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Design, Analysis, and Optimization of a Process to Produce Dimethyl Ether from Methanol

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DESIGN, ANALYSIS, AND OPTIMIZATION OF A PROCESS TO PRODUCE DIMETHYL ETHER FROM METHANOL

By

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A thesis submitted to the faculty of The University of Mississippi in partial fulfillment of the requirements of the Sally McDonnell Barksdale Honors College.

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ABSTRACT

THOMAS GRADY MATHWIG: Design, Analysis, and Optimization of a Process to Produce Dimethyl Ether from Methanol (Under the direction of Dr. Adam Smith)

The company that the engineering team works for is facing a contract loss with one of its customers of methanol. To avoid economic losses, a process has been proposed for converting the unused methanol to dimethyl ether (DME) through a dehydration reaction. After a preliminary simulation of the base case and optimization of the distillation column, an Equivalent Annual Operating Cost (EAOC) of $140,000 was calculated for the column. The EAOC was the sum of the annualized capital investment and the annual operating cost. Determining the process to be worth pursuing, a Toller was brought in to provide rental equipment needed for production. Using the available equipment from the Toller, the team performed a new optimization, this time of the entire process, by changing the process conditions from the base case. Optimization was streamlined by creating equations to verify equipment viability and display rental costs, and by identifying constraints evident from comparing the available equipment to constants in the process. The best equipment set decided upon, with an overall yearly cost of $689,000, utilized the smallest reactor and distillation column by strategically sizing the condenser, reboiler, and other heat exchangers. The overall yearly cost was the sum of all yearly rental and utility costs. To improve process safety, the team recommended abiding by Process Safety Management (PSM) guidelines, placing a deluge system on the reactor, placing conservation valves on all tanks, and piping pressure relief valve outlets to catch tanks. To decrease the plant's environmental impact, the team recommended

implementing heat integration networks and targeting a higher conversion of methanol. By lowering feed purity to investigate the effect on process economics, the team found that the profit decreased by only 3% when purity was decreased by 1.8%. The process was found to have a profit margin of $6.14 million per year with the best equipment set in use. This was determined by subtracting the raw material cost ($6.9 million) and the overall yearly cost from the revenue generated ($13.7 million). The team therefore recommended progressing to the next phase of the project.

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Introduction

The goal of this project was to optimize a given chemical process with a team using AVEVA Process Simulation software. According to Turton, optimization is "the process of improving an existing situation, device, or system such as a chemical process" (2018). Since different levels of improvement can be achieved, the project lent itself well to the competition format that the team operated under. AVEVA stipulated that teams could win for creating the best simulation with the best solution in each part of the competition. In Part 1, the team was tasked with designing a base case process and optimizing the distillation unit operation. In Part 2, a set of possible equipment was provided, and the team was tasked with performing an overall process optimization.

The base case design was necessary because it is crucial to have a starting point to work from in optimization. Once that is in place to provide a solid foundation, the work of figuring out how to implement the most effective improvements can begin. It is important to note the different types of optimization that can be performed. Topological optimization is concerned with the arrangement of steps and equipment in the process. It could look at eliminating unwanted by-products, rearranging/eliminating equipment, changing a reaction or separation unit operation, and setting up heat exchanger networks. While recommendations were made on how process topology could be modified, this type of optimization was not performed, as it was outside the scope of the given competition scenario. Parametric optimization, on the other hand, was explored extensively in this project. This is concerned with modifying process conditions, such as stream temperatures and pressures, equipment sizes, reactor conversion, and number of column trays, for example. In Part 1, process conditions remained the same as the distillation column was optimized, while in Part 2, process conditions were changed by manipulating equipment sizes from the given list. Armed with reasoning skills and chemical engineering knowledge, the team was able to arrive at several optimized solutions through many iterations of testing equipment in the simulation software.

Chapter 1: Project Statement and Recommendations

The team's company is a producer of methanol that has historically been sold to two customers via contract, but one of these customers has suffered an economic downturn and has decided not to renew their methanol contract. This leaves the company in a precarious situation where more methanol is being produced than is contracted to be sold. At the same time, the market spot price for methanol is lower than that of the contract itself and has been on the decline for the last two years. This can be seen in Figure 1 below.

