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# Process Design and Optimization of a Once-Through Dimethyl Ether Process Using AVEVA Process Simulation

Jerrod Scott
*University of Mississippi*

# PROCESS DESIGN AND OPTIMIZATION OF A ONCE-THROUGH DIMETHYL ETHER PROCESS USING AVEVA PROCESS SIMULATION

By

Brandon Jerrod Scott

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Approved By

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Advisor: Dr. Adam Smith

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Reader: Professor Michael Gill

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Reader: Professor David Carroll

# DEDICATION

This thesis is dedicated to my friends and family who have supported and encouraged me throughout my time here at the University of Mississippi.

ACKNOWLEDGEMENTS

I would like to formally state my deepest thanks to Dr. Adam Smith, Professor David Carroll, and Professor Michael Gill. Each has taken the time to not only be an excellent professor but to be an amazing mentor to me throughout my time here at the University of Mississippi. Their constant support helped push me to be the person that I am today. Because of them, I feel confident and well equipped to pursue my professional career as an engineer.

In addition, I would like to thank Miranda Nolan, Joshua Peltan, and Levi Petix for their help in completing this project. I could not have asked for a better team. Each of them put in the time and effort to pursue this project wholeheartedly. We had to utilize a new software, AVEVA Process Simulation, to model and optimize this project. Joshua learned this software very quickly and provided his expertise in DOE to help us model our runs and find our most optimal solutions. Levi and Joshua did an excellent job at troubleshooting our simulation files and preparing them for optimization. Miranda was a huge assistance in helping me run the optimizations on all of our files. She also helped me in properly reporting our solutions and keeping all of our documentation neat and organized for status reports and submissions. Miranda, Joshua, and Levi have given me permission to utilize our findings in my thesis. They are all exemplary students, and I am excited to see them pursue their professional careers. I am honored to call them my friends.

ABSTRACT

The primary purpose of the project on which I wrote this thesis was to design an optimize a once-through dimethyl ether process utilizing a software called AVEVA Process Simulation. The process was initially modeled and optimized to minimize the EAOC of the distillation column. The result of that effort was an optimized column with six stages with the feed entering the column at stage six. It had a height of 3 m, diameter of 0.44 m, and an EAOC of $65,100. This optimized solution was submitted to a Toller. The Toller provided available equipment to model the plant. From here, another optimization was conducted to find the appropriate equipment combination that would have both the lowest rent and utility cost. This solution was then further optimized by manipulating process variables such as temperature, pressure, and feed stage. The most optimal configuration was reactor B and column A. The metric used to gauge the most optimal configuration is the total annual cost which includes rent and utilities. After optimization, the estimated utility and rent cost for the entire process was approximately $642,000 per year. Of course, there are other costs to consider such as raw materials and labor, but they are not included in this price. The final recommendation is to proceed with this project considering the fixed equipment cost and economic potential of $6.8 million per year. The next steps would be complete a more thorough economic analysis and purchase the equipment from the Toller to get the process running as soon as possible to increase potential profit.

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## LIST OF ABBREVIATIONS

| | |
|---|---|
| DME | Dimethyl Ether |
| EAOC | Equivalent Annual Operating Cost |
| MeOH | Methanol |
| RSM | Response Surface Methodology |

## Basics of Process Design and Optimization

Process design and optimization are two of the many tasks that are encompassed in chemical engineering. Chemical engineers utilize their knowledge of subjects such as biology, chemistry, mathematics, and physics to create and innovate manufacturing processes that provide useful resources such as specialty chemicals, fuels, pharmaceuticals, food, and so much more.

Process design refers to arranging and sizing various process equipment in order to turn raw materials into a desired product. The primary process equipment in the once-through dimethyl ether process is a reactor, a distillation column, and some heat exchangers. A reactor is a vessel in which chemical reactions occur. Feed streams introduce reactant into the vessel where they are converted to products. The products and unreacted reactants leave the reactor and proceed to the next piece of process equipment. Distillation columns are utilized to separate components based on their volatility and boiling points. Components with lower boiling points and higher volatility will vaporize, rise, and leave out of the top of the column. This top stream is condensed to a liquid and is referred to as the distillate. Components with higher boiling points and lower volatility will remain a liquid and leave through the bottom of the column. This bottom stream is referred to as the bottoms. Heat exchangers facilitate the transfer of thermal energy from one fluid to another. For example, a utility such as cooling water can be used to cool a process stream to a desired temperature.

