	KVL2
		LIQUID 1	LIQUID 2	LIQUID 2	TOTAL
	METHANOL	WATER	METHANOL	WATER	METHANOL
BAR					

!	1.0133	!	0.9000	!	1.5458	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	0.9200	!	1.5677	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	0.9400	!	1.5901	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	0.9600	!	1.6129	!	MISSING	!	MISSING	!	MISSING	!
!	1.0133	!	0.9800	!	1.6362	!	MISSING	!	MISSING	!	MISSING	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	1.0000	!	1.6600	!	MISSING	!	MISSING	!	MISSING	!
-----		-----		-----		-----		-----		-----		-----

!	PRES	!	MOLEFRAC	!	KVL2	!	BETA	!	MOLEFRAC	!	MOLEFRAC	!
!		!		!	TOTAL	!	TOTAL	!	VAPOR	!	VAPOR	!
!		!	METHANOL	!	WATER	!		!	METHANOL	!	WATER	!
!	BAR	!		!		!		!		!		!
=====		=====		=====		=====		=====		=====		=====
!	1.0133	!	0.0	!	MISSING	!	1.0000	!	0.0	!	1.0000	!
!	1.0133	!	2.0000-02	!	MISSING	!	1.0000	!	0.1286	!	0.8714	!
!	1.0133	!	4.0000-02	!	MISSING	!	1.0000	!	0.2247	!	0.7753	!
!	1.0133	!	6.0000-02	!	MISSING	!	1.0000	!	0.2996	!	0.7004	!
!	1.0133	!	8.0000-02	!	MISSING	!	1.0000	!	0.3598	!	0.6402	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	0.1000	!	MISSING	!	1.0000	!	0.4094	!	0.5906	!
!	1.0133	!	0.1200	!	MISSING	!	1.0000	!	0.4513	!	0.5487	!
!	1.0133	!	0.1400	!	MISSING	!	1.0000	!	0.4872	!	0.5128	!
!	1.0133	!	0.1600	!	MISSING	!	1.0000	!	0.5185	!	0.4815	!
!	1.0133	!	0.1800	!	MISSING	!	1.0000	!	0.5461	!	0.4539	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	0.2000	!	MISSING	!	1.0000	!	0.5707	!	0.4293	!
!	1.0133	!	0.2200	!	MISSING	!	1.0000	!	0.5929	!	0.4071	!
!	1.0133	!	0.2400	!	MISSING	!	1.0000	!	0.6132	!	0.3868	!
!	1.0133	!	0.2600	!	MISSING	!	1.0000	!	0.6317	!	0.3683	!
!	1.0133	!	0.2800	!	MISSING	!	1.0000	!	0.6489	!	0.3511	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	0.3000	!	MISSING	!	1.0000	!	0.6649	!	0.3351	!
!	1.0133	!	0.3200	!	MISSING	!	1.0000	!	0.6798	!	0.3202	!
!	1.0133	!	0.3400	!	MISSING	!	1.0000	!	0.6939	!	0.3061	!
!	1.0133	!	0.3600	!	MISSING	!	1.0000	!	0.7073	!	0.2927	!
!	1.0133	!	0.3800	!	MISSING	!	1.0000	!	0.7200	!	0.2800	!

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PHYSICAL PROPERTY TABLES SECTION

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

!	PRES	!	MOLEFRAC	!	KVL2	!	BETA	!	MOLEFRAC	!	MOLEFRAC	!
!		!		!	TOTAL	!	TOTAL	!	VAPOR	!	VAPOR	!
!		!	METHANOL	!	WATER	!		!	METHANOL	!	WATER	!
!	BAR	!		!		!		!		!		!
=====		=====		=====		=====		=====		=====		=====
!	1.0133	!	0.4000	!	MISSING	!	1.0000	!	0.7321	!	0.2679	!
!	1.0133	!	0.4200	!	MISSING	!	1.0000	!	0.7437	!	0.2563	!
!	1.0133	!	0.4400	!	MISSING	!	1.0000	!	0.7549	!	0.2451	!
!	1.0133	!	0.4600	!	MISSING	!	1.0000	!	0.7657	!	0.2343	!
!	1.0133	!	0.4800	!	MISSING	!	1.0000	!	0.7762	!	0.2238	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	0.5000	!	MISSING	!	1.0000	!	0.7863	!	0.2137	!
!	1.0133	!	0.5200	!	MISSING	!	1.0000	!	0.7962	!	0.2038	!
!	1.0133	!	0.5400	!	MISSING	!	1.0000	!	0.8059	!	0.1941	!
!	1.0133	!	0.5600	!	MISSING	!	1.0000	!	0.8154	!	0.1846	!
!	1.0133	!	0.5800	!	MISSING	!	1.0000	!	0.8246	!	0.1754	!
-----		-----		-----		-----		-----		-----		-----
!	1.0133	!	0.6000	!	MISSING	!	1.0000	!	0.8337	!	0.1663	!
!	1.0133	!	0.6200	!	MISSING	!	1.0000	!	0.8427	!	0.1573	!
!	1.0133	!	0.6400	!	MISSING	!	1.0000	!	0.8515	!	0.1485	!
!	1.0133	!	0.6600	!	MISSING	!	1.0000	!	0.8603	!	0.1397	!

1.0133	0.6800	MISSING	1.0000	0.8689	0.1311
1.0133	0.7000	MISSING	1.0000	0.8774	0.1226
1.0133	0.7200	MISSING	1.0000	0.8858	0.1142
1.0133	0.7400	MISSING	1.0000	0.8942	0.1058
1.0133	0.7600	MISSING	1.0000	0.9025	9.7482-02
1.0133	0.7800	MISSING	1.0000	0.9108	8.9222-02
1.0133	0.8000	MISSING	1.0000	0.9190	8.1006-02
1.0133	0.8200	MISSING	1.0000	0.9272	7.2829-02
1.0133	0.8400	MISSING	1.0000	0.9353	6.4683-02
1.0133	0.8600	MISSING	1.0000	0.9434	5.6563-02
1.0133	0.8800	MISSING	1.0000	0.9515	4.8463-02
1.0133	0.9000	MISSING	1.0000	0.9596	4.0377-02
1.0133	0.9200	MISSING	1.0000	0.9677	3.2300-02
1.0133	0.9400	MISSING	1.0000	0.9758	2.4229-02
1.0133	0.9600	MISSING	1.0000	0.9838	1.6158-02
1.0133	0.9800	MISSING	1.0000	0.9919	8.0830-03
1.0133	1.0000	MISSING	1.0000	1.0000	0.0

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PHYSICAL PROPERTY TABLES SECTION

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES	MOLEFRAC METHANOL	MOLEFRAC LIQUID 1 METHANOL	MOLEFRAC LIQUID 1 WATER	MOLEFRAC LIQUID 2 METHANOL	MOLEFRAC LIQUID 2 WATER
1.0133	0.0	0.0	1.0000	MISSING	MISSING
1.0133	2.0000-02	2.0000-02	0.9800	MISSING	MISSING
1.0133	4.0000-02	4.0000-02	0.9600	MISSING	MISSING
1.0133	6.0000-02	6.0000-02	0.9400	MISSING	MISSING
1.0133	8.0000-02	8.0000-02	0.9200	MISSING	MISSING
1.0133	0.1000	0.1000	0.9000	MISSING	MISSING
1.0133	0.1200	0.1200	0.8800	MISSING	MISSING
1.0133	0.1400	0.1400	0.8600	MISSING	MISSING
1.0133	0.1600	0.1600	0.8400	MISSING	MISSING
1.0133	0.1800	0.1800	0.8200	MISSING	MISSING
1.0133	0.2000	0.2000	0.8000	MISSING	MISSING
1.0133	0.2200	0.2200	0.7800	MISSING	MISSING
1.0133	0.2400	0.2400	0.7600	MISSING	MISSING
1.0133	0.2600	0.2600	0.7400	MISSING	MISSING
1.0133	0.2800	0.2800	0.7200	MISSING	MISSING
1.0133	0.3000	0.3000	0.7000	MISSING	MISSING
1.0133	0.3200	0.3200	0.6800	MISSING	MISSING
1.0133	0.3400	0.3400	0.6600	MISSING	MISSING
1.0133	0.3600	0.3600	0.6400	MISSING	MISSING
1.0133	0.3800	0.3800	0.6200	MISSING	MISSING
1.0133	0.4000	0.4000	0.6000	MISSING	MISSING
1.0133	0.4200	0.4200	0.5800	MISSING	MISSING
1.0133	0.4400	0.4400	0.5600	MISSING	MISSING
1.0133	0.4600	0.4600	0.5400	MISSING	MISSING
1.0133	0.4800	0.4800	0.5200	MISSING	MISSING
1.0133	0.5000	0.5000	0.5000	MISSING	MISSING
1.0133	0.5200	0.5200	0.4800	MISSING	MISSING
1.0133	0.5400	0.5400	0.4600	MISSING	MISSING
1.0133	0.5600	0.5600	0.4400	MISSING	MISSING
1.0133	0.5800	0.5800	0.4200	MISSING	MISSING

1.0133	0.6000	0.6000	0.4000	MISSING	MISSING
1.0133	0.6200	0.6200	0.3800	MISSING	MISSING
1.0133	0.6400	0.6400	0.3600	MISSING	MISSING
1.0133	0.6600	0.6600	0.3400	MISSING	MISSING
1.0133	0.6800	0.6800	0.3200	MISSING	MISSING

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PHYSICAL PROPERTY TABLES SECTION

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES	MOLEFRAC	MOLEFRAC	MOLEFRAC	MOLEFRAC	MOLEFRAC
	METHANOL	LIQUID 1	LIQUID 1	LIQUID 2	LIQUID 2
BAR		METHANOL	WATER	METHANOL	WATER
1.0133	0.7000	0.7000	0.3000	MISSING	MISSING
1.0133	0.7200	0.7200	0.2800	MISSING	MISSING
1.0133	0.7400	0.7400	0.2600	MISSING	MISSING
1.0133	0.7600	0.7600	0.2400	MISSING	MISSING
1.0133	0.7800	0.7800	0.2200	MISSING	MISSING
1.0133	0.8000	0.8000	0.2000	MISSING	MISSING
1.0133	0.8200	0.8200	0.1800	MISSING	MISSING
1.0133	0.8400	0.8400	0.1600	MISSING	MISSING
1.0133	0.8600	0.8600	0.1400	MISSING	MISSING
1.0133	0.8800	0.8800	0.1200	MISSING	MISSING
1.0133	0.9000	0.9000	0.1000	MISSING	MISSING
1.0133	0.9200	0.9200	8.0000-02	MISSING	MISSING
1.0133	0.9400	0.9400	6.0000-02	MISSING	MISSING
1.0133	0.9600	0.9600	4.0000-02	MISSING	MISSING
1.0133	0.9800	0.9800	2.0000-02	MISSING	MISSING
1.0133	1.0000	1.0000	0.0	MISSING	MISSING