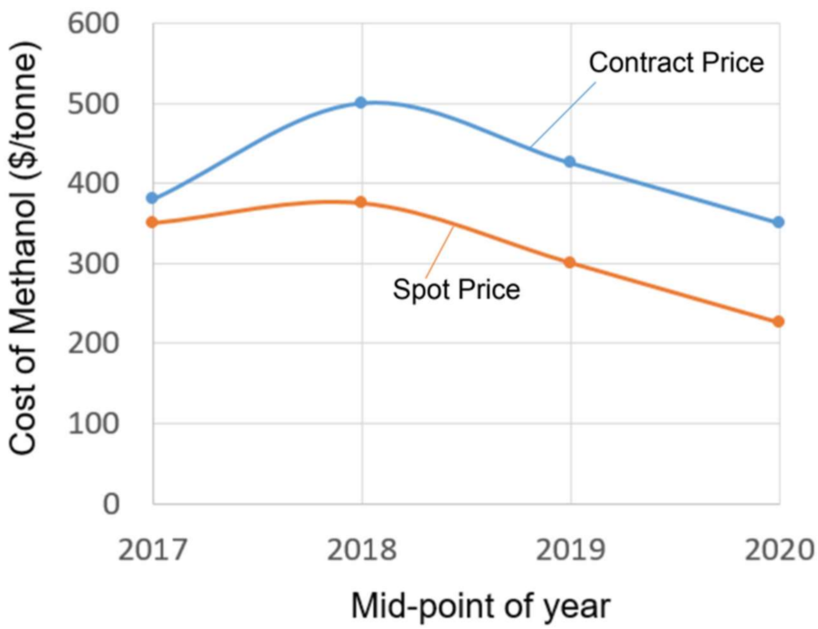

Figure 1: Spot Price vs Contract Price of Methanol

Due to this predicament, it has been proposed to produce dimethyl ether (DME) through dehydration of methanol. To create this process, the company is exploring the possibility of enlisting an outside contractor to provide skid-mounted rented equipment to avoid the fixed capital investment of a plant expansion. The plant design goal is to take a stream of 23,000 tonnes per year of 99.9 wt% methanol and produce a stream of at least 99.5 wt% DME. With a shortage of DME in the local market, there is potential for production to turn a profit. The reaction is carried out in the vapor phase in an adiabatic packed bed reactor.

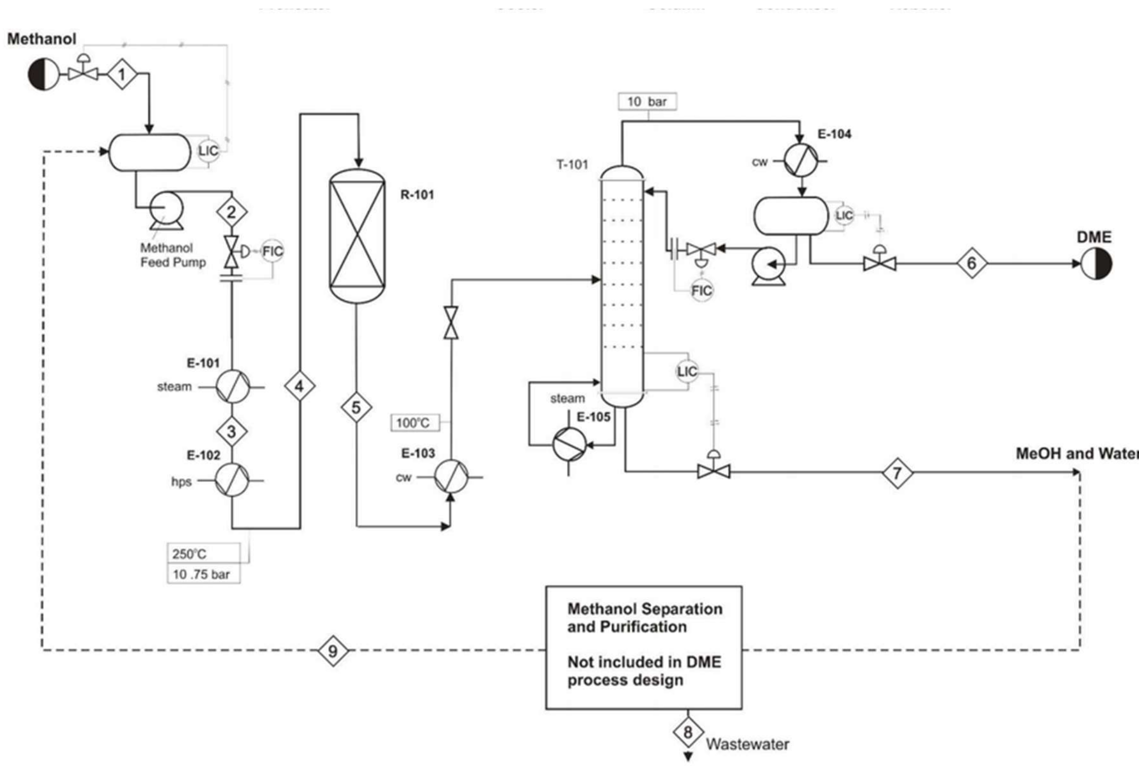

Figure 2: Process Flow Diagram

Methanol is fed into the process from a feed tank and goes through a vaporizer E-101 then into a reactor feed preheater E-102. The heated vaporized methanol is sent through an adiabatic packed bed reactor and the product stream is sent to an effluent cooler E-103 before entering the tower. The distillation column is used to produce a dimethyl ether rich overhead stream and to produce a bottoms stream of primarily unreacted methanol and water. The process water is sent to a wastewater and methanol separation unit, where the wastewater is removed and sent elsewhere for treatment, and the methanol is recycled to the feed tank, where it reenters the process with the fresh feed of 23,000 tonnes per year. The column was the primary focus of the preliminary optimization project.

After developing the steady-state simulation, the distillation column was optimized to reduce its equivalent annual operating cost (EAOC). The team used an optimizer tool within the AVEVA Process Simulation software to minimize the EAOC by varying boil-up ratio and column diameter. The number of trays was increased to 16, at which point the EAOC was minimized. Assuming an overall tray efficiency of 70%, this number of ideal trays was equated to 23 actual valve trays. The team changed tray spacing to a minimum heuristic value of 0.5 meters to minimize column volume and reduce the annualized fixed capital investment portion of the EAOC. Using a provided equation that used a present worth factor to annualize the cost of the column and adding the yearly utility cost, the team was able to get an initial EAOC of $173,000. After optimization, the team was able to bring down the EAOC to $140,000 providing a yearly savings of $33,000. The stream information for the process is shown in Table 1. The team created a base case equipment summary table, as shown in Table 2, which was used to identify recommendations for which selections from the Toller equipment to use.

Table 1: Stream Table

Stream	1	2	3	5	6	7	8	9
T (°C)	30.00	30.53	139.96	250.00	370.83	44.70	153.00	137.20
P (Bar)	1.01	11.00	10.85	10.75	10.56	10.00	10.23	10.23
VF	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00
Mass Flow (Tonne/H)	2.66	3.27	3.27	3.27	3.27	1.91	1.36	0.75
Mol Flow (Kmol/H)	83.09	102.21	102.21	102.21	102.21	41.62	60.59	41.47
DME Flow (Kmol/H)	0.00	0.03	0.03	0.03	41.36	41.32	0.03	0.00
CH3OH Flow (Kmol/H)	82.95	102.03	102.03	102.03	19.39	0.30	19.09	0.00
Water Flow (Kmol/H)	0.15	0.15	0.15	0.15	41.47	0.00	41.47	41.47

Table 2: Base Case Equipment Summary

Equipment Tag	Equipment Name	Length (m)	Diameter (m)	Catalyst Volume (m^3)
R-101	Reactor	7.72	1	3.64
Equipment Tag	**Equipment Name**	**Length (m)**	**Diameter (m)**	**Valve Trays**
T-101	DME Column	8	0.41	23
Equipment Tag	**Equipment Name**	**Area (m^2)**	**Duty (kW)**	**Utility**
E-101	Methanol Vaporizer	27.2	1184	150°C Saturated Steam
E-102	Reactor Feed Preheater	79.4	193	260°C Saturated Steam
E-103	Reactor Effluent Cooler	15.2	1176	Cooling Water
E-104	DME Column Condenser	23.2	368	Cooling Water
E-105	DME Column Reboiler	8.8	239	180°C Saturated Steam

From the base case, the team recommends moving forward with the project. Support for this recommendation comes from the determination of the economic potential of the process. By subtracting the annual cost of raw methanol ($6.9M) from the annual revenue of the product DME ($13.7M), an economic potential of $6.8M was found. This is, at the outset, a favorable indication to suggest progressing further with the DME plant. Additionally, the raw material cost is only 50% of the revenue, well below the 80% rule of thumb. Thus, the team began the optimization process using the provided Toller equipment.

Chapter II: Optimization Logic

After analysis of the base case process was completed, a third-party Toller was brought in to provide a list of available rental, skid-mounted equipment. This was in accordance with the wishes of management, who did not want to invest in a new plant for producing DME to maintain the option of future methanol contracts. The Toller had three reactors, three distillation columns, and eight heat exchangers available. The DME process also utilizes valves, pumps, and vessels, but the Toller was clear that there were plenty of these available, so that whatever our design required he would be able to accommodate. Therefore, the sizing and pricing of these auxiliary pieces of equipment were not included in this stage of the project. A possible exception might be if the column rental costs were negotiated to include the cost of the reflux drum and the reflux pump. The available reactors and columns are shown below in Table 3.