Optimization concerns the manipulation of various process variables and equipment to minimize the operating cost of the process. Manufacturing processes are expensive, so it is important to save money wherever possible in order to maximize profit. For this project, process variables such as temperature, pressure, and boil-up ratio (fraction of vapor returned to the bottom of the column to the bottom product removed) were manipulated using AVEVA Process Simulation's Optimization Tool. The tool essentially changes the specified process variables in order to meet the defined specifications. Those equipment and operating conditions are then evaluated to find the minimum EAOC. The desired result in this scenario would be minimized operating cost to produce the required DME.

## Introduction

The data for this project was acquired through participation in the AVEVA Academic Competition. The premise of this project is that there is a chemical company that produces commercial grade methanol (MeOH) that it sells to two customers through long term contracts. One of these customers has recently experienced a significant economic downturn and decided not to renew their contract for 23,000 tonnes per year of MeOH.

There are essentially three options available to mitigate this contract failure. Methanol production could be reduced, but this would obviously result in a reduction of profit. Another option, the methanol could be sold on the open market; however, the market for methanol is currently oversaturated and would require the methanol to be sold at a spot price that is low in comparison to the contract price. The final option would be to convert the excess methanol to dimethyl ether. This option makes the most sense due to the oversaturated market for methanol. This project is desirable because it has an economic potential of $6.8 million annually and will likely yield a high rate of return.

In Figure 1, a basic block flow diagram is provided that outlines that major unit operations in the once-through dimethyl ether process. The process shown is unusual in that the methanol is not directly recycled. The methanol-water separation unit already exists within the plant thus making this a once-through or single pass process.

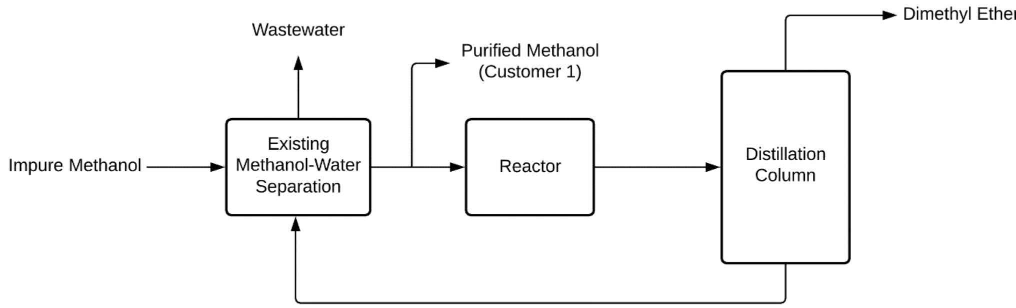


*Figure 1: Block Flow Diagram of Once-Through Dimethyl Ether Process*

After developing the optimized base case scenario, the design specifications were provided to the Toller who provided a list of equipment available to rent. From here, a secondary optimization utilizing the available equipment was done to find the optimal configuration. This provided a more realistic understanding of how much this process costs to operate.

# Chapter 1: Base Case

The base case of the once-through dimethyl ether process was modeled utilizing AVEVA Process Simulation. The tower within the process was optimized utilizing both the native optimization tool and manual calculations to find locally optimized areas. The most optimized tower has six trays, with the feed entering at tray six. This tower has an approximate equivalent annual operating cost (EAOC) of $65,100. A stream table and equipment data sheet are provided Table 1 and Table 2.

A base case model was created using the provided process flow diagram as a guide. The reaction kinetics data provided in the problem statement were used to generate a sub-model for the reactor. All relevant equipment was placed on the flowsheet, connected and specified properly, and equations were used to control the methanol recycle stream. Next, several additional heat exchanger trains were designed to simulate the different zones in the heat exchangers where a process stream undergoes both sensible and latent heat transfer. From these heat exchanger trains, which are multiple heat exchangers in a row, accurate heat exchanger areas were found. Finally, a series of equations were used to calculate EAOC, and once the simulation was confirmed to be square, spec, and solved the optimization process began.

