ChE 455
Major #1
Ethyl Benzene Process

Background

You have recently been assigned to the ethyl benzene (EB) plant at the XYZ petrochemical facility. This facility produces a wide range of monomers, polymers, and solvents, all derived from petroleum. The EB process produces 80,000 tonne/yr of 99.8 mol% ethyl benzene that is totally consumed by the styrene facility on site. Like most EB/styrene facilities, there is significant heat integration between the two plants. In order to decouple the operation of the two plants, the energy integration is achieved by the generation and consumption of steam within the two processes. The EB reaction is exothermic, so steam is produced, and the styrene reaction is endothermic, so energy is used in the form of steam.

Several changes are anticipated within the EB process, and your job is to evaluate the effect that each change will have on the processes (EB and styrene) and to recommend ways to minimize upsets in current operation and maximize the positive economic impact of each change.

Ethyl Benzene Production Reactions

The production of EB takes place via the direct addition reaction between ethylene and benzene:

$$\underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{ethyl benzene}}{C_6H_5C_2H_5} \tag{1}$$

The reaction between EB and ethylene to produce diethyl benzene (DEB) also takes place:

$$\underset{\text{ethyl benzene}}{C_6H_5C_2H_5} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{diethyl benzene}}{C_6H_4(C_2H_5)_2} \tag{2}$$

Additional reactions between DEB and ethylene yielding tri- and higher ethyl benzene are also possible. However, in order to minimize these additional reactions, the molar ratio of benzene to ethylene is kept high, at approximately 8:1. The production of diethyl benzene is undesirable, and its value as a side product is low. In addition, even small amounts of DEB in EB cause significant processing problems in the downstream styrene process. Therefore, the maximum amount of DEB in EB is specified as 2 ppm. In order to maximize the production of the desired EB, the DEB is separated and returned to a separate reactor in which excess benzene is added to produce EB via the following equilibrium reaction:

$$\underset{\text{diethyl benzene}}{C_6H_4(C_2H_5)_2} + \underset{\text{benzene}}{C_6H_6} \leftrightarrow \underset{\text{ethyl benzene}}{2C_6H_5C_2H_5} \tag{3}$$

The incoming benzene contains a small amount of toluene impurity. The toluene reacts with ethylene to form ethyl benzene and propylene:

$$\underset{\text{toluene}}{C_6H_5CH_3} + 2C_2H_4 \rightarrow \underset{\text{ethyl benzene}}{C_6H_5C_2H_5} + \underset{\text{propylene}}{C_3H_6} \tag{4}$$

The reaction kinetics are of the form:

$$-r_i = k_{o,i}\, e^{-E_i/RT}\, C_{ethylene}^a C_{EB}^b C_{toluene}^c C_{benzene}^d C_{DEB}^e \tag{5}$$

where *i* is the reaction number above, and

i	***E_i*** **kcal/kmol**	$k_{o,i}$	***a***	***b***	***c***	***d***	***e***
1	22,500	1.00×10^6	1	0	0	1	0
2	22,500	6.00×10^5	1	1	0	0	0
3	25,000	7.80×10^6	0	0	0	1	1
4	20,000	1.80×10^8	2	0	1	0	0

The units of r_i are kmol/s/m^3-reactor, the units of C_i are kmol/m^3-gas and the units of $k_{o,i}$ vary depending upon the form of the equation.

Process Description

The PFD is in Appendix 1. A refinery cut of benzene is fed from storage to an on-site process vessel (V-301) where it is mixed with the recycled benzene. From V-301, it is pumped to reaction pressure of approximately 2,000 kPa (20 atm) and sent to a fired heater (H-301) to bring it to reaction temperature (approximately 400°C). The preheated benzene is mixed with feed ethylene just prior to entering the first stage of a reactor system consisting of three adiabatic packed bed reactors (R-301 to R-303) with inter-stage feed addition and cooling. Reaction occurs in the gas phase and is exothermic. The hot, partially converted reactor effluent leaves the first packed bed, is mixed with more feed ethylene, and is fed to E-301, where the stream is cooled to 380°C prior to passing to the second reactor (R-302) where further reaction takes place. High-pressure steam is produced in E-301, which is subsequently used in the styrene unit. The effluent stream from R-302 is similarly mixed with feed ethylene and is cooled in E-302 (with generation of high-pressure steam) prior to entering the third and final packed bed reactor, R-303. The effluent stream leaving the reactor contains products, by-products, unreacted benzene, and small amounts of unreacted ethylene and other non-condensable gases. The reactor effluent is cooled in two waste-heat boilers (E-303 and E-304) in which high-pressure and low-pressure steam are generated, respectively. This steam is also consumed in the styrene unit. The two-phase mixture leaving E-304 is sent to a trim cooler (E-305), where the stream is cooled to 80°C, and then to a two-phase separator (V-302), where the light gases are separated and sent overhead as fuel gas to be consumed in the fired heater. The condensed liquid is then sent to the benzene tower, T-301, where the unreacted benzene is separated as the overhead product and returned to the front end of the process. The bottoms product from the first column is sent to T-302, where product ethyl benzene (at 99.8 mol% and containing less than 2 ppm DEB) is taken as the top product and is sent directly to the styrene unit. The bottom product from T-302 contains all the diethyl benzene and trace amounts of higher ethyl benzenes. This stream is mixed with recycle benzene and passes through fired heater (H-301) prior to being sent to a fourth packed bed reactor (R-304) in which the excess benzene is reacted with the DEB to produce EB and unreacted benzene. The effluent from this reactor is mixed with the liquid stream entering the waste heat boiler (E-303).

The PFD for this process is shown in Figure 1 in Appendix 1, and a stream table indicating current operation is given as Table 1 in Appendix 1. The utility summary is in Table 2 in Appendix 1. Pertinent equipment information is given in Table 3 in Appendix 1.

Proposed Changes and Improvements

Several changes to the process have been suggested and your job is to determine which of the proposed changes (if any) should be implemented.

Change 1: A new catalyst has been developed by your supplier that is claimed to suppress the ethylation of EB to give DEB. Information on this new catalyst along with information on the existing catalyst is given in Appendix 3. You are to determine what changes in the process are required in order to utilize this new catalyst and what economic benefits would be achieved.

Change 2: An opportunity has arisen to purchase a lower of grade of benzene that contains a significantly greater fraction of toluene than the existing feed. For this new feed (containing 10% toluene), you are to determine what changes, if any, are required to process this new feed and the reduction in price of the benzene feed stream (currently $1.22/kg) that would make a switch to the new feed economically attractive. You should assume an internal hurdle rate of 11% before taxes and a length of 5 years for these economic calculations.

