CH402 Capstone Design Problem

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Project Educational Objectives

- Enhanced understanding of unit and process operations.
- Understanding IT infrastructure and controller configurations in a process plant.
- Understanding of I/O, functions, process flow, and piping and instrumentation diagrams.
- Enhanced understanding of process economics.
- Use and understand process simulators.
- Development of communication ability.
- Enhanced understanding of safety issues confronting process engineers.

Introduction and Background

Ethylbenzene (EB) is an important molecule for the production of styrene and is synthesized commercially in large quantities. There are many proven methods for the industrial production of EB. Catalytic alkylation of benzene (B) with ethylene (E) using aluminum chloride has been used commercially since the 1930's. Another, totally different process involves running vapors of benzene and ethylene through a fixed bed of mixed oxide catalyst. The catalyst is usually a solid acid such as a zeolite. The solid-acid-catalyzed process is sometimes called "vapor-phase alkylation" since the reactants and products are in the vapor phase.

As a Process Design Engineer, you will provide a preliminary design for an EB fixed-bed reactor unit (FBR), including reactor effluent separation facilities, as part of a planned styrene plant. You are specifically requested to design a safe, environmentally clean, thermally integrated FBR with efficient capital and operating cost utilization. In addition, the FBR should be designed for optimum EB production. Furthermore, your design should be efficient and improve the operating expenses of the overall complex.

As an aid in producing a viable design, you will be provided with an EB plant simulation produced by Simulation Solutions, Incorporated (SSI). SSI is located in Shrewsbury, NJ, and makes computer programs known as "process simulators." A process simulator is a virtual chemical plant designed to assist in training plant operators, engineers, and supervisors. Some additional information about Simulation Solutions, Inc. can be found at: http://www.simulation-solutions.com.

The simulator software interfaces with the user in two ways. The first is a representation of the actual control room of the plant. It allows changes in the control variables in the plant and shows how all of the other process variables respond to that change. The second representation is an outside operator's view. This allows you to see a virtual 3D representation of the process equipment. Together, these two interfaces give a fairly realistic impression of what it is like to actually operate the real plant. The latest beta test version of the SSI software contains an EB FBR virtual chemical plant. This program consists of the control room and outside operator views of the plant, as discussed above.

When a new chemical plant is built, it must be started up for the first time and "shaken down" to find all the design issues. Just like in a real plant, a simulator must undergo the same process of initial cold startup. The EB FBR plant simulation you will be operating is very new, and you will be conducting a start up and shakedown of this process. Part of your assignment will be to execute a cold start and identify any issues you find along the way. This includes possible revisions of the start-up procedures as well as changes to the P&ID. The experiences you will go through are very similar to the issues that engineers and operators face when they start up a real plant. You will be faced with unknown technical questions, as well as incomplete procedures and diagrams. Your mission in this assignment is to develop a safe working start up procedure that will be used by operator and engineer trainees in the field. You will be provided old help menus as well as a preliminary start up procedure, but will need to make modifications as you work your way through the plant.

Design Objectives and Constraints

You must address and adhere to these specific objectives and constraints in the preliminary design:

1. Safety/Environmental – Design must not pose any environmental, health or safety hazards that should have been mitigated with better equipment, instrumentation or control. Additionally, no continuous flaring/venting of hydrocarbons is permitted in the design – if necessary, hydrocarbons can be reused in the process.

2. Energy Efficiency & Lowest Environmental Impact. The EEI is defined as: (mass of carbon in finished products/mass of carbon in feed) x 100%, where finished products = ethylbenzene (EB) + excess ethylene. Other than safety and environmental performance, energy efficiency is next most important attribute that will determine acceptance of your design by your company.

3. Optimum Finished EB Production – Appropriate cost/benefit balance is achieved.

4. Economic Analysis (Discounted Cash Flow Rate of Return) - Economic analysis should reflect not only the designed equipment capital investment and expense costs, but also the expense costs of process labor, financing, and utilities. For economic calculations assume:
   a. Project Life of 15 years
   b. 15 year Straight Line Depreciation
   c. 33% Tax Rate
   d. Projected 3% yearly inflation
   e. Total capital investment can be estimated by multiplying the equipment cost by using the percentage of delivered equipment method (Cost & Evaluation Spreadsheet). Multipliers in the spreadsheet will account for all associated direct costs, indirect costs and working capital.
   f. Total yearly operating expenses above and beyond financing, labor, and utilities can be estimated using 3% of the total capital investment. This estimate will cover fixed charges such as plant overhead costs, administrative costs, distribution & marketing and research & development
   g. The EB Unit will have a 1 month turnaround to coincide with catalyst replacement
   h. You may use equipment cost data from your textbook, ChemCAD, the McGraw-Hill Website, and other public sources.
5. Feasible Design – Even though you are not providing the final design, your preliminary design should be viable as specified.
6. Realistic and Adequate Process Control – Control valves, instrumentation, analyzers, etc. on required equipment to provide safety and minimize personnel. It is not necessary to specify each component in detail; simply identify what they are and where in the process they are required. (The process simulator will be invaluable here.)
7. You are required to execute a cold startup of the existing EB plant (virtual), and make safety walkthrough diagrams, changes to the P&ID, and identification of any malfunctioning equipment. Beyond the preliminary design, this is the most important aspect of your project.

Chemical Reaction Kinetics and Reaction Engineering

Determining the mass of catalyst is perhaps the most difficult part of any design problem. The reaction and the accompanying kinetics are defined for you below. In real world problems, you would be expected to research this information on your own. The chemical reactions are:

$$E(vap) + B(vap) \rightarrow EB(vap)$$

$$E(vap) + EB(vap) \rightarrow DEB(vap)$$

where E = ethylene, B = benzene, EB = ethylbenzene, and DEB = diethylbenzene (a side product).

The kinetic equations and rate constants are defined below:

$$-r_1 = \frac{k_r \cdot C_E}{1 + k_{EB} C_{EB}}, \text{ units are } \frac{kmol\ B}{kg\text{-}catalyst \cdot hr}$$

$$k_r = 0.69 \times 10^6 \exp\left(\frac{-6.344 \times 10^4}{RT} \right)$$

$$k_{EB} = -1.52 \times 10^{-2} \exp\left(\frac{-3.933 \times 10^3}{RT} \right)$$

$$r_2 = 2.80 \times 10^2 \exp\left(\frac{-4.7303 \times 10^4}{RT} \right) C_{EB} \cdot C_E, \text{ units are } \frac{kmol\ B}{kg\text{-}catalyst \cdot hr}$$

Reference: H. Ganji, J. Ahari, A. Farshi, and M. Makavand, *Petroleum & Coal*, 46(1), 55-63, 2004.

The reaction temperature will be determined by the feed temperature, the heat of reaction and heat transfer out of the tube and may vary along the length of the reactor. Information on heat transfer characteristics is provided below.

Product selectivity is defined as the rate of formation of the desired product divided by the rate of formation of the undesired product.

The catalyst you will be using has been formulated into 1/16 inch diameter extrudates, with a packed bulk density of 0.8 g/cc and a void fraction of 0.4. Equivalent diameter is 0.08 inches. Cost is $10/lb. Assume replacement every 4 years. The catalyst is an ultra stable formulation - with low deactivation rates - and the activity (as set by the kinetic equation) can be taken as the average activity for the life of the catalyst.

Because the reaction is highly exothermic you have selected a tubular fixed bed reactor. You have found that a practical limit for the size of these reactors is 20 ft in diameter and 60 ft in length (tangent to tangent). Prior company practice has been to build these types of reactors out of 2-inch Schedule 40 steel pipe, so that the reactor itself is in a shell-and-tube configuration. You need to determine the number of reactors needed and the optimum arrangement of the reactors (number of stages in series and number of tubes per stage).

Heat Transfer in the Reactor. The reaction is highly exothermic, and you will need to determine the heat of reaction. Temperature is controlled using the feed contacting pattern, but the shell-and-tube design allows cooling water to be used on the shell-side to reduce the probability of a runaway reaction. Normal operating conditions optimized to maximize process performance and minimize investment costs. You have determined that the heat transfer coefficient is controlled by process side conditions and found that an empirical relationship exists for the overall coefficient as follows:

$$U_{overall} = 0.385 \cdot G^{0.8} / D^{0.2}$$

where $U_{overall}$ = overall heat transfer coefficient, in units of $Btu \cdot hr \cdot ft^2$, G = inlet gas mass velocity, in units of $g/hr/cm^2$, and D = tube diameter in centimeters. You may assume the tubes are 2-inch Schedule 40, and that the minimum spacing between tubes is 1 inch.

Pressure Drop in the Reactor. Bed pressure drop should be calculated and pressure loss should be accounted for in the kinetics. Assume fluid properties are constant through the reactor and are equal to the properties at the inlet, neglecting the reaction. Maximum allowable pressure drop per reactor is 50 psi.

Mass Transfer in the Reactor. You have found that due to the particular formulation of your catalyst that mass transfer effects on the reaction kinetics are small and can be ignored.

Design Report Requirements [See Table 11-1 page 472]:

1. Cover Sheet
2. Table of Contents
3. Summary (w/ specific reference to design objectives)
4. Introduction (w/ specific reference to market economics)
5. Previous Work
6. Discussion
7. Recommended Design
    a. Preliminary I/O Analysis (diagram plus calculation)
    b. Functions Diagram
    c. Process Flow Diagram in ChemCAD
    d. Unit Control and Instrumentation Description
    e. Safety and Environmental Summary
    f. Equipment Information Summary – with enough design information to cost equipment
    g. Economics - In addition to DCF, include a summary of operating costs, utility requirements and energy efficiency
    h. Engineering Calculations, Computer Simulation Outputs
8. Conclusions and Recommendations

9. Acknowledgements
10. References

Additional Information (Use as Needed):

- Standard conditions, if needed, are 60F and 14.7PSIA.
- Use US Customary Units of Measure (see utility costs).
- G = 10^9, M = 10^6, K = 10^3
- Short ton = 2000lb; bbl = barrel of liquid at standard conditions = 42 gal
- Ambient Temperature: 75 ºF (Avg)

Utilities Available:

- 515 PSIG, 490 ºF HP Steam: Cost: $5/klb consumed, Credit: $4/klb produced
- 115 PSIG, 353 ºF MP Steam: Cost: $4/klb consumed, Credit: $3/klb produced
- 20 PSIG, 260 ºF LP Steam: Cost: $3.5/klb consumed Credit: $2.5/klb produced
- Electricity: Cost: $0.04/KW-h consumed, Credit: $0.03/KW-h produced
- Fuel Gas: Cost: $3/MBTU consumed, Credit: $2/MBTU produced
- Hydrogen: Cost: $0.06/lb consumed
- Carbon Dioxide: 100% pure (500PSIG & 100F): Cost: $400/MSCF consumed
- Steam Condensate (at least 99.9% v/v pure): Credit: $2/klb produced
- Process/Cooling Tower Water (at least 95% v/v pure): Cost: $0.5/kgal consumed, Credit: $0.35/kgal produced
- Waste Treatment (at least 75% v/v pure): Cost: $6/kgal produced

Hint: Steady-state design may not require all utilities.