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Process and design of a once-through dimethyl ether process using aveva process simulation

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

by

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ABSTRACT

In this project, an optimization and preliminary economic analysis based on the lowest rent and utility cost was performed on a dimethyl ether process plant. This process model was performed with AVEVA Process Simulation software. Basic chemical engineering design principles as well as 3D response surface modeling and the native AVEVA optimization tool were used to select the most cost-effective equipment by varying process specifications to minimize utility cost, finding the least expensive equipment combinations possible, and selecting the feed tray location. The rental prices were fixed, so only utility and limited process specifications such as feed tray location could be varied to find the minimum equivalent annual operating cost. It was found that dimethyl ether process has the ability to be profitable with an economic potential of $6.8 million annually and the rent and utility cost being about $642,000 annually. It is recommended based on the economic potential to continue the analysis of the project as outlined in this thesis.

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Chemical Engineering Design and Optimization Basics

One task chemical engineers face is taking a desired chemical reaction and designing a process that safely and efficiently creates the product as desired. It is important to minimize wastes and utilize fluid mechanic and thermodynamic principles to produce and separate product and biproducts, wastes, etc.. Chemical engineering design is the sizing and determining of specifications of a process, and optimization is essentially getting the most production for the lowest price. Some major equipment within chemical processes are reactors, distillation columns, and heat exchangers.

A reactor is a vessel in which a reaction takes place. The raw materials enter into the vessel, react within the vessel, and exit as product, byproduct, or unreacted reagents. A distillation column is a tower in which thermal energy and pressure are manipulated to separate components based on volatility into a liquid stream, known as the bottoms, and a vapor stream, known as the distillate. Heat exchangers are used to transfer thermal energy from one fluid to another.

Chemical processes and plants can be expensive, so it is crucial to economically optimize the process by altering the process utility use and design specifications to have the lowest operating cost. Some examples of factors that can be changed for this project specifically are the location of where the tower feed flows into the distillation column, also known as feed tray location, temperatures, pressures, and what equipment is rented for the project. The base case of this project exemplifies both chemical engineering design as well as optimization on the tower, whereas the secondary case exemplifies mainly chemical engineering optimization.

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 which is not a truly viable option, but this would obviously result in a reduction of sales. 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 third option would be to utilize the excess methanol to produce dimethyl ether. This alternative appears to be desirable because it has an economic potential of $6.8 million annually and will likely yield a large profit.

In Figure 1, a basic block flow diagram is provided that outlines the major equipment required for the dimethyl ether process as well as the flow of the process. This process utilizes existing equipment and unreacted methanol to create a new product for profit.

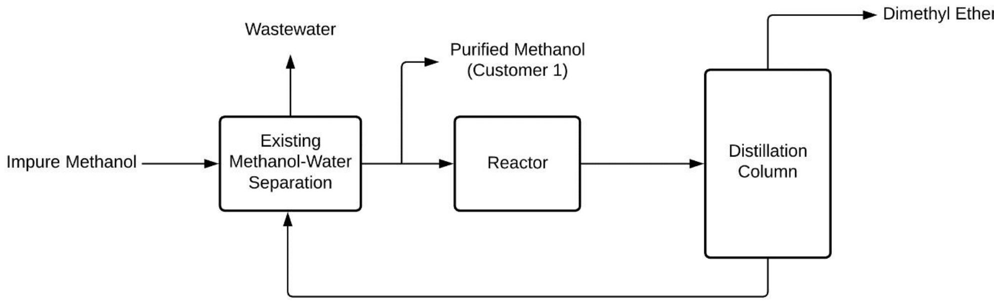

Figure 1: Block Flow Diagram of Once-Through Dimethyl Ether Process

After developing an optimized base case scenario, the design specifications are provided to the Toller who will provide a list of equipment available to rent. From here, a secondary optimization utilizing the available equipment is done to find the optimal configuration. This provides a more realistic understanding of how much this process will cost to operate.

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. These local minimums were used to ensure there were no other better options. The optimized tower has six trays, with the feed entering at tray six. This tower has an approximate equivalent annual operating cost (EAOC) $65,100. A stream table and equipment data sheet are provided Table 1 and Table 2.

