Portfolio 05: Multiple reactions

CHEN3010/ CHEN5040: chemical reaction engineering

Student ID:

General Instructions for in class Portfolios

1. The portfolio 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 time slot communicated earlier by the unit coordinator. Please refer to the portfolio schedule on blackboard for the portfolio dates and topics.
7. The tasks will be a mix of theory questions, short calculation type and long numerical examples.
8. You have **50 minutes** to complete the tasks in the portfolio.
9. The portfolios will be marked immediately after completion by your peers using a provided marking rubric.
10. The portfolios will be collected by the instructors to verify peer marking and record the marks. You will receive your portfolio back within a week.
11. When you are required to upload the portfolio 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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You are also expected to uphold the Student Charter and recognize 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/

Introduction

The direct vapor phase oxidation route to produce ethylene oxide (EO) from ethylene (E)

$$C_2H_4 + \frac{1}{2}O_2 \longrightarrow C_2H_4O \qquad \Delta H_{rxn,1} = -103.246\, kJ/mol \tag{1}$$

is usually accompanied by two main side reactions.

Ethylene combustion:

$$C_2H_4 + 3\,O_2 \longrightarrow 2\,CO_2 + 2\,H_2O \qquad \Delta H_{rxn,2} = -1321.716\, kJ/mol \tag{2}$$

Ethylene oxide combustion:

$$C_2H_4O + \frac{5}{2}O_2 \longrightarrow 2\,CO_2 + 2\,H_2O \qquad \Delta H_{rxn,3} = -1218\, kJ/mol \tag{3}$$

At reactor operating conditions (below 250 °C), EO combustion (Equation 3) is negligible.

The reaction rate expressions and their parameters for ethylene oxidation over silver catalyst on an alumina support were given by Borman and Westerterp (1992).

The rates of reactions (r_i) for reactions 1 and 2 are expressed using semi-empirical relations as:

$$r_i = \frac{k_r^i P_E P_O^{n_i}}{1 + K_E^i P_E + K_C^i P_C + K_W^i P_W + K_{EO}^i P_{EO}} \tag{4}$$

Where, r_i is the rate of production of EO or CO_2 in $mol/(kg - cat\ s)$. k_r^i is reaction rate constant for reaction i (in $mol/kg - cat\ s\ bar$); K_j^i is absorption rate constant for component j, reaction i, P_j is the partial pressure of component j in Pa, T is the temperature in K.

The subscripts E, O, C, W, and EO denote ethylene, oxygen, carbon dioxide, ethylene oxide, and water respectively. The values of all the constants is given in Table 1.

Table 1: Reaction rate data

	Reaction 1	Reaction 2
k_r	$0.2572\exp(-8068/T)$	$178\exp(-11381/T)$
n	0.13	0.14
K_E	0.30×10^{-3}	0.49×10^{-3}
K_C	0.87×10^{-3}	1.14×10^{-3}
K_{EO}	0.90×10^{-3}	0.49×10^{-3}
K_W	$3.68 \times 10^{-6}\exp(2370/T)$	$4.04 \times 10^{-7}\exp(3430/T)$

The reaction is carried out in vertical tubular packed bed reactor. Shell catalyst S882, which is silver impregnated on aluminum, in the form of Raschig rings of size 8mm $\times$ 8mm, is used. The tube diameter (d_t) is 0.0389 m and length (L) is 12.8 m. Catalyst density (ρ_s) is 890 kg/m^3 and void fraction (ϵ) is 0.6. Inlet superficial gas velocity (v) is 1 m/s (volumetric flow rate $v_0 = va_c = 1.188 \times 10^{-3} m^3/s$) and the feed enters at 180 °C.

The gases enter the reactor at the top and leave from the bottom. The shell side of the reactor has boiling kerosene. About top one third has kerosene vapour and the bottom has liquid kerosene. The vapour heats up the entering gases while the liquid at the bottom removes the heat generated in the exothermic reactions.

Inlet gas composition is given in Table 2.

Table 2: Inlet gas composition

Gas	volume fraction at inlet (%)
C_2H_4	31.36
O_2	6.30
C_2H_4O	0.03
CO_2	2.35
Inert	59.96

Questions

1. Write expressions for (6 marks)

   (a) instantaneous and overall yield of EO,
   (b) instantaneous and overall selectivity of EO w.r.t. CO_2, and
   (c) conversion of C_2H_4.

   You may use just r_i instead of expanding the expressions.

2. Comment on reactor selection and operating conditions to maximize yield of EO. Explain your answer with relevant equations. (6 marks)

3. Yield and selectivity of EO. (12 marks)

(a) Based on inlet conditions, calculate instantaneous yield and selectivity of EO.
(b) For the outlet composition given in Table 3 calculate instantaneous yield and selectivity of EO. The outlet temperature is 220 °C. Comment on the results.

Table 3: Outlet gas composition

Gas	volume fraction at outlet (%)
C_2H_4	28.84
O_2	4.26
C_2H_4O	2.45
CO_2	3.14
Inert	61.31

4. Write complete set of governing equations for calculating the conversion in the reactor. (6 marks)

References

Borman, P. C., and K. R. Westerterp. 1992. "An Experimental Study of the Selective Oxidation of Ethene in a Wall Cooled Tubular Packed Bed Reactor." *Chemical Engineering Science*, Twelfth International Symposium on Chemical Reaction Engineering Today, 47 (9): 2541–46. https://doi.org/10.1016/0009-2509(92)87090-D.