CHEM-E7150 Reaction Engineering
Exam 8 December 2020 at 13-18

Answer to four questions, all questions are worth 6 points. If you answer to all five questions, the question with least points is left out from the evaluation. The collection of equations has to be returned with the exam. More instructions on exam in MyCourses page in the exam submission box.

Question 1

You are studying the reaction A + B ⟷ C in a laboratory scale isothermal packed bed reactor. The reaction occurs isothermally in gas phase and is catalyzed by a metal catalyst in aluminum oxide support. Catalyst and support material are placed in the reactor and the reactants are fed to the reactor using a pump. The product composition is analyzed at the reactor outlet.

Your task is to plan a set of experiments, where you study the phenomena that might happen in the reactor (reaction system) and their effect to the reaction. What kind of experiments would you conduct in which order and what kind information would you obtain from these experiments?
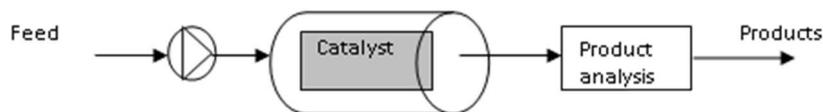
Question 2

The rate law for an irreversible gas-phase reaction (A_2 + B → C + D) is known to be

$$-r_{A2} = \frac{kP_AP_B}{\left(1 + \sqrt{K_AP_A} + K_CP_C\right)^2(1 + K_BP_B)}$$

What can be concluded about the reaction mechanism based on the given rate law?

a) Is the adsorption of reagent A_2 molecular or diccosiative? Answer with reasoning.
b) Is the adsorption of reagent B molecular or diccosiative? Answer with reasoning.
c) Is the adsorption of reagents A and B competitive or non-competitive? Answer with reasoning.
d) Which components react in the rate-limiting step? How many active sites are involved in the rate-limiting step? Answer with reasoning.
e) Are products C and D released directly to the gas-phase? Answer with reasoning.
f) Suggest the steps of the reaction mechanism. Indicate which of the steps is the rate-limiting step.

Question 3

An irreversible first order gas-phase isomerization rection (cyclopropane → propylene) takes place in a CSTR at 190 °C and atmospheric pressure. The feed to the reactor (150 mol/min of pure cyclopropane) is at the same temperature and pressure as the reactor is. The amount of catalyst in the reactor is 7 kg and the deactivation of the catalyst follows first order kinetics. The catalyst can be replaced every two weeks (= 336 h). In order to increase the conversion, you can either increase the temperature of the reactor (and the feed) by 10 °C degrees or double the amount of the catalyst. Which modification you should do? Support your answer with calculations.

Additional information:
Reaction rate constant at 190 °C: 1.3 m^3/(kg min)
Decay constant at 190 °C: $6 \cdot 10^{-4}$ 1/h
Activation energy for the main reaction: 160 kJ/mol
Activation energy for catalyst decay: 110 kJ/mol

Question 4

You are working as a production engineer in a process that produces a fine chemical C. The production takes place via an irreversible gas phase elementary reaction of A+ B → C in a packed bed reactor and external diffusion is known to limit the reaction rate. The catalyst particles are spherical (diameter 5 mm) and the reactor pipe has the length 0.30 m and diameter of 0.10 m. The total molar flow to the system is 50 mol/min with molar ratio A:B of 1:1. The reaction takes place at 150 °C and atmospheric pressure.

Now you would like to increase the production rate of C in your process. You think that decreasing the catalyst particle and increasing the feed flow would be worth a try. Are you able to increase the production of C, if you simultaneously decrease the particle size 20 % and double the total feed flow to the system? Assume that the porosity of the bed remains constant.

The following values are valid for the system at these conditions and ideal gas law can be applied:

Diffusivity $3.7 \cdot 10^{-6}$ m^2/s
Viscosity $8.0 \cdot 10^{-5}$ kg/(m·s)
Fluid density 1.20 kg/m^3
Bed porosity 0.45

Question 5

Dehydrogenation reaction of A → B + H_2 is studied in gas phase in a packed bed reactor (length of the reactor 0.75 m and inner diameter of the reactor pipe 15 cm) at 500 K and 101 kPa. The reactor is filled with spherical porous catalyst particles. Pure A is fed into the reactor 0.5 dm^3/s in the reaction conditions.

The reaction is first order with respect to A with the reaction rate coefficient k' = 0.018 dm^3/(kg$_{cat}$ ·s) at the studied conditions. Calculate the conversion of A in the system.

Information about the system at the reaction temperature of 500 K.

Concentration of A in the feed	C_{A0} = 24.3 mol/m^3
Dynamic viscosity of the gas	μ = 3.0·10^{-5} kg/(m·s)
Density of the gas	ρ_{fluid} = 0.4 kg/m^3
Bulk diffusion coefficient of the gas	D_{AB} = 2.0·10^{-5} m^2/s
Effective diffusion coefficient of the gas	D_e = 1.2·10^{-5} m^2/s
Diameter of the catalyst particles	d_p = 0.5 mm
Specific surface area of the catalyst particles	S_a = 90 m^2/g
Porosity of the catalyst bed	ε_b = 0.4
Bulk density of the catalyst	ρ_B = 1.2 g/cm^3
Mass transfer coefficient in the fluid	k_c = 0.096 m/s

$$\int_0^x \frac{dx}{1-x} = \ln\frac{1}{1-x}$$

$$\int_0^x x^n dx = \frac{x^{n+1}}{n+1}$$

$$\int_0^x \frac{dx}{(1-x)^2} = \frac{x}{1-x}$$

$$\int_0^x \frac{dx}{x} = \ln(x)$$

$$\int_0^x \frac{dx}{1+\varepsilon X} = \frac{1}{\varepsilon}\ln(1+\varepsilon x)$$

$$\int_0^x \frac{dx}{x^n} = \frac{x^{1-n}}{1-n}$$

$$\int_0^x \frac{1+\varepsilon x}{1-x}dx = (1+\varepsilon)\ln\frac{1}{1-x} - \varepsilon x$$

$$\int_0^x \frac{1+\varepsilon x}{(1-x)^2}dx = \frac{(1-\varepsilon)x}{1-x} - \varepsilon\ln\frac{1}{1-x}$$

$$\int_0^x \frac{(1+\varepsilon x)^2}{(1-x)^2}dx = 2\varepsilon(1+\varepsilon)\ln(1-x) + \varepsilon^2 x + \frac{(1+\varepsilon)^2 x}{1-x}$$

$$\int_0^x \frac{dx}{(1-x)(\theta_B - x)} = \frac{1}{\theta_B - 1}\ln\frac{\theta_B - x}{\theta_B(1-x)} \qquad \theta_B \neq 1$$

$$\int_0^x \frac{dx}{ax^2 + bx + c} = \frac{-2}{2ax+b} + \frac{2}{b} \qquad \text{when } b^2 = 4ac$$

$$\int_0^x \frac{a+bx}{c+gx}dx = \frac{bx}{g} + \frac{ag-bc}{g^2}\ln\frac{c+gx}{c}$$

$$\sinh x = \frac{e^x - e^{-x}}{2} \qquad\qquad \tanh x = \frac{\sinh x}{\cosh x} = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

$$\cosh x = \frac{e^x + e^{-x}}{2} \qquad\qquad \coth x = \frac{1}{\tanh x} = \frac{e^x + e^{-x}}{e^x - e^{-x}}$$