A base case model was created based on 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

The native optimizer utility and response surface methodology (RSM) for factors which could not be automatically adjusted in the optimizer were used to optimize the tower and heat exchanger system. 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 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.

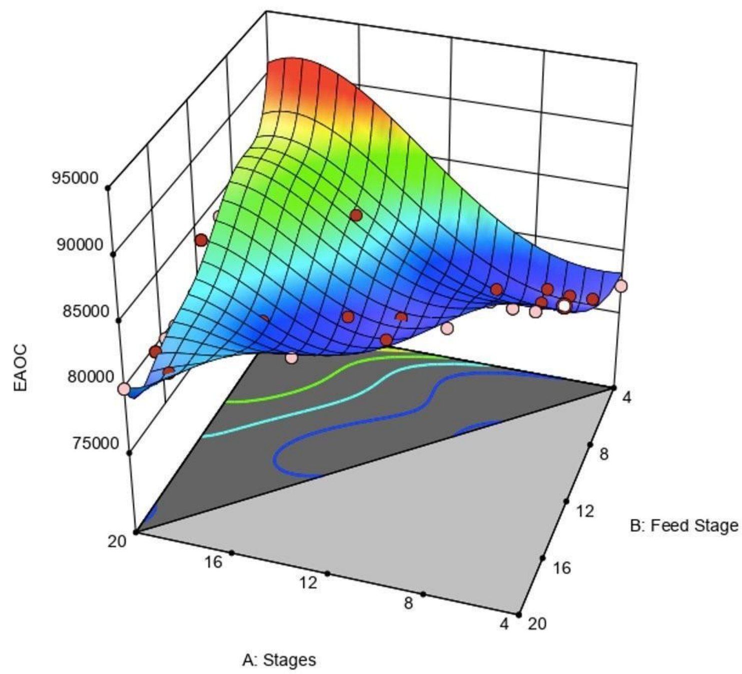

Figure 2: Response Surface Model Showing EAOC with Varying Stage Number and Feed Stage Location

Initially, a broad search from 20 to 3 stages, a reasonable range for a column, was performed to locate areas of interest using RSM. 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 that would solve, 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 extremely sensitive to small variation in reflux ratio. 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 which would require additional controls within the process, it is outside the current scope of analysis. While without a comprehensive search of feasible parameter space, it is impossible to conclude that the tower configuration found in this study is the most optimal, 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 identified 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: 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

Design Optimization Logic

The optimized design of the column was submitted to the Toller requesting a list of equipment that would potentially meet the operating specifications and product quality requirements. Unfortunately, the Toller did not have any equipment that exactly matched the design. However, the Toller responded with 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 enters the bottom stage, tray fourteen, as shown in Figure 3. It is important to note that the selected column has fourteen stages.