Table 3: Available Reactors and Columns from Toller

Equipment	Length (m)	Diameter (m)	Max Op Temp (°C)	Max Op Pressure (bar)	Catalyst Volume (m^3)	Rental Cost ($/mo.)
Reactor A	5	1	400	12	3.93	10.0 k
Reactor B	4	.8	400	12	2.00	6.31 k
Reactor C	7	1.4	400	12	10.74	20.3 k
	Length (m)	Diameter (m)	Max Op Temp (°C)	Max Op Pressure (bar)	No. of Valve Trays	Rental Cost ($/mo.)
Column A	9	.5	300	11	20	5.8 k
Column B	10	.6	300	7	24	7.9k
Column C	10	.8	300	15	24	11.9k

Each reactor maintains the same L/D ratio, max operating temperature, and max operating pressure. As reactor size increases, the rental cost increases, along with conversion of methanol to DME. Each column maintains the same max operating temperature, but varies in L/D ratio, max operating pressure, and the number of valve trays included. As column size increases, the rental cost increases and the separation capability improves. The available heat exchangers are shown below in Table 4.

Table 4: Heat Exchanger Toller Specifications

	Area (m^2)	Max - Tube P(bar)/T(°C)	Max - Shell P(bar)/T(°C)	Configuration Shell-pass	Tube-pass	Rental Cost ($/mo.)
Exchanger A	125	15/150	15/150	1	2	5.9 k
Exchanger B	90	15/300	50/300	1	2	4.5 k
Exchanger C	60	15/150	15/400	1	2	3.7 k
Exchanger D	40	20/300	15/180	1	1	3.4 k
Exchanger E	180	20/300	50/300	1	2	6.7 k
Exchanger F	100	15/150	15/150	2	4	6.1 k
Exchanger G	20	20/300	15/180	1	1	1.1 k
Exchanger H	150	50/300	15/300	1	1	6.1 k

Each exchanger has its own max specifications for the shell and tube side, as well as its own number of shell and tube passes. There was no dedicated submodel in the simulation software to investigate the effects of shell and tube passes, so it was not considered for this phase of the project. As exchanger size increases, the rental cost increases, except for Exchanger A.

To streamline the optimization process, the team decided to construct a set of equations, dubbed the "Equation World Model," using conditional statements in the simulation software. The goal of the model was to identify the rental costs based on the pieces of equipment used in the simulation, solve for the utility costs of the process, and check whether the process conditions associated with a given piece of equipment were below the specified maximums.

Equation World proved to be helpful in quickly determining the viability of a particular set, and it allowed the team to quickly evaluate the economic feasibility of a given set. Figure 3 below shows an example of the Equation World Model's evaluation of a heat exchanger in the process. Since the formulas created could only report numbers for various outcomes, the 100 specifies a parameter falling below a maximum threshold, and the -888 specifies a parameter exceeding the maximum. These numbers were simply chosen to be eye catching when looking through the flowsheet. Since three checks did not pass in this example, this would be an example of an exchanger that was not a viable option.

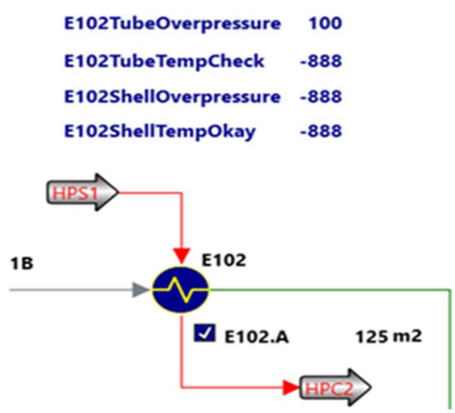

Figure 3: Example Operating Condition Checks from Equation World

To limit the number of equipment combinations that needed to be examined, the team identified several constraints in the given list before delving too greedily and too deep into optimization. Exchanger C was the only viable choice for E-103, the reactor effluent cooler, as it was the only exchanger that could handle the high temperature of the reactor effluent stream. The other exchangers were limited to 300 °C operating temperatures. At all examined reactor conditions, the product stream leaving the reactor was well above this 300 ºC cutoff. Also, Column B was not initially considered for optimization. The team would take a more rigorous analysis of this option later in the project, however. The tower pressure of the base case was well above the 7-bar limit of this column, and the simulation did not tend to converge below this pressure when process conditions were modified. Lastly, the reactor feed preheater (E-102) was narrowed down to either Exchangers B or E, as these had high enough shell pressure limits for the utility of high-pressure steam (HPS) that was used here. High Pressure Steam was the only available utility that was present in a higher temperature than the process stream in this exchanger. Exchanger H would have been a possible choice had the HPS been fed through the tube side, but when this change was implemented, the simulation would not converge. Changing heat exchanger configuration required breaking stream connectivity in the simulation, which resulted in it being not properly specified, so when the streams were reconnected, the simulation was unable to reach its prior solved state. With these constraints identified, the team was able to move more confidently into the optimization process.

