Energy Balances and Numerical Methods
Design Project

Production of Methyl Tertiary-Butyl Ether

Methyl Tertiary-Butyl Ether (MTBE) is a gasoline additive used to increase octane number that is produced from methanol and isobutylene. The purpose of this project is to continue a preliminary analysis to determine the feasibility of constructing a chemical plant to manufacture 60,000 tonne/y MTBE.

Methanol is purchased, and the isobutylene is obtained from a refinery stream. The stream contains 23% isobutene, 20% 1-butene, and 57% 2-butene, which is modeled as trans-2-butene. Only isobutene reacts with methanol; 1-butene and 2-butene are inert for this reaction.

A suggested process flow diagram (PFD) is shown in Figure 1. You should use this as a starting point only. Your primary task is to recommend operating conditions for the reactor and separators that maximize the equivalent annual operating cost, or EAOC (This term is defined later). Process improvements that increase the EAOC are also required. Any change that you can justify, and that does not violate the laws of nature, is allowed. Your assignment is to develop a "best" case, where "best" is dependent upon economic considerations, i.e., EAOC. In reporting your best case, clearly indicate the modified process and state not only the operating conditions for the (modified) process but also the corresponding values for the single-pass conversion of methanol, the overall conversion of methanol, and EAOC. Also, state any recommendations you have for additional process improvements that you were not able to incorporate into the process calculations.

Chemical Reaction

The chemical reaction to form MTBE is as follows:

$$CH_3OH + (CH_3)_2C = CH_2 \longrightarrow (CH_3)_3C - O - CH_3 \tag{1}$$

Process Description

The PFD for the (starting) process is given in Figure 1.