To optimize the tower and heat exchanger system, a strategy was used which combined the native optimizer utility and response surface methodology (RSM) for factors which could not be automatically adjusted in the optimizer. The optimizer utility was used to adjust the reflux ratio and column diameter while holding the flooding of the top stage between 0.3 and 0.8 of the flooding limit. For column setups where the feed stage was not the bottom stage, flooding on lower stages were brought into the specified range by adjusting stage diameter. A minimum stage height of 0.5 m was used, as recommended by the heuristics provided in *Analysis, Synthesis, and Design of Chemical Processes* (Turton). The number of stages and feed tray location were adjusted manually, and the output of minimized EAOC, for a given pair of stages and feed location, was plotted on a response surface.

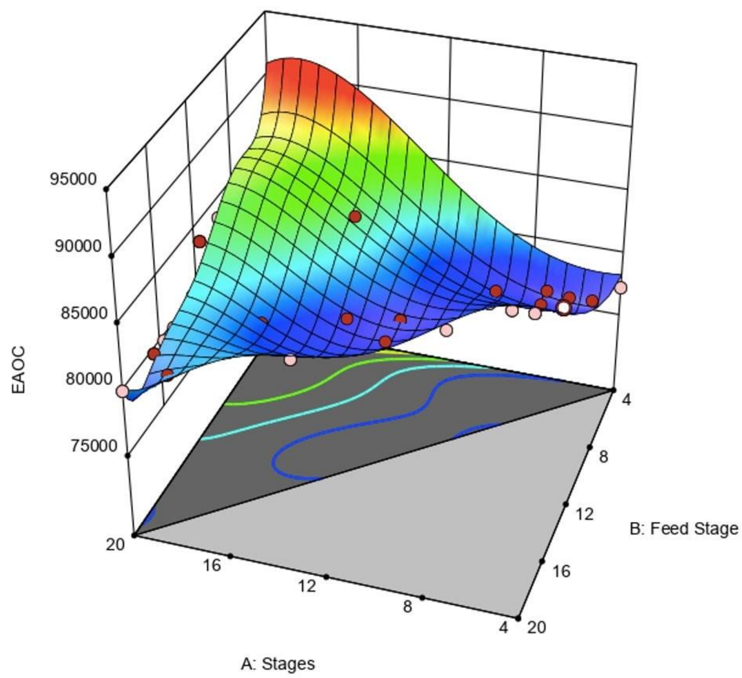


*Figure 2: Response Surface Model Showing EAOC with Varying Stage Number and Feed Stage Location*

Initially, a broad search from 20 to 3 stages was performed to locate areas of interest using RSM. This is reasonable range that will provide crude estimates as to where the minimum can be found. During this initial screening, three feed locations were used for each column with a given number of stages. The first feed location was the bottom stage, the second was the highest stage where the mass and energy transfer was sufficient to meet distillate specifications, and the last location was one approximately in the middle of the two extremes. An exception being the column with 3 stages, where the only solution found was where the feed tray was stage 3. Once the area of interest was identified, a more granular search between 4 and 8 stages found that the optimal tower has 6 stages with a feed tray location of 6. For each of these towers, every feasible feed tray location was examined. Figure 1 above shows the surface plot generated by this process, where the X-axis is the feed stage, the Y-axis is the number of stages, and the Z-axis is the minimized EAOC found using the native optimizer utility.

The optimized tower configuration has a diameter and reflux ratio of approximately 0.441 m and 0.662, respectively. The EAOC of the system is highly sensitive to small variations in reflux ratio. Adjusting the reflux directly impacts the duty of exchangers as well as the amount of utility required. A 1% increase of reflux ratio results in an EAOC increase of nearly 11%. Although this sensitivity is worth mentioning and is important in a practical sense, it is outside the current scope of analysis. While it is impossible to conclude with certainty that the tower configuration found in this study is the most optimal, without a comprehensive search of feasible parameter space, one can be reasonably confident that the solution is the most optimal configuration due to the use of both broad and narrow parameter searches. Barring any unaccounted-for discontinuities, the coarse response surface model should identify the approximate region where the optimal solution exists, and the comprehensive search of said region will reveal the local minimum. In principle, this minimum should correspond to the global minimum. Table 1 and Table 2 provided on the following page provided a detailed stream table and equipment data table, respectively. This is the data that was provided to the Toller.