Economic improvements: Although no specific recommendations or changes are suggested, if you see anywhere that process improvements can be made, these should be evaluated using the same hurdle rate and project time given above.

Deliverables

A written report of your results, an analysis of your results, your conclusions, and your recommendations is required by 9:00 am, Monday, November 14, 2005. There will be an oral presentation of your results which will be scheduled between Monday, November 14, 2005 and Friday, November 18, 2005. More details about the written and oral reports are given below.

Your report should address all of the following issues:

1. You should describe the changes in the process required in order to utilize the new catalyst and the economic benefits that would be achieved

2. For the new feed, you are to determine the changes, if any, required to process the new feed and the reduction in price of the benzene feed stream that would make a switch to the new feed economically attractive.

3. Chemcad reports (that include stream compositions, equipment summaries, and convergence results but without stream properties) for any new cases that you present should be included as separate, labeled appendices.

4. PFD and stream tables for any new cases that you present should be included in the main written report.

5. Cost-saving measures that you recommend for the plant should be suggested.

6. A written report, conforming to the guidelines, detailing the information in items 1-5 should be included.

7. A legible, organized set of calculations justifying your recommendations, including any assumptions made should be included as an appendix.

8. A signed copy of the attached confidentiality statement should be included as the last page of the report.

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 to XYZ's management representatives some time between November 14 and November 18, 2005. Your presentation should be 15-20 minutes, followed by about a 30 minute question and answer period. Make certain that you prepare for this meeting since it is an important part of your assignment. You should also prepare a hard copy of your transparencies to be handed in at the beginning of your report.

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 the 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

Figure 1 is a flowsheet of Unit 300 as it was designed. Table 2, the stream table, follows and identifies design operating conditions, which, as far as we know, reflect the actual operating conditions prior to the shut down. Table 3 provides a summary of available equipment specifications. If information is missing or incomplete for a particular piece of equipment, it is not available.