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PROBLEM STATUS SECTION

BLOCK STATUS

```

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

```


RUN CONTROL SECTION

RUN CONTROL INFORMATION

THIS COPY OF ASPEN PLUS LICENSED TO UNIVERSITY OF PENNSYLVAN

TYPE OF RUN: EDIT

INPUT FILE NAME: _1942wrf.inm

INPUT PROBLEM DATA FILE NAME : _1942wrf

OUTPUT PROBLEM DATA FILE NAME: _3154jyf

LOCATED IN:

PDF SIZE USED FOR INPUT TRANSLATION:

NUMBER OF FILE RECORDS (PSIZE) = 0
 NUMBER OF IN-CORE RECORDS = 256
 PSIZE NEEDED FOR SIMULATION = 1

CALLING PROGRAM NAME: apmain

LOCATED IN: C:\Program Files\AspenTech\Aspen Plus V11.0\Engine\Xe

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

ASPEN PLUS PLAT: WIN-X64 VER: 37.0

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FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
S-101	----	P-100	S-113	----	H-100
S-106	----	P-102	S-111	----	P-103
S-116	----	P-104	S-117	P-104	----
S-102	P-100	H-100	S-114	H-100	----
S-103	H-100	----	S-107	P-102	----
S-112	P-103	----			

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
P-100	S-101	S-102
H-100	S-113 S-102	S-114 S-103
P-102	S-106	S-107
P-103	S-111	S-112
P-104	S-116	S-117

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:

P-104 P-103 P-102 P-100 H-100

OVERALL FLOWSHEET BALANCE

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/HR)			
METHANOL	1542.89	1542.89	-0.147368E-15
WATER	1150.99	1150.99	-0.197547E-15
DIMET-01	1151.04	1151.04	0.00000
N-TRI-01	0.00000	0.00000	0.00000

TOTAL BALANCE			
MOLE (KMOL/HR)	3844.92	3844.92	0.00000
MASS (KG/HR)	123200.	123200.	0.00000
ENTHALPY (CAL/SEC)	-0.608356E+08	-0.608282E+08	-0.122615E-03

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	53027.2	KG/HR
PRODUCT STREAMS CO2E	53027.2	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

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PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME
METHANOL	C	CH4O	METHANOL
WATER	C	H2O	WATER
DIMET-01	C	C2H6O-1	DIMETHYL-ETHER
N-TRI-01	C	C30H62	N-TRIACONTANE

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U-O-S BLOCK SECTION

BLOCK: H-100 MODEL: HEATX

THIS BLOCK RUNS WITH ASPEN EDR 37.0 WITH ADVANCED METHOD FOR SHELL&TUBE HOT SIDE:

INLET STREAM: S-113
 OUTLET STREAM: S-114
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG
 COLD SIDE:

INLET STREAM: S-102
 OUTLET STREAM: S-103
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	2307.48	2307.48	0.00000
MASS (KG/HR)	63173.7	63173.7	0.00000
ENTHALPY (CAL/SEC)	-0.383274E+08	-0.383274E+08	0.00000

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.174509E-06	KG/HR
PRODUCT STREAMS CO2E	0.174509E-06	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

*** INPUT DATA ***

FLASH SPECS FOR HOT SIDE:
 TWO PHASE FLASH

MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

FLASH SPECS FOR COLD SIDE:
 TWO PHASE FLASH

MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

SHELL&TUBE INPUT FILE NAME
 SHELL&TUBE PROGRAM MODE

H-100_4.EDR
 SIMULATION

HEAT CURVE GENERATION

HOT HEAT CURVE GENERATED BY
 COLD HEAT CURVE GENERATED BY

ASPEN PLUS
 ASPEN PLUS

*** OVERALL RESULTS ***

ASPEN PLUS PLAT: WIN-X64 VER: 37.0

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U-O-S BLOCK SECTION

BLOCK: H-100 MODEL: HEATX (CONTINUED)
 STREAMS:

S-113	----->	HOT (SHELL)	-----> S-114
T=	4.3972D+02		T= 3.5838D+02
P=	7.2781D+00		P= 7.1727D+00
V=	0.0000D+00		V= 0.0000D+00
S-103	<-----	COLD (TUBE)	<----- S-102
T=	3.3320D+02		T= 2.9841D+02
P=	7.2630D+00		P= 7.4019D+00
V=	0.0000D+00		V= 0.0000D+00

UNIT RESULTS:

CALCULATED HEAT DUTY	CAL/SEC	346032.9319
CALCULATED (REQUIRED) AREA	SQM	8.2292
ACTUAL EXCHANGER AREA	SQM	8.2217
% OVER (UNDER) DESIGN		-0.0907
AVERAGE COEFFICIENT	CAL/SEC-SQCM-K	0.0517
UA	CAL/SEC-K	4255.0718
LMTD (CORRECTED)	K	81.3225
LMTD CORRECTION FACTOR		1.0037
NUMBER OF SHELLS IN SERIES		1
NUMBER OF SHELLS IN PARALLEL		1
HIGH RHOV2 INDICATION		YES
VIBRATION INDICATION		NO