Following the design “onion” strategy of optimization, the team began by analyzing the reactor and moving to other unit operations from there. The initial hypothesis was that renting a larger reactor would lead to reduced condenser and reboiler duties. This was true when comparing to the base case reactor but false when comparing between available reactors. As shown in Table 5, the duties generated when using the Toller reactors were lower than the base case, but they remained the same as reactor size increased from Reactor A to Reactor C. Reactor B was not able to be solved when put into the simulation, as it did not have a high enough conversion to produce the required amount of DME due to its small size. From these results, Reactor A was decided on because of its lower rental cost.

Table 5: Effect of Reactor Choice on Condenser & Reboiler

Reactor	Rental Cost	Conversion of Methanol	Reboiler Duty	Condenser Duty
Base Case	$10.0K	81.0%	302 kW	580 kW
Reactor A	$6.31 K	84.19%	285 kW	560 kW
Reactor B	Simulation Did Not Converge			
Reactor C	$20.3K	84.24%	285 kW	561 kW

The team then optimized the reboiler, column, and other heat exchangers. To reduce reboiler duty even more, the smallest available heat exchanger was selected (Exchanger G). This was also the best option for reducing column flooding, as each available column had an 80% flooding limit. Due to the column pressure exceeding 11 bar, Column C was the only viable selection. The rest of the heat exchangers were then sized by selecting the options most closely resembling each of their sizes in the base case model. Table 6 shows the first optimized equipment set, coming out to an overall yearly cost of $742,000.

Table 6: Equipment Set 1 Unit Operations and Yearly Expenses

Equipment Set 1			
Equipment on PFD	Toller's Equipment	Yearly Rental Cost	Yearly Utility Cost
R-101	Reactor A	$ 120,000	$ -
T-101	Column C	$ 142,800	$ -
E-101	Exchanger F	$ 73,200	$ 174,975
E-102	Exchanger B	$ 54,000	$ 34,414
E-103	Exchanger C	$ 44,400	$ 13,512
E-104	Exchanger D	$ 40,800	$ 3,539
E-105	Exchanger G	$ 13,200	$ 27,248
	Yearly costs	$ 488,400	$ 253,689
	Overall Yearly Cost	$ 742,089	

After the development of the first optimized design, the team optimized the alternate equipment sets and operating conditions. Going into subsequent equipment sets, the team decided Exchanger G, the smallest available option, should be reserved exclusively for reboiler service. This provides for two advantages: it minimizes the reboiler duty, keeping the utility cost associated with this exchanger low, and helps avoid the flooding limit of the column by sending less vapor up to the condenser. Upon deciding on this new constraint, the team set about the process of performing further process optimization.

For the design of the second equipment set, the team was able to reduce the size of both the packed bed reactor and the distillation column by manipulating the utility usage in the distillation column. By swapping the condenser with a larger heat exchanger, Exchanger B, the column was able to send more reflux from the overhead. By increasing the reflux flow rate returned to the column, the column was able to achieve a similar level of separation as in Set 1 with less valve trays. This enabled the use of a smaller packed bed reactor by allowing the process to achieve the specified product purity with less methanol conversion. Through reducing the size of both unit operations, the rental costs for the skid mounted equipment were significantly reduced. This strategy reduced the overall rental cost associated with the process from $488,000 for Set 1 to $408,000 for Set 2. The cost of implementing this change, however, was the increase of the plant's utility cost from $254,000 in Set 1 to $281,000 in Set 2. This is as expected, as the main optimization strategy explored for this equipment set was the reduction of rental cost by providing more reflux to the distillation column by installing a larger condenser.