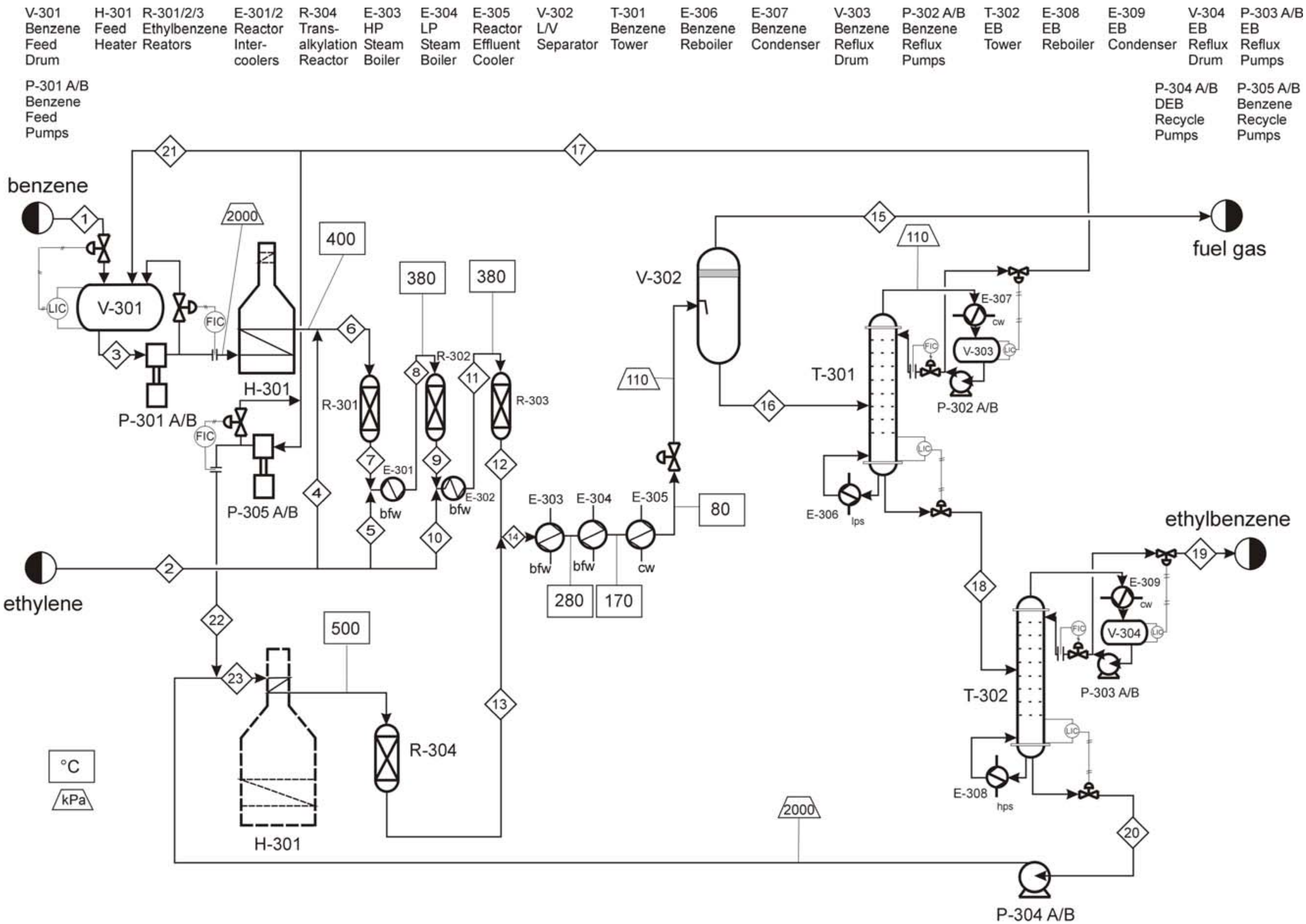


Figure 1: Unit 300 - Ethylbenzene Production Facility

Table 1: Stream Flow Table

Stream No.	**1**	**2**	**3**	**4**	**5**	**6**
Temp °C	25.0	25.0	58.5	25.0	25.0	383.3
Pres kPa	110.0	2000.0	110.0	2000.0	2000.0	1985.0
Vapor mole fraction	0.0	1.0	0.0	1.0	1.0	1.0
Total kmol/h	99.0	100.0	229.2	30.0	35.0	259.2
Total kg/h	7761.3	2819.5	17952.2	845.9	986.8	18797.9
Flowrates in kmol/h						
Ethylene	0.0000	93.0000	0.0000	27.9000	32.5500	27.9000
Ethane	0.0000	7.0000	0.0000	2.1000	2.4500	2.1000
Propylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	97.0000	0.0000	226.5099	0.0000	0.0000	226.5077
Toluene	2.0000	0.0000	2.0000	0.0000	0.0000	2.0000
Ethylbenzene	0.0000	0.0000	0.7003	0.0000	0.0000	0.7003
1,4-DiEthBenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Stream No.	**7**	**8**	**9**	**10**	**11**	**12**
Temp °C	444.1	380.0	453.4	25.0	380.0	449.2
Pres kPa	1970.0	1960.0	1945.0	2000.0	1935.0	1920.0
Vapor mole fraction	1.0	1.0	1.0	1.0	1.0	1.0
Total kmol/h	234.0	269.0	236.4	35.0	271.4	238.7
Total kg/h	18797.9	19784.7	19784.7	986.8	20771.5	20771.5
Flowrates in kmol/h						
Ethylene	0.8510	33.4010	0.6226	32.5500	33.1726	0.5407
Ethane	2.1000	4.5500	4.5500	2.4500	7.0000	7.0000
Propylene	1.8129	1.8129	1.9974	0.0000	1.9974	2.0000
Benzene	203.9113	203.9113	174.9631	0.0000	174.9631	148.3445
Toluene	0.1871	0.1871	0.0026	0.0000	0.0026	0.0000
Ethylbenzene	24.2827	24.2827	49.9541	0.0000	49.9541	70.5669
1,4-DiEthBenzene	0.8268	0.8268	4.2881	0.0000	4.2881	10.2963

Table 1: Stream Flow Table (cont'd)

Stream No.	**13**	**14**	**15**	**16**	**17**	**18**
Temp °C	497.9	458.1	73.6	73.6	81.4	145.4
Pres kPa	1988.0	1920.0	110.0	110.0	105.0	120.0
Vapor mole fraction	1.0	1.0	1.0	0.0	0.0	0.0
Total kmol/h	51.3	290.0	18.6	271.4	170.2	101.1
Total kg/h	4616.5	25387.9	1042.0	24345.9	13321.5	11024.5
Flowrates in kmol/h						
Ethylene	0.0000	0.5407	0.5407	0.0000	0.0000	0.0000
Ethane	0.0000	7.0000	7.0000	0.0000	0.0000	0.0000
Propylene	0.0000	2.0000	2.0000	0.0000	0.0000	0.0000
Benzene	29.5018	177.8462	8.3819	169.4643	169.2948	0.1695
Toluene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylbenzene	21.6875	92.2546	0.7128	91.5419	0.9154	90.6265
1,4-DiEthBenzene	0.0705	10.3668	0.0132	10.3536	0.0000	10.3536

Stream No.	**19**	**20**	**21**	**22**	**23**
Temp °C	139.0	191.1	82.6	82.6	121.4
Pres kPa	110.0	140.0	2000.0	2000.0	2000.0
Vapor mole fraction	0.0	0.0	0.0	0.0	0.0
Total kmol/h	89.9	11.3	130.2	40.0	51.3
Total kg/h	9538.6	1485.9	10190.9	3130.6	4616.5
Flowrates in kmol/h					
Ethylene	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000
Propylene	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	0.1695	0.0000	129.5100	39.7849	39.7849
Toluene	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylbenzene	89.7202	0.9063	0.7003	0.2151	1.1214
1,4-DiEthBenzene	0.0001	10.3535	0.0000	0.0000	10.3535

Table 2: Utility Summary

Stream Name	bfw to E-301	bfw to E-302	bfw to E-303	bfw to E-304	cw to E-305
Temp °C	115	115	115	115	30
Pressure kPa	4,200	4,200	4,200	600	400
Flowrate in 10^3kg/h	0.851	1.121	4.341	5.424	118.3
Duty (MJ/h)	-1,967	-2,592	-10,080	-12,367	-4,943
Stream Name	**lps to E-306**	**cw to E-307**	**hps to E-308***	**cw to E-309**	
Temp °C	160	30	254	30	
Pressure kPa	600	400	4200	400	
Flowrate in 10^3kg/h	4.362	174.1	3.124	125.9	
Duty (MJ/h)	9,109	-7,276	5,281	-5,262	

*throttled and desuperheated at exchanger

Table 3
Partial Equipment Specifications Summary

Heat Exchangers

E-301 *A* = 62.6 m^2 1-2 exchanger, floating head, carbon steel process stream in tubes *Q* = 1,967 MJ/h maximum pressure rating of 2,200 kPa	**E-302** *A* = 80.1 m^2 1-2 exchanger, floating head, carbon steel process stream in tubes *Q* = 2,592 MJ/h maximum pressure rating of 2,200 kPa
E-303 *A* = 546 m^2 1-2 exchanger, floating head, carbon steel process stream in tubes *Q* = 10,080 MJ/h maximum pressure rating of 2,200 kPa	**E-304** *A* = 1,567 m^2 1-2 exchanger, fixed head, carbon steel process stream in tubes *Q* = 12,367 MJ/h maximum pressure rating of 2,200 kPa
E-305 *A* = 348 m^2 1-2 exchanger, floating head, carbon steel process stream in shell *Q* = 4,943 MJ/h maximum pressure rating of 2,200 kPa	**E-306** *A* = 57.8 m^2 1-2 exchanger, fixed head, carbon steel process stream in shell *Q* = 9,109 MJ maximum pressure rating of 2,00 kPa
E-307 *A* = 54.6 m^2 1-2 exchanger, floating head, carbon steel process stream in shell *Q* = 7,276 MJ/h maximum pressure rating of 200 kPa	**E-308** *A* = 22.6 m^2 1-2 exchanger, fixed head, carbon steel process stream in shell *Q* = 5,281 MJ/h maximum pressure rating of 200 kPa
E-309 *A* = 17.5 m^2 1-2 exchanger, floating head, carbon steel process stream in shell *Q* = 5,262 MJ/h maximum pressure rating of 200 kPa	

Pumps

P-301 A/B Carbon steel – positive displacement Actual power = 15 kW Efficiency 75%	**P-302 A/B** Carbon steel - centrifugal Actual power = unknown Efficiency unknown
P-303 A/B Carbon steel - centrifugal Actual power = unknown Efficiency unknown	**P-304 A/B** Carbon steel - centrifugal Actual power = 1.4 kW Efficiency 80%
P-305 A/B Carbon steel - Positive displacement Actual power = 2.7 kW Efficiency 75%	

Fired Heater

H-301 required heat load = 22,376 MJ/h design (maximum) heat load = 35,000 MJ/h 75% thermal efficiency maximum pressure rating of 2,200 kPa	

Reactors

R-301 carbon steel packed bed, ZSM-5 mol. sieve catalyst $V = 20\ m^3$ 11 m long, 1.72 m diameter maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = 500°C	**R-302** carbon steel packed bed, ZSM-5 mol. sieve catalyst $V = 25\ m^3$ 12 m long, 1.85 m diameter maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = 500°C
R-303 carbon steel packed bed, ZSM-5 mol. sieve catalyst $V = 30\ m^3$ 12 m long, 1.97 m diameter maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = 500°C	**R-304** carbon steel packed bed, ZSM-5 mol. sieve catalyst $V = 1.67\ m^3$ 5 m long, 0.95 m diameter maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = 525°C

Vessels

V-301 7 m^3 Maximum operating pressure = 250 kPa horizontal height = 4.35 m Diameter = 1.45 m	**V-302** 10 m^3 Maximum operating pressure = 250 kPa vertical height = 4.90 m Diameter =1.62 m

Towers

T-301 carbon steel 45 sieve trays plus reboiler and total condenser 42% efficient trays feed on tray 19 additional feeds ports on tray 14 and 24 reflux ratio = 0.3874 24 in tray spacing column height 27.45 m diameter = 1.7 m maximum pressure rating of 300 kPa	**T-302** carbon steel 76 sieve trays plus reboiler and total condenser 45% efficient trays feed on tray 56 additional feeds ports on 50 and 62 reflux ratio = 0.6608 15 in tray spacing column height 28.96 m diameter = 1.5 m maximum pressure rating of 300 kPa

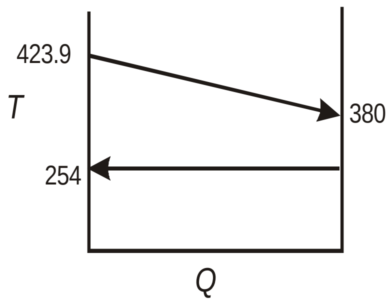
Appendix 2
Design Calculations

The following design calculations are available for this process. If information is not given, then it is not available.

Heat Exchangers

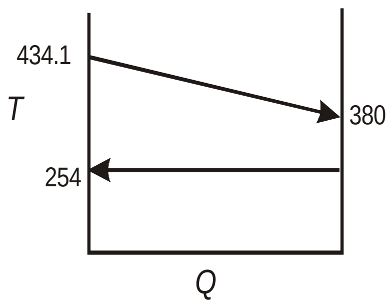
E-301

Q = 1,967 MJ/h
ΔT_{lm} = 146.9°C
process fluid h_i = 60 W/m^{2}K
bfw to hps h_o = 6000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 59.4 W/m^{2}K
A = 62.6 m^2



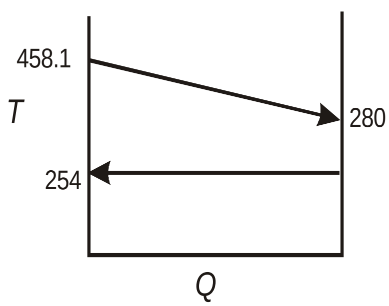
E-302

Q = 2,592 MJ/h
ΔT_{lm} = 151.4°C
process fluid h_i = 60 W/m^{2}K
bfw to hps h_o = 6000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 59.4 W/m^{2}K
A = 80.1 m^2



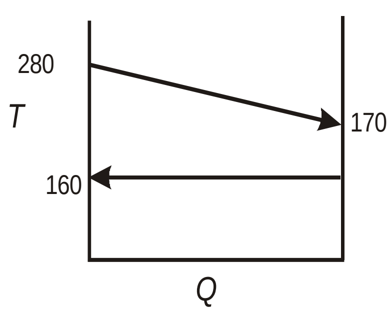
E-303

Q = 10,080 MJ/h
ΔT_{lm} = 86.4°C
process fluid h_i = 60 W/m^{2}K
bfw to hps h_o = 6000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 59.4 W/m^{2}K
A = 546 m^2



E-304

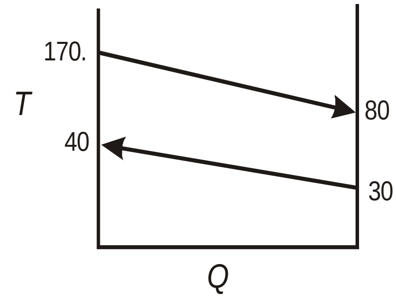
Q = 12,367 MJ/h
ΔT_{lm} = 44.3°C
process fluid h_i = 50 W/m^{2}K
bfw to lps h_o = 5000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 49.5 W/m^{2}K
A = 1567 m^2



NOTE: for E-301 – E-304 duties include specific heat change for bfw to saturation temperature but the shell side is assumed to be well mixed and at the temperature of the saturated steam.

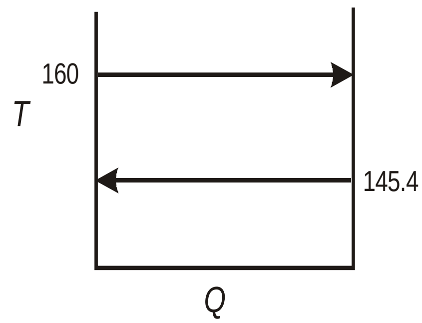
E-305

Q = 4,943 MJ/h
ΔT_{lm} = 83.7°C
process fluid h_o = 50 W/m^{2}K
cw h_i = 1000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 47.6 W/m^{2}K
P = 90/10 = 9
R = 10/140 = 0.07
F = 0.99
A = 348 m^2



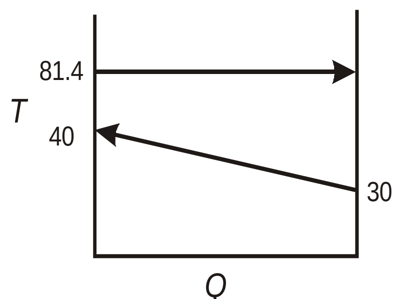
E-306

Q = 9,109 MJ/h
ΔT_{lm} = 14.6°C
process fluid h_o = 6000 W/m^{2}K
lps condensing h_i = 6000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 3000 W/m^{2}K
A = 57.8 m^2



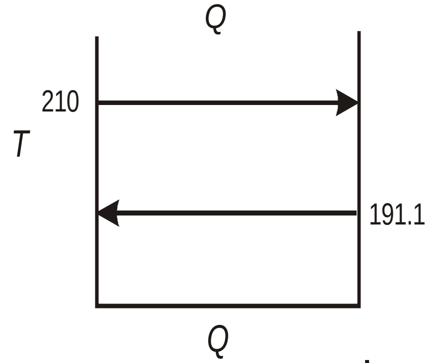
E-307

Q = 7,276 MJ/h
ΔT_{lm} = 46.2°C
process fluid h_o = 4000 W/m^{2}K
cw h_i = 1000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 800 W/m^{2}K
A = 54.6 m^2



