ChE 455
Fall 2012
Major 1

Cumene Production

Background

Cumene (isopropyl benzene) is produced by reacting propylene with benzene. During World War II, cumene was used as an octane enhancer for piston-engine aircraft fuel. Presently, most of the worldwide supply of cumene is used as a raw material for phenol production, a process that simultaneously produces most of the worldwide supply of acetone. Typically, cumene is produced at the same facility that manufactures phenol and acetone.

The plant at which you are employed currently manufactures cumene in Unit 800 by a vapor-phase alkylation process that uses a phosphoric acid catalyst supported on kieselguhr. Plant capacity is on the order of 100,000 tonne/y of 99 wt% purity cumene. Benzene and propylene feeds are brought in by tanker trucks and stored in tanks as liquids.

Cumene Production Reactions

The reactions for cumene production from benzene and propylene are given in Equations 1 and 2. The undesired product, p-DIPB, is p-diisopropyl benzene. Cumene is isopropyl benzene.

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{benzene}}{C_6H_6} \rightarrow \underset{\text{cumene}}{C_9H_{12}} \tag{1}$$

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{cumene}}{C_9H_{12}} \rightarrow \underset{\text{p - DIPB}}{C_{12}H_{18}} \tag{2}$$

Process Description

The PFD for the cumene production process, Unit 800, is given in Figure 1. The reactants are fed from their respective storage tanks. After being pumped up to the required pressure (dictated by catalyst operating conditions), the reactants are mixed, vaporized, and heated to the temperature required by the catalyst in the fired heater. The shell-and-tube reactor converts the reactants to desired and undesired products as per the reactions in Equations 1 and 2. The reactions are exothermic, and heat is removed using a co-current Dowtherm loop. The stream leaving the reactor is cooled, partially condensed, and enters the flash unit. The off-gas may be used for fuel credit. The liquid stream from the flash drum is sent to the first distillation column, which separates benzene for recycle. The second distillation column purifies cumene from the p-DIPB (p-diisopropyl benzene) impurity. Currently, the waste p-DIPB is used as fuel for a furnace.

Table 1 is the stream table for Unit 800. Table 2 shows the utility flows, and Table 3 provides some of the equipment specifications.

