Fluid Mechanics, Heat Transfer, Thermodynamics

Production of MTBE

We continue to investigate the feasibility of constructing a new, grass-roots, 60,000 tonne/y, methyl *tertiary*-butyl ether (MTBE) facility. As part of the feasibility study, we would like you to investigate some of the details of the proposed plant and of the thermodynamics of the components involved in the process.

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

Chemical Reaction

The chemical reaction to form MTBE is as follows:

$$CH_3OH + (CH_3)_2C = CH_2 \longrightarrow (CH_3)_3C - O - CH_3 \quad (1)$$

Process Description

The PFD for the process is given in Figure 1. Note that this is similar to the PFD as you were given last spring. It should be used as a starting point for this assignment.

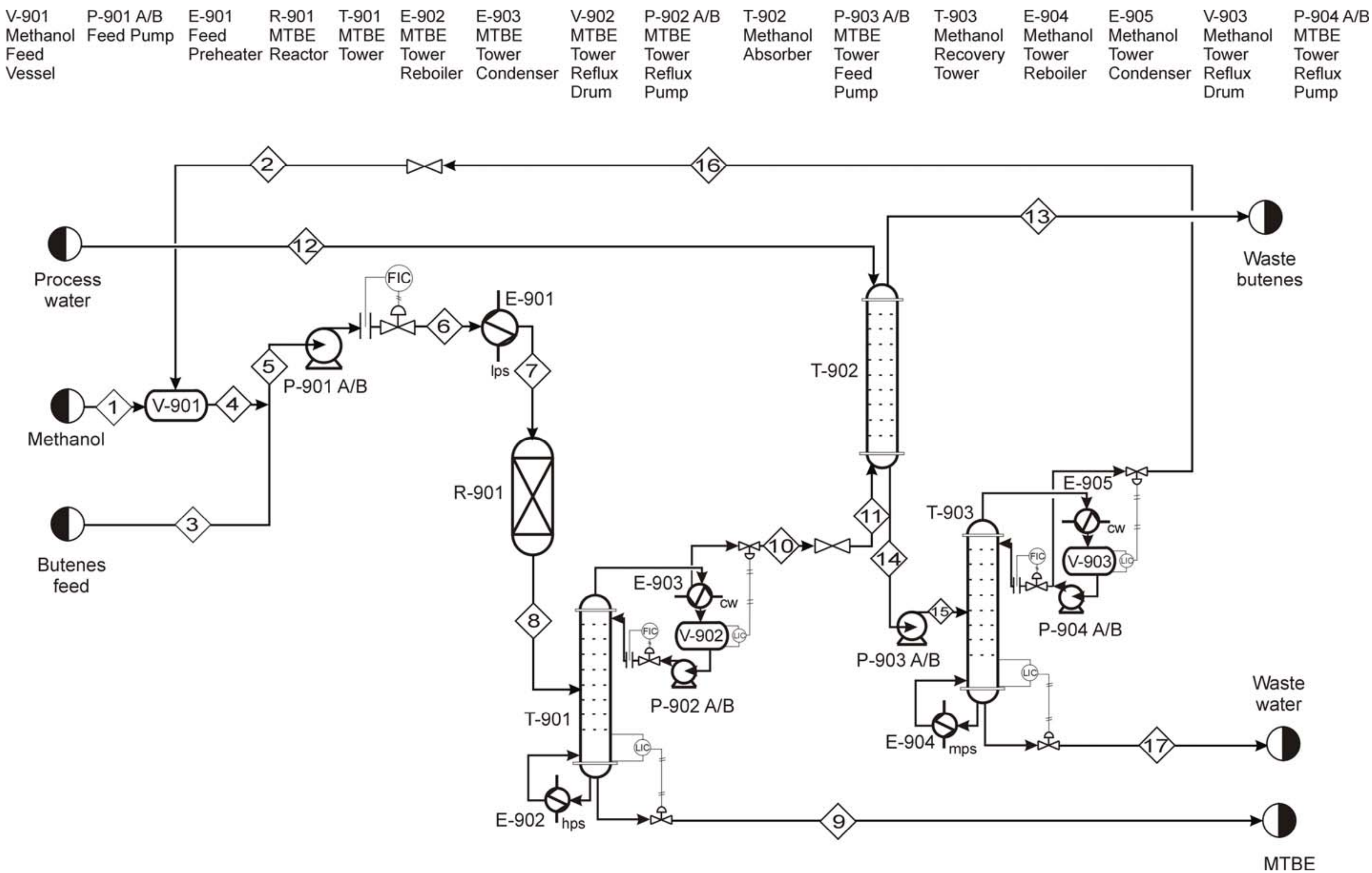


Figure 1: Unit 900 - MTBE Production Facility

Process Details

Feed Stream and Effluent Streams

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

Stream 2: Assume pure methanol

Stream 3: Mixed butene stream – 23% *iso*-butene, 20% 1-butene, 57% *trans* 2-butene.

Stream 9: MTBE product – must be 95 wt% pure.

Stream 12: Process water – see utility list for more information

Stream 13: Waste butenes – returned to refinery – contains 1-butene and 2-butene with less than 1 wt% other impurities.

Stream 17: 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 reactor feed pressure, which is 3000 kPa.

Heat Exchanger (E-901)

This heat exchanger heats the feed to the reactor feed temperature, which is 90°C.

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. However, for the required Chemcad simulation, you must enter a conversion. You should use a conversion of 90% of the limiting reactant.

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

Distillation Column (T-901)

This column runs at 19 atm. Separation of methanol and MTBE occurs in this column.

Heat Exchanger (E-902)

In this heat exchanger, some of the contents of the stream leaving the bottom of T-901 going to E-902 are vaporized and returned to the column.

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.

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 11 is absorbed into Stream 14. All other components enter Stream 13. Process water sent to the absorber is controlled so that 5.0 kmol of water are used for every 1.0 kmol of methanol entering the absorber.

Distillation Column (T-903)