Table 7: Equipment Set 2 Unit Operations and Yearly Expenses

Equipment Set 2			
Equipment on PFD	Toller's Equipment	Yearly Rental Cost	Yearly Utility Cost
R-101	Reactor B	$ 75,720	$ -
T-101	Column A	$ 69,600	$ -
E-101	Exchanger A	$ 70,800	$ 177,605
E-102	Exchanger E	$ 80,400	$ 36,392
E-103	Exchanger C	$ 44,400	$ 13,749
E-104	Exchanger B	$ 54,000	$ 5,398
E-105	Exchanger G	$ 13,200	$ 47,502
	Yearly costs	$ 408,120	$ 280,647
	Overall Yearly Cost	$ 688,767	

Upon completion of the second equipment set, the team moved into further optimization to determine the best possible equipment set. One of the primary optimization strategies for further equipment sets was a reduction of distillation column pressure. Reducing pressure would decrease the heating and cooling temperatures in the reboiler and condenser, respectively. If the reboiler's heat source could be changed from medium-pressure steam (MPS) to less expensive low-pressure steam (LPS), while maintaining the condenser's heat sink of cooling water, utility costs would decrease. The team had previously decided that Column B would not be considered for initial optimization; however, this was more closely analyzed at this stage of the project. It was observed that AVEVA Process Simulation did not allow for a high degree of manual control over column pressure, due to the "ignore inlet pressures" setting that had been enabled in the provided base case simulation. This setting precluded the team from simply using valves on the feed or reflux to reduce column pressure. Disabling this setting typically resulted in a failed solution state, but the team was able to converge the simulation once with reduced distillation column pressures. At a column pressure less than seven bar, the column tended to exceed the maximum flooding limit unless the largest distillation column was used. This flooding made for less effective separation, as the increased vapor flowrate up the column at this lower pressure led to more entrainment of the liquid flowing down the column. Since the reduction of pressure required the largest column, it was not determined to be economically attractive, so reducing column pressure was not considered an optimization strategy going forward.

One method of optimization examined by the team after completion of Set 2 was to reduce the duty on the reactor feed heat exchangers. This was accomplished by lowering the preheat temperature of the reactor feed and therefore the duty associated with the preheater. To reach our product purity specifications at this reduced reaction temperature, however, required the use of a larger reactor to achieve a comparable methanol conversion.

Table 8: Equipment Set 3 Unit Operations and Yearly Expenses

Equipment Set 3			
Equipment on PFD	Toller's Equipment	Yearly Rental Cost	Yearly Utility Cost
R-101	Reactor A	$ 120,000	$ -
T-101	Column A	$ 69,600	$ -
E-101	Exchanger A	$ 70,800	$ 175,051
E-102	Exchanger B	$ 54,000	$ 33,904
E-103	Exchanger C	$ 44,400	$ 13,610
E-104	Exchanger F	$ 73,200	$ 5,371
E-105	Exchanger G	$ 13,200	$ 48,799
	Yearly costs	$ 445,200	$ 276,734
	Overall Yearly Cost	$ 721,934	

By reducing the reactor preheat duty, the team was able to reduce the yearly utility cost by approximately $4,000. This came at the added expense of a larger reactor, however, which added $45,000 to the yearly rental cost. This set did not provide an economic advantage over the second set, because this increased rental cost offset the savings gained through reduction of preheat duty. This was the second-best optimized set developed during the optimization process. After exploring many avenues for optimizing the second set, it was determined Set 2 was the best equipment set that had been found by the team.

Chapter III: Process Safety and Environmental Concerns

Methanol and DME have several safety concerns for the proposed DME production process. The hazard diamonds for these two chemicals show that there are moderate health concerns due to possible irritation to exposed body parts while also being irritating to the respiratory tract if the fumes are inhaled. There are also concerns for the flammability of both chemicals due to the low flash points. However, DME has a low reactivity risk due to possible reactions with oxygen while methanol has no reactivity concerns. Taking these concerns into account, the team was able to provide safety recommendations that are relevant to the DME production process.

The first recommendation was to follow the OSHA guideline 1910.119, which places this process under PSM (Process Safety Management) standards. Although this guideline could be worked around, the recommendation stands that this should be a PSM operation in the interest of operator safety. Under these standards the plant personnel will be required to use personal safety equipment. The equipment involved will include hard hats, steel toe boots, arm coverings, leg coverings, and eye protection. From there, the next concern includes the temperature and pressure associated with the equipment in use. Because the reactor is operating at higher pressures and temperatures, a deluge system would be recommended to lower the risk of a runaway reaction caused by a potential fire. To decrease the risks of spills, the methanol feed tank and the DME storage tank should be fitted with high and low-level alarms which will indicate when the liquid level within the tank reaches 90% and 10% of the height of the tank, respectively. The DME will be produced and stored as a saturated liquid at 30 °C, requiring a pressure of about 7 bar. This storage tank would need to be insulated to avoid ambient temperature fluctuations and pressurized. Thus, the next stage of concern would be the possible over pressurization of certain pieces of equipment, such as this tank, of which there would need to be pressure relief valves included. Along with the DME storage tank, the pertinent equipment identified were the reactor, distillation column, methanol feed tank, and discharge line of both the methanol feed pump and the reflux pump. These pressure relief valves should be piped to catch tanks to contain the chemicals and prevent over pressurization. The next recommendation is to place conservation valves on every tank to maintain a nitrogen blanket within the tank. This will also lower the flammable vapor space and reduce the contact of oxygen with DME and methanol.