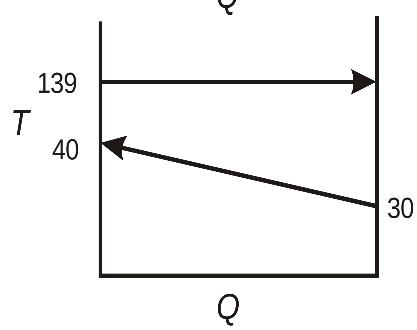
E-308

Q = 5,281 MJ/h
ΔT_{lm} = 18.9°C
process fluid h_o = 8000 W/m^{2}K
throttled hps condensing h_i = 6000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 3429 W/m^{2}K
A = 22.6 m^2



E-309

Q = 5,262 MJ/h
ΔT_{lm} = 103.92°C
process fluid h_o = 4000 W/m^{2}K
cw h_i = 1000 W/m^{2}K
$U \approx 1/h_i + 1/h_o$ = 800 W/m^{2}K
A = 17.5 m^2



T-301

tray/tower sizing done on Chemcad
efficiency from O'Connell correlation
run flash on distillate and bottom stream
at top $\alpha_{top} = K_{benzene}/K_{ethylbenzene} = 6.01$
at bottom $\alpha_{bottom} = K_{benzene}/K_{ethylbenzene} = 3.93$
$\alpha_{avg} = (\alpha_{top}\alpha_{bottom})^{0.5} = 4.9$
from Chemcad $\mu_{feed} = 0.003612$ Pa s = 0.3612 cp
See Figure 12-14 in Wankat
efficiency $\approx$ 0.42

21 stages = 19 trays + condenser + reboiler
19/0.42 = 45 actual trays + condenser + reboiler
feed on stage 9 = tray 8
8/0.42 = 19 so feed on tray 19

T-302

tray/tower sizing done on Chemcad
efficiency from O'Connell correlation
run flash on distillate and bottom stream
at top $\alpha_{top} = K_{ethylbenzene}/K_{di\text{-}ethylbenzene} = 3.84$
at bottom $\alpha_{bottom} = K_{ethylbenzene}/K_{di\text{-}ethylbenzene} = 3.2$
$\alpha_{avg} = (\alpha_{top}\alpha_{bottom})^{0.5} = 3.5$
from Chemcad $\mu_{feed} = 0.003612$ Pa s = 0.3612 cp
See Figure 12-14 in Wankat
efficiency $\approx$ 0.45

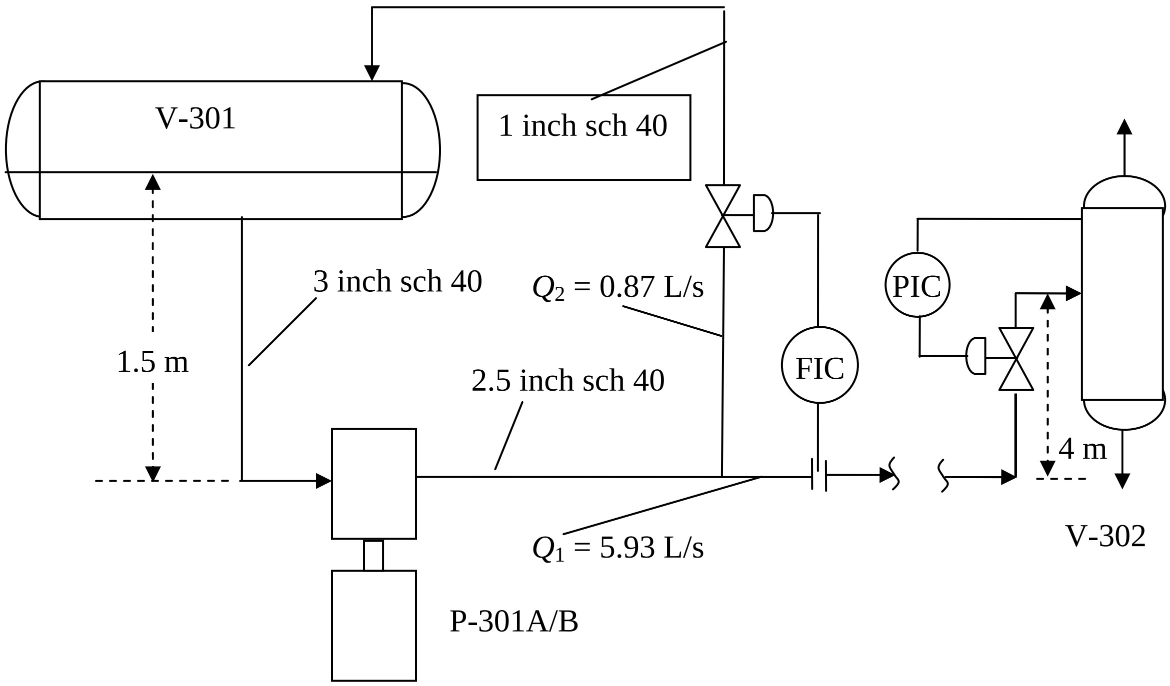
36 stages = 34 trays + condenser + reboiler
34/0.45 = 76 actual trays + condenser + reboiler
feed on stage 26 = tray 25
25/0.45 = 56 so feed on tray 56

V-301
from Chemcad, liquid throughput (volumetric rate of Stream 3) = 21.4 m^3/h = 0.3567 m^3/min
assume 10 min residence time, so volume = 3.567 m^3
assume vessel size is approximately double this volume = 7 m^3
horizontal vessel
$V = \pi D^2 L/4$, where D = diameter and L = length of vessel (as drawn on PFD)
$L/D = 3$

$$D = \sqrt[3]{\frac{(4)(7)}{\pi(3)}} = 1.45 \text{ m and } L = 3D = 4.35 \text{ m}$$

P-301

Flow of liquid at normal operating conditions, $\dot{m}$ =17,912 kg/h, T = 58.4°C, p_{ben}* = 50.6 kPa
Vol flow of liquid, Q = 21.36 m^3/h = 5.93 L/s
ρ_l = 839 kg/m^3, μ_l = 0.000404 kg/m s