This column runs at 5 atm. Separation of methanol and water occurs in this column.

Heat Exchanger (E-904)

In this heat exchanger, some of the contents of the stream leaving the bottom of T-903 going to E-904 are vaporized and returned to the column.

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.

Assignment

The assignment consists of four "mini-designs."

1. Design of P-904A/B MTBE Tower Reflux Pumps (ChE 310)

The purpose of the Process Fluid Mechanics mini-project is to design the piping and pumping system associated with the methanol tower reflux pumps, P-904A/B. The purpose of these pumps is to send the reflux stream back to T-903 and to return the unused methanol back to the methanol feed vessel, V-901. In order to complete this assignment, you have been provided with preliminary plot and elevation diagrams for Unit 900 (Appendix 1). Although complete piping isometric diagrams are not available (since the plant has not yet been built), you are to make your best estimate of the amount of piping, number of bends, and fittings that are required for each piping run. You should note that piping at ground level (except around pumps) should be avoided and that piping is generally placed on the pipe rack whenever possible.

For this part of the project, you should assume that Stream 16 contains 400 kmol/h of pure methanol at 500 kPa and that the reflux ratio, defined as the ratio of the flowrate of stream sent back to the tower and the flowrate of Stream 16, is 3.5.

In order to estimate the power requirements of the pumps, you must perform a mechanical energy balance for each part of leg of the piping run. These two piping legs consist of the piping needed to return reflux to the tower and the piping that returns recycled methanol back to the feed vessel. Each piping leg contains a control valve that regulates the flow of liquid. You should assume that both control valves are designed to have an 80 kPa pressure drop across them at the design (normal) flow condition.

The optimum pipe diameters for the suction line and both discharge legs are to be determined. The objective function for the optimization is the Equivalent Annual Operating Cost (EAOC) of the piping system including the pump ($/y). The EAOC is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + \text{annual operating costs} \tag{2}$$

where

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \tag{3}$$

where i = 0.15 (15% rate of return) and n = 10 (ten-year plant life).

