Design and Economic Analysis of a DME Synthesis and Separation Plant

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Abstract

We performed a preliminary design evaluation of a process based around a PBR packed with the catalyst Amberlyst 35, which produced a DME product flow rate of approximately 250,000 gal/day, with a minimum product purity of 98.5 mass% DME and an estimated value of $2.32/gal, from a methanol feed stream of approximately 295,000 gal/day, with a product purity of 98% MeOH and an estimated value of $1.53/gal. Based on our economic analysis, we predict that our proposed process, over it's 20 year project life, will result in a ROR of 65% with an NPV of approximately $141 million. This process will require an initial capital investment of approximately $20 million, with a payback period from 2018 to 2020. Based on our economic estimations we consider this process to be economically attractive.

In addition to the design of a Amberlyst 35 PBR process, we explored the application of reactive distillation using Amberlyst 35 to meet the design specifications of this project. We were able to appropriately simulate a reactive distillation process and analyze our results. Based on our economic analysis, we predict that the production of DME, as described in the design basis, by reactive distillation would result in an NPV of $182 million with an ROR of 240.5%. We found that the application of reactive distillation to accomplish the design basis, to be the most attractive of the two designs. The ability to separate the products from the reaction zone, through reactive distillation, and meet the design specification with a single column, significantly reduces operating costs and capital costs. Therefore, we recommend further detailed design of the reactive distillation process.

We found the specifications of our reactive distillation column to be as follows: The DME reactive distillation column is a single feed system with a methanol stream fed to stage 10 at the top of the reactive zone. The column has 8 stripping stages (including the condenser), 22 packed reactive stages, and 9 rectifying stages (including the reboiler). The column operates at a pressure of 139.1 psia and with a reflux ratio of 2.0. The catalyst holdup on each reactive tray is 66.8 lbm. This corresponds to a total holdup of 1469.6 lbm in the column.

Introduction

DME as an Alternative Fuel

Dimethyl Ether, C_2H_6O (DME), is a volatile hydrocarbon with a structure of two methyl groups bonded to an oxygen atom. DME is currently being studied as an alternative transportation fuel to low sulfur diesel (Design Statement). DME is attractive as a fuel due to it's lack of carbon to carbon bonds and due to this property the implementation of DME as a fuel source seems to be a promising pathway to the invention of zero particulate emission vehicles. A good example of particulate emissions is the black smoke we see emitting from truck engines. Low diesel sulfur engines, currently in 3% of vehicles in the United State, emit several particulates related to global warming (Diesel Engine Pencentages). Emissions of diesel engines include carbon dioxide, nitrogen oxides, and methane, all of which have high global warming potentials (Diesel Emissions). Global warming potentials are defined by ratio of radiation energy one ton of a substance will absorb relative to one ton of carbon dioxide (Global Warming

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Potentials). Global warming potentials of diesel emissions are shown below, along with the global warming potential of DME in *Table 1*.

Table 1: Global Warming Potentials (Dimethyl ether (DME) as an alternative fuel)

	Time Horizon		
	20 Years	100 Years	500 Years
DME	1.2	.3	.1
CO2	1	1	1
CH4	56	21	6.5
N2O	280	310	170

As shown in *Table 1*, DME emissions have a lower global warming potential than CO_2 over the next 100 and 500 years. In contrast, CH_4 and N_2O have much higher global warming potentials, absorbing as much as 31,000% the amount of energy that CO_2 absorbs. Converting as many engines as possible from low sulfur diesel fuel to DME would likely have a significant, positive impact on the environment.

Another benefit of converting engines from low sulfur diesel to DME is the variety of sources from which DME can be produced. DME can be produced from sustainable biomass, municipal solid waste, natural gas, methanol, or CO2, making it a flexible product [Design Statement]. Low sulfur diesel, comparatively, can only be produced from crude oil. The inflexible production process of low sulfur diesel leads to the conclusion that it will no longer be producible once the Earth's crude oil reserves are depleted. This impending shortage of low sulfur diesel will eventually need to be offset with another fuel. Switching to DME as soon as possible will ease the transition once diesel is no longer producible.

Design Basis

Our group was tasked with the preliminary design and evaluation of a DME production process, which includes an analysis of technical feasibility, economic feasibility and control system design. The key deliverables and design basis are shown in *Table 2* and *Table 3*.

Table 2: Key Deliverables

DME Production Rate	250,000 US gal/day
DME Composition	ASTM D7901.144734
Project Life	20 Years
Discount Rate	8%

Table 3: ASTM D7901.144734 Fuel-Grade DME Composition Requirements

DME (mass %), min	98.5

Methanol (mass %), max	.005
Water (mass %), max	.003
Methyl Formate (mass %)	report

Process Description

Our assumption at the beginning of the process is that the source methanol, of 96 mol% CH_3OH and 4 mol% H_2O, is stored at 75 psia (approximately 58 psi above the pure vapor pressure of CH_3OH at 77°F)*. In *Stream 1* the liquid methanol is pressurized to 261 psia and pumped into the process at 2601 lbmole/hr, by *P-101A/B*. In *Stream 2,* the feed *Stream 1* combines with the recycle *Stream 12,* resulting in a flow rate of 4402 lbmol/hr with 94 mol% CH_3OH. *Stream 2* enters E-101 where it is heated to 284°F, the driving force being HP Steam at 485°F from *Stream 26*. We found that the optimal temperature for maximum conversion of MeOH to DME, was 284°F and this temperature is maintained in R-101 through heat exchange with cooling water, as described by *Stream 25*. *Stream 4* exits R-101 with a conversion of approximately 59% of MeOH, resulting in a composition of 29 mol% DME, 33 mol% water and 38 mol% MeOH. *Stream 4* enters T-101 for fractionation resulting in a fuel grade DME product of 99 mol% DME in the distillate, with a flow rate of 1230 lbmole/hr and a pressure of 188.6 psia, as described by *Stream 6*. We assume that *Stream 6* contains enough pressure and head for transport to storage. The bottoms product of T-101, *Stream 10*, with the composition of 53 mol% MeOH and 45 mol% water enters T-102 to separate the MeOH from Water. The resulting purified MeOH in the distillate with a composition of 91 mol% MeOH, and 6 mol% water is recycled back into the beginning of the process, as described by *Stream 12.* The bottoms product of T-102, with a composition of 97 mol% water and 3 mol% MeOH and at the temperature of 255°F, as described by *Stream 16,* is sent to E-106 to be cooled down to 113°F before being sent to waste water treatment.

Control Strategy

Challenges associated with the control of this process

An ideal control strategy, would allow the operator to adjust the production of DME by simply increasing or decreasing the set point of FCV-101 and *Stream 1*, without any additional attention. It is important to note here, however, that effective control of the process to respond appropriately to feed flow rate changes and to accommodate a large operating range, is a significant challenge, and would require further detailed analysis and design beyond what we provide here.

 For example, in a situation that would call for an increase in the flow rate of methanol feed into the process, this would likely affect the composition of *Stream 4* exiting R-101. In this situation, the residence time of *Stream 3* entering R-101 would decrease, resulting in a reduced time for adsorption of MeOH on the Amberlyst 35 catalyst. Therefore, the component fraction of DME in *Stream 4* would be reduced as it enters T-101.

In addition, an increased flow rate in *Stream 1* would call for control adjustments in the reflux flow rate, boil-up flow rate and distillate flow rates in T-101 as well as T-102, for the process to function properly. With an increased flow rate, since DME is significantly more volatile than MeOH (as well as the heavy non-key component water), the resulting distillate product purity and flow rate out of T-101 may not be affected *immediately*. However, without

control adjustments, after several recycles of *Stream 12*, the performance of T-101 would eventually be affected. This problem would occur because the performance of T-102 would drop off rapidly. For example, without adjustments in the reflux flow rates and boil-up flow rates of T-102, the component fraction of water in the distillate, *Stream 12,* would increase, as well as the component fraction of MeOH in the bottoms, *Stream 16* (here, potentially causing issues on the water treatment end, or an ignition hazard). And, after several recycles of *Stream 12* combining with *Stream 1* into *Stream 2*, the component fraction of water in *Stream 3* would eventually accumulate to a point where water saturates adsorption sites on the Amberlyst 35 in R-101, preventing DME from forming, and resulting in no distillate product in T-101.

Likewise, under a decreased flow rate condition, without adjustments in the control system of T-101 and T-102, would result (at the very least), in the waste of unnecessary utility use of cooling water and high pressure steam. A more serious result of due to the lack of proper control adjustment, here, would cause increased boil up flow rates in T-101 and T-102, possibly resulting in a significant rise in vapor flow across column trays and flooding of the columns, as well as, a drop in bottoms product.

Ideally, we would like to establish an understanding with the composition of Stream 4 and the proper operation of T-101 and T-102, however, a composition analyzer placed directly on Stream 4 would be wildly inaccurate due to the presence of two-phase flow and would need to be condensed first. A solution may be found by establishing an understanding of the flow rate and composition of Stream 2 with the extent of reaction of R-101, so that we may be able to predict, effectively tune and control the optimal operating conditions of T-101 and T-102.

On the PFD of this process, we propose that a *flow element* placed on *Stream 3*, through a yet to be established mathematical relationship, needs to determine the set point of the boil up flow rate of *Stream 9*, the set point of the distillate flow rate of *Stream 6,* as well as, the reflux ratio and resulting reflux flow rate of *Stream 7*. In the same manner, a *flow element* placed on *Stream 10*, would need to determine the set points of the operation of T-102.

In sum, we note, that further analysis, design and work must be done to develop a comprehensive control strategy to accommodate a large operating range. Since this area is beyond our current competence. Moving forward, in the following description of the basic control strategy, we assume that the operation of the process is limited to slight oscillations and variations from our steady-state simulation data.

Pressure of T-101 and T-102

The pressure of T-101 and T-102 is controlled by throttling PCV-104 and PCV-110 through feedback control loops.

Control of E-101

The temperature of *Stream 3* entering R-101 must be maintained at or near the temperature of 284°F, to ensure the maximum possible conversion of MeOH to DME in R-101, as well as, to avoid degradation of the Amberlyst 35 catalyst. Thus, effective control of E-101 is critical. E-101, is controlled by throttling the steam condensate out of E-101 with TCV-102. This

strategy determines the amount of heat transfer surface area available in E-101 for latent heat transfer from *Stream 26 (*high pressure steam) to *Stream 3*. TCV-102 is governed through feedback control from temperature control equipment mounted on *Stream 3*. It is important to note, however, that if the flow rate of *Stream 2* is abruptly reduced, the temperature of *Stream 3* may enter R-101 at a dangerously high temperature. Therefore, in further detailed design, if the possibility of an abrupt change in flow rate is expected, we recommend an additional a by-pass stream from *Stream 2* directly to *Stream 3*.

Control of E-103

The flow rate of *Stream 9* by E-103, the column reboiler for T-101, is controlled by throttling FCV-108, in the same manner, as with the control and operation of E-101. In E-103, the pressure of the shell side of the reboiler is determined by the column and the vaporization temperature of the mixture is determined by it's composition. Thus, the heat duty supplied directly governs the rate of vaporization of the liquid at the bottom of the column. In addition, the bottoms flow rate is determined by a level controller on the weir side of the kettle reboiler, governing LCV-109.

Control of E-105

The control of E-105 is arranged in the same manner as E-103, with FCV-114 as the steam condensate throttle, and with LCV-115 regulating the flow rate of the bottoms.

Control of E-102 and E-104

The condenser of T-101, E-102, is controlled by throttling the flow rate of cooling water with TCV-107, as described by *Stream 26*, governed by a temperature controller placed on *Stream 7*. In the same manner the condenser of T-102, E-104, is controlled by TCV-113 with a temperature controller placed on *Stream 13*.

Control of E-106

The bottoms product cooler, E-106 is controlled in the same manner as E-102 and E-104 with TCV-116 governed by a temperature controller placed on *Stream 17*.

R-101 Design

The packed bed reactor (PBR) in our proposed design is the key unit in the process, as this is where all DME production occurs. We assumed that the MeOH feed would be supplied in liquid form. Therefore, we chose to design our process using the heterogeneous catalyst Amberlyst 35, which has been shown to be effective in facilitating the formation of DME from MeOH. The reaction occurs when liquid phase MeOH adsorbs onto the surface of the solid catalyst. Amberlyst 35 is a high acid resin catalyst with a void fraction of .6 and a bulk density of 607 kg/m3. Since this is a heterogeneous catalytic reaction, a PBR was chosen for this process.

We designed a PBR to maximize the conversion of MeOH to DME as much as technically feasible, and we predict a conversion of approximately 59% in our design. The reaction that occurs in the PBR is shown below (Eq. 1).

$$2CH_3OH \rightarrow DME + H_2O$$
<div align="right">*Eq. 1*</div>

Since, the reaction that occurs in the PBR is exothermic and requires a cooling fluid to maintain an isothermal environment.

R-101 was designed using a governing material balance equation. The reaction of MeOH to DME is to only reaction occurring in R-101, therefore, we used the following design equation, see Eq.2

$$\frac{d(X)}{d(W)} = \frac{-r'_{MeOH}}{F_{MeOH,0}}$$
<div align="right">*Eq. 2*</div>

Factors in the design equation include the rate of consumption of MeOH and the weight of catalyst located in the PBR. The rate of consumption of MeOH was determined to follow a Langmuir-Hinshelwood Mechanism. This type of mechanism assumes that the rate limiting step is the absorption of MeOH onto the surface of the catalyst. The rate of consumption of MeOH is modeled using the following rate law, see Eq. 3.

$$r'_{\square\square\square\square} = \frac{k}{(1+K1*[MeOH]^{-1}*[H_2O])^{\wedge}2}$$
<div align="right">*Eq. 3*</div>

Conversion Relationships

The rate of consumption of MeOH as described by Eq. 3, is not written in a form that is compatible with Eq. 2. Because of this, all molar fractions must be written in terms of conversion. The molar fraction of a component is as follows:

$$Component\ Molar\ Fraction = \frac{Component\ Flow\ Rate}{Total\ Flow\ Rate}$$

Therefore, we represent the molar fractions of MeOH and water as follows:

$$[MeOH] = \frac{F_{\text{▢▢▢▢}}}{F_{tot}}$$

$$[H_2O] = \frac{F_{H_2O}}{F_{tot}}$$

The molar fractions, written in terms of molar flow rate, can now be written in terms of conversion:

$$F_{\text{▢▢▢▢}} = F_{MeOH,0} * (1 - X) \qquad \text{Eq. 4}$$

$$F_{H_2O} = F_{MeOH,0} * (\frac{F_{MeOH,0}}{F_{H_2O,0}} - .5 * X) \qquad \text{Eq. 5}$$

Eq. 4 and Eq. 5 are then substituted into the rate of consumption of methanol, via the molar fraction equations. Combining these equations, a plot of reactor volume in m^3 vs conversion was created, see *Figure 1*.

Figure 1: PBR Volume vs Conversion
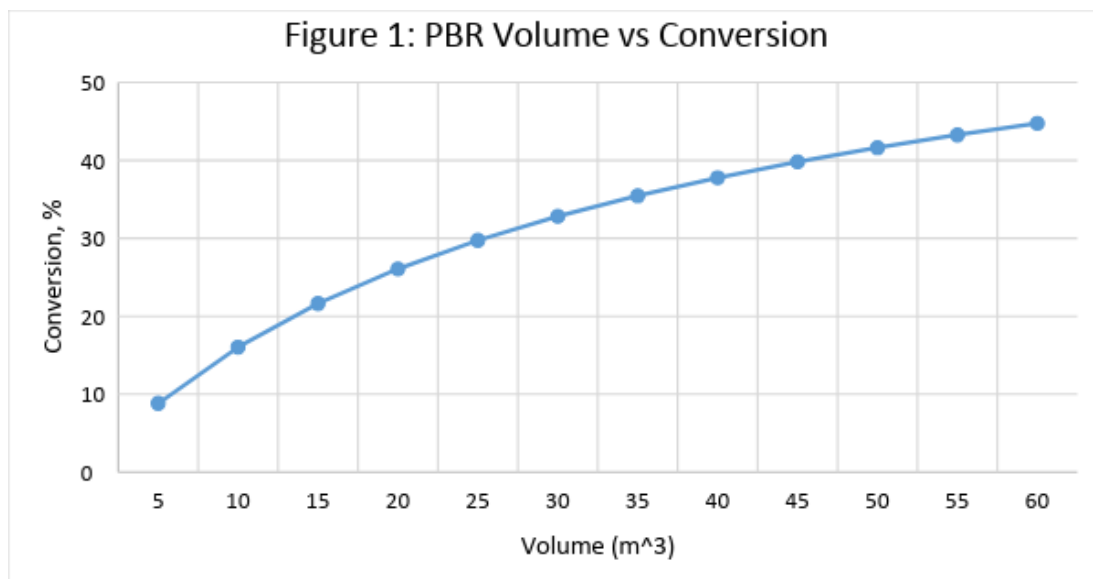
Determination of R-101 Volume and Optimal Operating Conditions

The high acid resin catalyst begins to degrade in reactors that exceed 9 meters in length. Therefore, we set the reactor length at 9 meters. Since, the most common diameter for vertical process vessels, including reactors and towers, is 2.5 meters, we chose this diameter as we judged that this would maximize the size of the reactor, while remaining a technically feasible solution. These dimensions result in a total reactor volume of 45 m^3 (1589 ft^3). Our decision is further supported by *Figure 1*, which shows a diminishing increase in conversion as reactor volume increases. We expect that a further increase in diameter of the PBR (and volume of the PBR), would incur a significant increase in capital cost, not offset by an appreciable increase in performance.

The maximum operating temperature for R-101 is 327.6 °F. Above this temperature, the high acid resin catalyst begins to desulfonate in a way that forms H_2SO_4 in aqueous solutions.

We found that a temperature of 284°F is near the most optimal operating temperature, after which, the increased heat duty requirement to preheat the reactor feed stream and corresponding operating cost, is not offset by appreciable gains in conversion. In addition this temperature is blow the maximum operation temperature for R-101 and allows for fluctuations in temperature due to imperfect temperature control, avoiding the risk of catalyst degradation.

We found that the pressure of 235 psia to be near the most optimal operating pressure. This prevents MeOH from vaporizing in R-101 at 284°F, which would lead to reduced conversion, as MeOH must contact the Amberlyst 35 catalyst in the liquid phase.

The capital and operating costs of R-101 are summarized in *Table 4*.

Table 4: Capital and Operating Costs of R-101	
Capital Cost	Operating Cost
$196,506	$35,338

R-101 was priced as a vertical process vessel with tower packing, added to the cost of a equivalent shell and tube heat exchanger that would provide the duty. The individual capital costs for the different components are summarized in *Table 5*.

Table 4: Capital Cost Breakdown of R-101	
	Capital Cost
Vertical Process Vessel	$111,844
Tower Packing	$476
Cooling Tubes	$85,185

The high acid resin catalyst was not included in the capital cost for R-101 because of the frequency at which we need to purchase it. The catalyst has a lifespan on ~10 years, so we kept the purchase price for the catalyst as a separate cost.

