MTBE Production

You work in a facility that produces about 100,000 tonne/y of methyl tertiary butyl ether (MTBE). MTBE is an oxygenated fuel additive that is blended with gasoline to promote CO_2 formation over CO formation during combustion. The facility manufactures MTBE from methanol and isobutylene. Isobutylene is obtained from a refinery cut, and it also contains 1-butene and 2-butene, both of which do not react with methanol.

Process Description

The process flow diagram is shown in Figure 1. Methanol and the mixed butylenes feed is pumped and heated to reaction conditions. Both the methanol and the mixed butylenes are made in on-site units, and are sent to this unit at the desired conditions. The reactor operates in the vicinity of 30 bar, to ensure that the reaction occurs in the liquid phase. The reaction is reversible. The feed temperature to the reactor is usually maintained below 90°C to obtain favorable equilibrium behavior. Any side reactions involving 1-butene and 2-butene form small amounts of products with similar fuel blending characteristics, so side reactions are assumed to be unimportant. Other side reactions are minimized by keeping the methanol present in excess. The reactor effluent is distilled, with MTBE as the bottom product. Methanol is recovered from the mixed butylenes in a water scrubber, and the methanol is subsequently separated from water so that unreacted methanol can be recycled. Unreacted butylenes are sent back to the refinery for further processing. The MTBE product is further purified (not shown), mostly to remove the trace amounts of water. The product stream from Unit 900 must contain at least 94 mol % MTBE, with the MTBE portion of the stream flowrate at specifications.

Tables 1 and 2 contain the stream and utility flows for the process as designed. Table 3 contains an equipment list. Other pertinent information and calculations are contained in the appendix.

Possibility of Changing Process Feed Conditions

This plant receives the mixed butylenes feed from a neighboring refinery, which has recently changed ownership. The new owners are planning to implement changes based on their proprietary technology. The changes will occur after a regularly scheduled plant shut down (for both plants) within the next six months. The effect on our plant is that they have proposed that the mixed butylenes feed that we receive will contain 23 wt% isobutylene (isobutene), 20 wt% 1-butene, and 57 wt% 2-butene. Our current contract for mixed butylenes expires at the next plant shut down, so we are in the process of negotiating a new contract with the new owners. An additional complication is that MTBE is in the process of being phased out as a fuel additive because of ground water contamination from leaky gasoline storage tanks.

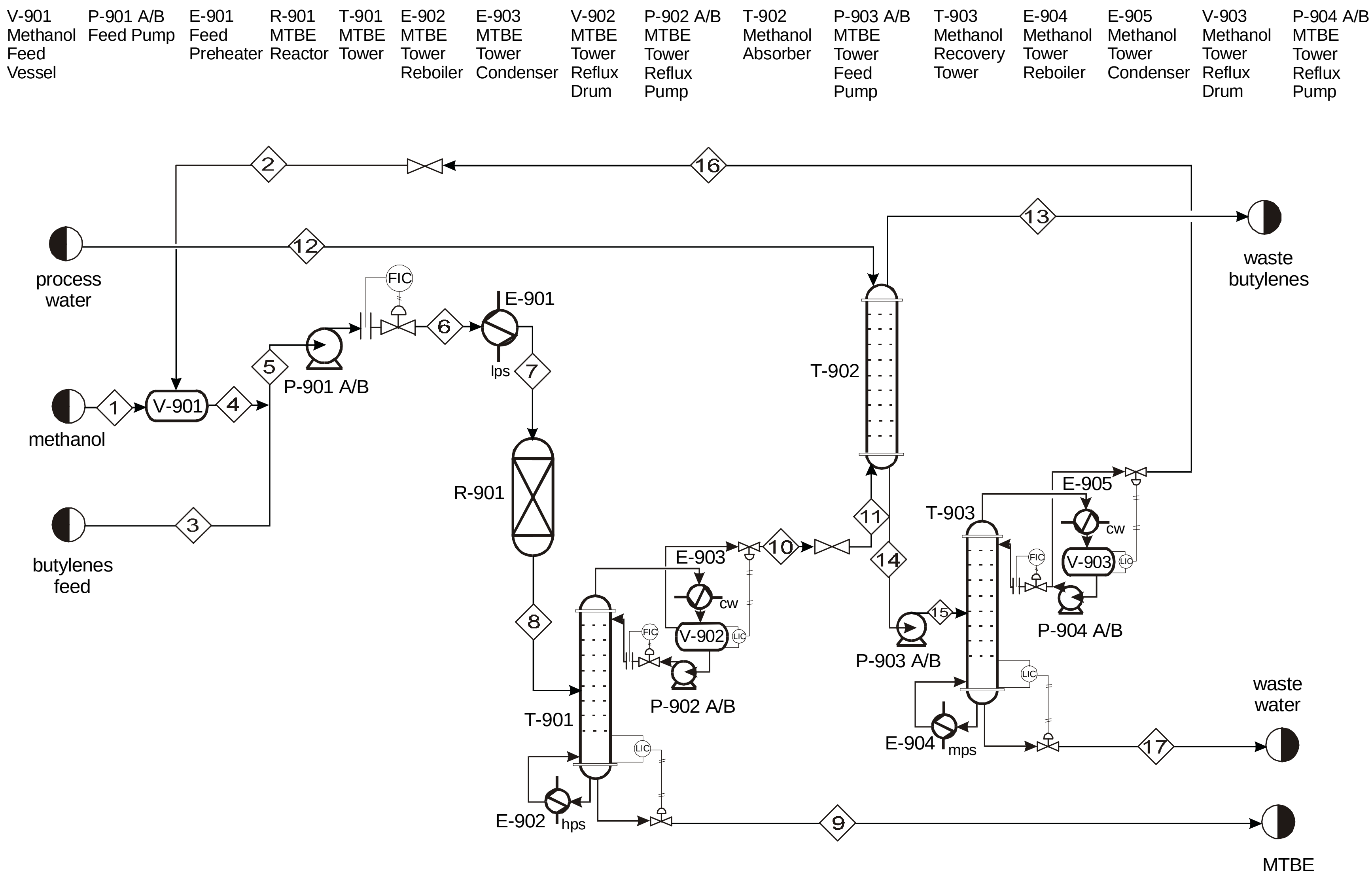


Figure 1: Unit 900 - MTBE Production Facility

Table 1
Stream Tables for Unit 900

Stream No	1	2	3	4
Temp °C	25.00	49.84	25.00	45.70
Pres kPa	400.00	400.00	390.00	390.00
Vapor fraction	0.00	0.045	0.00	0.00
Total kg/h	5600.00	16590.16	21875.00	22190.70
Total kmol/h	174.77	427.75	389.88	602.54
Component kmol/h				
Methanol	174.77	322.15		496.96
i-Butene		3.73	155.95	3.73
1-Butene		14.59	46.79	14.59
Trans-2-Butene		74.43	187.14	74.43
MTBE		11.86		11.86
Water		0.98		0.98

Stream No.	5	6	7	8
Temp °C	25.93	26.91	85.00	127.57
Pres kPa	380.00	3000.00	2965.00	2915.00
Vapor fraction	0.00	0.00	0.00	0.00
Total kmol/h	992.42	992.42	992.42	848.70
Total kg/h	44065.70	44065.70	44065.70	44065.70
Component kmol/h				
Methanol	496.96	496.96	496.96	353.23
i-Butene	159.68	159.68	159.68	15.95
1-Butene	61.38	61.38	61.38	61.38
Trans-2-Butene	261.58	261.58	261.58	261.58
MTBE	11.86	11.860	11.86	155.59
Water	0.97	0.97	0.97	0.97

Stream No.	9	10	11	12
Temp °C	178.46	134.37	110.36	30.00
Pres kPa	1925.00	1900.00	500.00	450.00
Vapor fraction	0.00	1.00	1.00	0.00
Total kg/h	12973.05	31272.80	31272.80	21618.00
Total kmol/h	150.40	698.30	698.30	1200.00
Component kmol/h				
Methanol	7.06	346.17	346.17	
i-Butene	0.00	15.95	15.95	
1-Butene	0.00	61.38	61.38	
Trans-2-Butene	0.00	261.58	261.58	
MTBE	142.36	13.22	13.22	
Water	0.97	0.00	0.00	1200.00