During the course of normal operation, it may be necessary to change the amount of reflux returning to T-903. For the optimal pump and piping system that you propose, determine the maximum amount of reflux that can be returned to the column when the flow of recycled methanol remains at the normal operating condition. For this part of the project, you may assume that the pump curve is described by the "standard" pump curve equation given below:

$$\frac{P}{P_{design}} = 1.1 - 0.1\left[\frac{Q}{Q_{design}}\right]^{7.1265} \tag{4}$$

where P_{design} is the pressure rise across the pump at the design volumetric flowrate of Q_{design}, and Q is the volumetric flowrate at any pressure rise, P, across the pump. In addition, the NPSH-required curve should be assumed to follow the following form:

$$NPSH_R(\text{m of liquid at } 20^{\text{o}}\text{C}) = 5 + 2\left(\frac{Q}{Q_{design}}\right)^2 \tag{5}$$

2. Heat Exchanger Design (ChE 311)

You should perform a detailed design of the reactor preheater, E-901. Assume that the inlet temperature to E-301 is 27°C and the outlet temperature is 90°C. You should assume that steam is available at the conditions specified in Appendix 2 of this problem statement. For this heat-exchanger design, you should report the following information, as needed for the design:

- Diameter of shell
- Number of tube and shell passes
- Number of tubes per pass
- Tube pitch and arrangement (triangular/square/..)
- Number of shell-side baffles and their arrangement (spacing, pitch, type)
- Diameter, thickness, and length of tubes
- Calculation of both shell- and tube-side film heat transfer coefficients
- Calculation of overall heat transfer coefficient (you may assume that there is no fouling on either side of the exchanger)
- Heat transfer area of the exchanger
- Shell-side and tube-side pressure drops
- Materials of construction
- Approximate cost of the exchanger

A detailed sketch of the exchanger should be included along with a set of comprehensive calculations in an appendix to the mini-project.

3. Thermodynamics (ChE 320)

You will consider the properties of Stream 8, leaving Reactor R-901, in terms of the composition of Stream 7, entering R-901. For the purpose of this mini-design, consider that Stream 7 (inlet) is a liquid at 30 atm and 90°C, and has the following composition and molar flow rates:

Component	Molar Flow Rate [kmol/h]
Methanol	497
Iso-butene	160
1-Butene	61
Tert 2-butene	262

For safety purposes, we are concerned that the reactor effluent stream might become a vapor, and we wish to avoid two-phase flow. To assist in this analysis, we need to know the properties of liquid and vapor phases if Stream 8 (outlet) were to be flashed adiabatically to 1 atm.

Your solution should address the following:

- The composition and temperature of Stream 8 after adiabatic reaction (assume the pressure stays at 30 atm; recall that the conversion is 90%).

- The temperature, composition, and molar flow rates of the vapor phase (call it Stream 101) and the liquid phase (call it Stream 102) obtained by flashing Stream 8 to 1 atm. Compute these manually, assuming the vapor phase to be an Ideal Gas and the liquid phase to be an Ideal Mixture. Compare these results to those obtained from the ideal model in Chemcad (*K*-value VAP and enthalpy LATENT HEAT).
- Similar to the above, but using Peng-Robinson and the software provided by Sandler [1]. Compare these results to those obtained from the Peng-Robinson model in Chemcad.
- Similar to the above, but using the predictive SRK model in Chemcad.
- A comparison and discussion of the three results from Chemcad, and a recommendation of which to use.
- Why these calculations are of interest.

4. Safety Analysis Report

When designing a chemical process, it is important to know the properties of the chemicals being consumed and produced in the process. The reactivity and toxicity of the reactants and products will not only affect the design but will also affect the procedures that might be implemented during an unscheduled event such as an emergency shutdown. The purpose of the safety analysis report is to make management aware of risks to personnel due to the flammability and toxicity of all chemicals consumed or produced in the process. As a minimum, the MSDS (material and safety data sheets) for all these chemicals should be provided in an appendix, and a brief discussion of the major concerns for each chemical should be given as a separate section of the report. In addition, briefly discuss possible safety hazards for each piece of equipment in your process. Finally, a feature of your process design that addresses one of these concerns should be explained.