The dehydration of MeOH is an exothermic reaction, releasing 11,712 kJ/kmol of energy. To maintain a constant temperature in R-101, 272.6 m^3/hr of cooling water is sent through cooling tubes. The annual cost for this amount of cooling water is $35,338.

The high acid resin catalyst provides the driving force behind the reaction. The catalyst has a bulk density of 607 kg/m^3. In the 45 m^3 reactor, this comes out to 27,315 kg of catalyst. At $33.07/kg, it costs $903,361 to purchase the amount of catalyst necessary to fill the reactor. The catalyst has a lifespan of ~10 years, so this cost need only be accounted for in 2019 and 2029.

Since DME formed in R-101 becomes gaseous in R-101, it is important to note that in order to ensure that the two phase (liquid and vapor) *Stream 4* flows properly - the orientation of R-101 relative to T-101 is critical. The top of R-101 must be below the feed stage at the 10th tray of T-101, to avoid the accumulation of gas in R-101 and process piping.

T-101 Design and Optimization

T-101 is the distillation column which separates the DME from MeOH and water. T-101 was designed to separate and produce 250,000 US gal/day of 98.5% DME by mass. T-101 consists of 13 trays with a tray spacing of 2.3ft. The feed from R-101 enters the column above Stage 10.

The design pressure and temperature of T-101 are the factors that affect the number of stages required, reflux ratio, and other tower parameters. Therefore, either temperature or pressure needed to be determined. A total condenser was utilized in the column, therefore, all vapor needed to be condensed in the overhead streams. To use cooling water in the condenser, a 10°C (20°F) difference between the overhead vapor stream and the cooling water outlet (or the approach temperature), needed to be maintained. The maximum cooling water return temperature is 113°F, therefore the minimum overhead temperature is 131°F. At 131°F, the pressure of the condenser was found to be 188.6 psia. The condenser pressure was calculated as the sum of the weighted vapor pressures of the components at 55 °C, see *Table 5*.

Table 5: Data used to Determine Operating Pressure of T-101 (at 131°F)			
Component	Mol%	Vapor Pressure at 55 °C (psia)	Weighted Vapor Pressure (psia)
DME	99.93%	188.5	188.37
MeOH	.07%	9.96	.0069
		Total	188.4

Once the condenser pressure was determined, the next step was to determine the minimum number of stages and minimum reflux ratio, we found these parameters to be 4 stages and .452, respectively. The Fenske and Underwood equation were used to determine these minimum parameters (*Eq. 6* and *Eq. 7*).

$$N_{min} = \frac{log(\frac{LK_D}{HK_D} * \frac{HK_B}{LK_B})}{log(\alpha_{avg})}$$

Eq. 6

To determine the minimum number of stages, the distillate and bottoms purities as well as the average volatility must be known. These parameters are summarized below (*Table 6 and Table 7*).

Table 6: Data used for Determination of N_{min}						
Component	DME	MeOH	DME	MeOH	DME	MeOH
K-Value	3.338	0.6612	1.007	0.04182	4.198	0.8217

Relative Volatility	5.048	24.079	5.109
Average Volatility	8.532		

Table 7: Data used for the Determination of N_{min}			
Fenske Equation	Molar Fraction		
	Distillate	Feed	Bottoms
DME	0.9928	0.2495	0.0878
MeOH	0.0072	0.5329	0.6473
N_{min}	4		
$N_{f,min}$	3		

Once the minimum number of stages was determined, the minimum reflux ratio needed to be determined. We calculated the minimum reflux ratio using the Underwood equation.

$$F * (1 - q) = \sum_{i} \frac{F * \alpha_{i,HK} * z_i}{\alpha_{i,HK} + \varphi}$$ *Eq. 7*

Table 8: Data Used for the Determination of the Minimum Reflux Ratio						
Underwood Equation	Feed			Distillate		
	T(K)	413		T(K)	323	
	P(bar)	16.78		P(bar)	11.47	
Component	DME	MeOH	Water	DME	MeOH	Water
Mole Fraction	0.2495	0.5329	0.2175	0.9928	0.0072	0.0000
K-Value	3.33800	0.66120	0.31430	1.00700	0.04182	0.01604
Relative Volatility	10.6	2.1	1.0	62.8	2.6	1.0
Single Term	911.3	4264.4	-2722.9	3262.1	44.8	0.0
V_{feed}	2453					
V_{min}	3307					
L_{min}	2732					
R_{min}	0.45					

The Underwood equation was solved with a value of $\varphi = 1.257$. This solution also satisfies the following criterion:

$$1 < \varphi = 1.257 < 62.8$$

This criterion ensures that the value of φ does not exceed the lowest or greatest relative volatility. Solving both the Fenske and Underwood equation gave us a starting point for determining the

number of stages in the actual tower. In order to determine the optimum number of stages, the net present cost (NPC) was calculated for different tower configurations. This takes into account both the capital cost and annual operating costs for the tower, and returns an equivalent value at present day pricing. The NPC for several tower configurations is shown in *Figure 2*.

Figure 2: T-101 Stages vs NPC
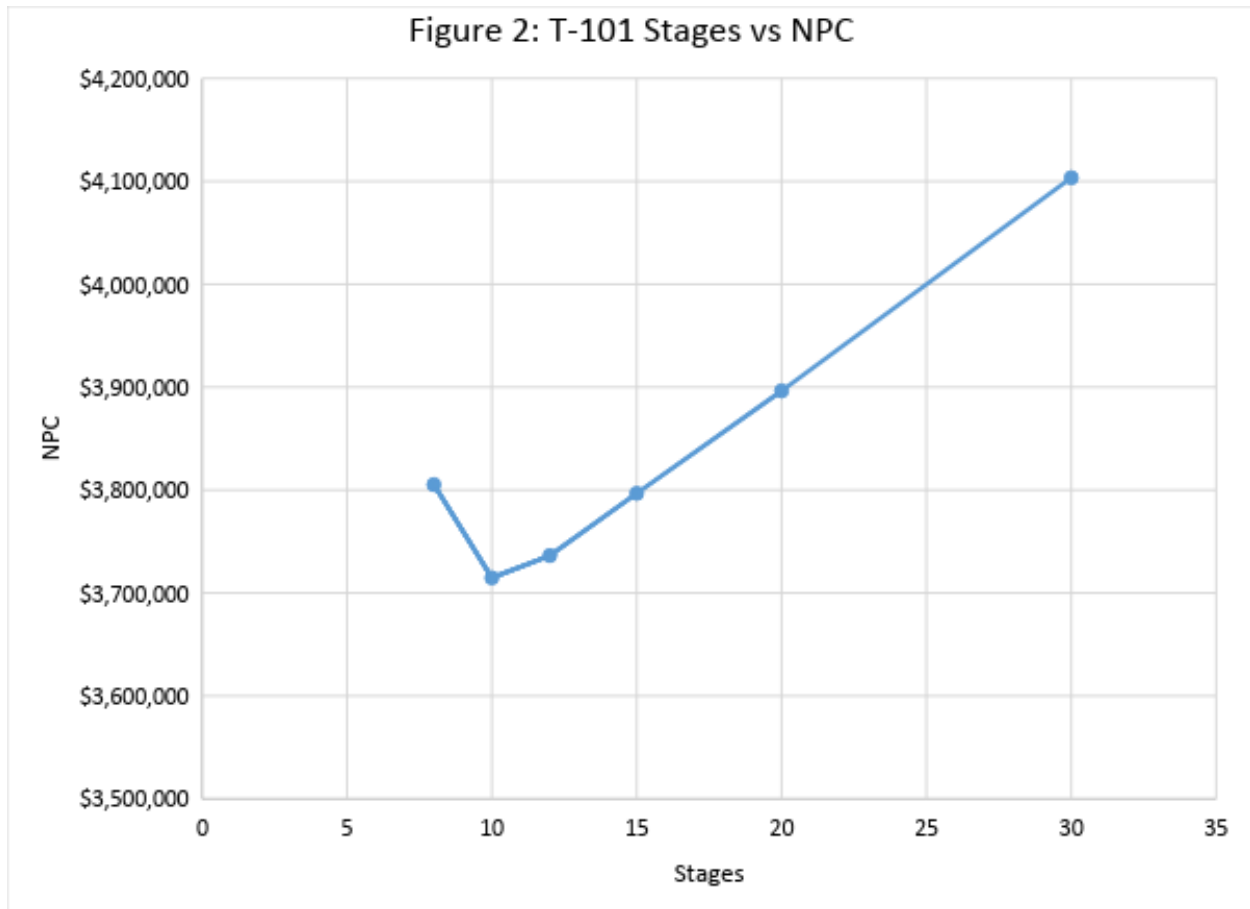
From *Figure 2,* the optimal number of theoretical stages was determined to be 10. Accounting for a 80% tray efficiency, this gives 13 actual stages. This configuration yields an NPC of $3,714,748. The last tower parameter that we optimized was the location of the feed stage. The feed stage was altered and the reflux ratio was measured at each location. The reflux ratio at each stage was plotted as a function of the feed location, see *Figure 3*.

Figure 3: T-101 Feed Stage vs Reflux Ratio
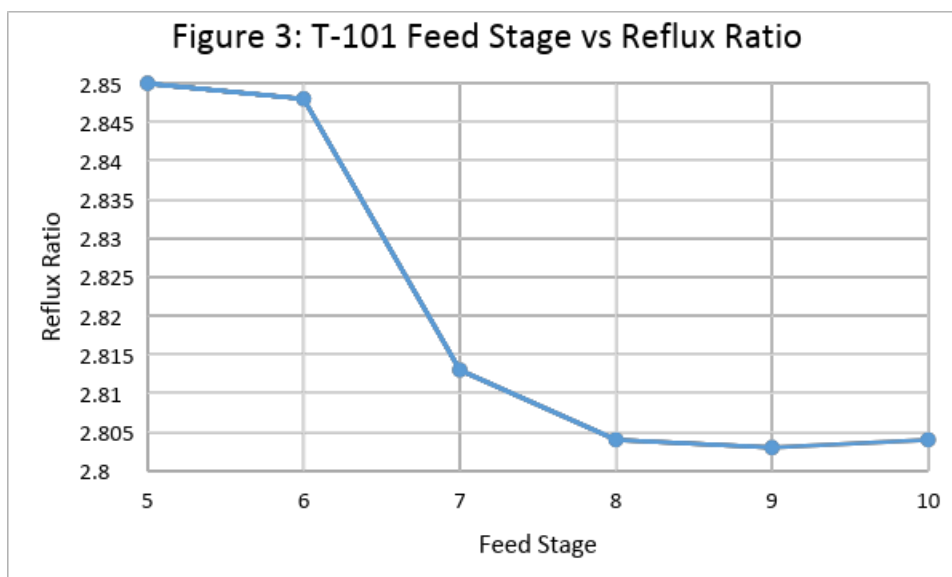
From *Figure 3*, the optimum feed stage was determined to be theoretical stage 9. This places the actual feed location above stage 10 when accounting for 80% tray efficiency. This results in a reflux ratio of 2.803. We note that the likely reason that the most efficient feed stage is near the bottom of the column due to the presence of DME vapor in the feed *Stream 4*, and that the relative volatility of DME to MeOH (and water) is high.

T-101 Summary

T-101 was designed to operate at a pressure of 188.6 psia with 13 stages at a reflux ratio of 2.803. These tower parameters result in the lowest NPC throughout the project life. The tower results in a total installed cost of $1,414,432. We report the operating cost for delivering the duties to the condenser (E-102) and reboiler (E-103) in a later section.

T-102 Design and Optimization

T-102 was designed to separate the unreacted MeOH from the water produced. The bottom water product will be sent to a waste water treatment plant, and the MeOH will be recycled (*Stream 12*), mixed with feed (*Stream 1*) from the MeOH tanks, and sent through R-101. The waste water composition was the design spec that needed to be met. The waste water could not exceed 6% MeOH by mass. This concentration is the low explosive limit of MeOH/water mixtures. T-102 was designed to have 50 actual trays, with a tray spacing of 2 ft. The feed enters T-102 above stage 43.

T-102 was designed following the same method as T-101, discussed above. The operating pressure was calculated to be 30.4 psia. This was calculated assuming a condenser temperature of 45 °C. The partial vapor pressures for each component are summarized in *Table 9*.

Table 9: Data used to Determine Operating Pressure of T-102

Component	Mol %	Vapor Pressure at 55 °C (psia)	Weighted Vapor Pressure (psia)
DME	3.45%	188.5	6.50
MeOH	90.47%	9.96	9.01
Water	6.08%	2.28	.139
		Total	30.4

Once the operating pressure and temperature were determined, the Fenske and Underwood equation were solved to obtain the minimum number of stages and reflux ratio. The Fenske equation resulted in 4 stages required to obtain the desired separation.

$$N_{min} = \frac{log(\frac{LK_D}{HK_D} * \frac{HK_B}{LK_B})}{log(\alpha_{avg})}$$

Eq. 6

The compositions and relative volatilities of the components are summarized below in *Tables 10 and 11*.

Table 10: Data used for Determination of N_{min}						
K-Values and Relative Volatilities for Fenske Equation	Feed		Distillate		Bottom	
	T (K)	397.7	T (K)	52.28	T (K)	394.2
	P (Bar)	11.58	P (Bar)	2.36	P (Bar)	2.45
Component	MeOH	Water	MeOH	Water	MeOH	Water
K-Value	0.6392	0.2978	0.2571	0.1047	5.4	0.8421
Relative Volatility	2.146		2.456		6.413	
Average Volatility	**3.233**					

Table 11: Data used for Determination of N_{min}			
Fenske Equation	Molar Fraction		
	Distillate	Feed	Bottoms
MeOH	0.8006	0.631 1	0.0346
Water	0.0155	0.225 6	0.9654
N_{min}	**3.72**		
$N_{f,min}$	**2.49**		

After the minimum number of stages was determined, the minimum reflux ratio was calculated using the Underwood equation. The method for determining the minimum reflux ratio is summarized below.

$$F * (1 - q) = \sum_i \frac{F * \alpha_{i,HK} * z_i}{\alpha_{i,HK} + \varphi}$$

Eq. 7

Table 12: Data used for Determination of the Minimum Reflux Ratio						
Underwood Equation	Feed			Distillate		
	T(K)	397.7		T(K)	52.28	
	P(bar)	11.58		P(bar)	2.36	
Component	DME	MeOH	Water	DME	MeOH	Water
Mole Fraction	0.1433	0.6311	0.2256	0.184	0.8006	0.0155
K-Value	3.695	0.6392	0.2978	4.308	0.2571	0.1047
Relative Volatility	12.408	2.146	1.000	41.146	2.456	1.000
Single Term	456.711	3927.016	- 4383.726	547.412	4350.856	- 301.187
V_{feed}	0					
V_{min}	4597					
L_{min}	2345					
R_{min}	**0.51**					

The Underwood equation was solved with a value of $\varphi = 1.15$. This solution also satisfies the following criterion:

$$1 < \varphi = 1.15 < 41.1$$

Solving both the Fenske and Underwood equations results in a minimum number of stages of 4 and a minimum reflux ratio of .51. These values provide a starting point in determining the optimal tower parameters. The optimal number of stages was again determined by altering the number of stages and reporting the NPC for each configuration. The NPC was plotted as a function of number of stages, *Figure 4.*

Figure 4: T-101 Stages vs NPC
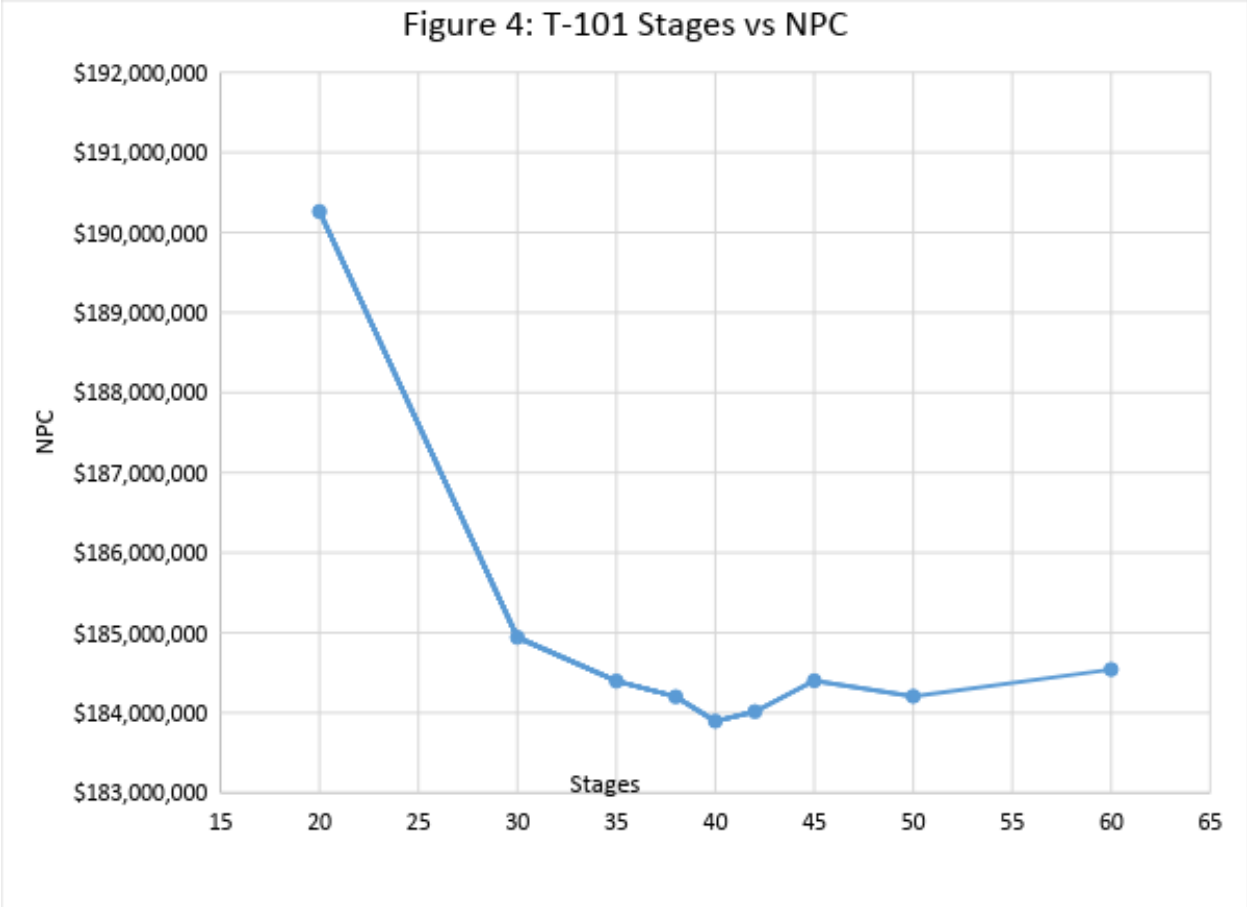
The optimal number of stages was determined to be 40 theoretical stages. This results in 50 actual stages with a stage efficiency of 80%. The 40 theoretical stage configuration results in an NPC of $183,895,827. The next tower parameter to be determined was the optimal feed location. The reflux ratio was reported at varying feed locations and plotted as a function of feed location, see *Figure 5*.