SHELLSIDE RESULTS:

MEAN SHELL METAL TEMPERATURE	K	394.4922
TOTAL PRESSURE DROP	ATM	0.1053
WINDOW PRESSURE DROP	ATM	0.0444
CROSSFLOW PRESSURE DROP	ATM	0.0453
BULK FILM COEFFICIENT	CAL/SEC-SQCM-K	0.1869
WALL FILM COEFFICIENT	CAL/SEC-SQCM-K	0.1869
THERMAL RESISTANCE	SEC-SQCM-K/CAL	5.3493
FOULING RESISTANCE	SEC-SQCM-K/CAL	0.0000
CROSSFLOW VELOCITY	M/SEC	0.5297
WINDOW VELOCITY	M/SEC	0.3432
MIDPOINT VELOCITY	M/SEC	0.4364
SHELL ENTRANCE RHOV^2	KG/M-SQSEC	303.8734
SHELL EXIT RHOV^2	KG/M-SQSEC	274.4842
BUNDLE ENTRANCE RHOV^2	KG/M-SQSEC	305.5102
BUNDLE EXIT RHOV^2	KG/M-SQSEC	275.9459
FOULING % OF OVERALL RESISTANCE		0.0000
FILM % OF OVERALL RESISTANCE		27.6595
FRICTIONAL PRESSURE DROP	ATM	0.1055

TUBESIDE RESULTS:

MEAN TUBE METAL TEMPERATURE	K	368.2560
TOTAL PRESSURE DROP	ATM	0.1389
BULK FILM COEFFICIENT	CAL/SEC-SQCM-K	0.0000

BULK FILM COEFFICIENT	CAL/SEC-SQCM-K	0.0830
WALL FILM COEFFICIENT	CAL/SEC-SQCM-K	0.0830
THERMAL RESISTANCE	SEC-SQCM-K/CAL	12.0542
FOULING RESISTANCE	SEC-SQCM-K/CAL	0.0000
INPUT VELOCITY	M/SEC	2.1264
OUTLET VELOCITY	M/SEC	2.2478
FOULING % OF OVERALL RESISTANCE		0.0000
FILM % OF OVERALL RESISTANCE		62.3287
FRICTIONAL PRESSURE DROP	ATM	0.1369

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U-O-S BLOCK SECTION

HEATX COLD-TQCU H-100 TQCURV INLET

 PRESSURE PROFILE: CONSTANT2
 PRESSURE DROP: -0.1389 ATM
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

DUTY	PRES	TEMP	VFRAC
CAL/SEC	ATM	K	
0.0	7.4019	333.1940	0.0
1.6478+04	7.4019	331.6571	0.0
3.2956+04	7.4019	330.1102	0.0
4.9433+04	7.4019	328.5529	0.0
6.5911+04	7.4019	326.9851	0.0
8.2389+04	7.4019	325.4065	0.0
9.8867+04	7.4019	323.8168	0.0
1.1534+05	7.4019	322.2157	0.0
1.3182+05	7.4019	320.6029	0.0
1.4830+05	7.4019	318.9781	0.0
1.6478+05	7.4019	317.3410	0.0
1.8126+05	7.4019	315.6913	0.0
1.9773+05	7.4019	314.0285	0.0
2.1421+05	7.4019	312.3523	0.0
2.3069+05	7.4019	310.6624	0.0
2.4717+05	7.4019	308.9583	0.0
2.6364+05	7.4019	307.2396	0.0
2.8012+05	7.4019	305.5059	0.0
2.9660+05	7.4019	303.7567	0.0
3.1308+05	7.4019	301.9916	0.0
3.2956+05	7.4019	300.2100	0.0
3.4603+05	7.4019	298.4114	0.0

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U-O-S BLOCK SECTION

HEATX HOT-TQCUR H-100 TQCURV INLET

 PRESSURE PROFILE: CONSTANT2
 PRESSURE DROP: 0.0 ATM
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

DUTY	PRES	TEMP	VFRAC
!	!	!	!
!	!	!	!

CAL/SEC	ATM	K		
0.0	7.2781	439.7200	0.0	
1.6478+04	7.2781	436.0576	0.0	
3.2956+04	7.2781	432.3735	0.0	
4.9433+04	7.2781	428.6678	0.0	
6.5911+04	7.2781	424.9407	0.0	
8.2389+04	7.2781	421.1923	0.0	
9.8867+04	7.2781	417.4226	0.0	
1.1534+05	7.2781	413.6318	0.0	
1.3182+05	7.2781	409.8199	0.0	
1.4830+05	7.2781	405.9869	0.0	
1.6478+05	7.2781	402.1330	0.0	
1.8126+05	7.2781	398.2582	0.0	
1.9773+05	7.2781	394.3626	0.0	
2.1421+05	7.2781	390.4462	0.0	
2.3069+05	7.2781	386.5090	0.0	
2.4717+05	7.2781	382.5512	0.0	
2.6364+05	7.2781	378.5727	0.0	
2.8012+05	7.2781	374.5737	0.0	
2.9660+05	7.2781	370.5542	0.0	
3.1308+05	7.2781	366.5143	0.0	
3.2956+05	7.2781	362.4541	0.0	
3.4603+05	7.2781	358.3737	0.0	