The pump curve and NPSH curves for P-301 are attached as Figures 2 and 3. Under normal operating conditions, approximately 15% of the flow through P-301 A/B is recycled back to V-301. The normal operating level of liquid is 1.5 m above the pump inlet. Pipe calculations for 100 ft of suction and discharge piping are

variable	2.5"sch 40	3" sch 40	units
D	2.469	3.0680	inch
D	0.062713	0.0779	m
Q	0.0068	0.0068	m^3/s
v	2.207766	1.4298	m/s
μ	4.04×10^{-4}	4.04×10^{-4}	kg/m s
ρ	839	839	kg/m^3
Re	287,533	231,395	
e/D	0.000718	0.000577	
f	0.004582	0.0044	
L	30.48	30.48	m
ΔP_f	9,107	2,937	Pa

NPSHA = $P_{supply} + h\rho g - (-\Delta P_f) - P^*$ = 101,000 + (1.5)(839)(9.81) – 2937 – 50,600 = 59,810 Pa
= (59,810)/(839)/(9.81) = 7.3 m of liquid – cavitation is not a problem

Equivalent length of suction piping ($L_{eq,suct}$) is approx 100 ft, discharge piping ($L_{eq,disch}$) = 500 ft

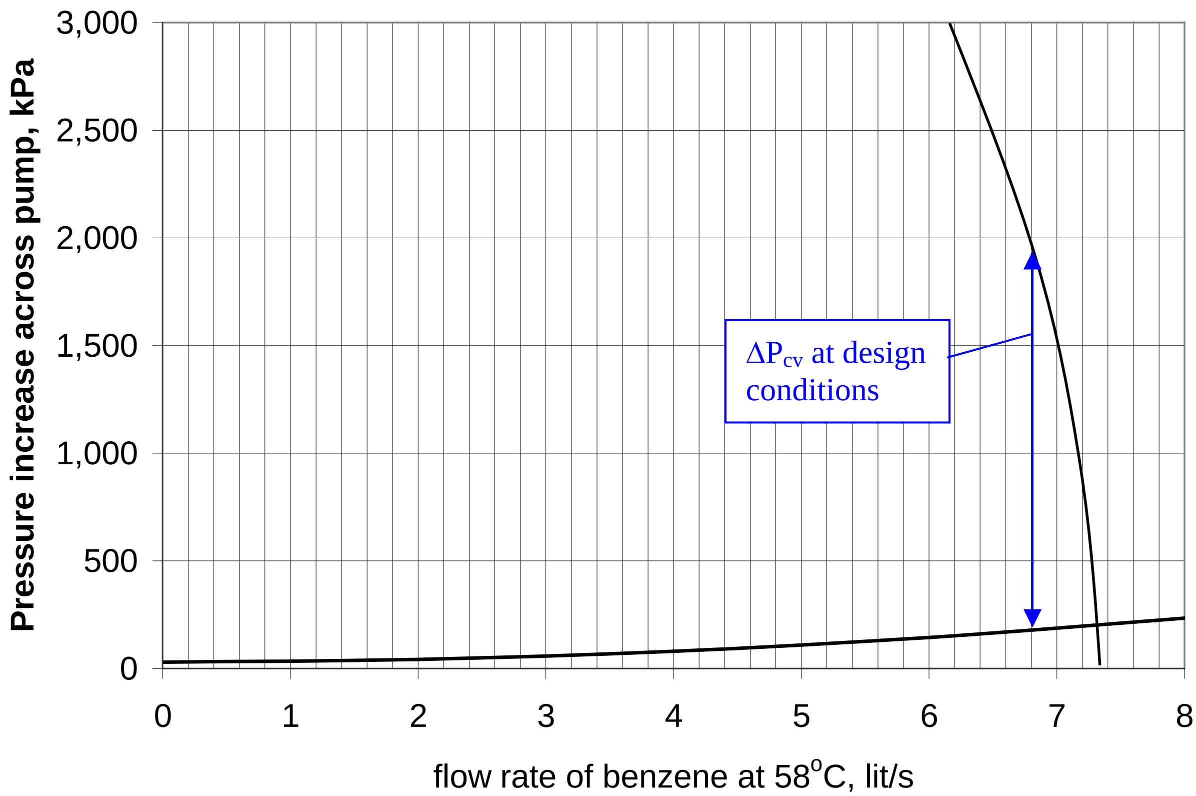
$-\Delta P_f = 2{,}937 + (500)(9{,}107)(5.93/6.8)^2/(100) + \Delta P_{H\text{-}301} + \Delta P_{R\text{-}301} + \Delta P_{R\text{-}302} + \Delta P_{R\text{-}303} + \Delta P_{E\text{-}301} + \Delta P_{E\text{-}302} + \Delta P_{E\text{-}303} + \Delta P_{E\text{-}304} + \Delta P_{E\text{-}305} = 2{,}937 + 34{,}627 + 15{,}000 + 15{,}000 + 15{,}000 + 15{,}000 + 10{,}000 + 10{,}000 + 10{,}000 + 10{,}000 + 10{,}000 = 147{,}560$ Pa