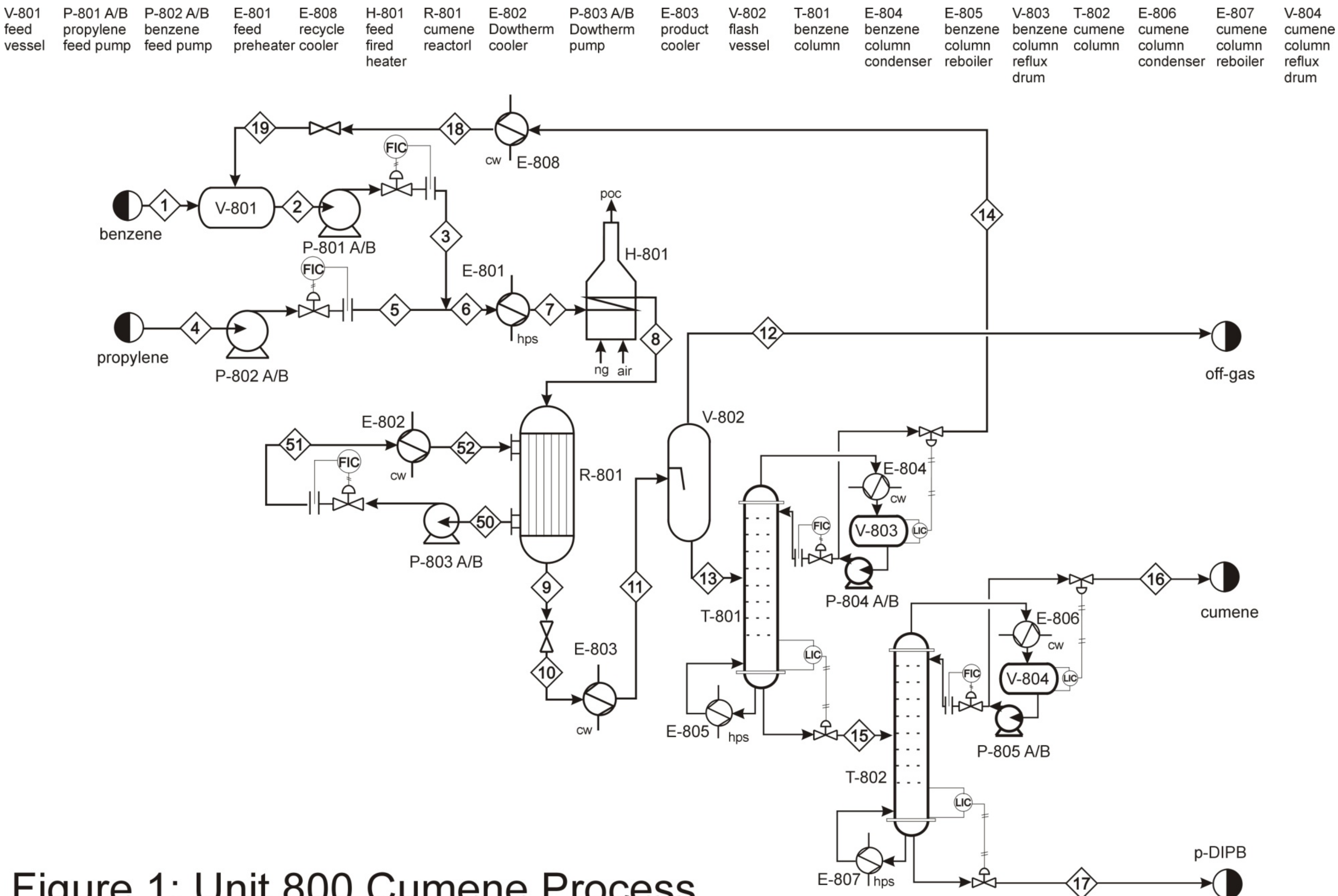

Figure 1: Unit 800 Cumene Process

Table 1
Stream Tables for Unit 800

Stream No.	**1**	**2**	**3**	**4**	**5**
Temperature (°C)	25.00	38.33	39.52	25.00	27.23
Pressure (kPa)	130.00	130.00	3150.00	1200.00	3150.00
Vapor Mole Fraction	0.00	0.00	0.00	0.00	0.00
Total Flow (kmol/h)	135.00	647.77	647.77	160.00	160.00
Total Flow (kg/h)	10,545.39	49,530.30	49,530.30	6,749.08	6,749.08
Component Flows (kmol/h)					
propane	0.00	30.42	30.42	8.00	8.00
propylene	0.00	1.09	1.09	152.00	152.00
benzene	135.00	616.14	616.14	0.00	0.00
cumene	0.00	0.11	0.11	0.00	0.00
p-diisopropyl benzene	0.00	0.00	0.00	0.00	0.00

Stream No.	**6**	**7**	**8**	**9**	**10**
Temperature (°C)	38.23	231.57	350.00	343.77	323.56
Pressure (kPa)	3125.00	3095.00	3075.00	3025.00	225.00
Vapor Mole Fraction	0.00	1.00	1.00	1.00	1.00
Total Flow (kmol/h)	807.77	807.77	807.77	656.07	656.04
Total Flow (kg/h)	56,279.38	56,279.38	56,279.38	56,279.16	56,276.69
Component Flows (kmol/h)					
propane	38.42	38.42	38.42	38.42	38.42
propylene	153.09	153.09	153.09	1.39	1.39
benzene	616.14	616.14	616.14	484.34	484.31
cumene	0.11	0.11	0.11	112.02	112.02
p-diisopropyl benzene	0.00	0.00	0.00	19.89	19.90

Stream No.	**11**	**12**	**13**	**14**	**15**
Temperature (°C)	65.00	65.00	65.00	44.81	185.81
Pressure (kPa)	200.00	200.00	200.00	170.00	200.00
Vapor Mole Fraction	0.017	1.00	0.00	0.00	0.00
Total Flow (kmol/h)	656.04	11.04	645.00	512.77	132.23
Total Flow (kg/h)	56,276.69	581.92	55,694.77	38,984.92	16,709.85
Component Flows (kmol/h)					
propane	38.42	8.00	30.42	30.42	0.00
propylene	1.39	0.30	1.09	1.09	0.00
benzene	484.31	2.69	481.62	481.14	0.48
cumene	112.02	0.05	111.96	0.11	111.85
p-diisopropyl benzene	19.90	0.00	19.89	0.00	19.89

Table 1
Stream Tables for Unit 800 (cont'd)

Stream No.	**16**	**17**	**18**	**19**
Temperature (°C)	167.50	235.86	40.00	39.62
Pressure (kPa)	150.00	180.00	135.00	130.00
Vapor Mole Fraction	0.00	0.00	0.012	0.011
Total Flow (kmol/h)	112.32	19.91	512.77	512.77
Total Flow (kg/h)	13,484.31	3225.54	38,984.92	38,984.92
Component Flows (kmol/h)				
propane	0.00	0.00	30.42	30.42
propylene	0.00	0.00	1.09	1.09
benzene	0.48	0.00	481.14	481.14
cumene	111.74	0.11	0.11	0.11
p-diisopropyl benzene	0.10	19.79	0.00	0.00

Stream No.	**50**	**51**	**52**
Temperature (°C)	338.67	338.70	300.00
Pressure (kPa)	1000.00	1070.00	1035.00
Vapor Mole Fraction	0.00	0.00	0.00
Total Flow (kmol/h)	1000.00	1000.00	1000.00
Total Flow (kg/h)	166,000.00	166,000.00	166,000.00
Component Flows (kmol/h)			
Dowtherm A	100.00	1000.00	1000.00

Table 2
Utility Summary for Unit 800
(all units of kg/h)

E-801	**E-802**	**E-803**	**E-804**
hps	Dowtherm	cw	cw
21,600	383,000	1,120,000	518,000

E-805	**E-806**	**E-807**	**E-808**
hps	cw	hps	cw
13,200	146,000	3470	4810

Table 3
Partial Equipment Summary

Heat Exchangers

H-801 fired heater – refractory-lined, stainless-steel tubes design Q = 15.03 GJ/h max Q = 18.00 GJ/h P_{design} = 3100 kPa P_{max} = 3300 kPa	**E-801** carbon steel A = 195 m^2 boiling in shell, condensing in tubes 1 shell – 2 tube passes Q = 36,531 MJ/h P_{design} = 3135 kPa P_{max} = 3300 kPa
E-802 carbon steel A = 84.77 m^2 cw in shell, process fluid in tubes 1 shell – 2 tube passes Q = 16,042 MJ/h P_{design} = 1070 kPa P_{max} = 1400 kPa	**E-803** carbon steel A = 473 m^2 process fluid in shell, cw in tubes 1 shell – 2 tube passes Q = 46,963 MJ/h P_{design} = 225 kPa P_{max} = 300 kPa
E-804 carbon steel A = 195 m^2 condensing in shell, cw in tubes 1 shell – 2 tube passes Q = 21,683 MJ/h P_{design} = 170 kPa P_{max} = 300 kPa	**E-805** carbon steel A = 60 m^2 boiling in shell, condensing in tubes 1 shell – 2 tube passes Q = 24,454 MJ/h P_{design} = 185 kPa P_{max} = 300 kPa
E-806 carbon steel A = 11.4 m^2 condensing in shell, cw in tubes 1 shell – 2 tube passes Q = 6097 MJ/h P_{design} = 150 kPa P_{max} = 250 kPa	**E-807** carbon steel A = 30.6 m^2 boiling in shell, condensing in tubes desuperheater – steam saturated at 150°C 1 shell – 2 tube passes Q = 5916 MJ/h P_{design} = 180 kPa P_{max} = 250 kPa
E-808 carbon steel A = 21.2 m^2 process fluid in tubes, cooling water in shell 1 shell – 2 tube passes Q = 201.3 MJ/h P_{design} = 170 kPa P_{max} = 250 kPa	