Figure 5: T-101 Feed Stage vs Reflux Ratio
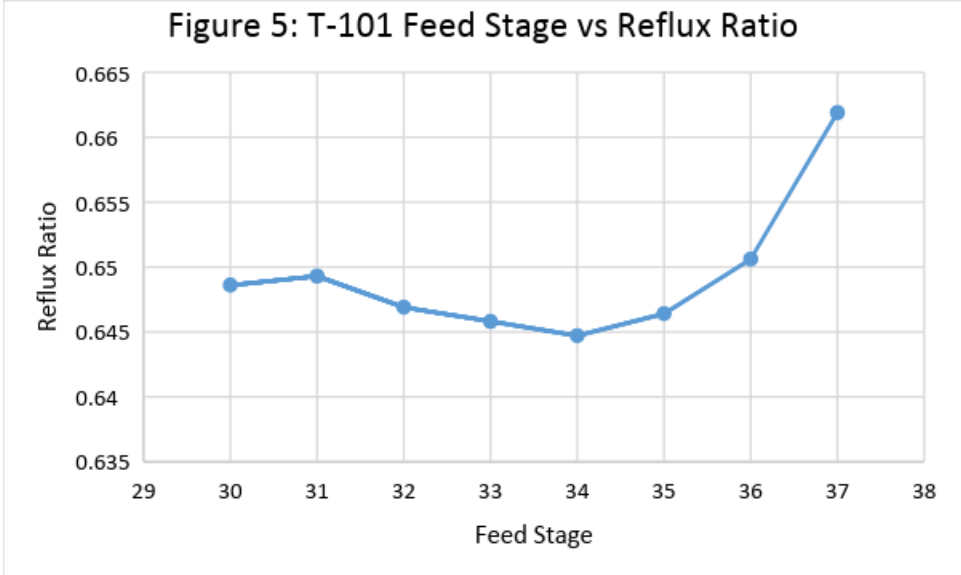
Placing the feed to T-102 above stage 34 resulted in a reflux ratio of .645. Taking tray efficiency into account, the feed to T-102 will be placed above stage 42.

T-102 Summary

T-102 was designed to operate at a pressure of 30.4 psia with 40 stages at a reflux ratio of .645. These tower parameters result in the lowest NPC throughout the project life. The tower results in a total installed cost of $1,441,452. We report the operating cost for delivering the duties to the condenser (E-104) and reboiler (E-105) in a later section.

Heat Exchanger Design

We determined the approximate heat transfer area required for the heat exchangers E-101, E-102, E-103, E-104, E-105, E-106, as well as, for the PBR R-101, based on the procedures outlined in the CRC Handbook of Thermal Engineering(X). Please see *Eq. 8.* Where, Q is the required duty, Uo is the overall heat transfer coefficient, F is the configuration correction factor and ΔLMTD is the counter-current log mean temperature difference.

$$Q = Uo*A*F*LMTD$$

Eq. 8

For each heat exchanger in this process, we obtained the required duty, Q, and the counter-current log mean temperature difference, ΔLMTD, from HYSYS output or by hand calculation. We assumed that the configuration correction factor, F to be 0.9 for every calculation, as the heat exchangers would likely have a mixed flow configuration (deviating from counter-current flow).

To obtain a reasonable estimate of the overall heat transfer coefficient, Uo, we assumed the heat transfer resistance due to conduction to be negligible (also known as the thin-walled assumption), reducing the overall heat transfer equation to *Eq. 9*. Where, hi is the inner (tube-side) convection coefficient, ho is the outer convection coefficient, Rfi is the inner fouling resistance, and Rfo is the outer fouling resistance. We used the data presented in Table 4.1.1: Typical Film Heat Transfer Coefficients for Shell-and-Tube Heat Exchangers contained in the CRC Handbook of Thermal Engineering, to obtain conservative estimates of convection coefficients and fouling resistances.

$$U_o = \frac{1}{\frac{1}{h_i} + R_{fi} + R_{fo} + \frac{1}{h_o}}$$

Eq. 9

We determined the ΔLMTD for E-102 and E-104, the tower condensers, as well as E-106, the bottoms product cooler, based on the assumption that cooling water would enter the heat

exchangers at 86°F and exit the exchanger at 95°F. This assumption allows for sufficient control of ∆LMTD, the driving force of heat transfer, by increasing or decreasing the flow rate of cooling water with our control strategy. It's important to note that the typical maximum return temperature of cooling water into the cooling water recovery system is 113°F, and was an important consideration in our design philosophy (Turton). We assumed that heat exchanger design based on a return temperature of 95°F was a good balance to maximize the design ∆LMTD and minimize the resulting calculated heat transfer area to reduce capital cost, while obtaining an acceptable operating flow rate of cooling water to mitigate operating costs.

We determined the ∆LMTD of E-103 and E-105, the tower reboilers, as well as E-101, the reactor preheater based on the assumption that high pressure steam will be supplied to the heat exchangers at 453°F and 436 psia. We note that a typical supply temperature and pressure of high pressure steam is 488°F at 610 psia (Turton). We assumed that heat exchanger design based on a steam temperature of 453°F would allow for a sufficient supply of heat energy to drive the process and allow operation and proper control over a large operating range. Our resulting ∆LMTD calculations are well above acceptable minimum heuristics due to the supply of this high-grade heat source, and also minimize the required heat exchanger surface area.

Pump Design

Since we found that the optimal operating pressure of R-101 was 235 psia (so that the MeOH remains in liquid phase and the DME bubbles out), we needed to ensure that P-101A/B and P-102A/B would supply the appropriate amount of pressure to *Stream 1* and *Stream 12 (*combining in *Stream 2)*, to overcome the pressure drop through E-101, R-101 as well as a change in elevation. We sized P-101A/B to supply a pressure of 261psia at a flow rate of 210 gal/min. Likewise, we sized P-102A/B to supply a pressure of 266psia at a flow rate of 157 gal/min. We chose a single stage centrifugal pump based on guidelines outlined in the GPSA Data Book.X

P-101A/B Feed Pumps

Identification	Item		Feed Pumps
	PFD Name		P-101 A/B
	No. Required		2
Function	Pump MeOH from storage tanks to process		
Operation	Continuous		
Type	Centrifugal		

	PFD notation	**Pump Design**	
Stream In	From Tanks		
Stream Out	1	Fluid Power	22.62 kW
		Material of Constr.	Cast Iron
Inlet Pressure (psia)	74.7		
Outlet Pressure (psia)	261		

Driver Design	Power		30.16
	Material of Constr.		Carbon Steel
	Type		Electric Explosion Proof

Annual Operating Cost			
	Power Consumed	30.16	kW/hr
	Cost of Electricity	0.0476	$/kW*hr
Purchase Cost	each		$2,941
Bare Module Cost	each		$22,517
Total Capital Cost			$45,034
Total Annual Operating Cost			$23,894
Comments			

E-101 Reactor Preheater

Identification	Item	Preheater
	PFD Name	E-101
	No. Required	1
Function	Preheat reactor feed stream	
Operation	Continuous	
Type	Shell and Tube	

	PFD notation	Tube Side	Shell Side
Stream In		2	1
Stream Out		3	18
Inlet Temp (F)		120	453.2
Outlet Temp (F)		284	453.2

Design Data	Surface Area (ft^2)	each	595
	Tube length	each	29.5
	LMTD (F)	each	242
	Material of Constr.	each	Carbon Steel

Annual Operating Cost		
High Pressure Steam		$3,297,749

Purchase Cost	each	$22,464
Bare Module Cost	each	$147,300
Total Capital Cost		$147,300
Total Annual Operating Cost		$3,297,749
Comments		

R-101 Packed Bed Reactor

Identification			
	Item		Packed Bed Reactor
	PFD Name		R-101
	No. Required		1
Function	Convert MeOH feed stream to DME		
Operation	Continuous		
Type	Packed Bed		

	PFD notation		
Stream In	3	Reactor Volume (ft^3)	1589
Stream Out	4	Reactor Length (ft)	29.5
Max Operating Temperature (°F)	327.6		
Design Temperature (°F)	284		

Stream	Feed	Products	Catalyst Information	
PFD Notation	3	4	Type	High Acid Resin
			Diameter (in)	2.73E-03
Mol% DME	0.0130	0.2921	Bulk Density (lb/ft^3)	37.59
Mol% MeOH	0.9406	0.3823	Weight (lb)	59730
Mol% Water	0.0464	0.3256	Cost	$902,400

Annual Operating Cost	
Cooling Water	$35,338

Purchase Cost	each	$17,088
Bare Module Cost	each	$196,506

Total Capital Cost	$196,506
Total Annual Operating Cost	$35,338

Comments	The high acid resin catalyst has a lifespan of ~10 years. New catalyst need only be purchased every ~10 years

T-101 DME Splitter

Identification	Item			DME Splitter
	PFD Name			T-101
	No. Required			1
	Achieve desired separation of components			
Operation	Continuous			
Type	Tray - Seive			
Stream	Feed	Top		Bottom
PFD notation	**4**	**6**		**10**
Mol% DME	0.2900	1.0000		0.0200
Mol% MeOH	0.3800	0.0000		0.5300
Mol% Water	0.3300	0.0000		0.4500
Design Data	Height, ft			40
	# of Trays			10
	Tray Spacing ft			2.3
	Material of			
	Constr.			Carbon Steel
Annual Operating Cost				
N/A			N/A	
Purchase Cost				$42,699
Bare Module Cost				$1,414,432
Total Capital Cost				$1,414,432
Total Annual Operating Cost				N/A
Comments				

E-102: T-101 Condenser

Identification		Item	Condensor
		PFD Name	E-102
		No. Required	1
Function		Condenses remaining vapors in the overhead stream	
Operation		Continuous	
Type		Floating Head, shell and tube	

	PFD notation	Tube Side	Shell Side
Stream In		1	5
Stream Out		22	7
Inlet Temp (F)		86	134
Outlet Temp (F)		95	133

Design Data	Surface Area (ft^2)	4510
	Tube length	20
	LMTD (F)	42.8
	Material of Constr.	Carbon Steel

Annual Operating Cost	
Cooling Water	$233,236

Purchase Cost	$77,504
Bare Module Cost	$439,870
Total Capital Cost	$439,870
Total Annual Operating Cost	$233,236
Comments	

E-103: T-101 Reboiler

Identification	Item		Reboiler
	PFD Name		E-103
	No. Required		1
Function	Boils the bottom stream of the column		
Operation	Continuous		
Type	Kettle Reboiler		

	PFD notation	**Tube Side**	**Shell Side**
Stream In		1	8
Stream Out		19	9
Inlet Temp (F)		453.2	297
Outlet Temp (F)		453.2	307

Design Data	Surface Area (ft^2)	each	216
	Tube length	each	20
	LMTD (F)	each	151
	Material of Constr.	each	Carbon Steel

Annual Operating Cost		
High Pressure Steam		$2,892,600

Purchase Cost	**each**	$28,096
Bare Module Cost	**each**	$309,178
Total Capital Cost		$309,178
Total Annual Operating Cost		$2,892,600
Comments		

T-102 MeOH Splitter

Identification	Item			MeOH Splitter
	PFD Name			T-102
	No. Required			1
Function	Achieve desired separation of components			
Operation	Continuous			
Type	Tray - Seive			
Stream	Feed	Top		Bottom
PFD notation	**10**	**11**		**16**
Mol% DME	0.0200	0.0318		0.0000
Mol% MeOH	0.5300	0.9052		0.0300
Mol% Water	0.4500	0.0631		0.9700
Design Data	Height, ft			110
	# of Trays			40
	Tray Spacing ft			2
	Material of			
	Constr.			Carbon Steel
Annual Operating Cost				
	N/A		N/A	
Purchase Cost			$92,026	
Bare Module Cost			$1,441,452	
Total Capital Cost			$1,441,452	
Total Annual Operating Cost			N/A	
Comments				

E-104: T-102 Condenser

Identification		Item	Condenser
		PFD Name	E-104
		No. Required	1
Function		Condenses remaining vapors in the overhead stream	
Operation		Continuous	
Type		Floating Head, shell and tube	
	PFD notation	**Tube Side**	**Shell Side**
Stream In		1	11
Stream Out		23	13
Inlet Temp (F)		86	192
Outlet Temp (F)		95	179
Design Data		Surface Area (ft^2)	17067
		Tube length	20
		LMTD (F)	95
		Material of Constr.	Carbon Steel
Annual Operating Cost			
	Cooling Water		$399,096
Purchase Cost			$256,461
Bare Module Cost			$1,420,967
Total Capital Cost			$1,420,967
Total Annual Operating Cost			$399,096
Comments		Due to the surface area exceeding the limit for the costing method, we recommend purchasing two condensers.	

P-102A/B Recycle Pumps

Identification	Item		Recycle Pumps
	PFD Name		P-102 A/B
	No. Required		2
Function	Pump MeOH recycle stream		
Operation	Continuous		
Type	Centrifugal		

	PFD notation	**Pump Design**	
Stream In	13		
Stream Out	12	Fluid Power	21.16 kW
		Material of Constr.	Cast Iron
Inlet Pressure (psia)	34.23		
Outlet Pressure (psia)	235		

Driver Design	Power		28.21
	Material of Constr.		Carbon Steel
	Type		Electric Explosion Proof

Annual Operating Cost		
Power Consumed	28.21	kW/hr
Cost of Electricity	0.0476	$/kW*hr

Purchase Cost	each	$2,930
Bare Module Cost	each	$22,540
Total Capital Cost		$45,080
Total Annual Operating Cost		$22,352
Comments		

E-105: T-102 Reboiler

Identification	Item	Reboiler
	PFD Name	E-105
	No. Required	1
Function	Boils the bottom stream of the column	
Operation	Continuous	
Type	Kettle Reboiler	

	PFD notation	Tube Side	Shell Side
Stream In		1	14
Stream Out		20	15
Inlet Temp (F)		453.2	238
Outlet Temp (F)		453.2	254.5

Design Data	Surface Area (ft^2)	each	296
	Tube length	each	20
	LMTD (F)	each	206.9
	Material of Constr.	each	Carbon Steel

Annual Operating Cost		
	High Pressure Steam	$5,427,825

Purchase Cost	each	$33,442
Bare Module Cost	each	$368,012
Total Capital Cost		$368,012
Total Annual Operating Cost		$5,427,825
Comments		

29

E-106 Waste Water Cooler

Identification		Item	Heat Exchanger
		PFD Name	E-106
		No. Required	1
Function		Cool waste water stream	
Operation		Continuous	
Type		Floating Head, shell and tube	

	PFD notation	Tube Side	Shell Side
Stream In		1	16
Stream Out		24	17
Inlet Temp (F)		86	255
Outlet Temp (F)		95	113

Design Data		Surface Area (ft^2)	223
		Tube length	20
		LMTD (F)	74.7
		Material of Constr.	Carbon Steel

Annual Operating Cost		
Cooling Water		$23,226

| Purchase Cost		$15,885
Bare Module Cost		$96,902
Total Capital Cost		$96,902
Total Annual Operating Cost		$23,226
Comments		

Necessary Fixed Capital Investment Summary

Table 13: Necessary Fixed Capital Investment Summary

Unit	Capital Cost ($)
P-101A/B: Feed Pump x2	$ 22,500
P-102A/B: MeOH Recycle Pump x2	$ 22,500
E-101: Reactor Preheater	$ 147,000
R-101: Water Cooled PBR	$ 1,100,000
T-101: DME Splitter	$ 1,410,000
E-102: T-101 Condenser	$ 439,000
E-103: T-101 Reboiler	$ 309,000
T-102: MeOH Splitter	$ 1,440,000
E-104: T-102 Condenser	$ 1,420,000
E-105: T-102 Reboiler	$ 368,000
E-106: Bottoms Cooler	$ 96,900
MeOH Storage Tanks x2	$ 3,350,000
DME Storage Tanks x2	$ 9,980,000
Pricing Method	CAPCOST
Total Capital Costs (2018)	$ 20,200,000

Figure 6: Relative Capital Costs of Components
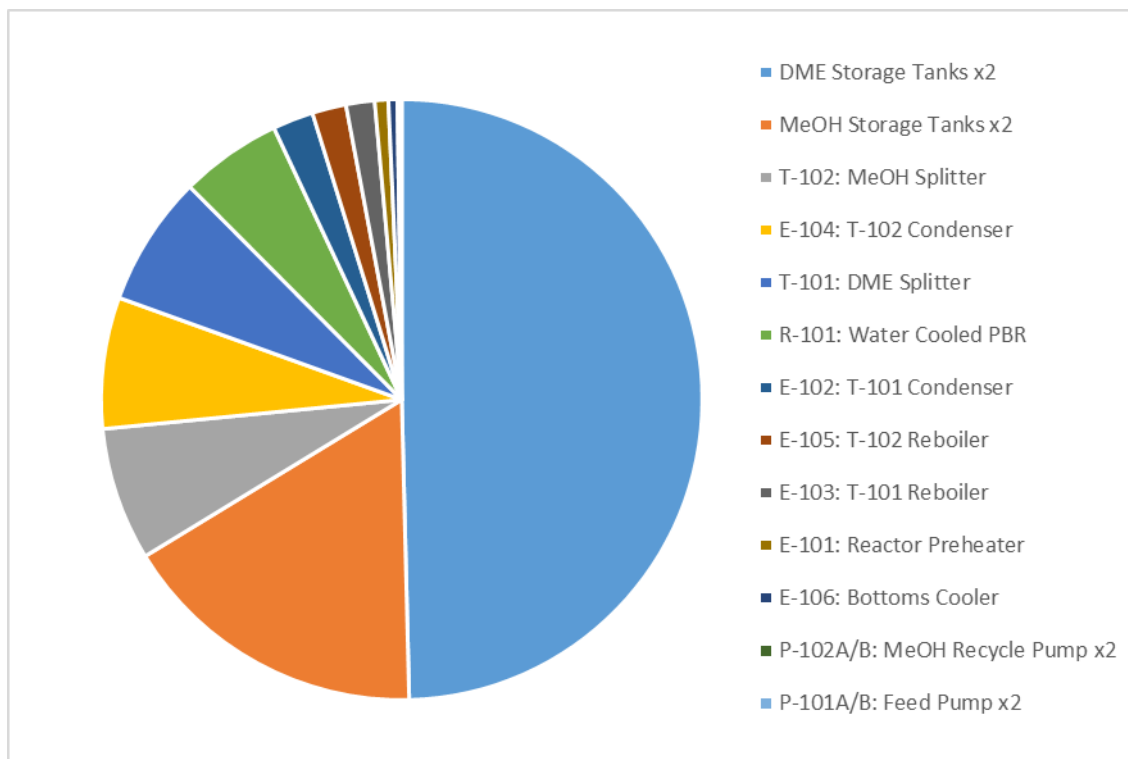
Safety, Health, and Environmental Considerations

The constant production of DME for sales is the primary driving force for the success of this project. With that in mind, the following safety and preventative measures were taken to ensure the well-being of the operators, and to reduce the risk of an incident:

Operator Training: The operators must be given the proper training on both the process controls system and how to identify hazards associated with the process. The process controls system, put in place to ensure production specs are met, is also an instrument to avoid incidents. Operators must have a working knowledge of each aspect of the controls system and how to identify hazards. Pressure in T-101 and T-102, as well as temperatures in the condensers and reboilers of each tower, must be monitored to ensure an incident does not occur.