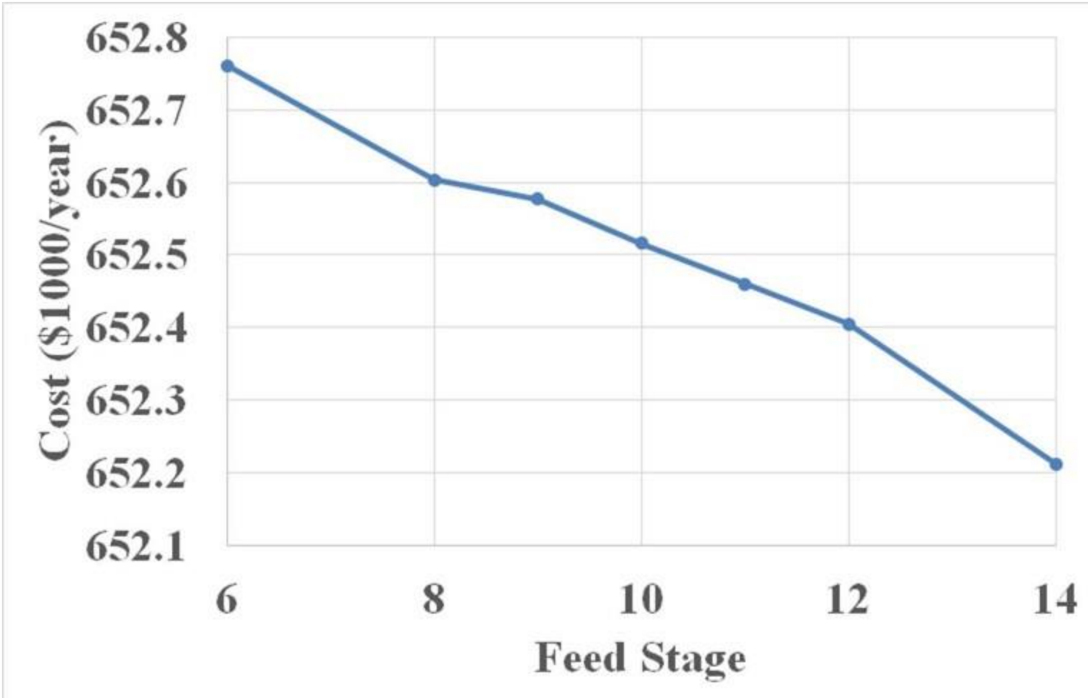

Figure 3: Total Rent and Utility Cost vs. Feed Stage Location

The Optimized Design

The 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	

Sensitivities

Given that equipment is being provided through a Toller that only has limited equipment available for rent; 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, although this is unlikely to occur if the equipment is rented in a timely fashion. This means that our overall cost is heavily dependent on equipment availability as shown in Figure 4.

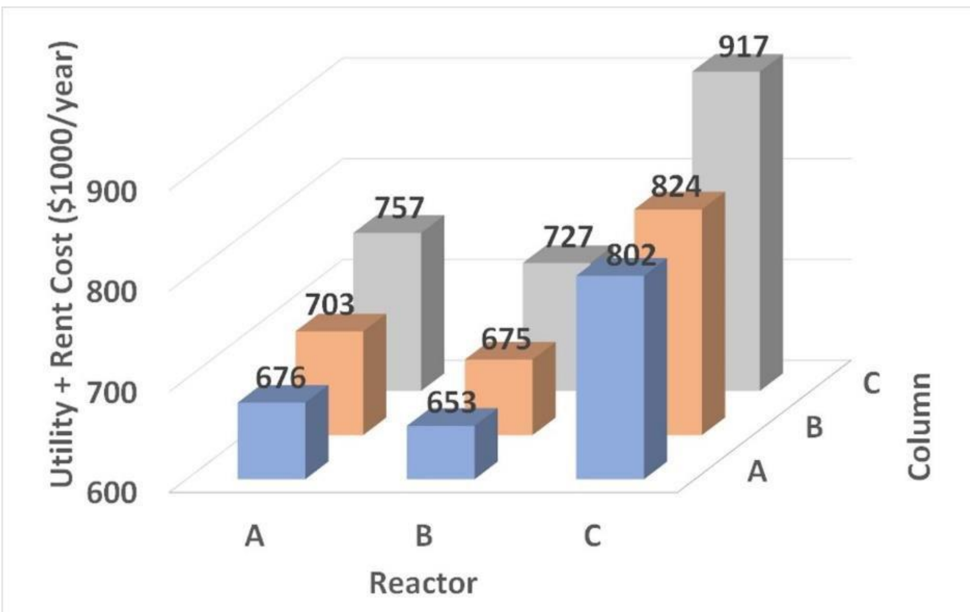

Figure 4: Annual Utility and Rent Cost vs. Reactor-Column Configuration

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.

This project is also sensitive to how soon the DME operations can start. If operations are delayed, due to delivery, installation and start-up of operations, the incentive to pursue this alternative may be significantly reduced. However, since the equipment is available now and ready to be delivered 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 a matter of months to make a reasonable profit.

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. The contract could also affect the profitability of this project if the rental costs are not fixed over the term of the contract.

Process Safety and Environmental Considerations

Dimethyl ether and methanol are highly flammable; therefore, 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. This will minimize damages 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 and safe distance from occupied buildings and residential areas.

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

Methanol is miscible in water and spills 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 such as concrete pads or dikes to drain to wastewater treatment to prevent the leakage of methanol into 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. This 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 treatment available for methanol poisoning.

Report Recommendation

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, with a profit potential of $6.1 million annually, 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. 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 additional employees required, the amount of time required to get the process online, and the flexibility of the rental contract from the Toller.

Works Cited

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APPENDIX

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