Several safety recommendations have been developed to minimize the effect of any incidents that go unprevented. The first recommendation is to place containment dikes around equipment for spillage risks and to contain and prevent the spread of fires. This will include the methanol feed tank, DME storage tank, and the distillation column. The next recommendation is to include dry chemical fire extinguishers within the process site. This is a recommendation from NIOSH guidelines, as these extinguishers are more effective than water for fighting small methanol fires. It is also suggested that Toller equipment be placed in the coverage zone of existing fire monitors, if any are present in the methanol plant, or that fire monitors be installed near the Toller equipment if none are present. This will provide an emergency firefighting option for plant personnel in case of a large fire.

An area of significant environmental concern for this plant is the presence of large aboveground storage tanks that will be used to contain the methanol feed and DME product.

Spill prevention needs to be accounted for in all storage tank loading or unloading operations. The wastewater treatment facility used to treat the process water coming out of the distillation column is another aspect of the chemical process with heavy environmental impact potential. The chemical fate of the impurities removed from the wastewater stream should be decided based upon relevant environmental regulations and best engineering practices. A certain amount of fugitive emissions will be present within this chemical process, as they are inherent in all chemical plants, and these should be considered when making any environmental evaluations.

To create a more sustainable process, heat integration networks could be set up between the existing methanol plant and the DME plant. This would reduce the utilities needed for heat transfer operations. Also, a larger conversion of methanol, which was targeted for in the team's optimization strategies, would mean less unreacted methanol would be present downstream. This is defined as an example of the most desirable waste management strategy, source reduction, under the Pollution Prevention Act of 1990. This would reduce the load on the methanol separation and purification process, which is outside the scope of the DME plant, as well as reduce the amount of wastewater coming from the process that would need to be treated. The team's optimization of condenser and reboiler duties is also environmentally beneficial, as it minimizes the energy consumption and utility usage needed for separation.

Chapter IV: Sensitivity Analysis

The effect of the incoming methanol purity on the economics of the proposed DME production process was evaluated. As shown in Figure 4, as the purity of the feed methanol decreased, the overall utility cost increased. This was expected due to the increased duties for all heat exchangers that exist downstream. The most notable increase came from the condenser and reboiler because of the much larger duties required to maintain the same purity of product DME. It should also be noted from Figure 4 that the lower limit of the purity was found to be roughly 98 mol%. This was the lowest purity that was able to be solved within the simulation, so if a lower purity feed were to be used, an additional distillation column would be required. This column would likely be located just after the methanol feed. Alternatively, one could be placed sequentially to the original column, or the number of trays in the present column could be increased.

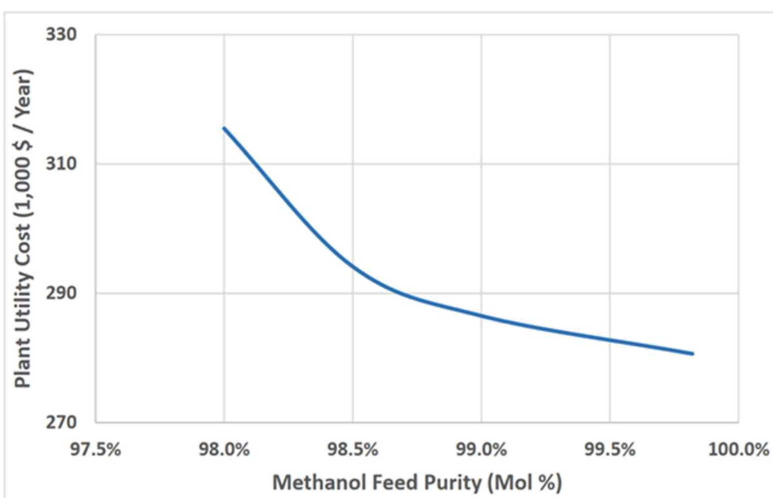

Figure 4: Effect of Methanol Feed Purity on Plant Utility Cost

The team was also able to analyze the effect of the methanol purity on the overall profit margin from selling DME as shown in Figure 5. Because there was no way to quantify the change in methanol price as compared to the drop in purity, it was assumed the price remained constant. In a real-world scenario, it would be expected that a less pure methanol feed would cost less to produce or purchase. Therefore, Figure 5 shows a worse-case scenario on the affected profit margin. The data showed that the overall drop in profit was roughly 3%, which was partially due to the increased duty costs presented in Figure 4.