Knowledge of Hazards: The operators must be given proper training on the hazards associated with materials in this process. Methanol and DME are both flammable and toxic. Any loss of containment could cause serious health problems for the operators in the vicinity. In the case of loss of containment, proper firefighting and first aid techniques must be followed.

Equipment Specific Considerations

R-101: The largest hazard associated with R-101 is the temperature and pressure of the inlet and outlet streams. Although the streams are not considered high temperature or pressure, a loss of containment could cause health problems for those in the immediate area. The other hazard present is a loss of cooling water flow rate. Should this occur, the temperature in R-101 would rise uncontrolled, leading to several problems. The first problem is the degradation of the high acid resin catalyst. At temperatures above 150 °C, the catalyst starts to degrade, leading to a lower conversion of MeOH. The other problem is an increase in pressure. If the flow of cooling water is lost, a higher production rate of gaseous DME would increase pressure, leading to a possible loss of containment.

T-101 and T-102: T-101 and T-102 do not have many hazards in this process. The corrosive nature of MeOH could lead to reduced separation in both T-101 and T-102. With this in mind, the condition of the trays in both towers must be monitored to ensure the desired separation is met in each column.

Pumps: Pumps must be placed in a well-ventilated, spacious area to avoid intake of vapors, and to prevent explosions. The pumps must not be allowed to run dry, as this would damage the pump and lead to possible health issues. Suction and discharge hoses for each pump must be positioned so that they are not damaged in any way.

Condensers and Reboilers: The temperature of the reboilers must be monitored to ensure the desired separation of the components. Likewise, the pressure of the condensers must also be monitored for the same reason. Should either the temperature of the reboilers or the pressures of the condensers differ significantly from the design specs, only a loss of production would occur.

Environmental Concerns:

We do not expect any significant environmental effects will occur during this process. Only loss of containment in any of the streams would lead to environmental effects. Should loss of containment occur, MeOH, DME and water would all be exposed to the atmosphere. The MeOH in the atmosphere would result in the creation of CO_2 in the atmosphere, leading to an increase in global warming.

Economic Analysis

We estimated the capital cost of our conventional liquid phase reaction process according to the CAPCOST program. We estimated all equipment costs using the Engineering Plant Cost Index (CPECI) of 391 in 2001. We used a 2017 CEPCI of 566.6 to account for current equipment costs relative to 2001. We note that the use of the CEPCI Index to account for inflation beyond a time period of 5-years is generally not recommended as this is likely to be inaccurate. Moreover, we acknowledge that our confidence in the following economic conclusions is limited. We would prefer the obtainment of vendor quotes to properly conduct an economic analysis. However, due to lack of data we proceeded in this manner.

Utility and Operating Costs

Table 14: List of Utility costs and Operating costs

| Utility		Annual Costs
P-101A/B: Feed Pump *Electricity*	$	11,900
P-102A/B: MeOH Recycle Pump *Electricity*	$	11,100
E-101: Reactor Preheater *HP Steam*	$	3,290,000
R-101: PBR *Cooling Water*	$	35,300
E-102: T-101 Condenser *Cooling Water*	$	233,000
E-103: T-101 Reboiler *HP Steam*	$	2,890,000
E-104: T-102 Condenser *Cooling Water*	$	399,000
E-105: T-102 Reboiler *HP Steam*	$	5,430,000
E-106: Bottoms Waste *Cooling Water*	$	23,200
Other Operating Costs		
MeOH Transportation	$	2,270,000
Additive Total Cost	$	760,000
Waste Water Treatment	$	5,720
Operating Labor	$	775,000
Annual Utilities Cost	$	15,400,000
Annual Utilities Cost (2018)	$	19,200,000
		w/ 25% Contingency
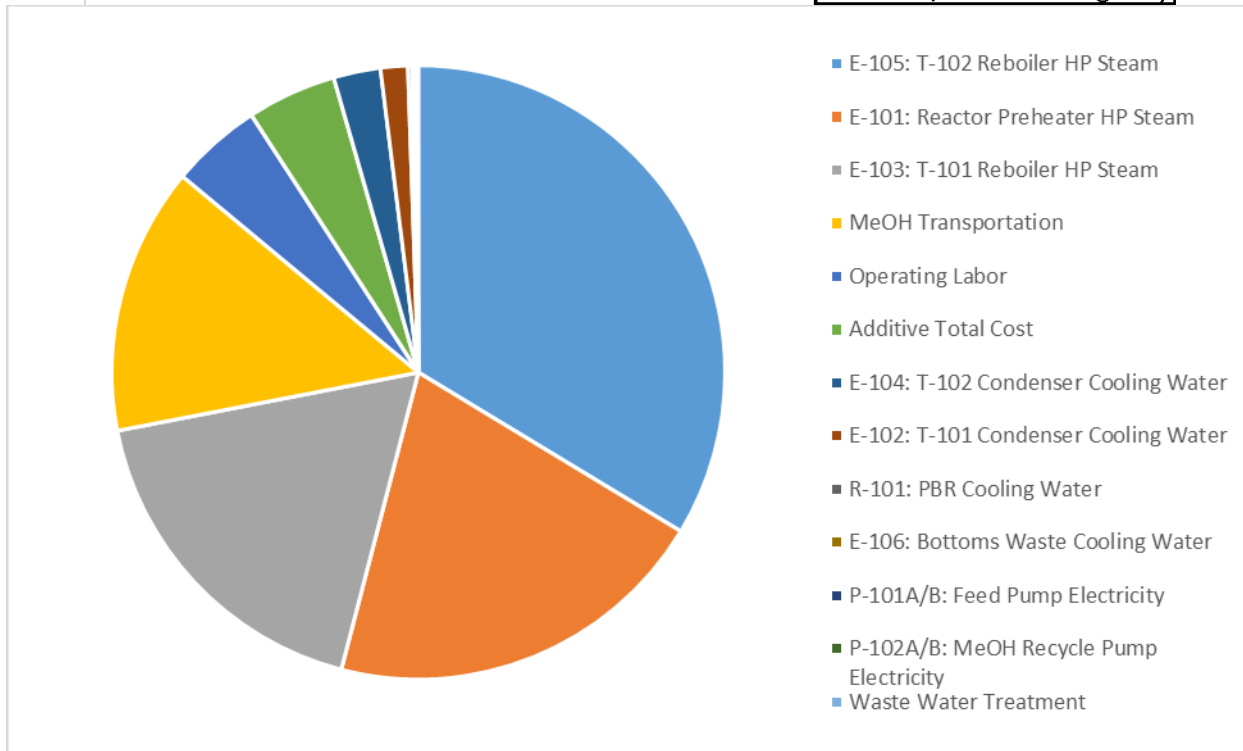
Figure 7: A Pie graph that shows the distribution of operating costs from highest to lowest cost.

We assumed that all utilities used, including high pressure steam, cooling water, and electricity, will be provided on site, at the rates outlined by *Turton et. al.* To determine NPV and ROR, we assumed that the operation costs would remain constant through the life of the project.

Other operating costs we considered include, MeOH transport, the cost of the lubricant additive to DME fuel product, waste water treatment, and labor costs. The lubrication additive cost was provided as $1.65/lb at a concentration of 900 ppm. We determined that 460,000 lb/year of the lubrication additive is needed. The waste water treatment is based on a volumetric flow rate out of the bottom of the methanol tower of 11.7 m^3/hr, y using a correlation generated by Alkhayat and Gerrard(X). We assumed that this process would require 13 employees working 8 hour shifts, 245 shifts a year.

Working capital was assumed to be 20% of total depreciable capital for project start up liability in the first year.

Figure 8: Cumulative cash position diagram: NPV per by year for the project life. We illustrate that the payback period is from 2018 to 2020
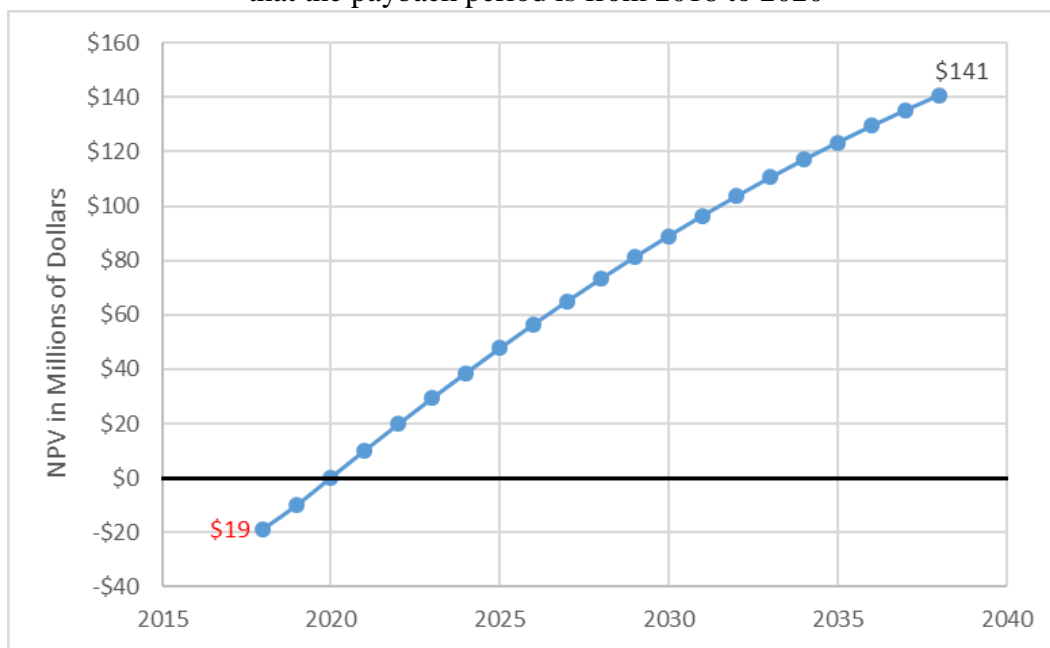

In the initial year, this project requires an investment of approximately $20 million. We predict the process will generate a revenue stream of more than $200 million each year. *Figure 8* illustrates that the payback period will end on the second year of operation, in 2020. After 2020 this process would generate a net positive cash flow throughout the project's 20 year life with a NPV of $140 million.

The revenue stream, is dependent on the market price of DME. There is minimal pricing information for DME and as a result we estimate the projected market value over the future 20 year project life based on the gasoline market trend over the past 30 years. As reported by the,

International DME Association, it's reasonable to estimate the value of DME to be 75%-90% the market price of gasoline.

Figure 9: Estimated Market Price of DME over the past 30 years. The high, medium and low linear regressions correspond to the predicted market value of DME, based on the assumption that DME was valued at 90%, 83% and 75% of the market value of gasoline, respectively.
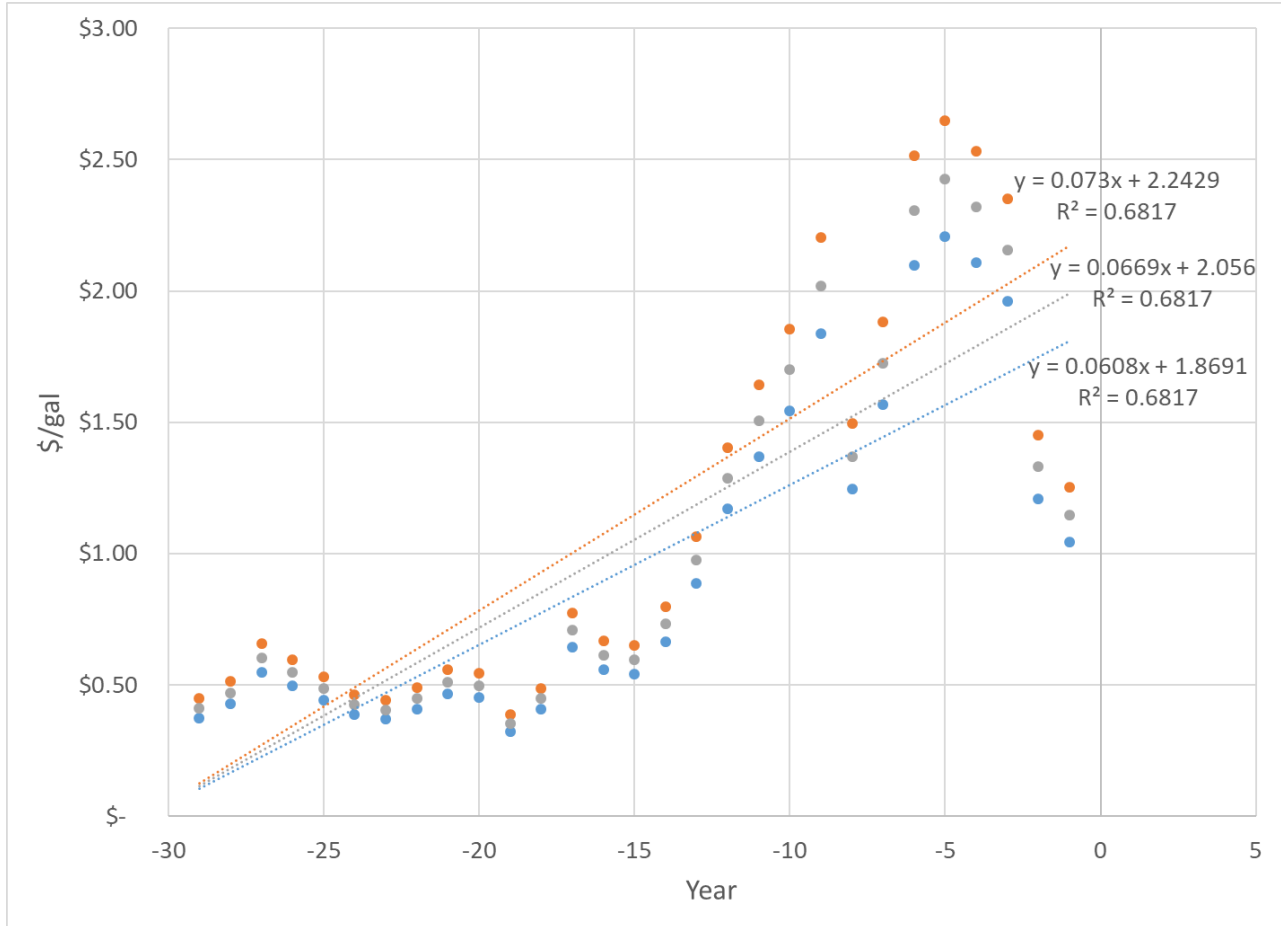
We took the data provided in *Figure 9* to predict the future market value trend of DME over the 20 year project life. We selected the trend line which represents 83% of the market value of gasoline over the past 30 years and assumed that the market value of DME will follow this trend. For example, we assume that the average price of DME in 2019 will be $2.32 and will increase approximately $0.06/year.

We performed a similar analysis to estimate the market value of MeOH, which will be needed for this process as feed material. We obtained MeOH price data from *Methanex Monthly Average Regional Posted Contract Price History*, took an average trend line as shown in *Figure 10* and extrapolated it to determine future sales price. We assume that the market value of MeOH will be $1.53 in 2019 and will increase approximately $0.04/year.

Figure 10: MeOH average price Per Year from 2000 to present, with an average trend plot.
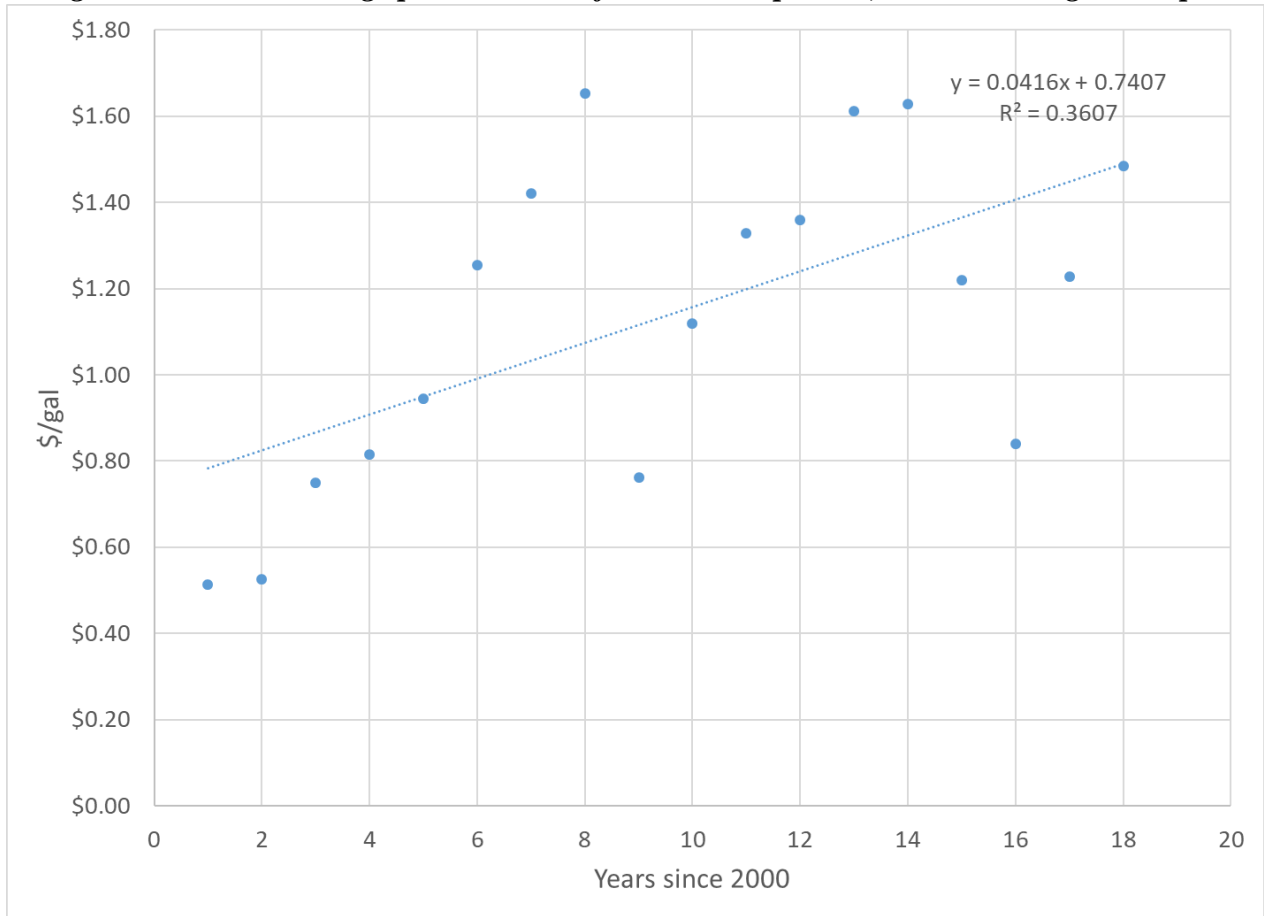
We observe that the past market values of MeOH and estimated market values of DME have fluctuated over the past 20 to 30 years. To analyze the effect of different market conditions on the economics of this project, we performed a sensitivity analysis. We chose the minimum and maximum values relative to the average trend line calculated the percent difference from the trend line and incorporated this into our sensitivity analysis. We also determined the effect of a 10% fluctuation in our estimated capital and operating costs.

