UDYOG

Hydrodesulfurization Reactor Design

Background

Just as you arrive at work one morning, your supervisor, Dr. Jones, says he needs to speak with you and your design group. He seems concerned about something, so you locate your group members and hurry into his office. As the last member of your group shuffles in, you turn to your supervisor and ask, “Alright, we are all here. What did you want to talk to us about?”

“Well, one of the processes recently proposed by the Process R&D group produces a by-product stream consisting of nearly pure benzothiophene, and since benzothiophene contains sulfur and an aromatic ring, we cannot vent this stream into the atmosphere. The engineers in Catalyst Development believe that we can use a hydrodesulfurization reaction to convert benzothiophene into ethylbenzene with a cobalt-molybdenum catalyst supported on alumina. If we can design a reactor to do this efficiently, we could sell the ethylbenzene as a commodity chemical. The other product, hydrogen sulfide, could be sent to the sulfur treatment facilities. I know that your group's specialty is reactor design, so I'm assigning the hydrodesulfurization reactor project to you. I would like a progress report in three weeks and a final design report four weeks after that. I've compiled a list of items that you should include in each of these reports. I know it has been a while since most of you designed a reactor from start to finish, so I've included a partial list of references that may help you. They will be especially helpful with the selection of the materials of construction. I know this assignment is open-ended and requires a lot of engineering judgment, but just remember to use your common sense and BE CREATIVE! Any questions?”. We unanimously reply, “No, we’ll get started right away”.

Problem Statement

As your supervisor told you, the engineers in Catalyst Development think that benzothiophene could be converted to ethylbenzene by a hydrodesulfurization reaction. Before you commit the company's time and money to design a reactor for this reaction, you may want to attempt to verify that the production of ethylbenzene is economically feasible. In other words, are the products worth more than the reactants and energy required to make them? If you discover the answer is no, you may have saved your company thousands of dollars in design fees. Research this issue and discuss your findings in your progress report. (See the Additional Information section for some references that may help in answering these questions.) If you knew that your supervisor supported the design of the new reactor and you discovered that producing ethylbenzene from benzothiophene was not cost effective, how would you inform your supervisor of this?

In the progress report i.e., ppt, be sure that your group provides support for your choice of -

- Reactor (i.e., PFR, fluidized CSTR, etc.)
- Adiabatic vs. isothermal reactor operation
- Reactor temperatures and pressures ***(Hint:*** Single-phase reactions are less complicated than multiple-phase reactions)
- Feed ratio of hydrogen to benzothiophene
- Effluent conditions and compositions
- The weight of catalyst required

Also include

- A qualitative discussion of the effect that operating conditions and the method of operation have on capital and operating costs
- Justification for any assumptions made
- Appendices summarizing your calculations

In the final presentation, you should also provide support for your choice of -

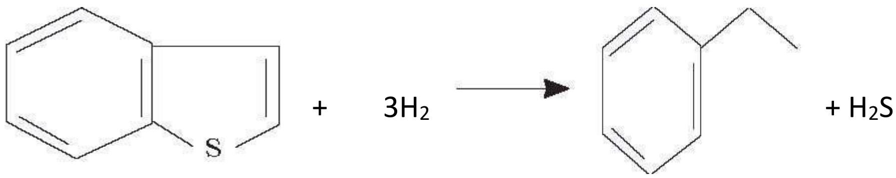
- Materials of construction for the reactor ***(Hint:*** Is the material susceptible to accelerated corrosion due to the presence of sulfur or hydrogen?)
- Reactor shape and dimensions
- Reactor wall thickness

Also include

- Support for any changes in the initial reactor design presented in your progress report
- Any environmental or safety concerns that may be relevant to your design
- Diagram of the reactor
- Justification for any assumptions made
- Appendices summarizing ALL calculations

Problem Information

The reaction is



Benzothiophene Ethylbenzene

In past research studies, the proposed reaction has been run in the vapor phase with reactor temperatures of 240-300°C, total pressures of 2-30 atm, and hydrogen to benzothiophene feed ratios of 4:1 to 9:1. These experiments resulted in the development of the following rate law *(**Note**:* You may assume that the rate law holds for conditions outside this range. Therefore, you are in no way constrained to using these operating ranges and should use them only as guides)