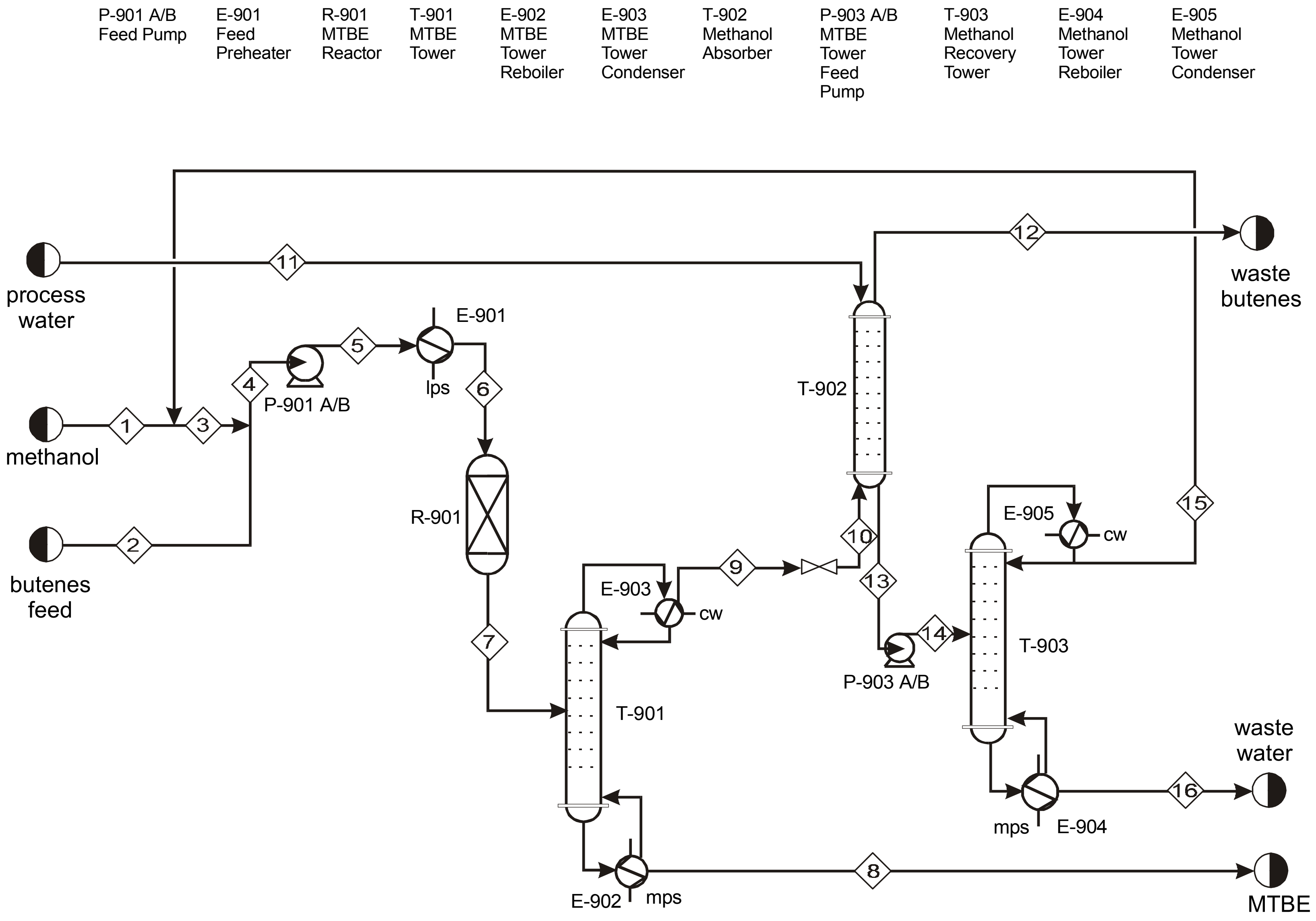

Figure 1: Unit 900 - MTBE Production Facility

Process Details

Feed Stream and Effluent Streams

Stream 1: Methanol – stored as a liquid at the desired pressure of the reaction.

Stream 2: Mixed butene stream – 23% isobutene, 20% 1-butene, 57% 2-butene.

Stream 8: MTBE product – must be 95 wt% pure.

Stream 11: Process water – see utility list for more information

Stream 12: Waste butenes – returned to refinery – contains 1-butene and 2-butene with less than 1 wt% other impurities.

Stream 16: Waste water – must be treated – must contain 99 wt% water – See the utility list for more information.

Equipment

Pump (P-901 A/B, includes spare pump)

The pump increases the pressure of the mixed feed to the reaction conditions. The liquid density may be estimated using a linear average of the pure component densities, weighted by their mass fractions in the mixture. The cost of electricity to run the pump is a utility cost based on the required power for the pump. The required power is the work multiplied by the mass flowrate of Stream 4.

Heat Exchanger (E-901)

This heat exchanger heats the feed to the reactor feed temperature. Each component must remain in the liquid phase at the chosen pressure. The cost of the heat source is a utility cost.

Reactor (R-901)

This is where the reaction occurs. The reactor is adiabatic, and the reaction is exothermic. Therefore, the heat generated by the reaction raises the temperature of the exit stream. The exit temperature is a function of the conversion. The reaction must be run at a pressure and temperature to ensure that all components remain in the liquid phase in the reactor.

Methanol must be present in the reactor feed at a minimum 200% excess to suppress undesired side reactions that produce undesired products.

The reactor operating conditions (feed and exit temperatures, pressure) are to be optimized. An operating pressure must be chosen. An optimum temperature and conversion must be determined.

Distillation Column (T-901)

This column runs at 19 atm. (The pressure is controlled by a valve, that is not shown on the PFD, in the product stream from R-901.) Separation of methanol and MTBE occurs in this column. Of the methanol in Stream 7, 98% enters Stream 9. Similarly, 99% of MTBE in Stream 7 enters Stream 8.

Heat Exchanger (E-902)

In this heat exchanger, the some of the contents of the stream leaving the bottom of T-901 going to E-902 are vaporized and returned to the column. The amount returned to the column is equal to the amount in Stream 8. The temperature of these streams is the boiling point of MTBE at the column pressure. There is a cost for the amount of steam needed to provide energy to vaporize the stream; this is a utility cost. The steam temperature must always be higher than the temperature of the stream being vaporized.

Heat Exchanger (E-903)

In this heat exchanger, the contents of the top of T-901 are partially condensed from saturated vapor to saturated liquid at the column pressure. 99% of the MTBE and water condense and 99% of all other components remain in the vapor phase. The remaining 1% of all other components condense with the MTBE. It may be assumed that this stream condenses at the boiling point of methanol at the column pressure. There is a cost for the amount of cooling water needed; this is a utility cost. The cooling water leaving E-903 must always be at a lower temperature than that of the stream being condensed.