BLOCK: P-100 MODEL: PUMP

INLET STREAM: S-101
 OUTLET STREAM: S-102
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 IN OUT RELATIVE DIFF.
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U-O-S BLOCK SECTION

BLOCK: P-100 MODEL: PUMP (CONTINUED)

TOTAL BALANCE
 MOLE (KMOL/HR) 1538.00 1538.00 0.00000
 MASS (KG/HR) 49280.8 49280.8 0.00000
 ENTHALPY (CAL/SEC) -0.243283E+08 -0.243242E+08 -0.168489E-03

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

OUTLET PRESSURE ATM 7.40192
 DRIVER EFFICIENCY 1.00000

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

TOLERANCE 0.00010000

*** RESULTS ***

VOLUMETRIC FLOW RATE	L/MIN	1,035.85
PRESSURE CHANGE	ATM	6.41500
NPSH AVAILABLE	M-KGF/KG	10.6964
FLUID POWER	KW	11.2217
BRAKE POWER	KW	17.1619
ELECTRICITY	KW	17.1619
PUMP EFFICIENCY USED		0.65387
NET WORK REQUIRED	KW	17.1619
HEAD DEVELOPED	M-KGF/KG	83.5916

BLOCK: P-102 MODEL: PUMP

INLET STREAM: S-106
 OUTLET STREAM: S-107
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	384.254	384.254	0.00000
MASS (KG/HR)	17694.3	17694.3	0.00000
ENTHALPY (CAL/SEC)	-0.516784E+07	-0.516653E+07	-0.251880E-03

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/10/2020 PAGE 9

U-O-S BLOCK SECTION

BLOCK: P-102 MODEL: PUMP (CONTINUED)

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	17676.6	KG/HR
PRODUCT STREAMS CO2E	17676.6	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

*** INPUT DATA ***

OUTLET PRESSURE	ATM	10.8562
DRIVER EFFICIENCY		1.00000

FLASH SPECIFICATIONS:

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

*** RESULTS ***

VOLUMETRIC FLOW RATE	L/MIN	457.179
PRESSURE CHANGE	ATM	3.94951
NPSH AVAILABLE	M-KGF/KG	0.0
FLUID POWER	KW	3.04926
BRAKE POWER	KW	5.44985
ELECTRICITY	KW	5.44985
PUMP EFFICIENCY USED		0.55951
NET WORK REQUIRED	KW	5.44985
HEAD DEVELOPED	M-KGF/KG	63.2620

BLOCK: P-103 MODEL: PUMP

INLET STREAM: S-111
 OUTLET STREAM: S-112
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	384.731	384.731	0.00000
MASS (KG/HR)	6946.25	6946.25	0.00000
ENTHALPY (CAL/SEC)	-0.700144E+07	-0.700138E+07	-0.997442E-05

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.872174E-07	KG/HR
PRODUCT STREAMS CO2E	0.872174E-07	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

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U-O-S BLOCK SECTION

BLOCK: P-103 MODEL: PUMP (CONTINUED)

*** INPUT DATA ***

PRESSURE CHANGE ATM	0.49346
DRIVER EFFICIENCY	1.00000

FLASH SPECIFICATIONS:

LIQUID PHASE CALCULATION

NO FLASH PERFORMED

MAXIMUM NUMBER OF ITERATIONS

30

TOLERANCE

0.000100000

*** RESULTS ***

VOLUMETRIC FLOW RATE L/MIN	137.456
PRESSURE CHANGE ATM	0.49346
NPSH AVAILABLE M-KGF/KG	0.0
FLUID POWER KW	0.11455
BRAKE POWER KW	0.29239
ELECTRICITY KW	0.29239
PUMP EFFICIENCY USED	0.39177
NET WORK REQUIRED KW	0.29239
HEAD DEVELOPED M-KGF/KG	6.05362

BLOCK: P-104 MODEL: PUMP

 INLET STREAM: S-116
 OUTLET STREAM: S-117
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	768.450	768.450	0.00000
MASS (KG/HR)	35385.9	35385.9	0.00000
ENTHALPY (CAL/SEC)	-0.103348E+08	-0.103328E+08	-0.192439E-03

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	35350.5	KG/HR
PRODUCT STREAMS CO2E	35350.5	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

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U-O-S BLOCK SECTION

BLOCK: P-104 MODEL: PUMP (CONTINUED)

*** INPUT DATA ***

OUTLET PRESSURE ATM	10.8562
DRIVER EFFICIENCY	1.00000

```

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

```

*** RESULTS ***

```

VOLUMETRIC FLOW RATE L/MIN          914.300
PRESSURE CHANGE ATM                  3.45423
NPSH AVAILABLE M-KGF/KG             7.91966
FLUID POWER KW                       5.33342
BRAKE POWER KW                       8.32682
ELECTRICITY KW                       8.32682
PUMP EFFICIENCY USED                 0.64051
NET WORK REQUIRED KW                   8.32682
HEAD DEVELOPED M-KGF/KG              55.3295
ASPEN PLUS PLAT: WIN-X64 VER: 37.0  04/10/2020 PAGE 12

```

STREAM SECTION

S-101 S-102 S-103 S-106 S-107

```

-----
STREAM ID          S-101      S-102      S-103      S-106      S-107
FROM :            -----      P-100      H-100      -----      P-102
TO   :            P-100      H-100      -----      P-102      -----