5. Chemcad

A Chemcad simulation for the feed section of the process (through Stream 8) shown in Figure 1 should be provided. Use the results from all mini designs, including the recommended thermodynamics package.

Other Information

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

Deliverables

Written Reports

Each group must deliver a report written using a word processor. Three identical copies should be submitted, one for each instructor. The written project reports are due by 11:00 a.m. Thursday, December 1, 2005. Late projects will receive a minimum of a one letter grade deduction.

The report should be clear and concise. For the correct formatting information, refer to the document entitled *Written Design Reports*. The report must contain a labeled process flow diagram (PFD) and a stream table, each in the appropriate format. The PFDs from Chemcad are generally unsuitable unless you modify them significantly. Figure 1 should be used as a template for your PFD. When presenting results for different cases, graphs are superior to tables. For the optimal case, the report appendix should contain details of calculations that are easy to follow. There should be separate appendices for each "mini-project." These may be hand written if done neatly. Alternatively, Excel spreadsheets may be included, but these must be well documented so that the reader can interpret the results. Calculations that cannot be easily followed and that are not explained will lose credit.

Since this project involves "mini-designs," it is suggested that the report be organized as follows. There should be a general abstract and introduction. Then, there should be a results section followed by a discussion section for each "mini-design." General conclusion and recommendation sections should follow. At a minimum, there should be one appendix for each of the "mini-designs."

In order to evaluate each group member's writing skills, the results and discussion sections for each mini-design should be written by a different group member. The authorship of each of these mini-reports should be clearly specified in the report. For groups with four members, the member not authoring a mini-report should author the safety analysis report, which is described below. The remainder of the report, namely the general abstract, general introduction, general results (including Chemcad simulation), general conclusions, and general recommendations sections should be a group effort.

Although the individual written portions of the reports must be authored by a single group member, it is the intent of the instructors that group members should help each other in writing different sections. To this end, we recommend that you seek input, such as proofreading and critiques, from other members of your group. The reports will be evaluated as follows:

- section technical content – 50%
- oral presentation – 20%
- written report – 20%
- technical quality of general sections (safety, simulation, etc.) – 10%

A historical account of what each group did is neither required nor wanted. Results and explanations should be what are needed to justify your choices, not a litany of everything that was tried. Each mini-report should be limited to 4-5 double space pages plus figures and tables.

Oral Reports

Each group will give an oral report in which the results of this project will be presented in a concise manner. The oral report should be between 15-20 minutes, and each group member must speak. Each group member should speak only once. A 5-10 minute question-and-answer session will follow, and all members must participate. Refer to the document entitled *Oral Reports* for instructions. The oral presentations will be Thursday December 1, 2005, from 11:00

a.m. to 2:00 pm. Attendance is required of all students during their classmates' presentations (this means in the room, not in the hall or the computer room). ***Failure to attend any of the above-required sessions will result in a decrease of one-letter grade (per occurrence) from your project grade in ChE 310, ChE 311, and ChE 320***.

Groups

You will work on this project in groups of 3 or 4. More details of group formation and peer evaluation will be discussed in class.