Figure 11 below indicates that fluctuations of 10% could have a large impact on the return on investment. For example a market high for MeOH could cause a loss on investment. If this happens a syngas process could be devised were a hydrogen and carbon monoxide gas are used to produce methanol. For this process however the gas phase kinetics in a plug flow reactor might be favored as the MeOH produced in this way would already be in gas phase and would require an extra condensation step to be processed in the packed bed reactor.

Figure 11: Sensitivity Analysis: The effect of fluctuations in the market price of MeOH, DME, as well as, fluctuations from our estimated operating and capital costs on the rate of return of this project.
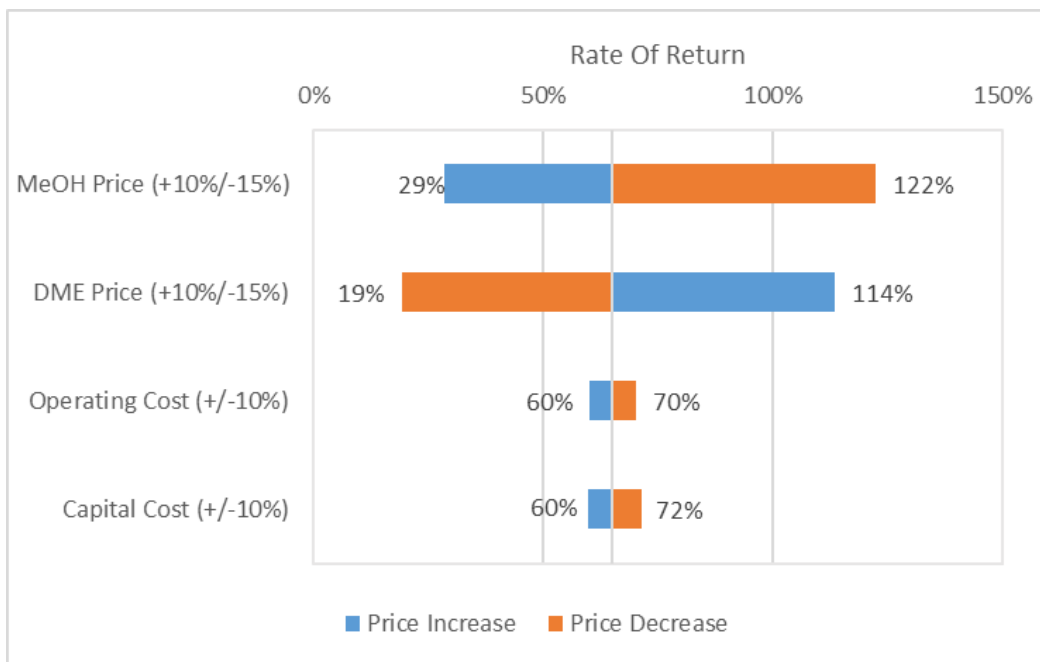
Figures 12 and 13 compares the ROR of our proposed process (based on the *Amberlyst 35* catalyst), with a process we simulated and analyzed based around the use of gamma-aluminum-oxide (a heterogeneous catalyst with MeOH reacting in the gas phase), as well as an reactive distillation process we explored utilizing Amberlyst 35. We observe that the ROR's and NPV's of the vapor phase and liquid phase processes are similar. We chose not to recommend the vapor phase process within the context of this project, mainly, because a PBR with gamma-aluminum-oxide catalyst would require servicing and replacing the catalyst every 9-12 months. We perceived that this would be inconvenient. Interestingly, based on our estimation data, the reactive distillation process seems to be the superior option to meet the design basis. We summarize our work in considering a reactive distillation process in the next section.

Figure 12: A comparison of RORs for the liquid phase reaction process, vapor phase reaction process, and the reactive distillation process.
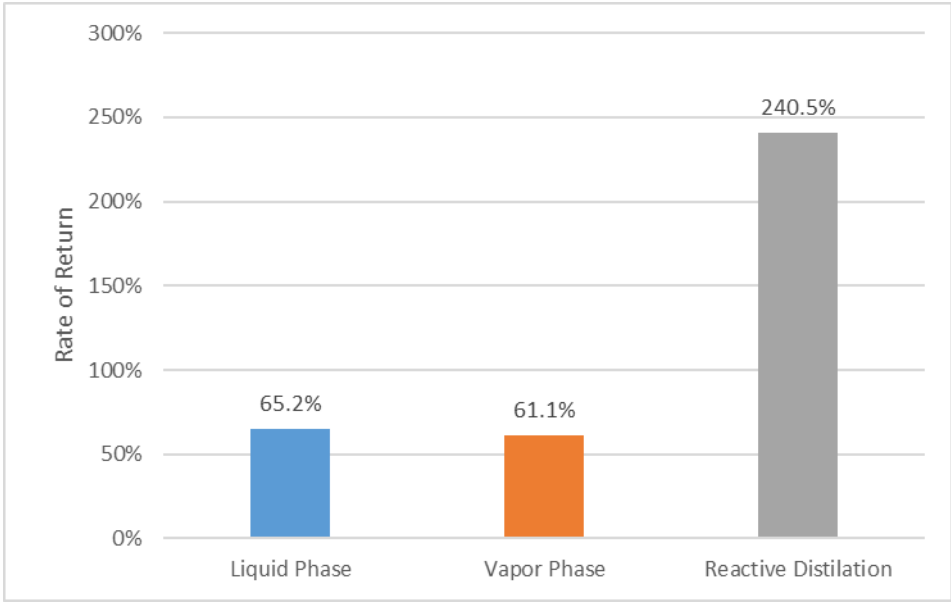

Figure 13: A comparison of NPVs for the liquid phase reaction process, vapor phase reaction process, and the reactive distillation process.
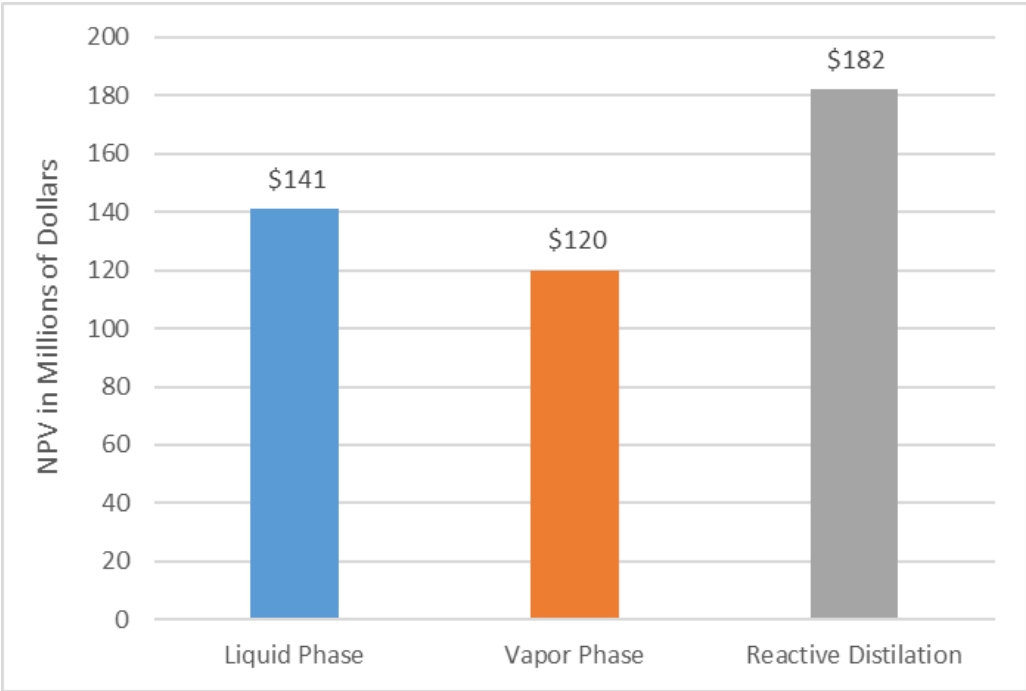
From a side by side comparison of capital cost and operating cost in *Figure 14* we can clearly see where the advantages and disadvantages are in each design. The vapor phase reaction favors a high operating cost because it needs a lot of energy from the preheater to be vaporized before entering the plug flow reactor. This results in the very high annual operating cost as seen in *Figure 15*. However the kinetics of the gas phase reaction allows for better conversion of MeOH into DME in the plug flow reactor. This allows for more efficient and smaller distillation towers, condensers and reboilers as seen in *Figure 15*.

Figure 15: Capital Cost   Operating Cost
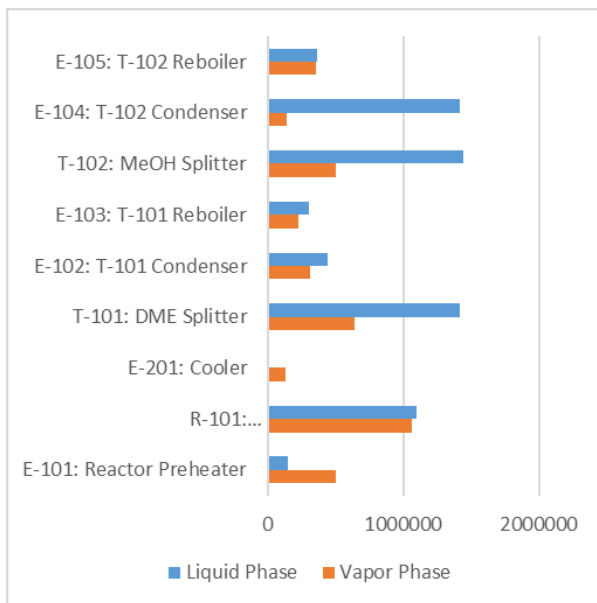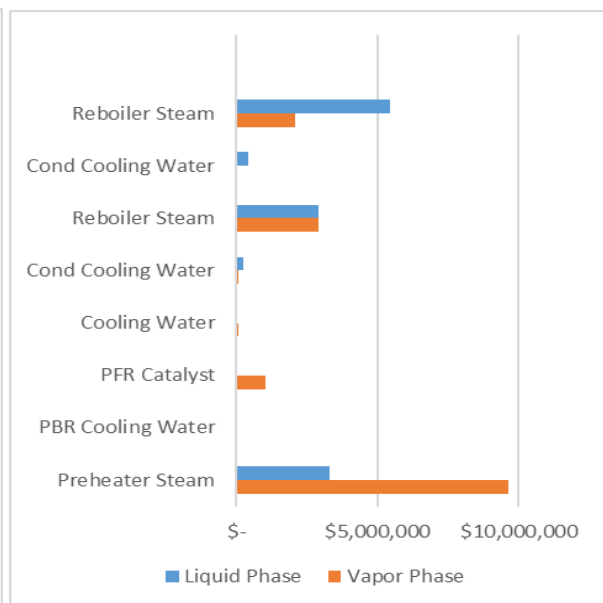
To decide between two mutually exclusive projects the NPV that is great is the one to be considered further. The liquid phase reaction has both higher NPV and ROR. Because the liquid phase reaction has a lower initial capital cost it is likely to keep its economic attractiveness as NPV weights money on hand higher than money in the future.

An Exploration of Reactive Distillation to meet the Design Basis

The DME reactive distillation column is a single feed system with a methanol stream fed to stage 10 at the top of the reactive zone. The methanol stream is 99.85 mass% methanol and 0.0015 mass% water. The column has 8 stripping stages (including the condenser), 22 packed reactive stages, and 9 rectifying stages (including the reboiler). A simple process flow diagram (PFD) can be seen in Appendix. The column operates at a pressure of 139.1 psia and with a reflux ratio of 2.0. The catalyst holdup on each reactive tray is 66.8 lbm. This corresponds to a total holdup of 1469.6 lbm in the column. The steady-state conditions and design parameters for the optimum design case is summarized in *Table 15*. The operating performance for the optimum design is given in *Table 16.*

Table 16: Steady-State Conditions and Design Parameters for Optimum Case

Fresh feed flowrate of MeOH (mol/s)	308.2
Distillate flowrate (mol/s)	154.3
Bottoms flowrate (mol/s)	154.3
Vapor boilup (mol/s)	242.0
Reflux flowrate (mol/s)	308.7
Stripping trays	8
Reactive trays	22
Intermediate trays	21
Rectifying trays	7
Tower height (ft)	175
Tower diameter (ft)	6.56
Liquid holdup on reactive trays (lbm)	1469.6
Pressure (psia)	139.1

Table 16: Operating Performance for Optimum Case

DME product purity (mass%)	98.59
Distillate flowrate (US-gal/day)	255,806
Total methanol conversion (%)	98.14
Water purity at the bottom (mass%)	97.00
Heat duty (kW)	
Condenser	-8417.3
Reboiler	8929.3
Pump duty (kW)	

Feed	35
Distillate	10
Bottoms	10

Conventionally, dimethyl-ether has been synthesized in a similar manner to the process presented. This process contains its own reaction sections and separation sections. Each section contains their respective vessels and equipment, and are linked together by energy material streams. An alternative to the conventional chemical plant design is to apply reactive distillation. In this process unit, separation and synthesis of dimethyl-ether occur simultaneously. The result from applying this innovative technology should be reduced equipment cost as well as a reduction in operating expenses.

Reactive distillation technology should, in theory, improve the reaction chemistry with respect to the equilibrium behavior. In the particular reaction of methanol decomposition, our reactant, methanol, is charged simultaneously. The product, dimethyl ether, vaporizes and is continuously withdrawn from the reaction zone. Water forms at the same rate as dimethyl ether, but due to its polar characteristics will compete with methanol for reaction sites. As water escapes from the bottom of a reactive stage and dimethyl ether from the top, the reaction equilibrium shifts toward the right which increases the conversion of methanol. Reactive distillation aims to convert virtually all the reactants entering the column. As the conversion increases, the operating costs (mainly the cost of cooling water and steam) will also increase significantly. This is why it is important to design an optimum which meets the specification without exceeding the necessary operating requirements.

The reaction kinetic parameters that were used to develop and model the designed column are given in *Table 17*. These parameters fit into Eq.10 , which is the reaction rate used to describe the amount of dimethyl ether produced. This reaction rate was developed by *Hosseininejad et al.* Data given in the AIChE design problem statement is comparable to the data described by this independent study. However, it was concluded that Eq. 10 was more applicable and more easily programmed for the development of our simulation model, which is presented later. It should also be noted that since we are removing products from the reaction zone, and DME is formed as a gas, equilibrium behavior is significantly diminished, the reverse reaction is not considered as concluded by *An et al.* The catalyst that is used for this reaction is Amberlyst 35, which is the same catalyst utilized in the presented conventional liquid process design.

$$r_{DME}[\frac{kmol}{kgcat \cdot s}] = \frac{1}{(\frac{1}{\sqrt{k_s}} + \frac{1}{\sqrt{k_s}} \frac{K_W}{K_M} \frac{C_W}{C_M})^2} \qquad \text{Eq. 10}$$

Methanol decomposing into water and dimethyl ether is an exothermic reaction, hence the negative heat of reaction value. The reactive distillation design uses this to its advantage. The more exothermic the reaction, the less the energy input has to be to maintain product specifications.

Table 17: Kinetic and Vapor-Liquid Equilibrium Parameters

Catalyst	Amberlyst 35
Activation energy, E (kJ/kgmol)	
Forward	98000.
Heat of reaction (kJ/kgmol)	-11712.0
Molecular weights (B/A/C) (g/mol)	46.07/32.04/18.02
k_0 (kmol/kgcat·s)	6.12×10^7
k_s	$k_0 exp\left(\frac{-E}{RT}\right)$
K_W/K_M	$exp\left(-6.46 + \frac{2964}{T}\right)$
Maximum temperature, °C	150

Reactive distillation is only applicable and economically attractive for when certain chemical conditions exist. For it to work, dimethyl ether must be removed by distilling it from water and any remaining methanol. In terms of the relative volatilities of the three components, dimethyl ether is the lightest product and water is the heaviest. This places methanol as an intermediate between the two. We can also make the comparison based on the vapor pressures of each component at a given temperature.

$$\alpha_{DME} > \alpha_{MEOH} > \alpha_{H2O}$$

Considering that dimethyl ether and water are products from the reaction and also defined as the discharged products from the process, reactive distillation is a favorable method for dimethyl ether production. According to the boiling point ranking, the components can be identified as light key (LK), intermediate key (IK), and heavy key (HK). In this case the reaction would be as follows:

$$IK \rightarrow LK + HK$$

This ranking is extremely important and has a significant impact on the way the process is configured and designed. The present design places the reactive zone in the middle of the column so that the light key component (DME) and the heavy key component (H_2O) can be removed from the top and bottom of the column, respectively. Designing the column this way allows the methanol concentration to remain high in the reactive zone.