```

SUBSTREAM: MIXED

```

PHASE:              LIQUID      LIQUID      LIQUID      LIQUID      LIQUID
COMPONENTS: KMOL/HR
METHANOL            1538.0000  1538.0000  1538.0000   0.5476      0.5476
WATER                0.0        0.0        0.0        8.1602-03   8.1602-03
DIMET-01             0.0        0.0        0.0        383.6982    383.6982
N-TRI-01             0.0        0.0        0.0        0.0         0.0
TOTAL FLOW:
KMOL/HR              1538.0000  1538.0000  1538.0000  384.2540    384.2540
KG/HR                4.9281+04  4.9281+04  4.9281+04  1.7694+04   1.7694+04
L/MIN                1035.8505  1036.2568  1095.4581  457.1793    457.6265

```

STATE VARIABLES:

```

TEMP K              298.1500  298.4114  333.1971  304.0755    304.4562
PRES ATM            0.9869   7.4019   7.2630   6.9066     10.8562
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:

```

CAL/MOL             -5.6945+04 -5.6936+04 -5.6126+04 -4.8416+04 -4.8404+04
CAL/GM              -1777.1970 -1776.8976 -1751.6196 -1051.4236 -1051.1588
CAL/SEC             -2.4328+07 -2.4324+07 -2.3978+07 -5.1678+06 -5.1665+06

```

ENTROPY:

```

CAL/MOL-K           -57.3929  -57.3826  -54.9208  -75.2875   -75.2702
CAL/GM-K            -1.7912  -1.7908  -1.7140  -1.6350   -1.6346

```

DENSITY:

```

MOL/CC              2.4746-02  2.4736-02  2.3400-02  1.4008-02   1.3994-02
GM/CC               0.7929   0.7926   0.7498   0.6451     0.6444
AVG MW              32.0422  32.0422  32.0422  46.0485    46.0485

```

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/10/2020 PAGE 13

STREAM SECTION

S-111 S-112 S-113 S-114 S-116