Table 1 (cont'd)
Stream Tables for Unit 900

Stream No.	13	14	15	16
Temp °C	83.49	83.12	70.73	56.27
Pres kPa	110.00	160.00	500.00	500.00
Vapor mole fraction	1.00	0.00	0.00	0.00
Total kg/h	18828.85	34061.93	34061.93	16590.16
Total kmol/h	500.96	1397.34	1397.34	427.75
Component kmol/h				
Methanol	23.69	322.48	322.48	322.16
i-Butene	12.23	3.72	3.72	3.72
1-Butene	46.78	14.60	14.60	14.60
Trans-2-Butene	187.13	74.44	74.44	74.44
MTBE	1.36	11.86	11.86	11.86
Water	229.76	970.24	970.24	0.97

Stream No.	17
Temp °C	155.61
Pres kPa	550.00
Vapor mole fraction	0.00
Total kg/h	17471.77
Total kmol/h	969.60
Component kmol/h	
Methanol	0.32
i-Butene	
1-Butene	
Trans-2-Butene	
MTBE	
Water	969.27

Table 2
Utility Stream Flow Summary for Unit 900

E-901	E-902	E-903
lps	hps	cw
3572 kg/h	25,828 kg/h	6.31×10^5 kg/h

E-904	E-905
mps	cw
32,433 kg/h	1.44×10^6 kg/h

Table 3
Partial Equipment Summary

Heat Exchangers

E-901 A = 44.6 m^2 1-2 exchanger, floating head, carbon steel process stream in tubes Q = 7502 MJ/h maximum pressure rating of 35 bar	**E-904** A = 209 m^2 1-2 exchanger, fixed head, carbon steel process stream in shell Q = 64,542 MJ/h maximum pressure rating of 6.5 bar
E-902 A = 50.9 m^2 1-2 exchanger, fixed head, carbon steel process stream in shell Q = 43,908 MJ/h maximum pressure rating of 23 bar	**E-905** A = 1003 m^2 1-2 exchanger, floating head, carbon steel process stream in shell Q = 60,347 MJ/h maximum pressure rating of 6.5 bar
E-903 A = 92.4 m^2 1-2 exchanger, floating head, carbon steel process stream in shell Q = 26,417 MJ/h maximum pressure rating of 23 bar	

Reactors and Vessels

R-901 carbon steel packed bed, Amberlyst 15 catalyst V = 9.35 m^3 10 m long, 1.1 m diameter maximum pressure rating of 32 bar	**V-901** stainless steel V = 11.215 m^3 maximum pressure rating of 5 bar

Pumps

P-901 A/B carbon steel power = 220.53 MJ/h (actual) 80% efficient	**P-903 A/B** carbon steel power = 18.65MJ/h (actual) 80% efficient

Table 3 (cont'd)
Partial Equipment Summary

Towers

T-901 carbon steel 97 sieve trays plus reboiler and partial condenser 70% efficient trays feed on tray 27 additional feeds ports on 23 and 30 reflux ratio = 1.62 12 in tray spacing, 2 in weirs column height 30 m diameter = 2.8 m above feed, 4.7 m below feed maximum pressure rating of 23 bar	**T-903** carbon steel 42 sieve trays plus reboiler and total condenser 48% efficient trays feed on tray 21 additional feed ports on 16 and 23 reflux ratio = 3.44 24 in tray spacing, 6.8 in weirs column height = 26 m diameter = 2.6 m maximum pressure rating of 6.5 bar
T-902 carbon steel 7.3 m of packing 5 theoretical stages 6.86 kPa/m pressure drop diameter = 2.9 m packing factor – 500 maximum pressure rating of 5 bar	

Your assignment is first to determine the maximum flowrate of the new feed stream the plant can process and the operating conditions needed for this plant to use the new feed stream and meet the required MTBE production rate and specifications without any capital investment. You must also determine whether these are feasible operating conditions. Any change in the cost of manufacture should be documented. Then, you are to determine the cost of any process modifications (capital and operating) needed for our plant to use this new feed to maintain the current production rate and specification of MTBE.

Cost Saving Strategies

Since we are expecting to implement process modifications during the upcoming shut down, please recommend any cost-saving strategies that we can also implement.

Economics

For all process modifications, use a 15%, before-tax rate of return and a 5-year lifetime. Use an EAOC or an INPV as the measure of profitability.