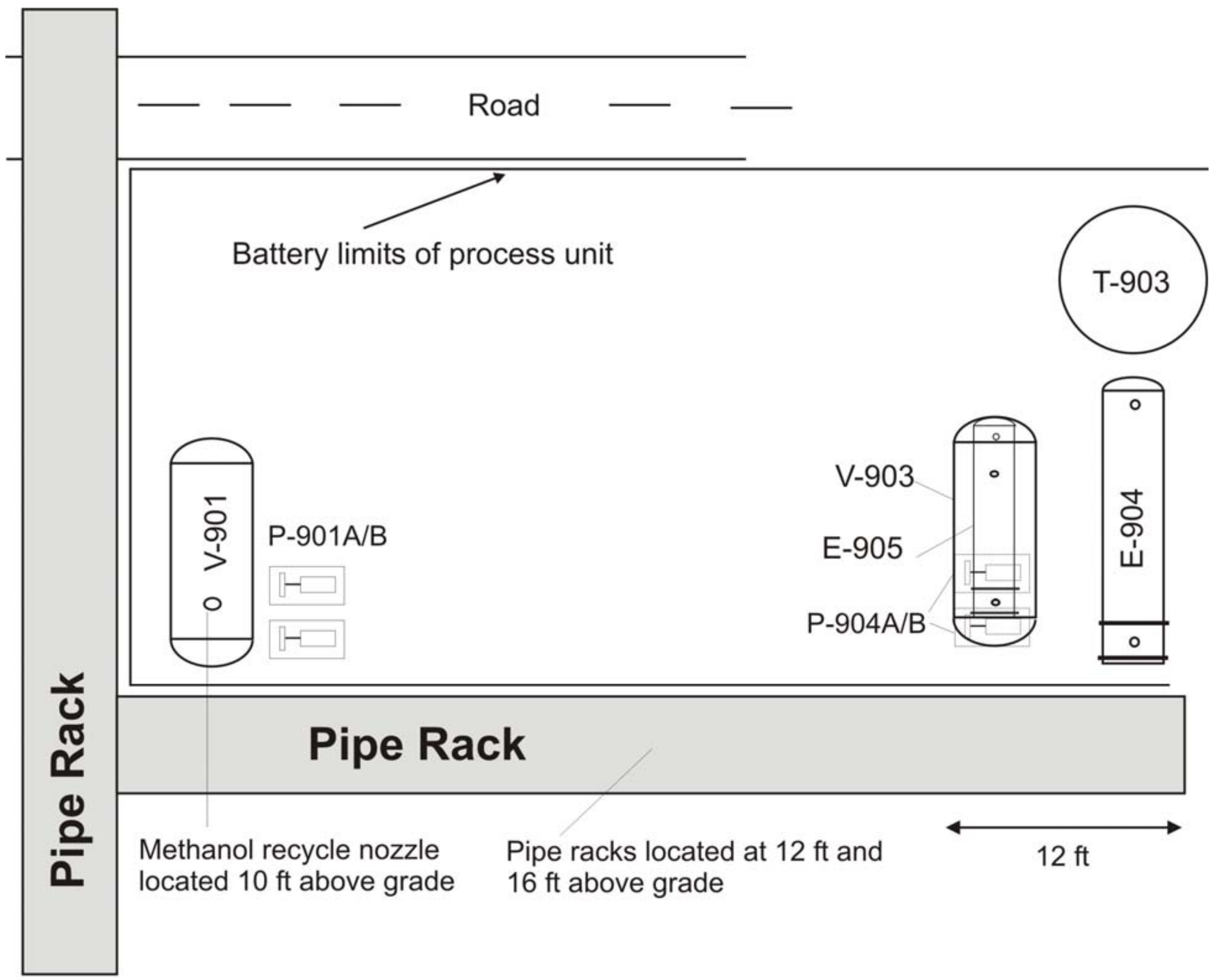
Revisions

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.