*Table 1: Stream Table for Optimized Base Case Scenario*

| | Stream 1 | Stream 2 | Stream 3 | Stream 4 | Stream 5 | Stream 6 | Stream 7 | Stream 8 | Stream 9 |
|---|---|---|---|---|---|---|---|---|---|
| Temperature (°C) | 30.0 | 30.5 | 140.0 | 250.0 | 376.5 | 30.0 | 97.9 | 30.0 | 30.0 |
| Pressure (bar) | 1.01 | 10.95 | 10.85 | 10.75 | 10.59 | 6.79 | 10.11 | 1.01 | 1.01 |
| Vapor Fraction | 0.00 | 0.00 | 1.00 | 1.00 | 1.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| Mass flow (tonne/h) | 2.66 | 3.28 | 3.28 | 3.28 | 3.28 | 1.89 | 1.39 | 0.75 | 0.62 |
| Molar flow (kmol/h) | 83.14 | 102.35 | 102.35 | 102.35 | 102.35 | 41.13 | 61.22 | 41.50 | 19.21 |
| Component flows | | | | | | | | | |
| DME (kmol/h) | 0.00 | 0.00 | 0.00 | 0.00 | 41.38 | 40.84 | 0.54 | 0.00 | 0.00 |
| Methanol (kmol/h) | 83.00 | 102.17 | 102.17 | 102.17 | 19.41 | 0.24 | 19.17 | 0.00 | 19.17 |
| Water (kmol/h) | 0.15 | 0.18 | 0.18 | 0.18 | 41.56 | 0.06 | 41.50 | 41.50 | 0.03 |

*Table 2: Equipment Data for Base Case Scenario*

| Equipment | L (m) | D (m) | Max Op Temp (°C) | Max Op Pressure (bar) | Catalyst Volume ($m^3$) | Pressure Drop (kPa) |
|---|---|---|---|---|---|---|
| Reactor (R-101) | 6.19 | 1.00 | 376.5 | 10.8 | 2.91 | 15.9 |
| | L (m) | D (m) | Max Op Temp (°C) | Max Op Pressure (bar) | #Trays/Feed Tray | Pressure Drop (kPa) |
| Column (T-101) | 3.3 | 0.44 | 97.8 | 10.08 | 6 / 6 | 13.5 |
| | A ($m^2$) | Max - Tube P(bar)/T(°C) | Max - Shell P(bar)/T(°C) | Configuration S-Pass T-Pass | | Pressure Drop (kPa) |
| Exchanger (E-101) | 34.3 | 10.0/180 | 11.0/140 | 1-1 | | 10.0 |
| Exchanger (E-102) | 73.9 | 46.9/260 | 10.9/250 | 1-1 | | 10.0 |
| Exchanger (E-103) | 206.2 | 3.0/40 | 10.6/377 | 1-1 | | 10.0 |
| Exchanger (E-104) | 25.9 | 3.0/15 | 10.0/30 | 1-1 | | 5.0 |
| Exchanger (E-105) | 10.0 | 4.8/150 | 10.1/97.9 | 1-1 | | 5.0 |

## Chapter 2: Design Optimization Logic and the Optimized Design

The optimized design of the column was submitted to the Toller in order to acquire a list of equipment available for rent that could accommodate the process. Unfortunately, the Toller did not have any equipment that exactly matched the design. However, the Toller identified three available reactors, three available columns, and eight available heat exchangers listed in Table 3. This response changed the task from designing the best column to optimizing the process with readily available equipment.

The strategy for optimization consisted of four phases. In the first phase, working Process Simulation files were developed for each of the nine combinations of reactor and column. In the second phase, each of those nine models were broken into two sub-models. One sub-model was optimized for lowest utility cost. The other sub-model was optimized to fit all of the cheapest heat exchangers to the process. This yields eighteen scenarios; however, it just happened that all of the lowest utility scenarios were also lowest rent scenarios. Thus, only nine unique scenarios remained after this phase. In the third phase, the combination of reactor and column with the lowest combined rent and utility cost was chosen to move continue forward with. The effect of feed tray location on overall cost was then tested. The fourth and final phase of the optimization strategy consisted of using the native optimization tool to change all allowable variables while meeting required design constraints.