Deliverables

Specifically, you are to prepare the following by 9:00 a.m., Monday, November 8, 2004:

1. Determine the maximum flowrate of the new feed stream the plant can process and the operating conditions needed for this plant to use the new feed stream and meet the required MTBE production rate and specifications without any capital investment

2. Determine the cost of any process modifications (capital and operating) needed for our plant to use this new feed to maintain the current production rate and specification of MTBE

3. Suggest cost-saving measures that you recommend for the plant. All recommendations should be accompanied by an economic analysis that accounts for the savings and cost of implementing the changes.

4. Prepare a written report, conforming to the guidelines, detailing the information in items 1, 2, and 3, above.

5. Include a legible, organized set of calculations justifying your recommendations, including any assumptions made.

6. Attach a signed copy of the attached confidentiality statement.

Report Format

This report should be brief and should conform to the guidelines. It should be bound in a folder that is not oversized relative to the number of pages in the report. Figures and tables should be included as appropriate. An appendix should be attached that includes items such as the requested calculations. These calculations should be easy to follow. The confidentiality statement should be the very last page of the report.

The written report is a very important part of the assignment. Reports that do not conform to the guidelines will receive severe deductions and will have to be rewritten to receive credit. Poorly written and/or organized written reports may also require re-writing. Be sure to follow the format outlined in the guidelines for written reports.

Oral Presentation

You will be expected to present and defend your results some time between November 11, 2004 and November 18, 2004. Your presentation should be 15-20 minutes, followed by about a 30-minute question and answer period. Make certain that you prepare for this presentation since it is an important part of your assignment. You should bring at least one hard copy of your slides to the presentation and hand it out before beginning the presentation.

Other Rules

You may not discuss this major with anyone other than the instructors. Discussion, collaboration, or any other interaction with anyone other than the instructors is prohibited. Violators will be subject to the penalties and procedures outlined in the University Procedures for Handling Academic Dishonesty Cases (begins on p. 47 of 2003-05 Undergraduate Catalog).

Consulting is available from the instructors. Chemcad consulting, *i.e.*, questions on how to use Chemcad, not how to interpret results, is unlimited and free, but only from the instructors. Each individual may receive five free minutes of consulting from the instructors. After five minutes of consulting, the rate is 2.5 points deducted for 15 minutes or any fraction of 15 minutes, on a cumulative basis. The initial 15-minute period includes the 5 minutes of free consulting.

Late Reports

Late reports are unacceptable. The following severe penalties will apply:

- late report on due date before noon: one letter grade (10 points)
- late report after noon on due date: two letter grades (20 points)
- late report one day late: three letter grades (30 points)
- each additional day late: 10 additional points per day

Appendix 1
Reaction Kinetics

The reactions and reaction kinetics are as follows:

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

$$-r = k_f \frac{C_{isobutylene}}{C_{methanol}} - k_r \frac{C_{MTBE}}{C_{methanol}^2} \quad (2)$$

where

$$k_f = 6.05 \times 10^{16} \exp\left(-\frac{85{,}400}{RT}\right) \quad (3)$$

$$k_r = 1.464 \times 10^{22} \exp\left(-\frac{129{,}600}{RT}\right) \quad (4)$$

The units of reaction rate, r_i, are mol/m^{3}h, and the activation energy is in J/mol. These kinetics are only valid when excess methanol is present.

Appendix 2
Chemcad Hints

If you choose to use Chemcad, here are some hints.

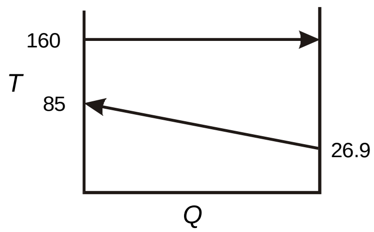
Use PSRK for the *K*-value and SRK for the enthalpy. However, for the absorber (T-902), use ideal vapor pressure for the *K*-value.

If you want to simulate the towers, use TOWR for T-901. Use SCDS for T-902 and T-903.

If you want to simulate the reactor, make sure that you set the flag for a liquid-phase reaction.