The reactive catalytic distillation process for kinetically-controlled dimethyl ether production was modelled in ASPEN Plus (V9.0). However, trying to simulate the reactive distillation column using the standard ASPEN Plus model has significant issues. One of the main issues was that the reaction rate, when applied to reactive distillation, is limited to a power law model. To overcome this issue, a user kinetic subroutine was developed to model the rate expression as a Langmuir-Hinshelwood reaction. The kinetic subroutine was built using a template provided by ASPEN Technology and examples provided by *Luyben et al. and Segovia-Hernandez et al.* The user subroutine used to model the optimum reactive distillation design is presented in *Appendix B.* Results from the simulation that utilized the user supplied kinetic subroutine are represented visually in *Figures 16-22.*
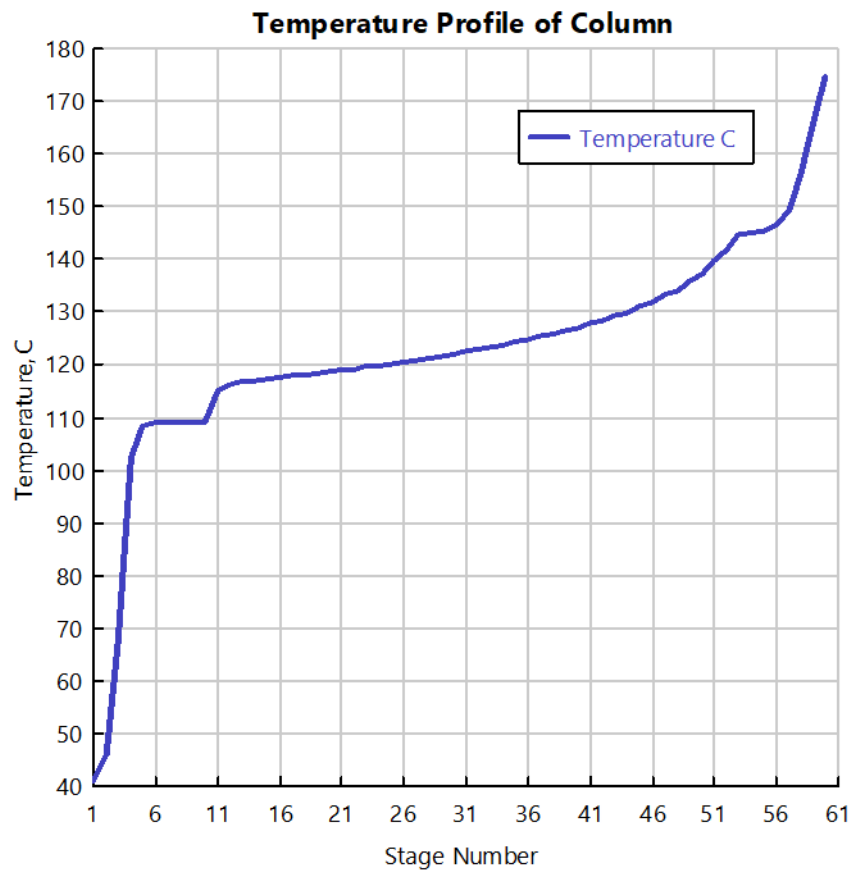
Figure 16: Temperature profile of DME reactive distillation column
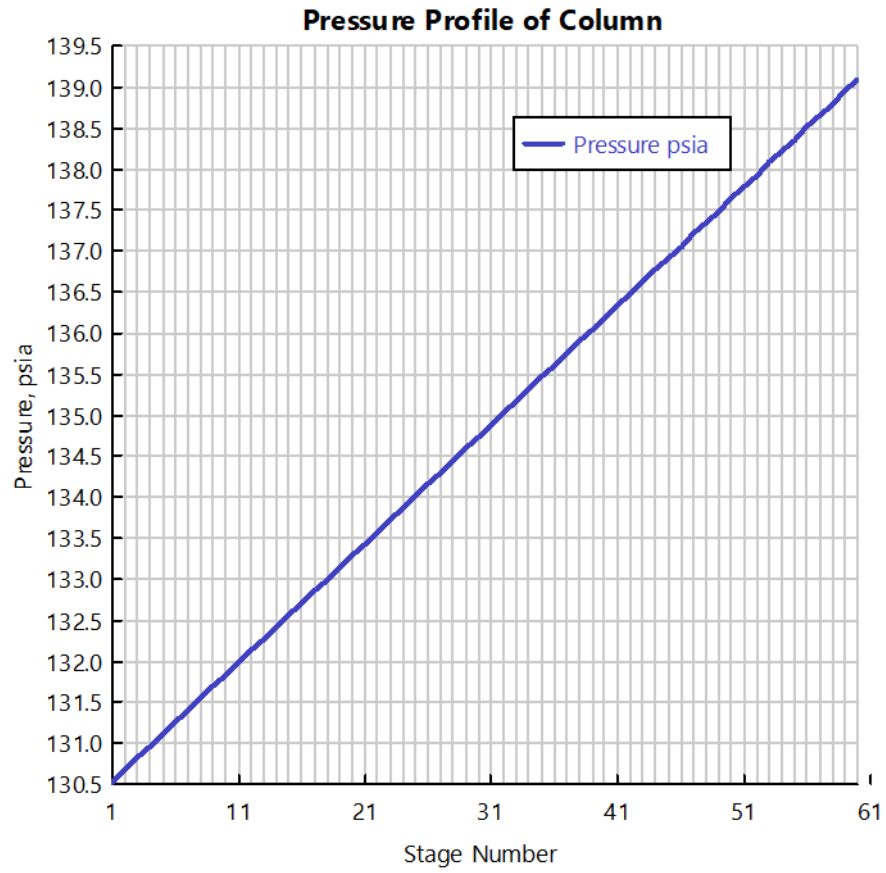
Figure 17: Pressure profile of DME reactive distillation column
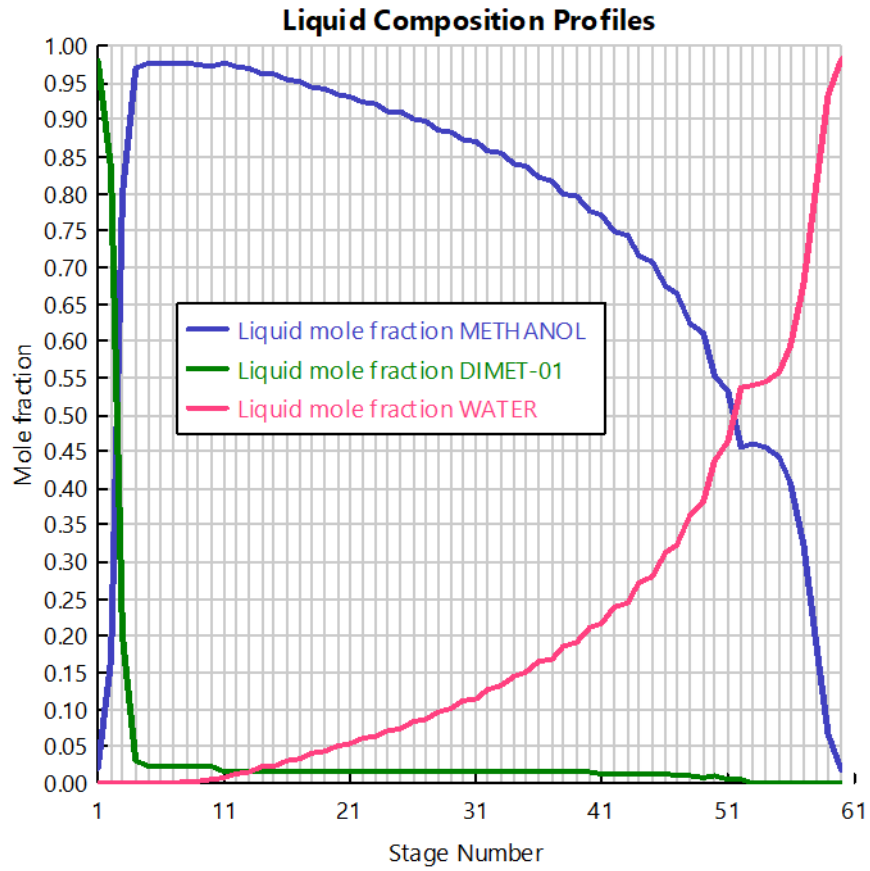
Figure 18: Liquid composition profile of DME reactive distillation column
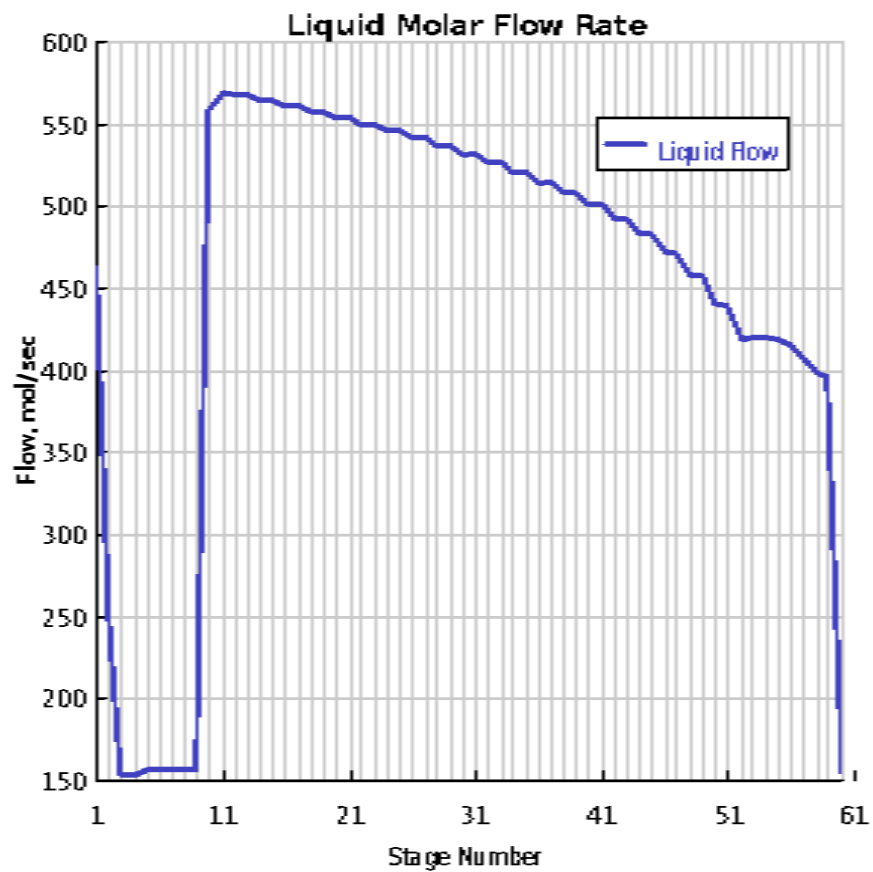
Figure 19: Liquid molar flow in DME reactive distillation column
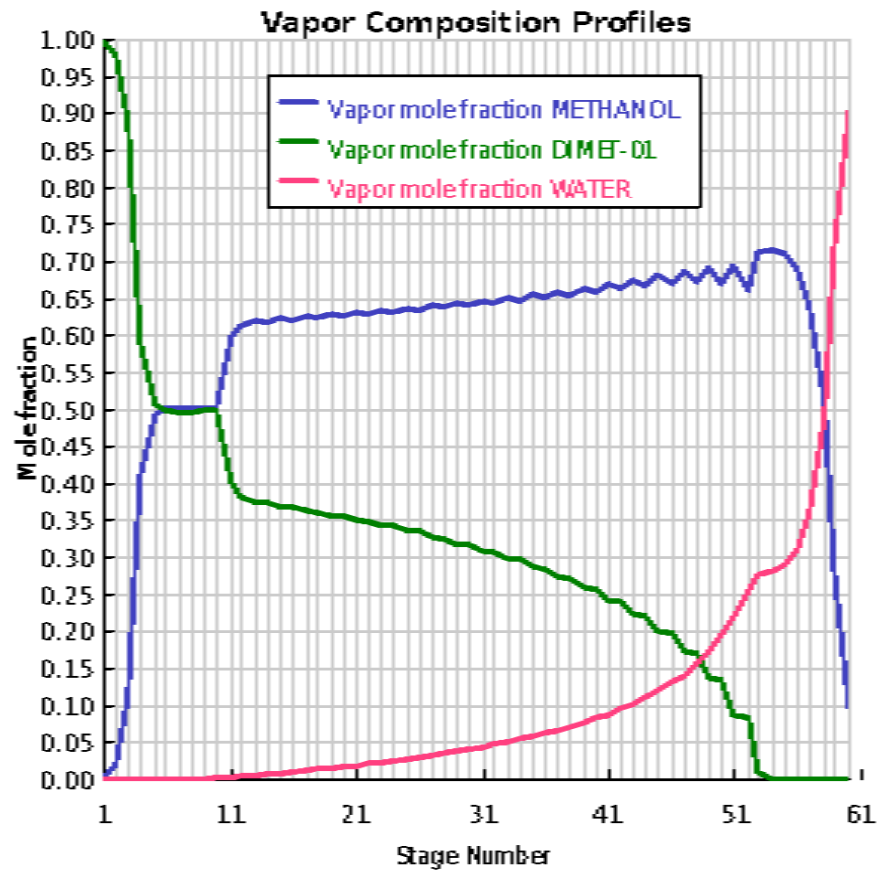
Figure 20: Vapor composition profiles in DME reactive distillation column
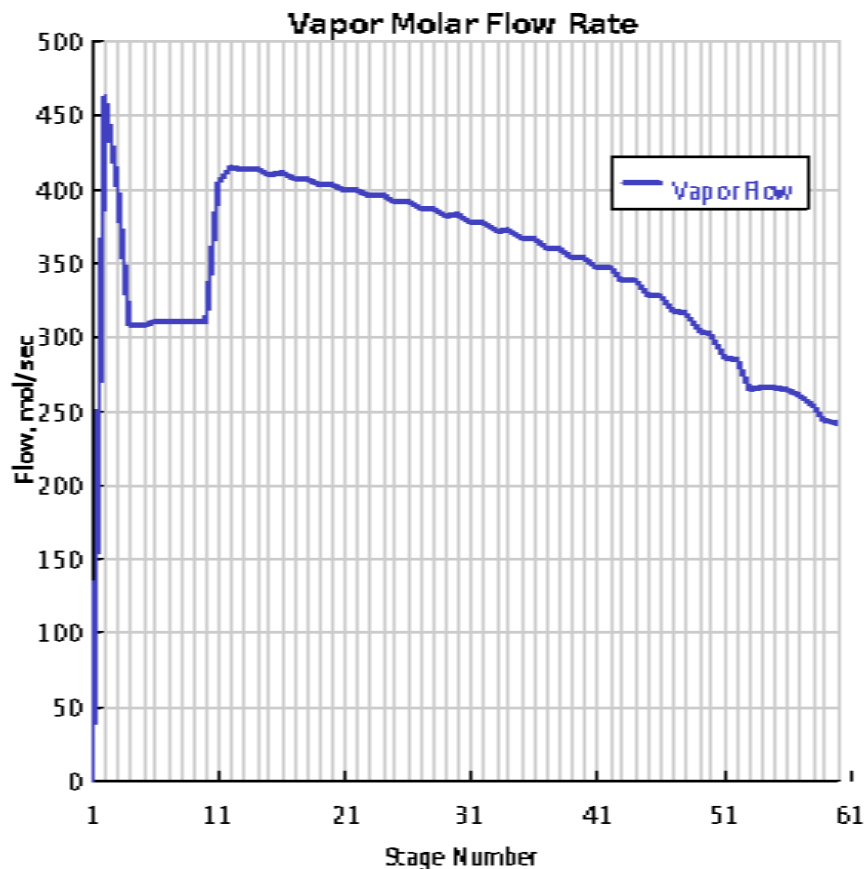
Figure 21: Vapor molar flow in DME reactive distillation column

To attempt to validate the simulated model, a comparison between the results of the presented user kinetic subroutine and published simulation results was carried out. The first comparison using identical reaction parameters and matching the column characteristics to the one presented by *Lei et al* showed promising results. However, the simulation utilizing the presented user subroutine would not converge when a pre-reactor configuration was used. More specifically, it would not converge when dimethyl ether was present in the feed stream and the product spec was greater than 97.6 mass% DME. The pre-reactor had no effect on the overall conversion of methanol, but it had a significant impact on the reboiler duty. Which will be shown later, has a significant impact on operating cost. Results from the comparison are summarized in Table 18.

Table 18: Comparison of the Operating Performance among Process Model from Z. Lei et al. and the Generated User Model

Contents	Process A	User A	Process C	User C
DME product purity (mol%)	99.55	98.66	99.5	99.99
DME mass flowrate (kg/h)	206.27	204.54	102.96	103.43
MeOH conversion (%)	99.55	98.66	49.66	49.89
H2O purity in bottoms (mol%)	99.50	98.66	99.50	99.93
Heat duty (kW)				
Fixed-bed reactor	24.42	0.00	0.00	0.00
Condenser	-100.27	-101.88	-313.85	-314.53
Reboiler	78.23	104.88	316.33	317.08