*Table 3: Available Equipment Provided by Toller*

| Equipment | Length (m) | Diameter (m) | Max Op Temp (°C) | Max Op Pressure (bar) | Catalyst Volume* ($m^3$) | Rental Cost ($/mo)** |
|---|---|---|---|---|---|---|
| Reactor A | 5 | 1 | 400 | 12 | 3.93 | 10.0 k |
| Reactor B | 4 | 0.8 | 400 | 12 | 2.00 | 6.31k |
| Reactor C | 7 | 1.4 | 400 | 12 | 10.74 | 20.3 k |
| | Length*** (m) | Diameter**** (m) | Max Op Temp (°C) | Max Op Pressure (bar) | No. of Valve Trays***** | Rental Cost ($/mo.) |
| Column A | 9 | 0.5 | 300 | 11 | 20 | 5.8 k |
| Column B | 10 | 0.6 | 300 | 7 | 24 | 7.9 k |
| Column C | 10 | 0.8 | 300 | 15 | 24 | 11.9 k |

| | 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 |

The feed location analysis focused on the lowest cost portion of the column, which is the bottom nine stages, stages six through fourteen. The lowest utility cost occurs when the feed enter is the bottom stage, tray fourteen, as shown in Figure 3.

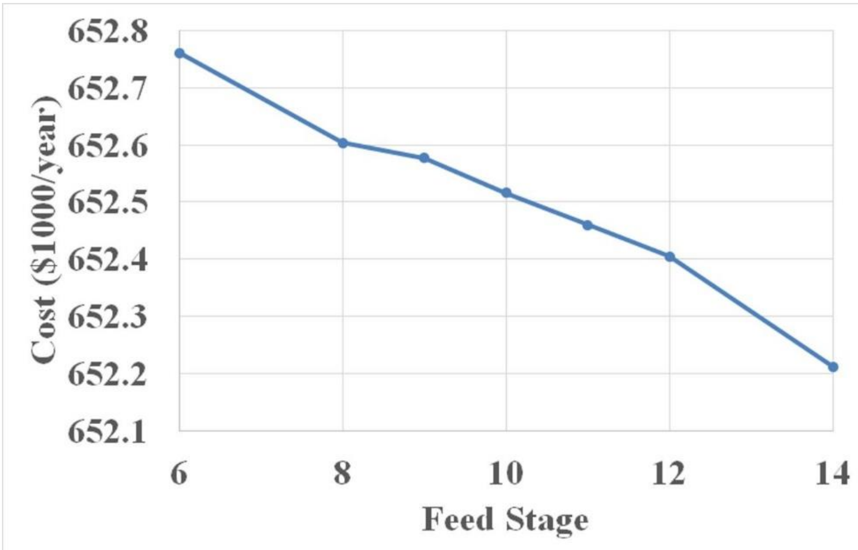


*Figure 3: Total Rent and Utility Cost vs. Feed Stage Location*

The recommended optimized configuration uses Reactor B and Column A. The column has fourteen trays with the feed entering on tray fourteen. The total rent and utility cost is $642,000 per year. The price break down is outlined in Table 4.

*Table 4: Optimized Equipment Configuration with Yearly Costs*

| **Equipment Set 1** | | | |
|---|---|---|---|
| **Equipment on PFD** | **Toller's Equipment** | **Yearly Rental Cost** | **Yearly Utility Cost** |
| R-101 | Reactor B | $ 75,720.00 | |
| T-101 | Column A | $ 69,600.00 | |
| E-101 | Exchanger A | $ 70,800.00 | $ 171,800.00 |
| E-102 | Exchanger B | $ 54,000.00 | $ 38,000.00 |
| E-103 | Exchanger C | $ 44,400.00 | $ 12,700.00 |
| E-104 | Exchanger D | $ 40,800.00 | $ 50,800.00 |
| E-105 | Exchanger G | $ 13,200.00 | $ 100.00 |
| | **Total yearly Cost** | $ 368,520.00 | $ 273,400.00 |
| | **Overall Yearly Cost** | $ 641,920.00 | |

## Chapter 3: Sensitivities

Given that equipment is being provided through a toller that only has limited equipment; the rent cost is heavily dependent on the toller having the specified equipment. For instance, if the toller happened to not have reactor B and column A, then there would be at least a $22,000 increase in cost to the next most optimal solution. This means that our overall cost is heavily dependent on equipment availability as shown in Figure 4.