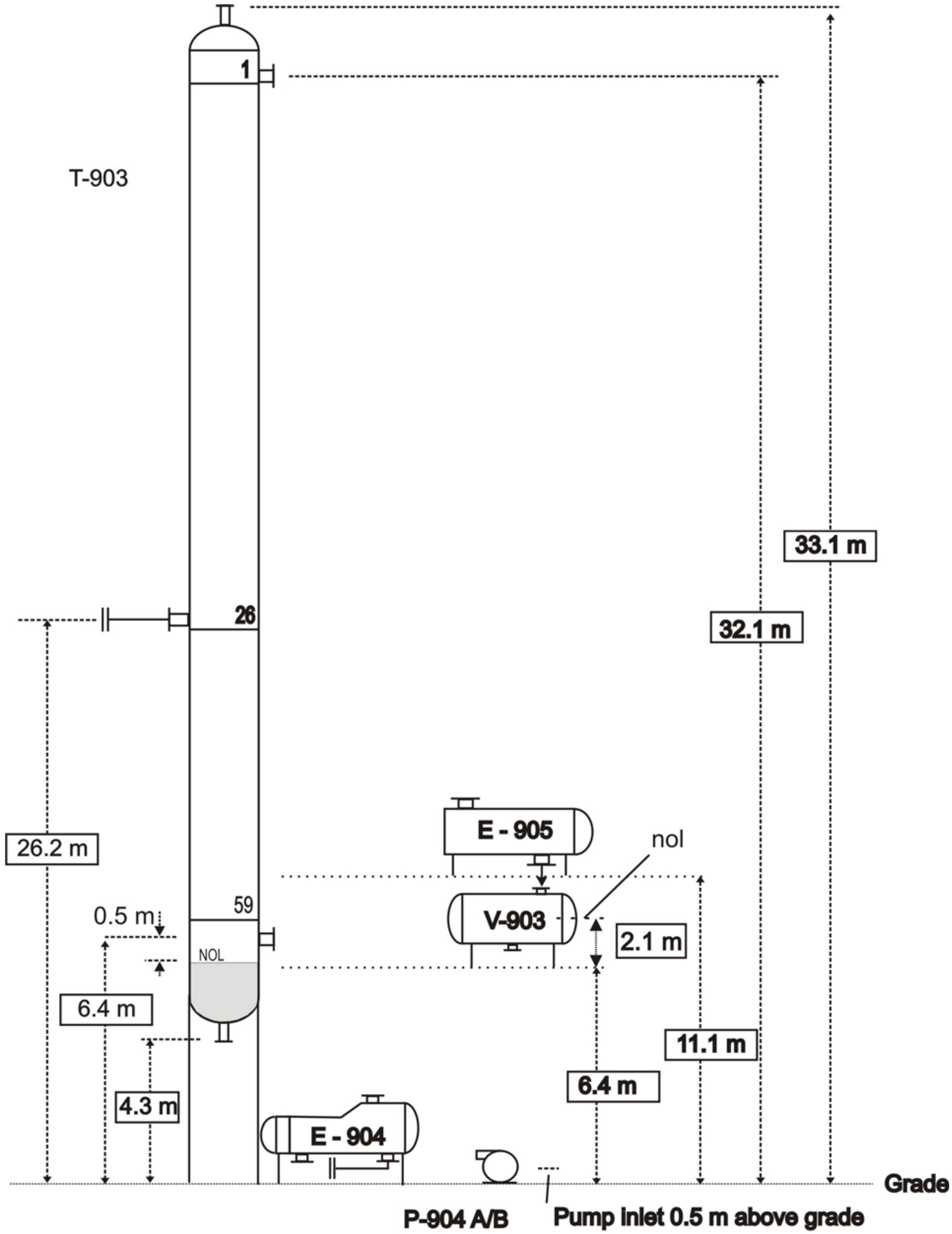
References

1. Sandler, S.I., *Chemical and Engineering Thermodynamics* (*3rd ed.*), Wiley, New York, 1999.

Appendix 1
Plot plan and Elevation Diagram for ChE 310 mini-project



Preliminary Plot Plan for MTBE Production Facility



Vessel Sketch for T-903 and Associated Equipment (not to scale)

Appendix 2
Economic Data

Equipment Costs (Purchased)

Note: The numbers following the attribute are the minimum and maximum values for that attribute. For a piece of equipment with a lower attribute value, use the minimum attribute value to compute the cost. For a piece of equipment with a larger attribute value, extrapolation is possible, but inaccurate. To err on the side of caution, you should use the price for multiple, identical smaller pieces of equipment.