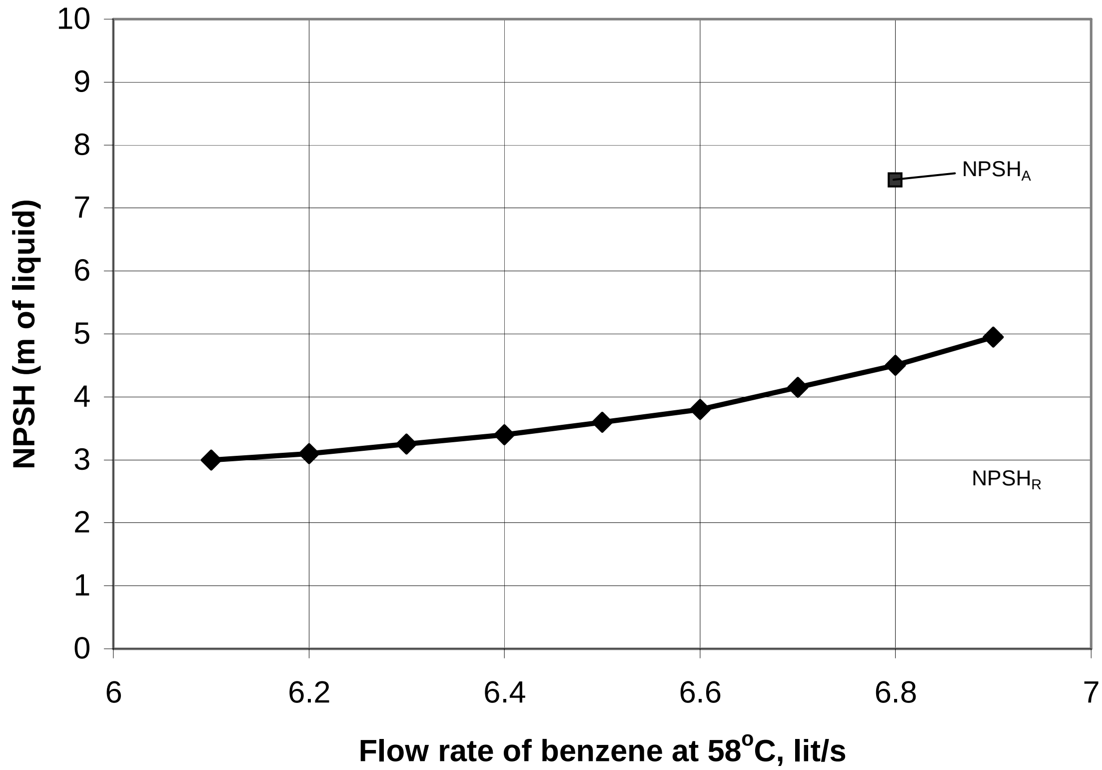
M E Balance from V-301 to V-302

$\Delta P_{12} + \rho g \Delta z_{12} + 0.5\rho\Delta v_{12} + (-\Delta P_f) + \Delta P_{cv} = -\rho w_s$

We require 2000 kPa at pump outlet thus $(-\rho w_s)$ + 101 + (1.5)(9.81)(839)/1000 – 2.937 = 2,000
$-\rho w_s$ = 1890 kPa

System Curve at normal flow = (110 - 101) + (839)(9.81)(4.0 - 1.5)/1000 + (0) + 147.6 = 177.2 kPa
$\therefore\ \Delta P_{cv}$ = 1890 – 177 = 1,723 kPa





V-302

from Chemcad, liquid throughput (volumetric rate of Stream 16) = 29.7 m^3/h = 0.495 m^3/min
assume 10 min residence time, so volume = 4.95 m^3
assume vessel size is approximately double this volume = 10 m^3
Vapor flow (Stream 15) = 476 m^3/h = 0.1322 m^3/s, ρ_g = 2.17 kg/m^3
vertical vessel
$V = \pi D^2 h/4$, where D = diameter and L = height of vessel (as drawn on PFD)
Assume $L/D = 3$

$$D = \sqrt[3]{\frac{(4)(10)}{\pi(3)}} = 1.62\,\text{m and } L = 3D = 4.90\text{ m}$$

Check gas velocity

$$v_{gas} = \frac{4Q}{\pi D^2} = \frac{(4)(0.1322)}{\pi(1.62)^2} = 0.064\text{ m/s}$$

Criterion for phase separators is $v_{gas} \le 0.11\sqrt{\frac{\rho_l}{\rho_g} - 1} = 0.11\sqrt{\frac{821}{2.17} - 1} = 2.14$ m/s - no problem

Design of Fuel gas feed line from V-302 to H-301

Vapor from V-302 (Stream 15) is fuel gas that is consumed in H-301.
Available pressure drop across line from V-302 to H-301 is 10 kPa.

Assume 2 kPa across regulating flow valve at heater.
Equivalent length of pipe from V-302 to H-301 is 110 ft.

$$-\Delta P_f = 8{,}000 = \frac{2\rho_g f v^2 L_{eq}}{D} = 2(2.17)(110)(0.3048)\frac{f v^2}{D}$$

Choose values of D and calculate $-\Delta P_f$

Variable	Units	2"sch 40	3" sch 40	4" sch 40
D	inch	2.067	3.068	4.026
D	m	0.0525	0.07792	0.10226
Q	m^3/s	0.1322	0.1322	0.1322
v	m/s	61.0651	27.7181	16.0963
μ	kg/m s	9.51×10^{-6}	9.51×10^{-6}	9.51×10^{-6}
Re		7.32×10^{5}	4.93×10^{5}	3.76×10^{5}
e	m	0.000045	0.000045	0.000045
e/D		0.000857	0.000577	0.000440
f		0.004748	0.004346	0.004108
$-\Delta P_f$	Pa	49,068	6,235	1,515

Choose 3” sch 40 carbon steel

R-301
packed bed
Volume of reactor containing catalyst, $V_{reac} = 20\ m^3$
$V_{reac} = 20 = V_{cat}/(1-\varepsilon)$
Voidage, $\varepsilon = 0.4$
$V_{cat} = 12\ m^3$ of catalyst
Catalyst size = 2 mm approx spherical
Vertical vessel
$V = \pi D^2 L/4$, where D = diameter and L = height of vessel containing catalyst
Assume an $L/D = 5$

$$D = \sqrt[3]{\frac{(4)(20)}{\pi(5)}} = 1.72\ \text{m}$$

$$L = 5D = 8.6\ \text{m}$$

Add 1 m either end for vapor distribution, giving $L = 11$ m

R-302
packed bed
Volume of reactor containing catalyst, $V_{reac} = 25\ m^3$
$V_{reac} = 25 = V_{cat}/(1-\varepsilon)$
Voidage, $\varepsilon = 0.4$
$V_{cat} = 15\ m^3$ of catalyst

Catalyst size = 2 mm approx spherical
Vertical vessel
$V_{reac} = \pi D^2 L/4$, where D = diameter and L = height of vessel containing catalyst
Assume an $L/D = 5$

$$D = \sqrt[3]{\frac{(4)(25)}{\pi(5)}} = 1.85\,\text{m}$$

$L = 5D = 9.27$ m
Add 1 m either end for vapor distribution, giving L = 12 m

R-303
packed bed
Volume of reactor containing catalyst, $V_{reac} = 30$ m^3
$V_{reac} = 30 = V_{cat}/(1-\varepsilon)$
Voidage, $\varepsilon = 0.4$
$V_{cat} = 18$ m^3 of catalyst
Catalyst size = 2 mm approx spherical
Vertical vessel
$V_{reac} = \pi D^2 L/4$, where D = diameter and L = height of vessel containing catalyst
Assume an $L/D = 5$

$$D = \sqrt[3]{\frac{(4)(30)}{\pi(5)}} = 1.97\,\text{m}$$

$L = 5D = 9.85$ m
Add 1 m either end for vapor distribution, giving L = 12 m

R-304
packed bed
Volume of reactor containing catalyst, $V_{reac} = 1.67$ m^3
$V_{reac} = 1.67 = V_{cat}/(1-\varepsilon)$
Voidage, $\varepsilon = 0.4$
$V_{cat} = 1$ m^3 of catalyst
Catalyst size = 2 mm approx spherical
Vertical vessel
$V = \pi D^2 L/4$, where D = diameter and L = height of vessel containing catalyst, assume an L/D = 2.5