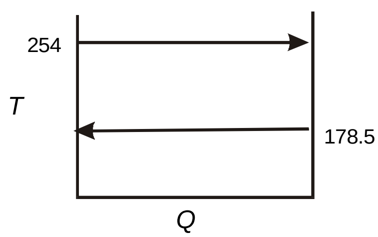
Appendix 3
Calculations and Other Pertinent Information

E-901



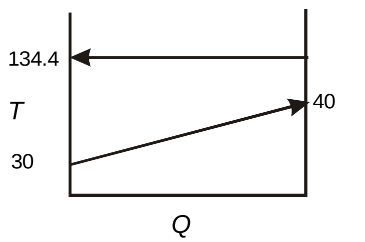
Q = 7502 MJ/h
ΔT_{lm} = 101.3°C
process fluid h_i = 500 W/m^{2}K
lps condensing h_o = 6000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 461.5 W/m^{2}K
A = 44.6 m^2
$Q = \dot{m}\lambda = \dot{m}$ (2100 kJ/kg)
lps flow in Table 2

E-902



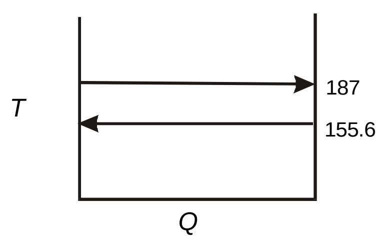
Q = 43,908 MJ/h
ΔT_{lm} = 75.5°C
process fluid boiling h_o = 5500 W/m^{2}K
hps condensing h_i = 7500 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 3173 W/m^{2}K
A = 50.9 m^2
$\dot{m}_{hps} = Q/\lambda = Q/(1700\,\text{kJ/kg})$
hps flow in Table 2

E-903



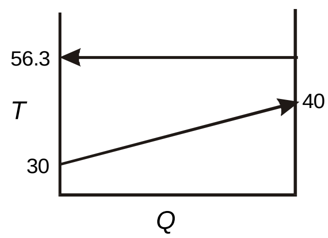
Q = 26,417 MJ/h
ΔT_{lm} = 99.3°C
cw h_i = 1000 W/m^{2}K
condensing organic process stream h_o = 4000 W/m^{2}K
$U \approx$ 800 W/m^{2}K
A = 92.4 m^2
$\dot{m}_{cw} = Q / C_p \Delta T = Q / [(4.184\,\text{kJ/kgK})(10\text{K})]$
cw flow in Table 2

E-904



Q = 64,542 MJ/h
ΔT_{lm} = 31.4°C
mps condensing h_i = 6000 W/m^{2}K
boiling process stream h_o = 5000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 2727 W/m^{2}K
A = 209 m^2
$\dot{m}_{mps} = Q / \lambda = Q / (1990\,\text{kJ/kg})$
mps flow in Table 2

E-905



Q = 60,347
ΔT_{lm} = 20.9°C
cw h_i = 1000 W/m^{2}K
condensing organic process stream h_o = 4000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 800 W/m^{2}K
A = 1003 m^2
$\dot{m}_{cw} = Q/C_p\Delta T = Q/[(4.184\,\text{kJ/kgK})(10\text{K})]$
cw flow in Table 2

R-901

V = 9.35 m^3

$V = (\pi D^2/4)(L)$ = 9.35
L = 10 m
D = 1.1 m

T-901

from Chemcad, 68 ideal trays, plus partial reboiler and partial condenser

above feed:
L = 45,000 kg/h, G = 75,000 kg/h
ρ_L = 480 kg/m^3
ρ_G = 28 kg/m^3
$(L/G)(\rho_G/\rho_L)^{0.5}$ = 0.145
from flooding graph for 12 in tray spacing (P. Wankat, *Equilibrium Staged Separations*, Prentice Hall, 1988, p. 387.)
C_{sb} = 0.18
u_{fl} = 0.72 ft/s
u_{act} = 0.165 m/s (75% of flooding)
if 75% active area
$A = (G/3600)/[(0.75)(\rho_G)(u_{act})]$ = 6.01 m^2
D = 2.8 m

below feed:
L = 244,000 kg/h, G = 231,000 kg/h
ρ_L = 509 kg/m^3
ρ_G = 64 kg/m^3
$(L/G)(\rho_G/\rho_L)^{0.5} = 0.375$
from flooding graph for 12 in tray spacing (P. Wankat, *Equilibrium Staged Separations*, Prentice Hall, 1988, p. 387.)
$C_{sb} = 0.13$
u_{fl} = 0.34 ft/s
u_{act} = 0.078 m/s (75% of flooding)
if 75% active area
$A = (G/3600)/[(0.75)(\rho_G)(u_{act})] = 17.1$ m^2
D = 4.7 m