Pumps

$$\log_{10}(\text{purchased cost}) = 3.4 + 0.05\log_{10} W + 0.15[\log_{10} W]^2$$

W = power (kW, 1, 300)
assume 80% efficiency

Heat Exchangers

$$\log_{10}(\text{purchased cost}) = 4.6 - 0.8\log_{10} A + 0.3[\log_{10} A]^2$$

A = heat exchange area (m^2, 20, 1000)

Compressors

$$\log_{10}(\text{purchased cost}) = 2.3 + 1.4\log_{10} W - 0.1[\log_{10} W]^2$$

W = power (kW, 450, no limit)
assume 70% efficiency

Compressor Drive

$$\log_{10}(\text{purchased cost}) = 2.5 + 1.4\log_{10} W - 0.18[\log_{10} W]^2$$

W = power (kW, 75, 2600)

Turbine

$$\log_{10}(\text{purchased cost}) = 2.5 + 1.45\log_{10} W - 0.17[\log_{10} W]^2$$

W = power (kW, 100, 4000)
assume 65% efficiency

Fired Heater

$$\log_{10}(\text{purchased cost}) = 3.0 + 0.66\log_{10} Q + 0.02[\log_{10} Q]^2$$

Q = duty (kW, 3000, 100,000)
assume 80% thermal efficiency
assume can be designed to use any organic compound as a fuel

Vertical Vessel

$$\log_{10}(\text{purchased cost}) = 3.5 + 0.45\log_{10} V + 0.11[\log_{10} V]^2$$

V = volume of vessel (m^3, 0.3, 520)

Horizontal Vessel

$$\log_{10}(\text{purchased cost}) = 3.5 + 0.38\log_{10} V + 0.09[\log_{10} V]^2$$

V = volume of vessel (m^3, 0.1, 628)

Additional Cost Information

Piping straight pipe $/m = 5.0 (nominal pipe diameter, in)$(1+(\text{sch }\#)/20)^{0.25}$
sch = schedule number for pipe
use the same sch number for fittings and valves

fittings (except valves) $/fitting = 50.0 (nominal pipe diameter, in)$(1+(\text{sch }\#)/20)^{0.25}$

Valves for gate (isolation) valves $100 (nominal pipe diameter, in)$^{0.8}$ $(1+(\text{sch }\#)/20)^{0.25}$
for control valve use $1000 (nominal pipe diameter, in)$^{0.8}$$(1+(\text{sch }\#)/20)^{0.25}$

Utility Costs

Low-Pressure Steam (618 kPa saturated)	$7.78/1000 kg
Medium-Pressure Steam (1135 kPa saturated)	$8.22/1000 kg
High-Pressure Steam (4237 kPa saturated)	$9.83/1000 kg
Natural Gas (446 kPa, 25°C)	$6.00/GJ
Fuel Gas Credit	$5.00/GJ
Electricity	$0.06/kWh
Boiler Feed Water (at 549 kPa, 90°C)	$2.45/1000 kg
Cooling Water available at 516 kPa and 30°C return pressure ≥ 308 kPa return temperature is no more than 15°C above the inlet temperature	$0.354/GJ
Refrigerated Water available at 516 kPa and 10°C return pressure ≥ 308 kPa return temperature is no higher than 20°C	$4.43/GJ
Deionized Water available at 5 bar and 30°C	$1.00/1000 kg
Waste Treatment of Off-Gas	incinerated - take fuel credit
Refrigeration	$7.89/GJ
Wastewater Treatment	$56/1000 m^3

Equipment Cost Factors

Total Installed Cost = Purchased Cost (4 + material factor (MF) + pressure factor (PF))

Pressure	< 10 atm, PF = 0.0	does not apply to turbines, compressors, vessels,
(absolute)	10 - 20 atm, PF = 0.6	packing, trays, or catalyst, since their cost
	20 - 40 atm, PF = 3.0	equations include pressure effects
	40 - 50 atm, PR = 5.0	
	50 - 100 atm, PF = 10	

Carbon Steel	MF = 0.0
Stainless Steel	MF = 4.0