In addition to the operating performance and heat duties required, temperature and liquid/vapor composition profiles were also compared. Process A, which contained a pre-reactor configuration, was the only process that Lei et al. presented temperature and composition profiles for. Since a higher mass fraction of water and DME was entering the column in Process A, it is expected that a higher liquid composition of water and DME compared to methanol would be seen at the feed stage. This is exactly what is seen. For the User A generated model, pure methanol is being fed into the column so the liquid composition of methanol is significantly higher than that of water and DME. This is the only discrepancy when comparing the liquid profiles. This also causes the water-DME vapor composition intersection to be shifted towards the bottom of the column in the User A generated model. The temperature profiles are close to a 1:1 match. The temperature, vapor composition, and liquid composition profiles for the User A generated model are represented by Figures 23, 24 and 25, respectively. The overall trends are very similar which provide validation that the user supplied kinetic subroutine can effectively model the process. Liquid composition profiles were also compared to the composition profiles generated by *An et al.* The same overall trend between the two models was identified.
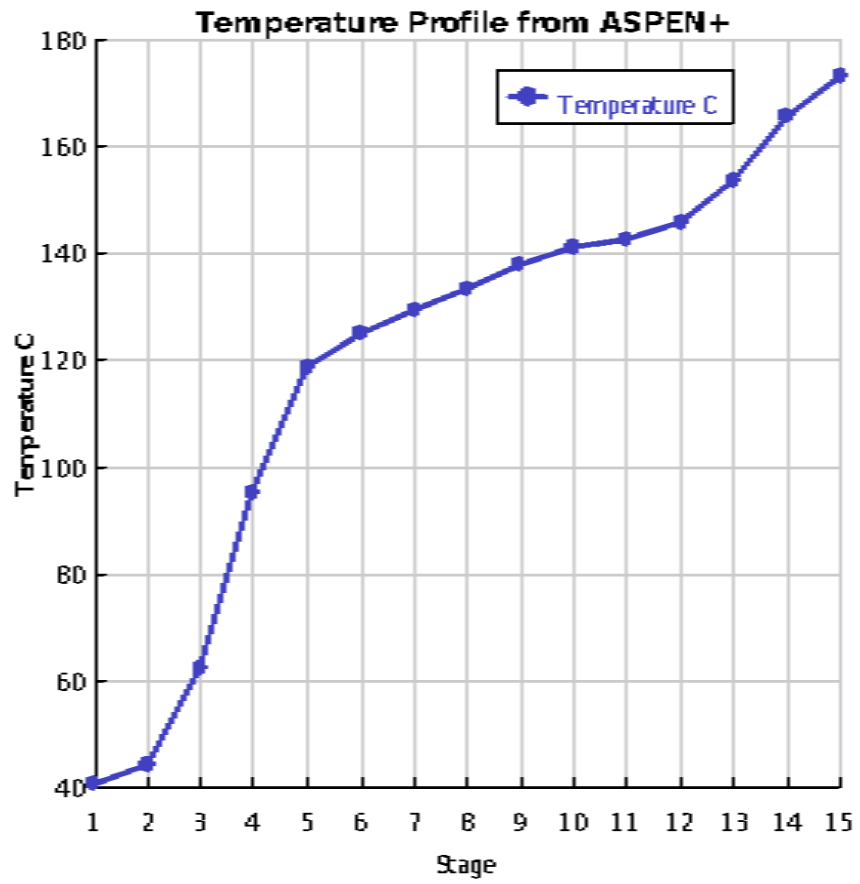
Figure 22: Temperature profile for the User A generated model
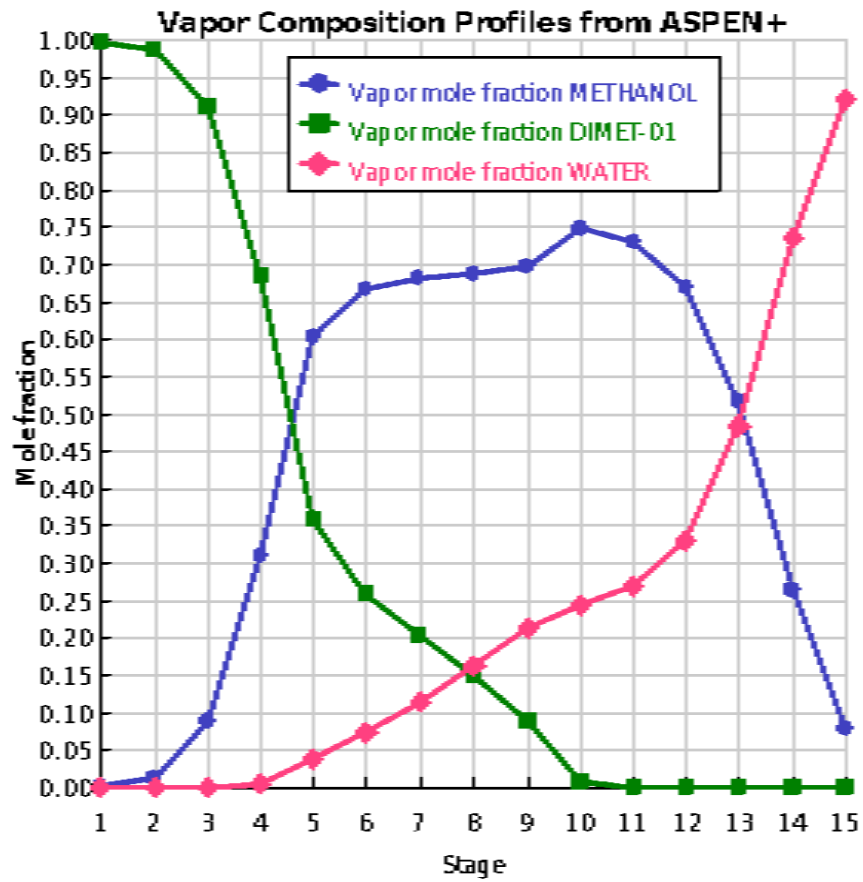
Figure 23: Vapor composition profile for the User A generated model
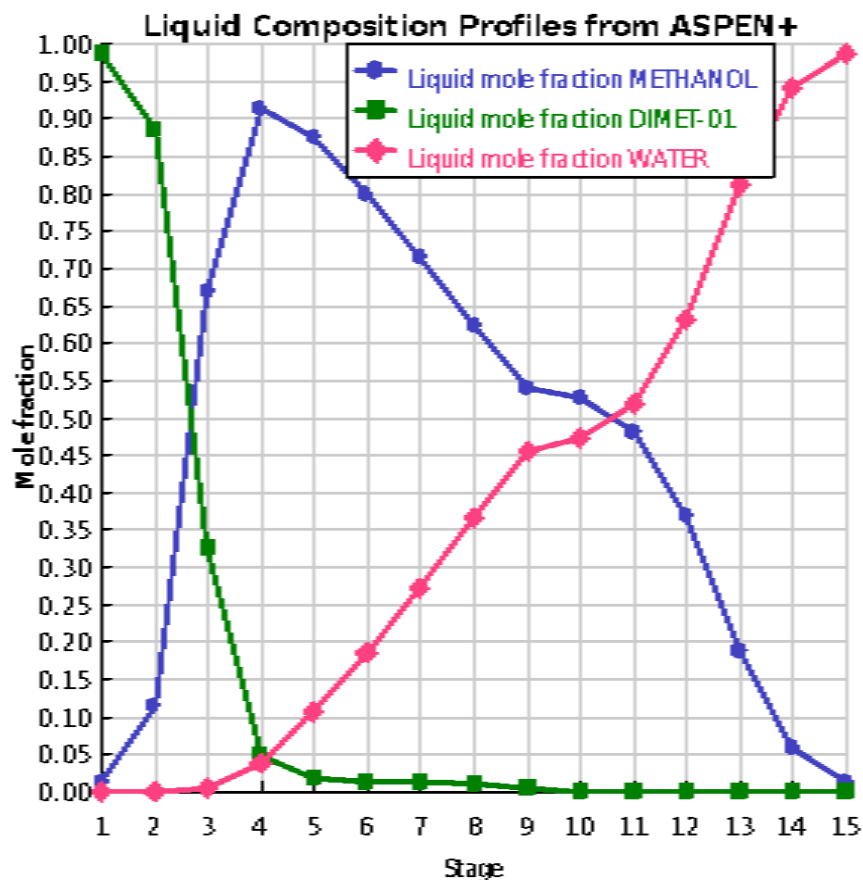
Figure 24: Liquid composition profile for the User A generated model

For the determination of the optimum design parameters, the steps laid out by *Luyben et al.* were followed. This mainly consisted of varying the number of rectifying, reactive, stripping trays, and reflux ratio independently to reduce the total annual cost. The total annual cost was determine by taking the operating cost and adding it to ratio of the total capital cost to the payback period. The payback period was assumed to be 3 years. Since a pre-reactor configuration could not be used due to the limitations of the user supplied subroutine, an exhaustive economic analysis could not be carried out. It was concluded to identify what the cost would be to incorporate the entirety of the conventional liquid process into one column. Based on published data, adding a pre-reactor before the reactive distillation column is beneficial in terms of lowering the annual operating cost [Lei et al.]. Even without the pre-reactor configuration, the reactive distillation process is the superior DME production method. By comparison, operating the reactive distillation column costs 59% and 68% less in utilities than the conventional liquid and vapor processes, respectively. The total capital cost can be reduced by more than 50% in both cases.

Table.19 Total Captial and Utility Cost Comparison of Liquid, Vapor, and Reactive Distillation Processes

	Coventional Liquid	Conventional Vapor	Reactive Distillation
Annual Utility Cost			
	$12,328,000	$15,849,000	$5,040,000
Total Capital Cost			
	$20,156,000	$17,300,000	$6,275,000

Conclusions and Recommendations

We performed a preliminary design evaluation of a process based around a PBR packed with the catalyst Amberlyst 35, which produced a DME product flow rate of approximately 250,000 gal/day, with a minimum product purity of 98.5 mass% DME and an estimated value of $2.32/gal, from a methanol feed stream of approximately 295,000 gal/day, with a product purity of 98% MeOH and an estimated value of $1.53/gal. Based on our economic analysis, we predict that our proposed process, over it's 20 year project life, will result in a ROR of 65% with an NPV of approximately $141 million. This process will require an initial capital investment of approximately $20 million, with a payback period from 2018 to 2020. Based on our economic estimations we consider this process to be economically attractive.

In addition to the design of a Amberlyst 35 PBR process, we explored the application of reactive distillation using Amberlyst 35 to meet the design specifications of this project. We were able to appropriately simulate a reactive distillation process and analyze our results. Based on our economic analysis, we predict that the production of DME, as described in the design basis, by reactive distillation would result in an NPV of $182 million with an ROR of 240.5%. We found that the application of reactive distillation to accomplish the design basis, to be the most attractive of the two designs. The ability to separate the products from the reaction zone, through reactive distillation, and meet the design specification with a single column, significantly reduces operating costs and capital costs. Therefore, we recommend further detailed design of the reactive distillation process.

We found the specifications of our reactive distillation column to be as follows: The DME reactive distillation column is a single feed system with a methanol stream fed to stage 10 at the top of the reactive zone. The column has 8 stripping stages (including the condenser), 22 packed reactive stages, and 9 rectifying stages (including the reboiler). The column operates at a pressure of 139.1 psia and with a reflux ratio of 2.0. The catalyst holdup on each reactive tray is 66.8 lbm. This corresponds to a total holdup of 1469.6 lbm in the column.

Acknowledgements

Aspen HYSYS V9
Aspen Plus V9
Intel Fortran Compiler 16/2016
Microsoft Visual Studio 14/2015
Microsoft Word
Microsoft Excel
Matlab

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P-101A/B Feed Pump			
Design Equation for Pumps:			
1) Select Pump using Table 21.1(page 4 of "Pumps")			
What we are Finding	Equation	Value	Units
Flow Rate:	From Simulation	209.40	gal/min
Head: go to "Pumps" on pg. 8 use eqn for Head Calc	( ) ——————	545.77	ft
Page 330: in textbook and fig 12-3 Pump Selection	We chose a single stage centrifugal pump		
Pg.927 Finding Fp	$\log_{10}(F_P)=C_1+C_2\log_{10}(P)+C_3(\log_{10}P)^2$	1.23	N/A
P	Discharge Pressure from Hysys Pump	16.99	barg
Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K_3[\log_{10}(A)]^2$	2941.02	$
Hydraulic hp, A	Given to us by HYSYS	22.62000	kW
Break hp	Hydraulic/efficiency	30.16	kW
Finding F_{BM}	FBM=B1+B2*FM*FP	$4.55	N/A
Finding C_{BM}	$C_{BM}=C_p^{\circ}*F_{BM}$	$13,370.85	$
C_{TM}	Adding Cbm, contingency, and Fees	$22,517.87	

E-101 Surface Area Calculator				
	—————————		—————————	Thin Walled Assumption
	— —			
Variable		Units	Source:	Assmptions:
h_i	20000	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	HP Steam Condensing Heat Transfer
R_{fi}	0.00005	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
h_o	1500	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Light Organic Sensible Heat Transfer
R_{fo}	0.0002	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
Uo=	1034.482759	W/(m^2)*K		
Variable		Units	Source:	Assumptions
Q	22609937.16	KJ/hr	HYSYS Output	
F	0.9	unitless	Flow Correction Factor	
LMTD	134.34	K	HYSYS Output	
A=	50.21410707	m^2		110% Fudge Factor, High Flux Copper
A*1.1=	55.23551778	m^2	Heat Transfer Area For Costing	Tubes, Low Carbon Steel Shell

E-101 Costing Calculator				
Variable	Equation	Input	Notes	Units
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K_3\log_{10}(A)]^2$	22464.46	*Max Size for Correlation 1000m^2*	$
Finding F_{BM}	FBM=B1+B2*FM*FP	3.89		N/A
Pg. 931 F_M	Using CS Tubes, CS Shell: Material factor FM	1.2		N/A
Fp (A.3)	log10(FP)=C1+C2log10(P)+(C3((log10(P))^2)	1.136291775		N/A
Pressure	Converting psia to barg	32.53		barg
C_{TM}		147300.2169		$

Packed Bed Reactor (Modeled as Vertical Process Vessel)				
Material	Carbon Steel			
Variable	Value	Units	Source/Equation	Assumptions
Cp^0	3144.4	N/A	( ) ( )	N/A
Volume	45	m^3	HYSYS Output	N/A
Fp	5.184176722	N/A	$$\frac{(\quad)}{(\quad)}$$	Thickness > .0063 m P in Barg
Pressure	18.64	Barg	HYSYS Output	N/A
Diameter	2.523	m	HYSYS Output	N/A
C_{bm}	66412	N/A		N/A
F_{bm}	21.12040327	N/A		N/A
Total Module Cost (2017)			$ 111,844.14	

Packed Bed Reactor Packing				
Variable	Value	Units	Source/Equation	Assumptions
Cp^0	283.0	N/A	( ) ( )	N/A
Volume	45	m^3	HYSYS Output	N/A
Fp	4.306807894	N/A	$$\frac{(\quad)}{(\quad)}$$	Thickness > .0063 m P in Barg
Pressure	15	Barg	HYSYS Output	N/A
Diameter	2.523	m	HYSYS Output	N/A
C_{bm}	283	N/A		N/A
F_{bm}	1	N/A	Table A.6: Turton Textbook	N/A
Total Module Cost (2017)			$ 476.62	

R-101 Cooling Tubes Surface Area Calculator				
				Thin Walled Assumption
Variable		Units	Source:	Assmptions:
h_i	6250	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Sensible Water Heat Transfer
R_{fi}	1.75E-04	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
h_o	1500	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Light Organic Sensible Heat Transfer
R_{fo}	1.00E-04	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
Uo=	907.7155825	W/(m^2)*K		
Uo*2=	1815.431165	W/(m^2)*K		~2X Improved Uo with High Flux Tubes
Variable		Units	Source:	Assumptions
Q	5.747E+06	KJ/hr	HYSYS Output	
F	0.9	unitless	Flow Correction Factor	
LMTD	107.48	K	HYSYS Output	
A=	97.85763296	ft^2		110% Fudge Factor, High Flux Copper
A*1.1=	107.6433963	ft^2		Tubes, Low Carbon Steel Shell

R-101 Cooling Tubes Costing Calculator				
Variable	Equation	Input	Notes	Units
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K3\log_{10}(A)]^2$	13661.63	*Max Size for Correlation 1000m^2*	$
Finding F_{BM}	FBM=B1+B2*FM*FP	3.66		N/A
Pg. 931 F_M	Using CS Tubes, CS Shell: Material factor FM	1.2		N/A
Fp (A.3)	log10(FP)=C1+C2log10(P)+(C3((log10(P))^2)	1.0185894		N/A
$C_{BM\ 2001}$	$C_{BM}=Cp^0*F_{BM}$	49988.3203		$
C_{TM}		84185.3679		$

T-101 Distillation Column			
Design Equation for Column:			
1) Select Carbon Steel			
What we are Finding	Equation	Value	Units
A, Volume	Volume=Area*Height (m^3)	54.53	m^3
Tray Spacing		0.70	m
Number of Theoretical Trays		10.00	
Height	Column Height= $h_{top}+h_{trays}+h_{btms}$	12.06	m
Diameter	From Hysys	2.4	m
Column Pressure	Simulation	189.6	psia
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K_3[\log_{10}(A)]^2$	39,831	$
Finding F_{BM}	FBM=B1+B2*FM*FP	9.06	N/A
Pg. 931 F_M	Using Carbon Steel: Material factor FM	1	N/A
Pg. 927 F_P	(((P+1)D)/(2(850-.6(P+1))+.00315)/.0063	3.74	N/A
Pressure	Converting psia to barg	15.51	barg
C_{TM} 2017	$C_{TM}=C_{BM}$+Contingency+Fees	607,827	$

T-101 Sieve Trays			
Design Equation for Sieve Trays: CBM=Cpo*FBM			
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K_3[\log_{10}(A)]^2$	2,868	$
Area, A	Area (m^2) from HYSYS	4.52	m^2
Diameter	From HYSYS	2.4	m
F_{BM}	For Carbon Steel Sieve Trays	1	N/A
C_{TM}	C_{TM}= C_{BM}+Contingency+Fees	565,164	$

T-101 Condenser Surface Area Calculator				
				Thin Walled Assumption
Variable		Units	Source:	Assmptions:
h_i	6250	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Cooling Water Sensible Heat Transfer
R_{fi}	1.75E-04	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
h_o	3000	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Condensing Light Organics Shell Side
R_{fo}	1.00E-04	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
Uo=	1301.518438	W/(m^2)*K		
Variable		Units	Source:	Assumptions
Q	3.79E+07	KJ/hr	HYSYS Output	
F	0.9	unitless	Flow Correction Factor	
LMTD	23.62	K	HYSYS Output	Assuming 30C Cooling Water
A=	380.8486188	m^2		
A*1.1=	418.9334807	m^2	Heat Transfer Area For Costing	110% Fudge Factor, Low Carbon Steel Shell

T-101 Condenser Costing Calculator				
Variable	Equation	Input	Notes	Units
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K3\log_{10}(A)]^2$	77504.94	*Max Size for Correlation 1000m^2*	$
Finding F_{BM}	FBM=B1+B2*FM*FP	3.37		N/A
Pg. 931 F_M	Using Cu/Ni Tubes, CS Shell: Material factor FM	1	CS Shell/CS Tube	N/A
Fp (A.3)	log10(FP)=C1+C2log10(P)+(C3((log10(P))^2)	1.048179799		N/A
Pressure	Converting psia to barg	15.44		barg
C_{TM}		$439,870.22		$

T-101 Reboiler Surface Area Calculator				
				Thin Walled Assumption
Variable		Units	Source:	Assmptions:
h_i	20000	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Steam Sensible Heat Transfer
R_{fi}	5.00E-05	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
h_o	4000	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Vaporizing Water/Organic Mixture Shell Side
R_{fo}	1.50E-04	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
Uo=	2000	W/(m^2)*K		
Uo*2=	4000		2x (High Flux Tubing to facilitate vaporization)	
Variable		Units	Source:	Assumptions
Q	1.99E+07	KJ/hr	HYSYS Output	
F	0.9	unitless	Flow Correction Factor	
LMTD	83.82	K	HYSYS Output	
A=	18.27754184	m^2		
A*1.1=	20.10529603	m^2	Heat Transfer Area For Costing	110% Fudge Factor, Low Carbon Steel Shell

T-101 Reboiler Costing Calculator				
Variable	Equation	Input	Notes	Units
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K3\log_{10}(A)]^2$	28096.13	*Max Size for Correlation 1000m^2*	$
Finding F_{BM}	FBM=B1+B2*FM*FP	6.53		N/A
Pg. 931 F_M	Using Cu/Ni Tubes, CS Shell: Material factor FM	2.6		N/A
Fp (A.3)	log10(FP)=C1+C2log10(P)+(C3((log10(P))^2)	1.136291775		N/A
Pressure	Converting psia to barg	32.53		barg
C_{TM}		$309,178.58		$