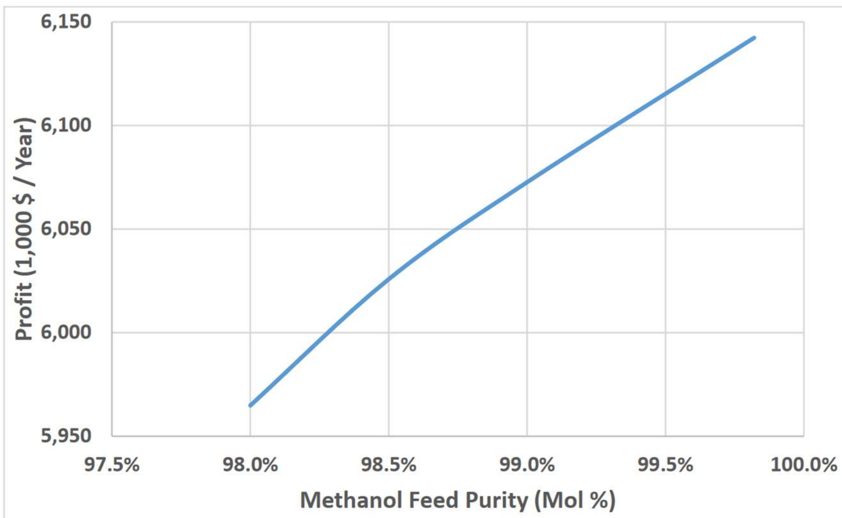

Figure 5: Effect of Methanol Feed Purity on Profit

Chapter V: Report Recommendation

The engineering team used the overall process economics to determine the final recommendation regarding the DME process based on the best optimized set presented in Table 7. As shown, the methanol cost was the largest deficit present in the proposed process. However, the revenue from the sale of the DME is projected to significantly offset the methanol cost. The team is projecting that the proposed process has a potential 6-million-dollar profit margin. Based on these projections and the feasibility of the proposed DME process, the engineering team is recommending the current process to move forward to the next step in the process design.

Table 9: Economics of Optimization

Expense / Sale	Amount ($/Year)	
Methanol Cost	$	(6,900,008)
Toller Equipment Cost	$	(408,120)
Utility Cost	$	(280,647)
DME Revenue	$	13,731,071
Total	$	6,142,296

To move forward with the design process, it is recommended that the next step is to look further into the DME column optimization by using an alternative process simulation software like ChemCAD or AspenPlus that would be able to examine the effects of column pressure on separation efficiency more accurately. This would attempt to find an option that would allow for a lower pressure within the column. Next, the process control loops and the piping and instrumentation diagrams for the process would need to be developed. Once all design decisions have been finalized, piping isometrics would need to be created to determine the layout of all process equipment. The engineering team has confidence in the proposed DME process and feels that a finalized design will be economically feasible. By setting the plans in motion now, the company can be ready for its impending methanol customer loss and can start producing DME as soon as that customer's current contract ends.

Conclusion

The completion of this project gave the team a greater understanding of process optimization. Personally, I learned a great deal about how to approach a large-scale problem and how to give effective status reports to management. I also honed my communication skills through this project – with my professors, my teammates, and technical support. While the work involved was mostly a team effort, I took leadership in several key areas. I was the group's designated note taker in the early stages of the project, when we constantly ran into technical problems and had to figure out how to resolve them. This also applied to recording status report feedback, which helped the team continuously improve our delivery of the key pieces of information surrounding our progress. This role transitioned into a keeper of the management of change document as we entered the actual optimization portion of the project. This proved to be helpful when checking that the recorded equipment sets matched up with the specified equipment sizes in our simulation files. On the simulation side, I was an early adopter in the power of the SELECT function as a substitute for a nested IF function, which helped in the creation of the EAOC-related equations in Part 1 and of the Equation World Model in Part 2. I also led the charge in pursuing the lower pressure column, Column B, which could have given us a new best optimized set. While this was ultimately unsuccessful, it helped the team decide to pursue other options to the end to ensure that there were not any lower cost sets we were missing. Lastly, I presented on and wrote the first half of the Optimization Logic section in our final presentation and final report, respectively.

Bibliography

Turton, R.; Shaewitz, J. A.; Bhattacharyya, D.; Whiting, W. B., Analysis, Synthesis, and Design of Chemical Processes, 5th edition, Prentice Hall, 2018.