$$D = \sqrt[3]{\frac{(4)(1.67)}{\pi(2.5)}} = 0.95\,\text{m}$$

$L = 2.5D = 2.37$ m

Add 1 m either end for vapor distribution, giving L = 5 m

Appendix 3

Pressure drop calculations for reactors R-301 – R-304 – Existing Conditions

Variable	Units	R-301	R-302	R-303	R-304
V_{cat}	m^3	12	15	18	1
Voidage, ε		0.4	0.4	0.4	0.4
volume of cat filled reactor, V_{reac}	m^3	20.00	25.00	30.00	1.67
L/D		5	5	5	2.5
D	m	1.72	1.85	1.97	0.95
L_{cat}	m	8.60	9.27	9.85	2.37
D_{cat}	m	0.002	0.002	0.002	0.002
gas density, ρ_g	kg/m^3	28.00	28.30	29.70	29.60
gas viscosity, $(\times10^{-5})\mu_g$	kg/m s	1.80	1.75	1.70	1.82
Volumetric gas flow, Q	m^3/s	0.1889	0.1939	0.1936	0.0433
Superficial gas vel, v	m/s	0.0812	0.0719	0.0636	0.0615
ΔP Ergun Equation	Pa	15,700	13,600	11,900	2,700

<u>Look at pore diffusion resistance in catalysts</u>

Consider the main reaction (Reaction 1) only since this is the fastest reaction and will provide the limiting case.
Since benzene is in high excess, we can consider this as pseudo-first-order reaction with respect to ethylene

Use highest temperature in reaction system which is approx. 450°C = 723K
Mole fraction of benzene at reactor R-301 inlet (Stream 6) = 226.34/259.3 = 0.8729
Mole fraction of ethylene at reactor R-301 inlet (Stream 6) = 27.9/259.3 = 0.1076
Total molar concentration at reactor inlet (Stream 6) = P/RT = (1985000)/(8.314)/(383+273) = 363.9 mol/m^3 = 0.3639 kmol/m^3
Benzene concentration at reactor inlet = (0.8729)(0.3639) = 0.3177 kmol/m^3
Pseudo first-order reaction rate constant, $k_1C_{benzene} = 1.00\times10^6$exp(-22,500/1.986/723)(0.3177) = 0.04974 m^3-gas/m^3-reactor/s
Changing the basis to the volume of catalyst $\Rightarrow k'_1 = k_1/(1-\varepsilon)$ = (0.04974)/(1-0.4) = 0.08290 m^3-gas/m^3-catalyst/s
Effective diffusivity of catalyst (from catalyst manufacturer) = 6×10^{-8} m^3-gas/m-catalyst/s

Thiele Modulus, $M_T = \dfrac{D_{cat}}{6}\sqrt{\dfrac{k_1'}{D_{eff}}} = \dfrac{0.002}{6}\sqrt{\dfrac{0.0829}{6\times10^{-8}}} = 0.39$

This gives an effectiveness factor of approximately 0.95 – close to 1, so use of intrinsic kinetics should be ok. Next, check for external mass transfer resistance.

External mass transfer to surface of catalyst

Particle Reynolds number, $\mathrm{Re}_p = \dfrac{D_{cat}\rho_g u_{bed}}{\mu_g} = \dfrac{(0.002)(28)(0.0812/0.4)}{(18\times 10^{-6})} = 632$

Estimate mass transfer coefficient from correlation due to Froessling [N. Froessling, Gerlands Beitr. Geophys., 52, 170 (1938).]

$$\frac{k_m D_{cat}}{y_A D_{AB}} = 2.0 + 0.552\,\mathrm{Re}_p^{0.5}\left(\frac{\mu}{\rho D_{AB}}\right)^{1/3}$$

At these conditions the diffusivity of ethylene in benzene, D_{AB}, is estimated to be 1×10^{-2} cm^2/s = 1×10^{-6} m^2/s

$$\therefore \frac{k_m(0.002)}{(0.1076)(1\times 10^{-6})} = 2.0 + 0.552(632)^{0.5}\left(\frac{(18\times 10^{-6})}{(28)(1\times 10^{-6})}\right)^{1/3} = 14.0$$

$k_m = 7.519\times 10^{-4}$ m/s

Fraction of resistance in the external film = $\dfrac{1}{1+\dfrac{k_m}{k_1^{'}(D_{cat}/6)}} = \dfrac{1}{1+\dfrac{7.519\times 10^{-4}}{(0.0829)(0.002/6)}} = 0.035$

Therefore, the external mass transfer resistance is only 3.5% of the total and can be safely ignored. Therefore, the reaction is controlled by the intrinsic kinetics of the reaction and these should be used in the simulation.

Properties of new Catalyst

The new catalyst is available as a cylindrical extruded pellet with diameter 4 mm and length 8 mm. For the sake of calculations, you may assume that the catalyst behaves like a spherical particle of diameter = 5.8 mm and packed bed voidage of 0.52. You should assume that the maximum allowable catalyst temperature = 500°C.

According to the manufacturer, the intrinsic rates of reaction are given in the following table:

i	***E$_i$*** **kcal/kmol**	***k$_{o,i}$***	***a***	***b***	***c***	***d***	***e***
1	22,500	1.50×10^{6}	1	0	0	1	0
2	22,500	6.00×10^{3}	1	1	0	0	0
3	25,000	7.80×10^{6}	0	0	0	1	1
4	20,000	1.80×10^{8}	2	0	1	0	0

The pore structure of the new catalyst is somewhat smaller than the existing catalyst and the manufacturer gives the effective diffusivity as 1×10^{-8} m^3-gas/m-catalyst/s. The bulk density of the new catalyst is 1,200 kg/m^3.

Appendix 4
Cost Information

Raw Materials

Ethylene	\$0.77/kg
Benzene	\$1.22/kg

Products

Ethyl Benzene	not available

Utility Costs

See Table 6.3 of text

Equipment Costs and Cost Factor

Use CAPCOST if needed

Appendix 5
Chemcad Simulation

A Chemcad simulation is provided to aid in the solution of the current problem. The simulation is for the current operating conditions. The thermodynamics models are K-val = UNIFAC and Enthalpy = Latent Heat, these should not be changed.

It should be noted that, in the simulation, a component separator is placed after the high-pressure flash drum (V-302) in order to remove non-condensables from Stream 16 prior to entering T-301. This is done in order to avoid problems in simulating this tower. In practice, the non-condensables would be removed from the overhead reflux drum, V-303 after entering T-301.

Both towers are simulated as Shortcut columns in the main simulation but each is separately simulated using the rigorous TOWER module. You should use the same approach in your simulations. The rigorous TOWER module provides accurate design and simulation data and should be used to assess column operation.