Reactors

R-801 carbon steel, shell-and-tube packed bed V = 22.7 m^3 4.0 m tall, 2800 tubes, 0.0508 m = 2 in diameter P_{design} = 3075 kPa P_{max} = 3300 kPa

Towers

T-801 carbon steel D = 2.5 m 32 sieve trays 41% efficient feed on tray 17 24 in tray spacing 4.90 in weirs column height = 64 ft = 19.5 m P_{design} = 205 kPa P_{max} = 300 kPa	**T-802** carbon steel D = 1.8 m 58 sieve trays 57% efficient feed on tray 44 12 in tray spacing 2.95 in weirs column height = 58 ft = 17.7 m P_{design} = 180 kPa P_{max} = 300 kPa

Other Equipment

V-801 carbon steel V = 15.3 m^3 horizontal D = 1.86 m, L = 5.59 m P_{design} = 130 kPa P_{max} = 200 kPa	**V-802** carbon steel V = 21.5 m^3 vertical D = 2.09 m, H = 8.35 m P_{design} = 200 kPa P_{max} = 250 kPa
P-801 A/B stainless steel W = 61.9 kW (actual) 80% efficient	**P-802 A/B** carbon steel W = 9.1 kW (actual) 80% efficient
P-803 A/B stainless steel W = 2.64 kW (actual) 80% efficient	

Problem

Due to an upset at another plant, production of cumene, phenol, and acetone must be increased at this plant (and all other company plants) to fulfill contracts for phenol and acetone. Your assignment is to determine the maximum possible scale-up for the cumene plant. Others are assigned the same task for the phenol and acetone plant. The bottleneck to scale-up must be identified. If a bottleneck can be removed by changing process conditions within acceptable parameters, these conditions should be defined. This process should be repeated until a bottleneck is reached that cannot be removed through changes in operating conditions. The conditions at this point define the maximum possible scale-up. New equipment cannot be purchased and installed unless there is a parallel unit (a pump for example), because shut down is not possible at this point in time.

Until phenol and acteone production can be increased to make up for the loss of cumene production at the other plant, some deliveries are being delayed. This will not make the customers happy, and they may not want to renew their contracts to purchase phenol and acetone. Therefore, it is important that cost-saving strategies (that could be passed on to our customers) be identified within the current plant. A thorough analysis to identify cost-saving strategies should be performed. Since this is a long-term project, it may be possible to purchase new equipment that could be installed during a typical two- to three-week annual shut down. The incremental profitability of any such equipment should be analyzed.

Additionally, there are some concerns about P-802 making unusual noises. Suggestions should be made regarding the cause and any possible remedy.

Finally, a summer intern wondered why E-808 was necessary, since it only changes the stream temperature by about 8°C. You should evaluate this idea for process feasibility and for incremental profitability.

Deliverables

Specifically, the following is to be completed by 9:00 a.m., Monday, November 12, 2012:

1. Prepare a written report, conforming to the guidelines, detailing the solution to the problem. Determine the maximum possible scale-up. Then, by removing bottlenecks to scale-up, state the maximum possible scale-up and provide clear explanations of the process changes required in order to accomplish the stated scale-up level. If additional equipment is needed, as stated above, it must be parallel equipment that can be installed without shut down. Determine the cost of such equipment, if it is recommended.