Absorber (T-902)

The absorber runs at 5 atm and 90°C (outlet streams and Stream 11). In the absorber, 99% of the methanol in Stream 9 is absorbed into the water. All other components enter Stream 12. The cost of Stream 9 is a raw material cost. Process water sent to scrubber is controlled so that 5.0 kmol of water are used for every 1.0 kmol of methanol.

Distillation Column (T-903)

This column runs at 5 atm. (The pressure is controlled by a valve in the product stream from T-903, which is not shown on the PFD.) Separation of methanol and water occurs in this column. Of the methanol in Stream 14, 99% enters Stream 15. Similarly, 99% of water in Stream 14 enters Stream 16.

Heat Exchanger (E-902)

In this heat exchanger, the some of the contents of the stream leaving the bottom of T-903 going to E-904 are vaporized and returned to the column. The amount returned to the column is equal to the amount in Stream 16. The temperature of these streams is the boiling point of water at the column pressure. There is a cost for the amount of steam needed to provide energy to vaporize the stream; this is a utility cost. The steam temperature must always be higher than the temperature of the stream being vaporized.

Heat Exchanger (E-905)

In this heat exchanger, the contents of the top of T-903 are completely condensed from saturated vapor to saturated liquid at the column pressure. It may be assumed that this stream condenses at the boiling point of methanol at the column pressure. The flowrate of the stream from T-902 to E-905 is three times the flowrate of Stream 15. There is a cost for the amount of cooling water needed; this is a utility cost. The cooling water leaving E-905 must always be at a lower temperature than that of the stream being condensed.

Economic Analysis

When evaluating alternative cases, the objective function to be used is the Equivalent Annual Operating Cost (EAOC), defined as

EAOC = -(product value - feed cost – utility costs – waste treatment cost - capital cost annuity)

A negative value of EAOC means there is a profit. It is desirable to minimize EAOC; *i.e.*, a large negative value of EAOC is very desirable.

Utility costs are those for steam, cooling water, boiler-feed water, natural gas, and electricity.

The capital cost annuity is an ***annual*** cost (like a car payment) associated with the ***one-time***, fixed capital cost of plant construction and installation. A list of fixed capital costs on an installed basis (“installed cost”) for all pieces of equipment will be provided by mid-March.

The capital cost annuity is defined as follows:

$$\text{capital cost annuity} = FCI\frac{i(1+i)^n}{(1+i)^n - 1} \tag{2}$$

where FCI is the installed cost of all equipment; i is the interest rate; and n is the plant life, in [y]. For accounting purposes, take $i = 0.15$ and $n = 10$.

Optimization

You will learn optimization methods in ChE 230. The objective function (EAOC) is defined above. You should consider both topological and parametric optimization.

Topological optimization involves considering different process configurations (such location of process equipment, adiabatic vs. isothermal reactor). Recall that you may alter the process configuration in any way that improves the economic performance, as long as it does not violate the laws of nature.

Parametric optimization involves determining the best operating parameters for the chosen process topology. It is your responsibility to define appropriate decision variables. If there are too many decision variables to do a reasonable parametric optimization, it is your responsibility to determine, with appropriate justification, which ones most significantly affect the objective function. Then you should focus on only those decision variables.

Utility Costs

Low-Pressure Steam (618 kPa, saturated, cost or credit)	\$7.78/1000 kg
Medium-Pressure Steam (1135 kPa, saturated, cost or credit)	\$8.22/1000 kg
High-Pressure Steam (4237 kPa, saturated, cost or credit)	\$9.83/1000 kg
Natural Gas or Fuel Gas (446 kPa, 25°C)	
cost	\$6.00/GJ
credit	\$5.00/GJ
Electricity	\$0.06/kWh
Boiler Feed Water (at 549 kPa, 90°C)	\$2.45/1000 kg
(There is a cost for boiler feed water only if the steam produced enters process streams. If, on the other hand, the steam produced is subsequently condensed, it can be made into steam again. In that case, there would be no net cost for boiler feed water.)	
Cooling Water	\$0.354/GJ
available at 516 kPa and 30°C	
return pressure ≥ 308 kPa	
return temperature should be no more than 15°C above the inlet temperature	
Refrigerated Water	\$4.43/GJ
available at 516 kPa and 5°C	
return pressure ≥ 308 kPa	
return temperature should be no higher than 15°C	
Process Water	\$0.067/1000 kg
available at desired pressure and 30°C	
Waste Water Treatment	\$56/1000 m^3
based on total volume treated	

Data

Data for methanol and H_2O are available in your textbook.[1] The following data are provided for the other components.

