Portfolio 02: Isothermal reactor design

CHEN3010/ CHEN5040: chemical reaction engineering

General Instructions for in class Portfolios

1. The portolio is an open-book task.
2. You can use textbooks, the resources provided during class/ workshop etc. to answer the questions.
3. The portfolio task is made available in both pdf format and as a print.
4. You are free to choose a solution technique. It is **not** required that you use the provided python code to answer the questions. You can use any tool (pen and paper, excel, ...) and any technique (graphical, numerical, analytical) that you are comfortable with.
5. Irrespective of your solution method, you are expected to write your answers on to the printed question paper provided. **This is what gets marked.**
6. The portfolio will take place during designated timeslot communicated earlier by the unit coordinator. Please refer to the portfolio schedule on blackboard for the portolio dates and topics.
7. The tasks will be a mix of theory questions, short calculation type and long numerical examples.
8. You have **90 minutes** to complete the tasks in the portfolio.
9. When you are required to upload the portolio answers on to blackboard:
   - Save your report as a pdf file.
   - Rename the file as STUDENTID_Portfolio_x.pdf (Where STUDENTID is your student ID, and x is the portfolio number) and
   - Upload it using assessment submission link on blackboard.

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Academic integrity at its core is about honesty and responsibility and is fundamental to Curtin's expectations of you. This means that all of your work at Curtin should be your own and it should be underpinned by integrity, which means to act ethically, honestly and with fairness.

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You are also expected to uphold the Student Charter and recognise that cheating, plagiarism collusion, and falsification of data and other forms of academic dishonesty are not acceptable.

For more information, visit https://students.curtin.edu.au/essentials/rights/academic-integrity/

Question 1: Indoor air quality (25 marks)

Room 402:220, where the reaction engineering lecture takes place, is designed for 100 students and has a mechanical ventilation system that supplies 60.00 m^3/min of fresh air and removes an equal amount of air to maintain well-mixed conditions. To help track air quality during lectures, CO_2 monitors are installed in the room. Since students continuously exhale CO_2, its concentration can build up over time. Monitoring these levels helps ensure the room is well-ventilated, keeps everyone comfortable and alert, and reduces the risk of spreading airborne illnesses.

The floor area of the room is 150.00 m^2, and the ceiling height is 4.00 m.

Assume:

- Fresh air contains 0.04% CO_2.
- The air within the room well-mixed.
- Temperature is 25.0°C, and pressure is 1.0 atm.

(a) Which ideal reactor model best represents the room and its ventilation system? Justify your choice. (2 marks)

Answer:

(b) Based on the reactor model identified in part (a), derive mole balance equation to describe how the CO_2 concentration in the room changes with time. Clearly state your variables, steps, and assumptions. Make sure to include generation from occupants and the effect of fresh air ventilation. The generation can be assumed to be uniform throughout the lecture room. (8 marks)

Answer:

(c) After 2 hours of lecture, the CO_2 concentration in the room reaches a steady state level of 0.30% CO_2. Assuming that CO_2 generation by students follows zeroth-order kinetics, and using the mole balance derived in part (b), determine the rate expression and calculate all relevant constants. (5 marks)

Answer:

(d) Once the lecture ends and the room is empty, how long will it take for the CO_2 concentration to return to atmospheric levels (y_{CO_2} = 0.04%)? Use the mole balance developed in (b). Assume ventilation continues as before. (10 marks)

Answer:

Question 2: Selectivity in complex reactions (25 marks)

A specialty chemicals manufacturer produces a high-value intermediate D from feedstock A through a multi-reaction system.

The following reactions occur in the process:

$$
\begin{array}{rll}
\text{desired reaction:} & 2\,\mathrm{A} \longrightarrow \mathrm{D} & -r_{1A} = k_1 C_A^2 \\
\text{undesired reaction:} & \mathrm{A} \longrightarrow \mathrm{U_1} & -r_{2A} = k_2 C_A^{1.2} \\
\text{undesired degradation:} & \mathrm{D} \longrightarrow \mathrm{U_2} & -r_D = k_3 C_D
\end{array}
$$

(a) Derive expressions for the conversion of A, the yield of D, and the selectivity toward D with respect to $\mathrm{U_1}$, $\mathrm{U_2}$, and overall selectivity ($S_{\mathrm{D/U_1U_2}}$) based on the kinetics. (5 marks)

Answer:

(b) Based on the reaction network, recommend a suitable reactor configuration to maximize the overall selectivity for D and justify your choice. (5 marks)

Answer:

The current manufacturing facility uses a tubular reactor consisting of a bank of 100 tubes. During maintenance, it is found that some tubes are blocked and no longer carry flow. Instead of halting production, the manager chooses to plug the inlets of the faulty tubes.

The reactor operates under isothermal, isobaric conditions. The total volumetric flow rate is 100.0 m^3/min. The concentration of A at inlet is 2 mol/m^3. Each tube in the reactor has a diameter of 10cm and a length of 10m.

At reactor temperature, the rate constants for the reaction are:

k_1 = 10.0 m^3/mol/min

k_2 = 5.0 $m^3/mol^{0.2}$/min

k_3 = 2.0 /min

(c) To evaluate the impact of tube plugging, follow the steps outlined in the reaction engineering algorithm. Develop a comprehensive set of model equations for the tubular reactor and describe the solution methodology. (10 marks)

Answer:

(d) What would be the effect of plugging 20%, 50%, and 80% tubes on the yield, overall selectivity, and conversion? Assume all unblocked tubes continue to operate under identical conditions. Comment on the implications of these blockages in active tubes for process performance and decision-making. (5 marks)

Answer:

% blockage	0%	20%	50%	80%
Conversion of A (X_A)				
Yield of D (Y_D)				
Selectivity S_{D/U_1}				
Selectivity S_{D/U_2}				
Selectivity S_{D/U_1U_2}				

Discussion: