NAME: ______________________________

Instructions: Parts I and II of the exam are closed book and notes. You may use anything you have on your laptops for both Part I and Part II.
Remove your wireless network card during the exam.
Part I does not require any numerical calculation using the laptop. Part I is worth 50 points and part II is worth 50 points. Write all answers on separate paper. Do not write any answers on the exam itself. Hand in your exam as well as your solution at the end. Make sure your name is on your solution and your exam.

Part I.

Problem 1. Packed-Bed Reactors. 25 pts.

A second order catalytic reaction

$$\mathrm{A} \longrightarrow \mathrm{B}$$

is carried out in an isothermal packed-bed reactor containing spherical catalyst pellets. The exit conversion is 85%. The reactant and product are gases. What happens to the required bed length to achieve 85% conversion if the feed pressure is doubled and the feed volumetric flowrate is held constant? You may assume that the flowrate is small enough that the pressure drop across the bed is unimportant. Consider the following two cases.

(a) What is the new required bed length if the overall pellet reaction rate is controlled by the intrinsic reaction rate?

(b) What is the new required bed length if the overall pellet reaction rate is controlled by the pellet diffusion rate?

You may assume the entire bed length is either in the intrinsic reaction rate or pellet diffusion rate limited regimes and that the external mass transfer resistance between the fluid and the solid catalyst is negligible.

Additional Data: The Thiele modulus is defined as:

$$\Phi = \frac{R}{3}\left[\frac{n+1}{2}\frac{kc_s^{n-1}}{D_e}\right]^{1/2}$$

in which c_s is the outer pellet surface concentration and k is the intrinsic rate constant on a per volume of catalyst basis.

The effectiveness factor for positive order reactions in a sphere can be approximated by

$$\eta = \frac{1}{\Phi}\left[\frac{1}{\tanh 3\Phi} - \frac{1}{3\Phi}\right]$$

Problem 2. Surface reactions. 25 pts.

Consider the overall reaction:

$$\mathrm{A} + \mathrm{B} \rightleftharpoons \mathrm{C}$$

A possible catalyst material contains two different types of reactive sites, X and Y. Both A and B adsorb on X and Y, but the reaction proceeds only if A adsorb on X and B on Y. This reaction is described by the following mechanism:

$$\mathrm{A} + \mathrm{X} \rightleftharpoons \mathrm{A} \cdot \mathrm{X} \tag{1}$$
$$\mathrm{A} + \mathrm{Y} \rightleftharpoons \mathrm{A} \cdot \mathrm{Y} \tag{2}$$
$$\mathrm{B} + \mathrm{X} \rightleftharpoons \mathrm{B} \cdot \mathrm{X} \tag{3}$$
$$\mathrm{B} + \mathrm{Y} \rightleftharpoons \mathrm{B} \cdot \mathrm{Y} \tag{4}$$
$$\mathrm{A} \cdot \mathrm{X} + \mathrm{B} \cdot \mathrm{Y} \rightleftharpoons \mathrm{C} + \mathrm{X} + \mathrm{Y} \tag{5}$$

(a) What is the production rate of C if Reaction 5 is irreversible and Reactions 1–4 reach equilibrium? Hint: you can assume you know the monolayer coverage amounts of both the X and Y available sites, $\bar{c}_{mX}$, $\bar{c}_{mY}$.

(b) If the equilibrium constants for Reactions 1–4 are of the same order of magnitude, what happens to the production rate of C if very large or very small ratios of A to B are feed to the reactor? Why?

(c) Two sets of experiments were performed to determine kinetic information for the overall reaction. These experiments were performed under the conditions that $K_1 c_A, K_2 c_A, K_3 c_B$, and $K_4 c_B \ll 1$. The effective rate constant for the production of C, k_{eff} was measured at various temperatures and the plots in Figure 1 were developed. Does this catalyst material promote or inhibit the production rate? Why do you think so?

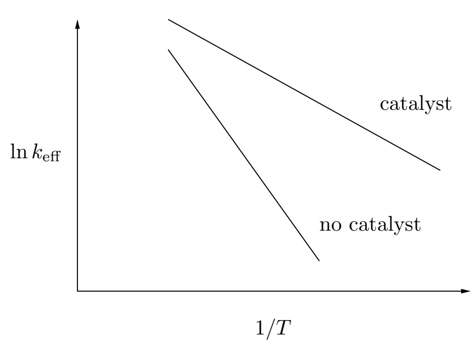


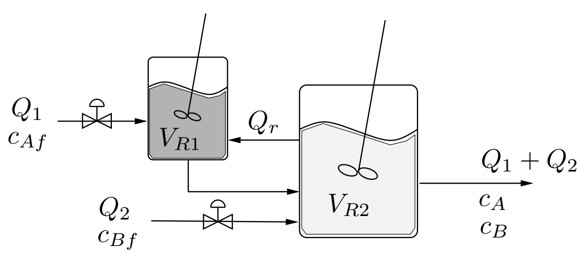
Figure 1: Effective rate constant versus inverse temperature.