T-102 Distillation Column			
Design Equation for Column:			
1) Select Carbon Steel			
What we are Finding	Equation	Value	Units
A, Volume	Volume=Area*Height (m^3)	138.81	m^3
Tray Spacing		0.61	m
Number of Trays		40.00	
Height	Column Height= $h_{top}+h_{trays}+h_{btms}$	33.43	m
CS Area of Column	Area= (pi/4)* (Diameter)^2	4.15	m^2
Diameter	From Hysys	2.3	m
Column Pressure	Simulation	38.29	psia
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K_3[\log_{10}(A)]^2$	89,381	$
Finding F_{BM}	FBM=B1+B2*FM*FP	4.63	N/A
Pg. 931 F_M	Using Carbon Steel: Material factor FM	1	N/A
Pg. 927 F_P	(((P+1)D)/(2(850-.6(P+1))+.00315)/.0063	1.31	N/A
Pressure	Converting psia to barg	5.07	barg
C_{TM} 2017	$C_{TM}=C_{BM}+Contingency+Fees$	697,567	$

T-102 Sieve Trays			
Design Equation for Sieve Trays: CBM=Cpo*FBM			
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K_{3[}\log_{10}(A)]^2$	2,645	$
Area, A	Area (m^2) from HYSYS	4.15	m^2
Diameter	From HYSYS	2.3	m
C_{TM}	$C_{TM}= C_{BM}+Contingency+Fees$	521,219	$

T-102 Condenser Surface Area Calculator

Variable		Units	Source:	Assmptions:
				Thin Walled Assumption
h_i	6250	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Cooling Water Sensible Heat Transfer
R_{fi}	1.75E-04	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
h_o	3000	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Condensing Light Organics Shell Side
R_{fo}	1.00E-04	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
Uo=	1301.518438	W/(m^2)*K		
Variable		Units	Source:	Assumptions
Q	1.95E+08	KJ/hr	HYSYS Output	
Q	54099774.24	W	Unit Conversion	
F	0.9	unitless	Flow Correction Factor	
LMTD	32.04	K	HYSYS Output	Assuming 30C Cooling Water
A=	1441.484945	m^2		
A*1.1=	1585.633439	m^2	Heat Transfer Area For Costing	110% Fudge Factor, Low Carbon Steel Shell

T-102 Condenser Costing Calculator

Variable	Equation	Input	Notes	Units
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K3\log_{10}(A)]^2$	256461.07	*Max Size for Correlation 1000m^2*	$
Finding F_{BM}	FBM=B1+B2*FM*FP	3.29		N/A
Pg. 931 F_M	Using Cu/Ni Tubes, CS Shell: Material factor FM	1	CS Shell/CS Tube	N/A
Fp (A.3)	log10(FP)=C1+C2log10(P)+(C3((log10(P))^2)	0.99999457		N/A
Pressure	Converting psia to barg	4.79		barg
C_{TM}		$1,420,967.78		$

P-102 Recycle Pumps A/B

Design Equation for Pumps:			
1) Select Pump using Table 21.1(page 4 of "Pumps")			
What we are Finding	Equation	Value	Units
Flow Rate:	From Simulation	157.30	gal/min
Head: go to "Pumps" on pg. 8 use eqn for Head Calc	( ) ————	678.98	ft
Page 330: in textbook and fig 12-3 Pump Selection	We chose a single stage centrifugal pump		
Page 933 in textbook and Figure A.18	Using Cast Iron: Material factor FM	1	N/A
Page 933 in textbook and Figure A.18	Using Carbon Steel: Material factor FM	1.6	N/A
Pg.927 Finding Fp	$\log_{10}(F_P)=C_1+C_2\log_{10}(P)+C_3(\log_{10}P)^2$	1.24	N/A
P	Discharge Pressure from Hysys Pump	17.33	barg
Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K_3[\log_{10}(A)]^2$	2930.52	$
Hydraulic hp, A	Given to us by HYSYS	21.16000	kW
Break hp	Hydraulic/efficiency	28.21	kW
Finding F_{BM}	FBM=B1+B2*FM*FP	$4.57	N/A
Finding C_{BM}	$C_{BM}=C_p^{0}*F_{BM}$	$13,384.39	$
C_{TM}	Adding Cbm, contingency, and Fees	$22,540.67	

T-102 Reboiler Surface Area Calculator

Variable		Units	Source:		Thin Walled Assumption
Variable		Units	Source:		Assmptions:
h_i	20000	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.		Steam Sensible Heat Transfer
R_{fi}	5.00E-05	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.		
h_o	4000	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.		Vaporizing Water/Organic Mixture Shell Side
R_{fo}	1.50E-04	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.		
$U_o=$	2000	W/(m^2)*K			
$U_o*2=$	4000		2x (High Flux Tubing to facilitate vaporization)		
Variable		Units	Source:		Assumptions
Q	3.73E+07	KJ/hr	HYSYS Output		
F	0.9	unitless	Flow Correction Factor		
LMTD	115.04	K	HYSYS Output		
A=	24.9892901	m^2			
A*1.1=	27.48821911	m^2	Heat Transfer Area For Costing		110% Fudge Factor, Low Carbon Steel Shell

T-102 Reboiler Costing Calculator

Variable	Equation	Input	Notes	Units
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K3\log_{10}(A)]^2$	33442.55	*Max Size for Correlation 1000m^2*	$
Finding F_{BM}	FBM=B1+B2*FM*FP	6.53		N/A
Pg. 931 F_M	Using Cu/Ni Tubes, CS Shell: Material factor FM	2.6		N/A
Fp (A.3)	log10(FP)=C1+C2log10(P)+(C3((log10(P))^2)	1.136291775		N/A
Pressure	Converting psia to barg	32.53		barg
C_{TM}		368012.1975		$

E-106 Surface Area Calculator

Variable		Units	Source:	Thin Walled Assumption
Variable		Units	Source:	Assmptions:
h_i	6250	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Cooling Water Sensible Heat Transfer
R_{fi}	1.75E-04	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
h_o	6250	W/(m^2)*K	Table 4.1.1 HEX Handout Ramsey et. al.	Water Sensible Heat Transfer
R_{fo}	1.75E-04	((m^2)*K)/W	Table 4.1.1 HEX Handout Ramsey et. al.	
$U_o=$	1492.537313	W/(m^2)*K		
Variable		Units	Source:	Assumptions
Q	3.776E+06	KJ/hr	HYSYS Output	
F	0.9	unitless	Flow Correct Factor	
LMTD	41.44	K	HYSYS Output	
A=	18.84140078	m^2		
A*1.1=	20.72554086	m^2	Heat Transfer Area For Costing	110% Fudge Factor, High Flux Copper Tubes, Low Carbon Steel Shell

E-106 Costing Calculator				
Variable	Equation	Input	Notes	Units
C_{po} Pg. 910	$\log_{10}(C_P^0)=K_1+K_2\log_{10}(A)+K3\log_{10}(A)]^2$	15885.83	*Max Size for Correlation 1000m^2*	$
Finding F_{BM}	FBM=B1+B2*FM*FP	3.62		N/A
Pg. 931 F_M	Using CS Tubes, CS Shell: Material factor FM	1.2		N/A
Fp (A.3)	log10(FP)=C1+C2log10(P)+(C3((log10(P))^2)	1.000034227		N/A
Pressure	Converting psia to barg	5.07		barg
C_{TM}		96902.3984		$

Appendix B : Reactive Distillation Fortran Code

```
C
C
C    User Kinetics Subroutine for RADFRAC
C    (REAC-DIST type Reactions)
C
    SUBROUTINE DMEPRO (N,    NCOMP, NR,   NRL,   NRV,
   2           T,    TLIQ,  TVAP, P,    PHFRAC,
   3           F,    X,    Y,    IDX,  NBOPST,
   4           KDIAG, STOIC, IHLBAS, HLDLIQ, TIMLIQ,
   5           IHVBAS, HLDVAP, TIMVAP, NINT,  INT,
   6           NREAL, REAL,  RATES, RATEL, RATEV,
   7           NINTB, INTB,  NREALB, REALB, NIWORK,
   8           IWORK, NWORK,  WORK)
C
C
C    DESCRIPTION: TO CALCULATE REACTION RATES FOR KINETIC REACTIONS
C           USING USER SUPPLIED SUBROUTINE
C
C    VARIABLES IN ARGUMENT LIST
C
C    VARIABLE  I/O  TYPE    DIMENSION    DESCRIPTION AND RANGE
C    N       I  I    -      STAGE NUMBER
C    NCOMP    I  I    -        NUMBER OF COMPONENTS
C    NR      I  I    -        TOTAL NUMBER OF KINETIC
C                    REACTIONS
C    NRL     I  I    3       NUMBER OF LIQUID PHASE
C                    KINETIC REACTIONS.
C                    NRL(1): NUMBER OF
C                       OVERALL LIQUID
C                       REACTIONS.
C                    NRL(2): NUMBER OF
C                       LIQUID1 REACTIONS.
C                    NRL(3): NUMBER OF
C                       LIQUID2 REACTIONS.
C    NRV     I  I    -        NUMBER OF VAPOR PHASE
C                    KINETIC REACTIONS
C    T      I  R    -        STAGE TEMPERATURE (K)
C    TLIQ    I  R    -        LIQUID TEMPERATURE (K)
C                    * USED ONLY BY RATEFRAC **
C    TVAP    I  R    -        VAPOR TEMPERATURE (K)
C                    * USED ONLY BY RATEFRAC **
C    P     I  R    -        STAGE PRESSURE (N/SQ.M)
C    PHFRAC   I  R    3       PHASE FRACTION
C                    PHFRAC(1): VAPOR FRACTION
C                    PHFRAC(2): LIQUID1 FRACTIO
C                    PHFRAC(3): LIQUID2 FRACTIO
C    F      I  R    -        TOTAL FLOW ON STAGE
C                    (VAPOR+LIQUID) (KMOL/SEC)
C    X      I  R    NCOMP,3    LIQUID MOLE FRACTION
C    Y      I  R    NCOMP     VAPOR MOLE FRACTION
C    IDX    I  I    NCOMP     COMPONENT INDEX VECTOR
```

```
C     NBOPST   I   I      6      OPTION SET BEAD POINTER
C     KDIAG    I   I      -      LOCAL DIAGNOSTIC LEVEL
C     STOIC    I   R      NCOMP,NR   REACTION STOICHIOMETRY
C     IHLBAS   I   I      -      BASIS FOR LIQUID
C                               HOLDUP SPECIFICATION
C                               1:VOLUME,2:MASS,3:MOLE
C     HLDLIQ   I   R      -      LIQUID HOLDUP
C                               IHLBAS   UNITS
C                               1      CU.M.
C                               2      KG
C                               3      KMOL
C     TIMLIQ   I   R      -      LIQUID RESIDENCE TIME
C                               (SEC)
C     IHVBAS   I   I      -      BASIS FOR VAPOR
C                               HOLDUP SPECIFICATION
C                               1:VOLUME,2:MASS,3:MOLE
C     HLDVAP   I   R      -      VAPOR HOLDUP
C                               IHVBAS  UNITS
C                               1      CU.M.
C                               2      KG
C                               3      KMOL
C     TIMVAP   I   R      -      VAPOR RESIDENCE TIME (SEC)
C     NINT     I   I      -      LENGTH OF INTEGER VECTOR
C     INT      I/O I      NINT   INTEGER VECTOR
C     NREAL    I   I      -      LENGTH OF REAL VECTOR
C     REAL     I/O R      NREAL  REAL VECTOR
C     RATES    O   R      NCOMP  COMPONENT REACTION RATES
C                               (KMOL/SEC)
C     RATEL    O   R      NRLT   INDIVIDUAL REACTION RATES
C                               IN THE LIQUID PHASE
C                               (KMOL/SEC)
C                               NRLT =NRL(1)+NRL(2)+NRL(3)
C                               * RATE-BASED MODE ONLY *
C     RATEV    O   R      NRV    INDIVIDUAL REACTION RATES
C                               IN THE VAPOR PHASE
C                               (KMOL/SEC)
C                               * RATE-BASED MODE ONLY *
C     NINTB    I   I      -      LENGTH OF INTEGER VECTOR
C                               (FROM UOS BLOCK)
C     INTB     I/O I      NINTB  INTEGER VECTOR
C                               (FROM UOS BLOCK)
C     NREALB   I   I      -      LENGTH OF REAL VECTOR
C                               (FROM UOS BLOCK)
C     REALB    I/O R      NREALB REAL VECTOR
C                               (FROM UOS BLOCK)
C     NIWORK   I   I      -      LENGTH OF INTEGER WORK
C                               VECTOR
C     IWORK    I/O I      NIWORK INTEGER WORK VECTOR
C     NWORK    I   I      -      LENGTH OF REAL WORK VECTOR
C     WORK     I/O R      NWORK  REAL WORK VECTOR
C
C   IMPLICIT NONE
C
C   DECLARE VARIABLES USED IN DIMENSIONING
C
      INTEGER NCOMP, NR, NRL, NRV, NINT,
     + NINTB, NREALB,NIWORK,NWORK, N_COMP
C
C   DECLARE PARAMETERS & VARIABLES USED IN PARAMETERS
C
C    component order
C    ==============
C    this routine assumes that the components are in this order:
      INTEGER K_METHANOL,K_DME, K_H2O
      PARAMETER(K_METHANOL=1)
      PARAMETER(K_DME=2)
      PARAMETER(K_H2O=3)
      PARAMETER(N_COMP=3)
C----------------------------------------------------------------
C
```

```
C     DECLARE ARGUMENTS
C
      INTEGER IDX(NCOMP), NBOPST(6), INT(NINT),
     +     INTB(NINTB), IWORK(NIWORK),N,
     +     KDIAG, IHLBAS,IHVBAS,NREAL, KPHI,
     +     KER, L_GAMMA, J, K
      REAL*8 X(NCOMP,3), Y(NCOMP),
     +     STOIC(NCOMP,NR), RATES(NCOMP),
     +     RATEL(NRL), RATEV(NRV),
     +     REALB(NREALB),WORK(NWORK), B(1), T,
     +     TLIQ, TVAP, P, PHFRAC(1), F
      REAL*8 HLDLIQ,TIMLIQ,HLDVAP,TIMVAP,TZERO,
     +     FT
C
C
C     DECLARE SYSTEM FUNCTIONS
C
      REAL*8 DLOG
C
C     DECLARE LOCAL VARIABLES
C
      INTEGER IMISS, IDBG
      REAL*8 REAL(NREAL), RMISS, KWM, KS, am, ad, aw,
     +       RATE(4), RATNET(4)
      REAL*8 PHI(N_COMP)
      REAL*8 DPHI(N_COMP)
      REAL*8 ACTIV(N_COMP)
C
#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)
C
C
#include "dms_maxwrt.cmn"
#include "dms_ipoff3.cmn"
#include "dms_lclist.cmn"
      INTEGER FN
#include "dms_plex.cmn"
      EQUIVALENCE(B(1),IB(1))
      FN(J)=J+LCLIST_LBLCLIST
C
#include "dms_rglob.cmn"
C
C     DATA STATEMENTS
C
      DATA IDBG/0/
C     thermodynamic rate constant DKA
C     =============================
 9010 FORMAT(1X,3(G13.6,1X))
 9000 FORMAT(' fugly failed at T=',G12.5,' P=',G12.5,' ker=',I4)
 9020 FORMAT(' compo ',I3,' mole-frac=',G12.5,' activity=',G12.5)
 9030 FORMAT(' stage=',I4,' spec-rate=',G12.5,' net-rate=',G12.5)
C
C     BEGIN EXECUTABLE CODE
C
C Temperature dependent adsorption equilibrium constant ratio
      KWM = DEXP(-6.46 + 2964/T)
C Surface reaction rate constant
      KS = (6.12D+07)*DEXP(-98/(0.008314*T))
C
C     ====================
C
      IF(IDBG.GE.1)THEN
      WRITE(MAXWRT_MAXBUF(1),9010) KWM, KS
      CALL DMS_WRTTRM(1)
      ENDIF
C     calculation of components activities
C     ================================
C     calculate only fugacity coefficient
      KPHI=1
```

```fortran
C    fugacity coefficient of components in the mixture
     CALL PPMON_FUGLY(T,P,X(1,1)
    +     ,Y,NCOMP,IDX,NBOPST,KDIAG,KPHI,PHI,DPHI,KER)
     IF(KER.NE.0)THEN
      WRITE(MAXWRT_MAXBUF(1),9000) T,P,KER
      CALL DMS_WRTTRM(1)
     ENDIF
C    set offset to get activity coefficients
C    (see vol5, p 11-11 and asp$sor search for 'GAMMAL')
     L_GAMMA=IPOFF3_IPOFF3(24)
C    calculate activities for plex data
     DO J=1,NCOMP
      ACTIV(J)=DEXP(B(FN(L_GAMMA)+J))*X(J,1)
     END DO
C
     am = ACTIV(K_METHANOL)
     ad = ACTIV(K_DME)
     aw = ACTIV(K_H2O)
C
     IF(IDBG.GE.1)THEN
      DO J=1,NCOMP
       WRITE(MAXWRT_MAXBUF(1),9020) J,X(J,1),ACTIV(J)
       CALL DMS_WRTTRM(1)
      END DO
     ENDIF
C    reaction rate
C    =============
     RATE(1)=1/((1/dsqrt(KS))+((1/dsqrt(KS))*(KWM)*(aw/am)))**2
C
     DO K = 1,NRL
       RATE(K) = RATE(K) * HLDLIQ
     END DO
C    INITIALIZATION OF COMPONENT REACTION RATES
C
     DO J = 1,NCOMP
       RATES(J) = 0.D0
     END DO
C
C    COMPONENT REACTION RATES in kmol/sec
C
     DO K=1,NRL
      DO J=1,NCOMP
       IF (DABS(STOIC(J,K)) .GE. RGLOB_RMIN) RATES(J) = RATES(J) +
    1     STOIC(J,K) * RATE(K)
      END DO
     END DO

     IF(IDBG.GE.1)THEN
      WRITE(MAXWRT_MAXBUF(1),9030) N,RATE(1)
      CALL DMS_WRTTRM(1)
     ENDIF
c    write(1,*) N, k1, Keq, KW,
c    write(1,*) aw, ap, ae
c    write(1,*)
     RETURN
#undef P_MAX3
     END
```

Appendix C: Reactive Distillation Specifics

Operating Conditions for Processes A and C

	Process A	Process C
Feed stream		
Temperature (K)	298	298
Pressure (Mpa)	2.0	2.0
Flowrate (mol/s)	2.5	2.5
Composition (mole fraction)		
Methanol	1.0	1.0
Water	0	0
DME	0	0
Rgibbs (fixed-bed reactor)		
Temperature (K)	403	
Pressure (Mpa)	2.0	
RadFrac (catalytic distillation column)		
Total stages	15	30
Rectification zone	1-2	1-7
Reactive zone	3-9	8-25
Stripping zone	10-15	26-30
Feed stage	3	8
Catalyst loading (kg/stage)	15.0	15.0
Column Pressure (Mpa)	0.9	0.9
Reflux ratio (mole)	3.5	3.5
Distillate rate (kmol/h)	4.50	2.245
Radfrac (ordinary distillation column)		
Total stages		15
Feed stage		10
Column pressure (Mpa)		0.1
Reflux ratio (mole)		5
Distillate rate (kmol/h)		4.51

Reactive · Distillation