70% overall column efficiency (O'Connell correlation)
$\Rightarrow$ 97 trays (so column about 100 ft tall ≈ 30 m)
$\Delta P = \rho g h N$
25000 Pa = (520 kg/m^3)(9.8 m/s^2)(h_{weir})(97)
h_{weir} = 0.0505 m ≈ 2 in

T-902

from Chemcad, 5 ideal trays

use packed bed:
L = 32,000 kg/h, G = 26,500 kg/h
ρ_L = 760 kg/m^3
ρ_G = 2.8 kg/m^3
$(L/G)(\rho_G/\rho_L)^{0.5} = 0.073$
packing factor is 500
packing pressure drop is 6.86 kPa/m
from flooding (P. Wankat, *Equilibrium Staged Separations*, Prentice Hall, 1988, p. 421.)
G_{fl} = 0.3 lb/ft^{2}s = 1.48 kg/m^{2}s
if 75% of flooding
A = (26500 kg/3600 s)/((0.75)(1.48 kg/m^{2}s) = 6.63 m^2
D = 2.9 m

T-903

from Chemcad, 20 ideal trays, plus partial reboiler and total condenser

above feed:
L = 55,000 kg/h, G = 71,000 kg/h
ρ_L = 700 kg/m^3
ρ_G = 5.90 kg/m^3
$(L/G)(\rho_G/\rho_L)^{0.5} = 0.071$

from flooding graph for 24 in tray spacing (P. Wankat, *Equilibrium Staged Separations*, Prentice Hall, 1988, p. 387.)
C_{sb} = 0.35
u_{fl} = 3.80 ft/s
u_{act} = 0.87 m/s (75% of flooding)
if 75% active area
$A = (G/3600)/[(0.75)(\rho_G)(u_{act})] = 5.12\ m^2$
D = 2.6 m – use this value

below feed:
L = 49,000 kg/h, G = 31,000 kg/h
$\rho_L = 910\ kg/m^3$
$\rho_G = 2.9\ kg/m^3$
$(L/G)(\rho_G/\rho_L)^{0.5} = 0.089$
from flooding graph for 24 in tray spacing (P. Wankat, *Equilibrium Staged Separations*, Prentice Hall, 1988, p. 387.)
C_{sb} = 0.33
u_{fl} = 5.84 ft/s
u_{act} = 1.33 m/s (75% of flooding)
if 75% active area
$A = (G/3600)/[(0.75)(\rho_G)(u_{act})] = 2.98\ m^2$
D = 2.0 m

48% overall column efficiency (O'Connell correlation)
$\Rightarrow$ 42 trays (so column about 84 ft tall ≈ 26 m)
$\Delta P = \rho g h N$
$50000\ Pa = (700\ kg/m^3)(9.8\ m/s^2)(h_{weir})(42)$
$h_{weir} = 0.174\ m \approx 6.8\ in$

V-901

Use a 10 minute holding time for liquid to P-901
$V = (67.29\ m^3/h)(10\ min)/(60\ min/h) = 11.215\ m^3$
$L/D = 3$
$V = \pi D^2 L/4 = \pi D^3 (L/D)/4$ (assuming horizontal bullet of diameter D and length L)
$D = \{(4)(11.215)/[(\pi)(3)]\}^{1/3} = 1.68\ m$
L = 5.05 m

No calculations are available for following equipment items:

P 902 A/B
P-904 A/B
V-902
V-903

P-901 A/B

Pump Curve Equation: $\Delta P(\text{kPa}) = 3000 - 0.03974\dot{v}^2$ (m^3/h)

Stream conditions – Stream 5: $\dot{v} =$ 67.3 m^3/h, ρ = 655 kg/m^3
Stream 8: ρ = 523 kg/m^3

Pressure drops at design conditions

location	ΔP (kPa)
pump inlet to T-901 inlet	2535
E-901	35
R-901	50
~25 m head to T-901 inlet	128
frictional losses in pipes	22
control valve	50

Bubble point pressure of Stream 5 at 25.93°C is 2.78 bar
At zero flowrate, $NPSH_A$ = 3.5 bar

$$NPSH_R(\text{kPa}) = 30 + 0.011\,\dot{v}^2 \ (\text{m}^3/\text{h})$$