Part II.

Instructions: You will require your laptops for Part II of the exam.
Write any answers on separate paper. Do not write any answers on the exam itself. Hand in your exam as well as your solution at the end. Make sure your name is on your solution and your exam.
When you have finished, insert your wireless network card and **email to your TA the programs you have written to solve the problem and plot the solution. Your programs should generate the solutions for each problem.**

Problem 3. Pulse response of a mixing model. 20 pts.

Consider the mixing model depicted below. Suppose that a tracer is injected with the A feed stream with concentration profile given in Figure 2. You may assume that there is no tracer in the reactor up to time $t = 0$. The reactor parameters are given below. Plot the dynamic response of the effluent tracer concentration for $0 \leq t \leq 50$ minutes.



Parameter	Value	Units
$\theta_1 = V_{R1}/Q_2$	1	min
$\theta_2 = V_{R2}/Q_2$	2	min
$\theta = V_R/Q_2$		
$= \theta_1 + \theta_2$	3	min
$\alpha = Q_1/Q_2$	0.1	
$\rho = Q_r/Q_2$	0.1	

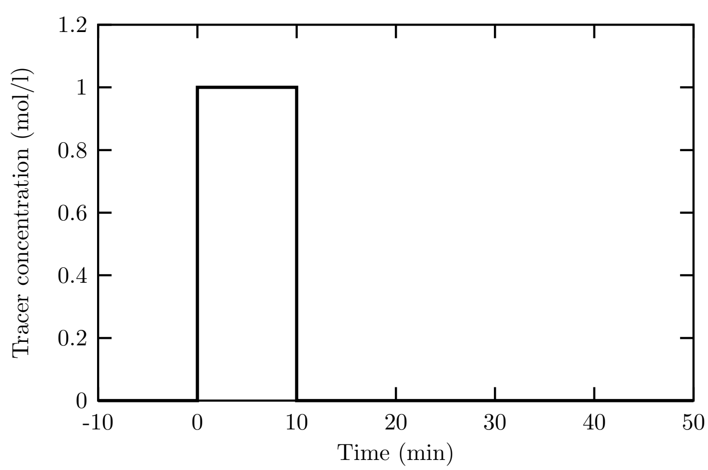


Figure 2: Tracer concentration profile

Problem 4. Benzene pyrolysis for different reactor configurations. 30 pts.

Hougen and Watson analyzed the rate data for the pyrolysis of benzene by the following two reactions. Diphenyl is produced by the dehydrogenation of benzene,

$$2C_6H_6 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C_{12}H_{10} + H_2 \tag{6}$$

Triphenyl is formed by the secondary reaction,

$$C_6H_6 + C_{12}H_{10} \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} C_{18}H_{14} + H_2 \tag{7}$$

The reactions are assumed to be elementary so that the rate expressions are

$$r_1 = k_1\left(c_B^2 - \frac{c_D c_H}{K_1}\right) \qquad r_2 = k_2\left(c_B c_D - \frac{c_T c_H}{K_2}\right) \tag{8}$$

in which the subscripts, B, D, T and H represent benzene, diphenyl, triphenyl and hydrogen, respectively. We would like to isothermally react benzene at 1033 K and 1.0 atm. The rate and equilibrium constants at $T = 1033$ K and $P = 1.0$ atm are given in Hougen and Watson,

$$k_1 = 7 \times 10^5 \text{ L/mol}\cdot\text{hr} \qquad K_1 = 0.31$$
$$k_2 = 4 \times 10^5 \text{ L/mol}\cdot\text{hr} \qquad K_2 = 0.48$$

The feed stream is 60 kmol/hr of pure benzene. The value of the gas constant is $R = 82.06$ atm$\cdot$cm^3/mol$\cdot$K.

(a) Write down the steady-state material balances for a PFR. Calculate the overall conversion of benzene for an 800 liter PFR.

(b) Write down the steady-state material balances for a CSTR. Calculate the overall conversion of benzene for an 800 liter CSTR.

(c) Calculate the overall conversion of benzene for the configuration given below. The volume of each reactor is 400 L.