```

-----
STREAM ID          S-111      S-112      S-113      S-114      S-116
FROM :            -----      P-103      -----      H-100      -----
TO   :            P-103      -----      H-100      -----      P-104

```

SUBSTREAM: MIXED
 PHASE: LIQUID LIQUID LIQUID LIQUID LIQUID
 COMPONENTS: KMOL/HR
 METHANOL 1.0839 1.0839 2.1679 2.1679 1.0952
 WATER 383.6476 383.6476 767.3141 767.3141 1.6305-02
 DIMET-01 1.8932-09 1.8932-09 3.7880-09 3.7880-09 767.3385
 N-TRI-01 0.0 0.0 0.0 0.0 0.0
 TOTAL FLOW:
 KMOL/HR 384.7315 384.7315 769.4820 769.4820 768.4500
 KG/HR 6946.2496 6946.2496 1.3893+04 1.3893+04 3.5386+04
 L/MIN 137.4565 137.4613 274.9197 248.3499 914.2999
 STATE VARIABLES:
 TEMP K 439.7200 439.7451 439.7200 358.3757 304.0800
 PRES ATM 7.2780 7.7715 7.2781 7.1727 7.4019
 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:
 CAL/MOL -6.5514+04 -6.5513+04 -6.5514+04 -6.7133+04 -4.8416+04
 CAL/GM -3628.6058 -3628.5696 -3628.6058 -3718.2720 -1051.4171
 CAL/SEC -7.0014+06 -7.0014+06 -1.4003+07 -1.4349+07 -1.0335+07
 ENTROPY:
 CAL/MOL-K -31.6508 -31.6498 -31.6508 -35.6531 -75.2893
 CAL/GM-K -1.7530 -1.7530 -1.7530 -1.9747 -1.6350
 DENSITY:
 MOL/CC 4.6649-02 4.6647-02 4.6649-02 5.1640-02 1.4008-02
 GM/CC 0.8422 0.8422 0.8422 0.9323 0.6450
 AVG MW 18.0548 18.0548 18.0548 18.0548 46.0485
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STREAM SECTION

S-116C S-117 U2-IN U2-OUT

STREAM ID	S-116C	S-117	U2-IN	U2-OUT
FROM :	----	P-104	----	----
TO :	----	----	----	----

SUBSTREAM: MIXED
 PHASE: LIQUID LIQUID LIQUID LIQUID
 COMPONENTS: KMOL/HR
 METHANOL 1.0952 1.0952 0.0 0.0
 WATER 1.6305-02 1.6305-02 555.0844 555.0844
 DIMET-01 767.3385 767.3385 0.0 0.0
 N-TRI-01 0.0 0.0 0.0 0.0
 TOTAL FLOW:
 KMOL/HR 768.4500 768.4500 555.0844 555.0844
 KG/HR 3.5386+04 3.5386+04 1.0000+04 1.0000+04
 L/MIN 914.2999 914.9705 164.8621 166.9400
 STATE VARIABLES:
 TEMP K 304.0800 304.3654 280.3722 293.5717
 PRES ATM 7.4019 10.8562 1.0000 1.0000
 VFRAC 0.0 0.0 0.0 0.0
 LFRAC 1.0000 1.0000 1.0000 1.0000
 SFRAC 0.0 0.0 0.0 0.0
 ENTHALPY:
 CAL/MOL -4.8416+04 -4.8407+04 -6.8575+04 -6.8343+04
 CAL/GM -1051.4171 -1051.2147 -3806.4851 -3793.6289
 CAL/SEC -1.0335+07 -1.0333+07 -1.0574+07 -1.0538+07
 ENTROPY:
 CAL/MOL-K -75.2893 -75.2786 -40.0416 -39.2388
 CAL/GM-K -1.6350 -1.6348 -2.2226 -2.1781
 DENSITY:
 MOL/CC 1.4008-02 1.3998-02 5.6116-02 5.5418-02
 GM/CC 0.6450 0.6446 1.0100 0.8884

GM/CC 0.6450 0.6446 1.0109 0.9984
AVG MW 46.0485 46.0485 18.0153 18.0153
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PROBLEM STATUS SECTION

BLOCK STATUS

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


TYPE OF RUN: EDIT

INPUT FILE NAME: _4625fhg.inm

INPUT PROBLEM DATA FILE NAME : _4625fhg

OUTPUT PROBLEM DATA FILE NAME: _0231qae

LOCATED IN:

PDF SIZE USED FOR INPUT TRANSLATION:

NUMBER OF FILE RECORDS (PSIZE) = 0
NUMBER OF IN-CORE RECORDS = 256
PSIZE NEEDED FOR SIMULATION = 1

CALLING PROGRAM NAME: apmain

LOCATED IN: C:\Program Files\AspenTech\Aspen Plus V11.0\Engine\req

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

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FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
U1-IN	----	C-100	DIST-IN	----	C-100
DIST-OUT	C-100	----	U1-OUT	C-100	----

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
C-100	DIST-IN U1-IN	DIST-OUT U1-OUT

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:

C-100

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/HR)			
WATER	15653.4	15653.4	0.00000
DIMET-01	1368.27	1368.27	0.00000
METHANOL	1.95285	1.95285	0.00000
TOTAL BALANCE			
MOLE (KMOL/HR)	17023.6	17023.6	0.00000
MASS (KG/HR)	345098.	345098.	0.00000
ENTHALPY (CAL/SEC)	-0.314940E+09	-0.314940E+09	0.00000

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	63034.8	KG/HR
PRODUCT STREAMS CO2E	63034.8	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

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PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME
WATER	C	H2O	WATER
DIMET-01	C	C2H6O-1	DIMETHYL-ETHER
METHANOL	C	CH4O	METHANOL

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U-O-S BLOCK SECTION

BLOCK: C-100 MODEL: HEATX

HOT SIDE:

INLET STREAM: DIST-IN
 OUTLET STREAM: DIST-OUT
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG
 COLD SIDE:

INLET STREAM: U1-IN
 OUTLET STREAM: U1-OUT
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	17023.6	17023.6	0.00000
MASS (KG/HR)	345098.	345098.	0.00000
ENTHALPY (CAL/SEC)	-0.314940E+09	-0.314940E+09	0.00000

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	63034.8	KG/HR
PRODUCT STREAMS CO2E	63034.8	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

*** INPUT DATA ***

FLASH SPECS FOR HOT SIDE:

TWO PHASE FLASH
 MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

FLASH SPECS FOR COLD SIDE:

TWO PHASE FLASH
 MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

FLOW DIRECTION AND SPECIFICATION:

COUNTERCURRENT HEAT EXCHANGER
 SPECIFIED HOT VAPOR FRACTION
 SPECIFIED VALUE 0.0000
 LMTD CORRECTION FACTOR 1.00000

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U-O-S BLOCK SECTION

BLOCK: C-100 MODEL: HEATX (CONTINUED)

PRESSURE SPECIFICATION:

HOT SIDE PRESSURE DROP BAR 0.0000
 COLD SIDE PRESSURE DROP BAR 0.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:

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

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

*** OVERALL RESULTS ***

STREAMS:

```

-----
DIST-IN  -----> |                HOT                | -----> DIST-OUT
T=  3.1540D+01 |                |                | T=  3.0926D+01
P=  6.9982D+00 |                |                | P=  6.9982D+00
V=  1.0000D+00 |                |                | V=  0.0000D+00
-----
U1-OUT   <----- |                COLD                | <----- U1-IN
T=  2.8948D+01 |                |                | T=  7.2222D+00
P=  1.0132D+00 |                |                | P=  1.0132D+00
V=  0.0000D+00 |                |                | V=  0.0000D+00
-----

```

DUTY AND AREA:

CALCULATED HEAT DUTY	CAL/SEC	1662834.4759
CALCULATED (REQUIRED) AREA	SQM	858.6170
ACTUAL EXCHANGER AREA	SQM	858.6170
PER CENT OVER-DESIGN		0.0000

HEAT TRANSFER COEFFICIENT:

AVERAGE COEFFICIENT (DIRTY)	CAL/SEC-SQCM-K	0.0203
UA (DIRTY)	CAL/SEC-K	174315.5787

LOG-MEAN TEMPERATURE DIFFERENCE:

LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	9.5392
NUMBER OF SHELLS IN SERIES		1

PRESSURE DROP:

HOTSIDE, TOTAL	BAR	0.0000
COLD SIDE, TOTAL	BAR	0.0000

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U-O-S BLOCK SECTION

BLOCK: C-100 MODEL: HEATX (CONTINUED)

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:

```

-----
HOT
-----
HOT IN |                COND                | HOT OUT
-----> |                |                | ----->
  31.5 |                |                |   30.9
-----
COLDOUT |                LIQ                 | COLDIN
<----- |                |                | <-----
  28.9 |                |                |   7.2
-----
COLD
-----

```

ZONE HEAT TRANSFER AND AREA:

ZONE HEAT DUTY AREA LMTD AVERAGE U UA
 CAL/SEC SQM C CAL/SEC-SQCM-K CAL/SEC-K
 1 1662834.476 858.6170 9.5392 0.0203 174315.5787
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U-O-S BLOCK SECTION

HEATX COLD-TQCU C-100 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
 PRESSURE DROP: 0.0 BAR
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

DUTY	PRES	TEMP	VFRAC
CAL/SEC	BAR	C	
0.0	1.0133	28.9482	0.0
7.9183+04	1.0133	27.9217	0.0
1.5837+05	1.0133	27.9217	0.0
2.3755+05	1.0133	26.8943	0.0
3.1673+05	1.0133	25.8661	0.0
3.9591+05	1.0133	24.8371	0.0
4.7510+05	1.0133	23.8072	0.0
5.5428+05	1.0133	22.7765	0.0
6.3346+05	1.0133	21.7450	0.0
7.1264+05	1.0133	20.7126	0.0
7.9183+05	1.0133	19.6795	0.0
8.7101+05	1.0133	18.6455	0.0
9.5019+05	1.0133	17.6108	0.0
1.0294+06	1.0133	16.5753	0.0
1.1086+06	1.0133	15.5390	0.0
1.1877+06	1.0133	14.5020	0.0
1.2669+06	1.0133	13.4642	0.0
1.3461+06	1.0133	12.4256	0.0
1.4253+06	1.0133	11.3864	0.0
1.5045+06	1.0133	10.3464	0.0
1.5837+06	1.0133	9.3057	0.0
1.6628+06	1.0133	8.2643	0.0

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U-O-S BLOCK SECTION

HEATX HOT-TQCUR C-100 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
 PRESSURE DROP: 0.0 BAR
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

DUTY	PRES	TEMP	VFRAC
CAL/SEC	BAR	C	
0.0	6.9982	31.5404	1.0000

7.9183+04	6.9982	31.2712	0.9537
1.5837+05	6.9982	31.1734	0.9066
2.3755+05	6.9982	31.1146	0.8591
3.1673+05	6.9982	31.0750	0.8116
3.9591+05	6.9982	31.0466	0.7640
4.7510+05	6.9982	31.0251	0.7163
5.5428+05	6.9982	31.0083	0.6686
6.3346+05	6.9982	30.9948	0.6209
7.1264+05	6.9982	30.9838	0.5732
7.9183+05	6.9982	30.9746	0.5255
8.7101+05	6.9982	30.9667	0.4777
9.5019+05	6.9982	30.9600	0.4300
1.0294+06	6.9982	30.9542	0.3822
1.1086+06	6.9982	30.9491	0.3344
1.1877+06	6.9982	30.9445	0.2867
1.2669+06	6.9982	30.9405	0.2389
1.3461+06	6.9982	30.9369	0.1911
1.4253+06	6.9982	30.9337	0.1433
1.5045+06	6.9982	30.9308	9.5565-02
1.5837+06	6.9982	30.9281	4.7784-02
1.6628+06	6.9982	30.9256	2.1118-10

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STREAM SECTION

DIST-IN DIST-OUT U1-IN U1-OUT

STREAM ID	DIST-IN	DIST-OUT	U1-IN	U1-OUT
FROM :	----	C-100	----	C-100
TO :	C-100	----	C-100	----
SUBSTREAM: MIXED				
PHASE:	VAPOR	LIQUID	LIQUID	LIQUID
COMPONENTS: KMOL/HR				
WATER	2.9101-02	2.9101-02	1.5653+04	1.5653+04
DIMET-01	1368.2680	1368.2680	0.0	0.0
METHANOL	1.9529	1.9529	0.0	0.0
TOTAL FLOW:				
KMOL/HR	1370.2500	1370.2500	1.5653+04	1.5653+04
KG/HR	6.3098+04	6.3098+04	2.8200+05	2.8200+05
L/MIN	7.4066+04	1630.3019	4649.1106	4746.8016
STATE VARIABLES:				
TEMP C	31.5404	30.9256	7.2222	28.9482
PRES BAR	6.9982	6.9982	1.0133	1.0133
VFRAC	1.0000	0.0	0.0	0.0
LFRAC	0.0	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0
ENTHALPY:				
CAL/MOL	-4.4048+04	-4.8416+04	-6.8575+04	-6.8192+04
CAL/GM	-956.5518	-1051.4235	-3806.4851	-3785.2574
CAL/SEC	-1.6766+07	-1.8429+07	-2.9817+08	-2.9651+08
ENTROPY:				
CAL/MOL-K	-60.9246	-75.2875	-40.0416	-38.7342
CAL/GM-K	-1.3231	-1.6350	-2.2226	-2.1501
DENSITY:				
MOL/CC	3.0834-04	1.4008-02	5.6116-02	5.4961-02
GM/CC	1.4199-02	0.6451	1.0109	0.9901
AVG MW	46.0485	46.0485	18.0153	18.0153
ASPEN PLUS	PLAT: WIN-X64	VER: 37.0	04/06/2020	PAGE 10

PROBLEM STATUS SECTION

BLOCK STATUS

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