2. Provide a list of suggested process improvements that can enhance the profitability of Unit 800. Provide a table that gives the purchased costs (use C_{BM} from Capcost) and specifications for any new equipment required. **DO NOT** include equipment from the original design.

3. Provide a diagnosis and potential solution to the problem with P-802.

4. Provide an analysis of the suggestion by the summer intern.

5. Submit a written report, conforming to the guidelines, detailing the information in items 1 through 4.

6. Include an updated PFD and stream table for the modified process for scale-up.

7. Include, in an appendix, a legible, organized set of calculations justifying your recommendations, including any assumptions made. In addition, a converged Chemcad simulation of a modified design **MUST** be included in a separate appendix.

8. Include a signed copy of the attached confidentiality statement

Report Format

One report should be submitted per team. This report should be brief and should conform to the guidelines, which are available at the end of the following web page: http://www.che.cemr.wvu.edu/publications/projects/index.php. It should be bound in a three-ring binder/folder that is not oversized relative to the number of pages in the report. Figures and tables should be included as appropriate. An appendix must be attached that includes items such as the requested calculations and a Chemcad consolidated report (required) of the converged simulation for your recommended case. Stream properties (viscosity, density, etc.) **ARE NOT** to be included in the Chemcad consolidated report, but stream compositions (component molar flowrates) must be included, and there will be a deduction if these rules are not followed. The calculations in the appendix 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 during the week of November 12, 2012 through November 16, 2012. Your presentation should be 15-20 minutes, followed by about a 30-minute question and answer period. Questions will be directed to a specific team member, and the other team member **may not** answer unless specifically asked to answer the question. Make certain that you prepare for this presentation since it is an important part of your assignment. You should bring two hard copies of your slides to the presentation and hand them out before beginning the presentation. Remember the guidelines regarding professional attire for this presentation.

Other Rules

Each team member will receive the same grade for the technical content of the report and for the written report. Different grades are possible for the oral presentation and for the response to questions. Therefore, it is possible that each team member will receive a different grade for this assignment.

You may not discuss this major with anyone other than the instructors and your partner. Discussion, collaboration, or any interaction with anyone other than the instructor or your partner is prohibited. This means that any cross talk among students about anything relating to this assignment, no matter how insignificant it may seem to you, is a violation of the rules and is considered academic dishonesty. Violators will be subject to the penalties and procedures outlined in the University Procedures for Handling Academic Dishonesty Cases (see p. 5 of 2012-13 Undergraduate Catalog (http://coursecatalog.wvu.edu/) or follow the link http://catalog.wvu.edu/undergraduate/coursecreditstermsclassification/#Integrity_and_Dishonesty or the link http://docs.facultysenate.wvu.edu/08Files/AcademicDishonestyFlowChart.pdf.

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 team 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 A
Reaction Kinetics

The kinetics for the reactions are as follows:

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{benzene}}{C_6H_6} \xrightarrow{k_1} \underset{\text{cumene}}{C_9H_{12}} \tag{A-1}$$

$$r_1 = k_1 c_p c_b \text{ mole/L reactor sec}$$
$$k_1 = 3.5\times 10^7 \exp\left(\frac{-24.90}{RT}\right) \tag{A-2}$$

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{cumene}}{C_9H_{12}} \xrightarrow{k_2} \underset{\text{p - DIPB}}{C_{12}H_{18}} \tag{A-3}$$

$$r_2 = k_2 c_p c_c \text{ mole/L reactor sec}$$
$$k_2 = 2.9\times 10^9 \exp\left(\frac{-30.15}{RT}\right) \tag{A-4}$$

where the units of the activation energy are kcal/mol, the units of concentration are mol/L, and the temperature is in Kelvin.

Appendix 2
Calculations and Other Pertinent Information

All of the pertinent calculations are on the embedded spreadsheet and Chemcad file, both of which are also posted on eCampus.

cumene calcs.xlsx

cumene 2012.cc6