Heat of Formation at 25°C, [kJ/kg] – all in gas phase

MTBE	isobutene	1-butene	2-butene
-3216.1	-301.3	-9.62	-199.1

Heat of Vaporization [kJ/kmol] at normal boiling point, T_b [°C]

	MTBE	isobutene	1-butene	2-butene
ΔH_v	2.81×10^4	2.22×10^4	2.24×10^4	2.29×10^4
T_b	55.2	-6.9	-6.25	0.88

Liquid-Phase Heat Capacity – use the following equation

$C_p = A + BT + CT^2 + DT^3 + ET^4$, **where T is in [K] and C_p is in [J/kmol K]**

	MTBE	isobutene	1-butene	2-butene
A	140,120	179,340	140,200	112,760
B	-9	-1467	-554.87	-104.7
C	0.563	10.323	2.6242	0.521
D		-0.03	-0.003	
E		3.395×10^{-5}		

Vapor-Phase Heat Capacity – use data from the CD accompanying the text[1]

Vapor Pressure Equation Constants – use the following equation

$\ln [P^*] = A - (B/T) + C\ln T + DT^E$, **where P^* is in [Pa] and T is in [K]**

	MTBE	isobutene	1-butene	2-butene
A	55.875	95.222	67.78	77.551
B	5132	4867	4429	4848
C	-4.96	-12.567	-7.2064	-8.7864
D	1.91×10^{-17}	0.0178	8.4×10^{-6}	1.172×10^{-5}
E	6	1	2	2

Additional Information

The equipment costs for the MTBE plant as follows. Each cost is for an individual piece of equipment, including installation.

Equipment	Installed Cost in millions of $
Reactor, R-901	0.5
Tower, T-901	2.0
Absorber, T-902	0.3
Tower, T-903	0.5
Any heat exchanger	0.15

Fired heater installed cost in dollars:

$$11 \times 10^{x}$$

where

$$x = 2.5 + 0.8 \log_{10} Q$$

where Q is the heat duty in kW

Additionally, the following raw material and product costs should be used:

Raw Material or Product	$/kg
methanol	0.50
i-butene	0.45
MTBE	0.50

Other Information

You should assume that a year equals 8000 hours. This is about 330 days, which allows for periodic shutdown and maintenance.

Deliverables

Each group must deliver a word-processed report. It should be clear, concise and adhere to the prescribed format. The format is explained in the written report guidelines, provided in a separate document. When presenting results for different cases, graphs are superior to tables. The body of the report should be short, emphasizing only the results and briefly summarizing computational strategies. The report appendix should contain details of calculations that are easy to follow. Calculations that cannot be followed easily will lose credit.

The project is due April 25, 2005, at the beginning of class. There will be oral presentations of project results on that day. Oral presentations will continue on April 27, 2005, if we are unable to complete all presentations on April 25, 2005. Oral presentation guidelines will be provided in a separate document.

Anyone not participating in this project will automatically receive an F for ChE 202 and ChE 230, regardless of other grades earned in this class.

Grading

The report grade for each class will be based on the technical content pertinent to that class, which includes the response to questions during the oral presentation (60%), the oral presentation (20%), and the written report (20%). The grade for the written report portion will include the quality of the writing, the quality of the presentation, and the adherence to the prescribed format. The grade for the oral presentation will be a composite grade for the entire team. Therefore, group preparation and feedback are recommended. The grade for the technical content is self explanatory.

The documents on the following web site provide an indication of the expected attributes of a design report.

http://www.che.cemr.wvu.edu/ugrad/outcomes/rubrics/index.php

Groups

You will work on this project in groups of 4. More details of group formation and peer evaluation will be discussed in class.

Revisions

As with any open-ended problem; i.e., a problem with no single correct answer, the problem statement above is deliberately vague. The possibility exists that, as you work on this problem, your questions will require revisions and/or clarifications. You should be aware that these revisions/clarifications may be forthcoming.

References

1. Himmelblau, D. M. and J. B. Riggs, *Basic Principles and Calculations in Chemical Engineering (7th ed.)*, Prentice Hall, Englewood Cliffs, NJ, 2004.