The rate law is -

$$-r_B' = \frac{k_B K_B K_{H_2} P_B P_{H_2}}{\left[1 + (K_{H_2} P_{H_2})^{0.5} + \left(K_{H_2S} \frac{P_{H_2S}}{P_{H_2}}\right) + (K_B P_B)\right]}$$

where

$k_B(260°C) = 6.65 \times 10^{-5}$ mol/gcat • s $\quad$ $k_B(300°C) = 1.80 \times 10^{-4}$ mol/gcat • s

$K_B(260°C) = 19.3$ atm^{-1} $\quad$ $K_B(300°C) = 9.90 \times 10^{-2}$ atm^{-1}

$K_{H_2}(260°C) = 0.358$ atm^{-1} $\quad$ $K_{H_2}(300°C) = 1.84 \times 10^{-3}$ atm^{-1}

$K_{H_2S}(260°C) = 211$ $\quad$ $K_{H_2S}(300°C) = 10.82$

*(**Note**:* The heat of adsorption was estimated at -80 kcal/mol for all three species.)

<u>Catalyst Properties</u>:

Particle diameter: 0.08 cm

For a packed bed reactor: φ = porosity = 0.30

α = pressure drop parameter = 0.34 kg^{-1}

For a fluidized CSTR: φ = porosity = 0.75

α = pressure drop parameter = 0.005 kg^{-1}

Feed (pure benzothiophene before the addition of hydrogen):

F_{B0} = 20 mol/h

T_0 = Entering temperature = 260°C

T_{melt} = melting temperature at 1 atm = 32°C

T_{boil} = boiling temperature at 1 atm = 221°C

References

M. J. GIRGIs and B. C. GATES. "Reactivities, Reaction Networks and Kinetics in High Pressure Catalytic Hydro processing." *Ind. Eng. Chem. Res.,* 30, 2021—2058

I. A. VAN PARIJS, L. H. HOSTEN, and G. F. FROMENT. "Kinetics of Hydrodesulfurization on a CoMo/J-AltO; Catalyst. 2. Kinetics of the Hydrogenolysis of Benzothiophene." *Ind. Eng. Chem. Prod. Re,s. Dev.,* 25, 437—443

RULES AND EVALUATION:

- You can participate in a group of at most 3 members. More than three is strictly not allowed.
- Solution submission format-
    - Make a PPT of maximum 10 slides (including introduction & thank you slide).
    - Create a video in which you will share your screen playing your presentation in slide show mode, with your voice included. You will be clearly and confidently pitching your key ideas mentioned in your presentation and approach to us.
    - Save your video file as a Google drive link using your institute Id for G-suite services. In case you use your personal Id, do not forget to give us the view access.
- The drive link along with your PPT should be mailed to osmoze@itbhu.ac.in. The filename of the drive should be "Osmoze_Udyog_Video_<Team_Name>. The filename of the PPT should be "Osmoze_Udyog_PPT_<Team_Name>.
- The deadline of PPT submission will be 17th April 2021 11:59 PM. Any changes in the scheduled deadline if made, will be communicated to you, unless you are made to follow this deadline strictly.
- You need to clearly state all the assumptions and methods of calculation used. The presentation will be evaluated on how well you have approached and analyse the problem, how much the solution is feasible in practical terms and how much practically innovative the designed processes and the strategies are.

- You are advised to strictly adhere to all the rules mentioned here. Violating the rules will lead you to pay heavy penalty of marks.
- You can contact any of the coordinators if you have any query/doubts regarding the event structure, evaluation and the problem statement.

EVENT COORDINATORS:

Rajesh Saha - +91-8640005433 - rajeshsaha.che18@itbhu.ac.in

Yash Balraj Ippakayal - +91-9325380133 - yashbalraji.che18@iitbhu.ac.in

Tejaswita Som - +91-8765001039 - tejaswitasom.che18@itbhu.ac.in

Suraj Kumar Maurya - +91-7860610532 - surajkmaurya.che18@itbhu.ac.in