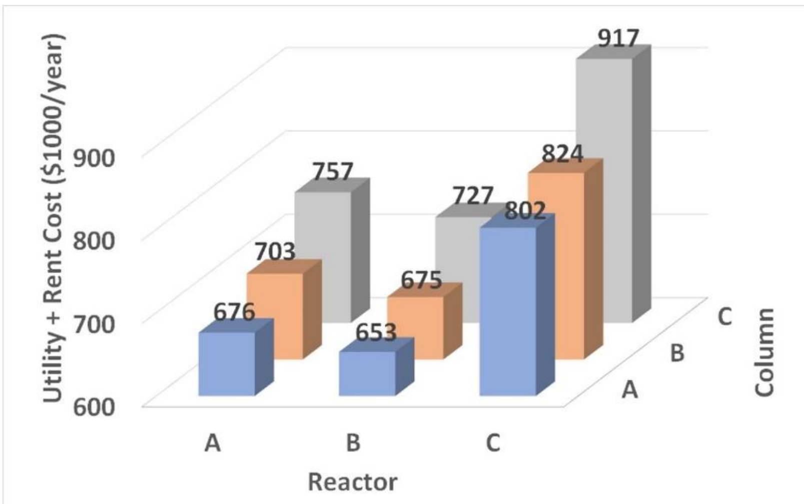


*Figure 4: Annual Utility and Rent Cost vs. Reactor-Column Configuration*

Another sensitivity of the success of this project is the supply and demand of the dimethyl ether market. There could be a point that shutting down the methanol sales all together and completely converting the plant to dimethyl ether production plant could be beneficial, and there could be a point where there is no longer a high rate of return in producing and selling dimethyl ether. There is currently not an estimate for these points, but they would be included in the detailed economic analysis included in the next phase of this project.

The start-up amount of time also is a sensitive part of this project. If the equipment and start up takes too long, this project may not be worth pursuing. For example, if the project life is seven years, but it takes two years to get the plant operating. There is a two-year window with no revenue. However, since the equipment is premade and rented from the Toller and are small enough to travel in the back of an eighteen-wheeler, it is likely this project can be put online in time to make a reasonable profit. The data acquired suggests this project would be highly profitable, so they equipment could be ordered from the Toller immediately. However, the Toller did not provide an estimation for how long it would take to ship the equipment.

The length of the contract is another sensitivity to consider. If the toller requires long term contracts, it may be determined that the risk associated with being tied to this project would outweigh the potential benefit. It is possible that the Toller would provide a better rental rate for longer term contracts, but the Toller would have to be contacted to discuss this possible discount. The contract could also affect the profitability of this project if the rental costs are not fixed over the term of the contract.

## Chapter 4: Process Safety and Environmental Considerations

Dimethyl ether and methanol are highly flammable; therefore, ignition sources should be limited and an alarm system should be included in the process to alert the employees when a fire occurs. Additionally, a deluge fire monitor system and containment dike should be installed in the plant. This will minimize damaged in the case of a fire or spill. It is important to provide the operators with proper personal protective equipment and training. It is also important that process is kept at a proper distance from occupied buildings and residential areas. Agencies such as NFPA and OSHA provide regulations for zoning, and these would need to referenced before installing the equipment onsite.

An environmental consideration is that methanol is an environmental toxin and will be removed from the wastewater using onsite wastewater treatment. To limit fugitive emissions, proper, high-quality equipment, especially valves, should be selected, installed, and properly maintained.

Methanol is miscible in water and can cause groundwater contamination. Methanol groundwater contamination is easily treated using biodegradation; however, this can be expensive (Malcolm Pirnie, Inc.). All storage vessels of methanol would need to have secondary containment to prevent the methanol leaks from entering the groundwater.

Methanol is toxic and can cause severe adverse health effects including death. For this reason, operators shall be trained on the dangers of working around such chemicals. Operator training is required to be refreshed and updated as changes are implemented in the process or standard operating conditions. Additionally, the site will need to have proper emergency systems in place such as eye wash and shower stations in the case of exposure to methanol.

## Conclusion

The process has the potential to be profitable, and it is recommended to continue the analysis. The economic potential is $6.8 million per year, and the utility and rent cost is estimated to be to $642,000 per year. The first thing to continue is perform a complete economic analysis. This will include identifying trigger prices that will determine when to either halt methanol production or consider switching to only DME production. Then, the next steps in the project would be to create a dynamic process model, draft a piping and instrumentation diagram, and develop necessary controls for the process. Some other necessary considerations are the number of employees required, the amount of time required to get the process online, and the flexibility of the rental contract from the Toller.

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## Appendix

Below is detailed process flow diagram of the once-through dimethyl ether process.