Design of a New, 100,000 Metric Ton Per Year, Cumene Production Facility

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. Since phenol is made from cumene, a grass-roots cumene plant would also be necessary. Given your experience in trouble-shooting our existing cumene process, we would like you to study the economics 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. We would also like you to consider the economics of us continuing to use propylene with 5% propane impurity at \$0.095/lb versus purer propylene feed. In preparing this preliminary design, you should assume that all steam made can be used elsewhere in the plant with the appropriate economic credit, that condensed steam can be returned as boiler feed water for the appropriate credit, and that fuel gas can be burned for credit at its LHV (lower heating value). Additional information is given in Table 2.

Assignment

Your assignment is to provide:

- 1. an optimized preliminary design of a plant to make cumene from benzene and propylene using the new catalyst
- 2. an economic evaluation of your optimized process, using the following information:

After-tax internal hurdle rate = 9% p.a. Depreciation = MACRS (6 year schedule see Prob. 4.18, Turton et al. [1]) Marginal taxation rate = 35% Construction period = 2 years Project plant life = 10 years after start-up.

Specifically, you are to prepare the following by (4 weeks from now)

1. a written report detailing your design and profitability evaluation of the new process

- 2. a clear, complete, labeled process flow diagram of your optimized process including all equipment and the location of all major control loops
- 3. a clear stream flow table including *T*, *P*, total flowrate in kg/hr and kmol/hr, component flowrate in kmol/hr, and phase for each process stream.
- 4. a list of new equipment to be purchased, including size, cost, and materials of construction
- 5. an evaluation of the annual operating cost for the plant.
- 6. an analysis of the after-tax *NPV* (10 years, 9%), and the discounted cash flow rate of return on investment (*DCFROR*) for your recommended process
- 7. a legible, organized set of calculations justifying your recommendations, including any assumptions made

Report Format

This report should be in the "standard" design report format, consistent with the guidelines given in Chapter 22 of Turton et al. [1]. It should include an abstract, results, discussion, conclusions, recommendations, and an appendix with calculations.

References

1. Turton, R., Bailie, R.C., Whiting, W.B., and J.A. Shaeiwitz, Analysis, Synthesis, and Design of Chemical Processes, Prentice-Hall, PTR, Upper Saddle River, NJ, 1997.

Table 1: Reaction Kinetics for Cumene Reactions (Unit 800)

The kinetics for the reactions are as follows:

$$C_3H_6 + C_6H_6 \xrightarrow{k_1} C_9H_{12}$$

propylene benzene cumene

$$r_{1} = k_{1}c_{p}c_{b} \quad \text{mole} / \text{g cat sec}$$
$$k_{1} = 3.5 \times 10^{4} \exp\left(\frac{-24.90}{RT}\right)$$

$$C_{3}H_{6} + C_{9}H_{12} \xrightarrow{k_{2}} C_{12}H_{18}$$
propylene cumene $p - diisopropyl benzene$

$$r_{2} = k_{2}c_{p}c_{c} \quad \text{mole / g cat sec}$$

$$k_{2} = 2.9 \times 10^{6} \exp\left(\frac{-35.08}{RT}\right)$$

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

Table 2: Additional Information (Unit 800)

Cost of Manufacture

In order to estimate the cost of manufacture (not including depreciation), COM_d , you should use the following equation:

$$COM_d = 0.180 \ FCI + 2.73 \ C_{OL} + 1.23 \ (C_{UT} + C_{WT} + C_{RM}) \tag{3.2}$$

The current MACRS method for depreciation should be used in your calculations (see Problem 4.18, Turton et al. [1]).

Hints for Process Simulator

The CHEMCADTM process simulator was used to generate the flow table given in Project 5. The hints given here are specifically directed to CHEMCADTM users but should also be applicable for other process simulators.

Use SRK (Soave-Redlich-Kwong) thermodynamics package for VLE and Enthalpy calculations for all the equipment in the process.

For heat exchangers with multiple zones, it is recommended that you simulate each zone with a separate heat exchanger. Actual equipment may include several zones, so costing should be based on the actual equipment specifications.

For the reactor, you may use an isothermal reactor to estimate the volume of catalyst and heat exchange area. For more accurate results the temperature profile in the reactor should be modeled by completing a differential heat and material balance on the reactor.

For the distillation columns, you should use the shortcut method (SHOR) to get estimates for the rigorous distillation simulation (TOWR or SCDS). The shortcut method may be used until an optimum case is near. It is then expected that everyone will obtain a final design using rigorous simulation of the columns.

When simulating a process using "fake" streams and equipment, it is absolutely necessary that the process flow sheet that you present not include any "fake" streams and equipment. It must represent the actual process.