Design Project
Fall 2005

Background

In the opinion of our marketing research department, the demand for phenol-derived plasticizers is on the rise. Therefore, we are investigating the possibility of a new, grass roots phenol plant to handle the anticipated increase. Because phenol is made from cumene, a grass roots cumene plant would also be necessary. With your expertise in design developed in ECH 4605, we would like you to study the feasibility of a new cumene plant. Specifically, we would like a complete, preliminary design of a grass roots, 100,000 metric ton/yr cumene process using benzene and propylene. We have a new, proprietary catalyst, and the kinetics are included in Table 1. The propylene feed has a 5% propane impurity.

Assignment

Your assignment is to a preliminary design of a plant to make cumene from benzene and propylene using the new catalyst. Specifically, you need to do the following:

1. Utilize the Douglas Hierarchy and develop a BFD for the process. Describe each step as well as the rationale for each alternative. Find out the cost prices of the reactants and the selling price of the products and perform a preliminary economic analysis. Convert this BFD into a skeleton PFD.

2. Compute the mass balances necessary to get the desired product specification. This part of the project is done *without* using CHEMCAD. You are allowed to use a spread-sheet to do calculations. Assume that the conversion in the reactor at 350 ^oC and 35 $bars$ is as follows:

$$\begin{array}{llll} C_3H_6 + C_6H_6 & \longrightarrow & C_9H_{12} & \eta_1(propylene) = 0.950 \\ C_3H_6 + C_9H_{12} & \longrightarrow & C_{12}H_{18} & \eta_2(propylene) = 0.012 \end{array} \quad (1)$$

   The feed entering the reactor has an excess of benzene to minimize the side reaction.

3. Utilize the PFD that you developed in Part 1 and compute the molar flowrate of each stream in the flowsheet using CHEMCAD. For this part, use the kinetics information given on page three of this document.

4. Compute the energy balance using CHEMCAD and determine the heating/cooling requirements for each unit.

5. Compare your CHEMCAD results with your spread-sheet calculations done in Part 3 and comment on the differences (if any). Use the kinetic reactor module in CHEMCAD (Table 1 has the necessary data) instead of the stoichiometric or equilibrium modules.

6. Specify which heuristics you used from TBWS to set pressure and/or temperature levels in the PFD.
7. Determine the size of each equipment in your PFD. Specify which heuristic you used from TBWS for sizing each unit.
8. Specify which type of equipment you are using and its material of construction.
9. Run simulations in CHEMCAD to determine what happens to the product quantity and quality if the reactor temperature is varied from 300^o C to 400^o C in increments of 10^o C. Assume that all equipment sizes and operating conditions (other than reactor temperature) are the same for all the cases.

Design Report Format

Write a design report using the instructions given in TBWS that include the answers to all the questions asked above. You need to back up all your results and conclusions with appropriate calculations and/or references to heuristics.

The kinetics for the reactions are as follows:

$$\underset{propylene}{C_3H_6} + \underset{benzene}{C_6H_6} \xrightarrow{k_1} \underset{cumene}{C_9H_{12}}$$

$$r_1 = k_1 c_p c_b \quad \text{mole/g cat sec}$$

$$k_1 = 3.5 \times 10^4 \exp\left(\frac{-24.90}{RT}\right)$$

$$\underset{propylene}{C_3H_6} + \underset{cumene}{C_9H_{12}} \xrightarrow{k_2} \underset{p\text{-diisopropyl benzene}}{C_{12}H_{18}}$$

$$r_2 = k_2 c_p c_c \quad \text{mole/g cat sec}$$

$$k_2 = 2.9 \times 10^6 \exp\left(\frac{-35.08}{RT}\right)$$

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

For a shell-and-tube packed bed, the recommended configuration, the following data may be assumed:

- catalyst particle diameter $d_p = 3$ mm
- catalyst particle density $\rho_{cat} = 1600$ kg/m^3
- void fraction $\varepsilon = 0.50$
- heat transfer coefficient from packed bed to tube wall $h = 60$ W/m^2°C
- use standard tube sheet layouts as for a heat exchanger
- if tube diameter is larger than in tube sheet layouts, assume that tube cross sectional area is 1/3 of shell cross sectional area

Table 1

Hints

1. Assume that the price of cumene is \$0.61/kg and that of propylene with 5% impurity is \$0.474/kg.

2. TBWS, Appendix C, Project 5, "Problems at the Cumene Production Facility, Unit 800" can serve as a base case. It provides considerable information to assist a newly assigned engineer on the design project to quickly come up to speed. While a useful starting point, the process design of Project 5 is not optimized. There are many ways that it can be significantly improved.

3. **Process Simulation Startup**: Early on, students may want to plug the process data from Project 5 into CHEMCAD. This exercise has several benefits.

   - Students can test their ability to use individual unit operations. By entering the appropriate input data for a unit operation, students can try to reproduce the same results for the output streams that are reported in Project 5 for that unit operation. As Project 6 progresses, students can update the input data to keep the CHEMCAD simulation current.
   - CHEMCAD screens often identify alternatives for setting up the unit operation. The screens also define the type of data needed for each option. Studying these screens can deepen understanding of the unit operation and may also stimulate the generation of new ideas on how to approach many aspects of the project. The Help section of CHEMCAD is also a valuable resource of technical guidance on process simulation.
   - Students may encounter idiosyncrasies when using a process simulator, particularly when starting up the project. One line of attack is to review pertinent instructional modules for CHEMCAD that have been developed for this course and explore variations on the module. Students may also want to read over portions of the TBWS chapter on process simulation to identify appropriate troubleshooting methods. In addition, textbooks on the corresponding unit operation may provide other test cases on which to try out the simulator and thereby furnish more clues.

4. **Reactor Design**: The heart of this project is the reactor. It is likely that students will conduct hundreds of simulation runs in CHEMCAD in order gain an understanding of the effect of various process variables. Students are encouraged to review their textbooks from their course in Kinetics & Reactor Design. Oftentimes, pertinent examples are presented. These can serve as test cases on which to learn CHEMCAD and to demonstrate its viability. More importantly, these cases can point to which variables might be important to examine in simulation runs. It is also suggested that students read the TBWS chapter on Reactor Performance. It contains a wealth of practical information.

5. **Equipment Sizing and Design**: The heuristics, presented in the TBWS chapter on Utilizing Experience-Based Principles to Confirm the Suitability of a Process Design, can be extremely useful for sizing equipment and for identifying (or eliminating) design options. The TBWS chapter on Understanding Process Conditions is similarly useful.

6. **Report Presentation**:

- The report should be readable by any faculty member of the Department of Chemical Engineering who has read the problem statement.
- TBWS Chapter 27 provides example tables and figures.
- On the BFD, feed streams are labeled by their commercial names.
- Include a page defining all nomenclature.