

1. An aqueous feed of A and B (400 liter/min, 100 millimol A/liter, 200 millimol B/liter) is to be converted to product in a mixed-flow reactor. The kinetics of the reaction are represented by



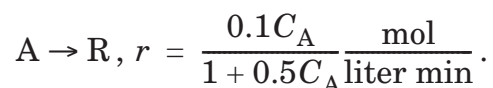
Find the volume of reactor needed for 99.9% conversion of A to product.

2. We are planning to operate a batch reactor to convert A into R. This is a liquid reaction, the stoichiometry is $A \rightarrow R$, and the rate of reaction is given in the table below. How long must we react each batch for the concentration to drop from $C_{A_0} = 1.3$ mol/liter to $C_{A_f} = 0.3$ mol/liter?

Table 1: Kinetics Data

C_A , mol/liter	r , mol/liter min
0.1	0.1
0.2	0.3
0.3	0.5
0.4	0.6
0.5	0.5
0.6	0.25
0.7	0.10
0.8	0.06
1.0	0.05
1.3	0.045
2.0	0.042

3. A specific enzyme acts as a catalyst in the fermentation of reactant A. At a given enzyme concentration in the aqueous feed stream (25 liter/min) find the volume of plug flow reactor needed for 95% conversion of reactant A ($C_{A_0} = 2$ mol/liter). The kinetics of fermentation at this enzyme concentration is given by



4. A laboratory-scale mixed reactor was used to study the kinetics of the reaction $A \rightarrow R$. The reactor has a volume of 10.0 liters. An aqueous mixture of 5.00 mol/liter of A was the feed. The output concentration was measured at several different input flowrates. The results are in the table below. Your company has a spare 2 m³ PFR which they wish to use to produce R. The boss wants 99% conversion of A in the reactor. How much R can you produce in mol/hr from a feedstock of 10.0 mol/liter A?

Table 2: CSTR Lab Data

\dot{V} , lit/min	C_{A_f} , mol/liter
71	4.75
35	4.5
16	4
7	3
4	2
3	1.6
2	1
1.3	0.5
0.9	0.25

5. R is presently produced by the decomposition of aqueous A according to the reaction $A \rightarrow 3R + S$, $r = 0.1C_A \frac{\text{mol}}{\text{liter s}}$. The present process uses a 10 m³ PFR with a feed rate of 1 m³/s of 5.00 molar A. The boss wants to retain the present reactor but increase the overall conversion of the process by installing a separator and a recycle loop. The separator can provide a product stream and a recycle stream. Essentially all of the R and S are recovered in the product stream. The split fraction of A and water with respect to the product stream can be varied from 0.05 to 1, but it is the same for both A and water. A, R, and S dissolve perfectly in water (no volume change for the aqueous phase upon solution).
- What is the production rate of R for the current setup?
 - At what split fraction of A in the separator would the production rate of R be maximized? Explain.

- (c) What possible modifications could be made to the recycle process to increase the production rate of R?
6. For a non-isothermal CSTR, the mass balance and the energy balance must be solved simultaneously to determine the operating temperature and conversion of the reactor. In this problem you are to derive the two equations and one variant. Assume that the density of the fluid, ρ , is constant, that the heat capacity, C_p , is constant with temperature, that the reaction kinetics are n -th order, i.e., $r = kC_A^n$, and that k has a Arrhenius form, i.e., $k = k_0 e^{-E_a/RT}$. Ignore the work of the stirrer, and assume that a specified amount of heat, \dot{Q} , can be added to or removed from the reactor. The inlet conditions are \dot{V} , C_{A_0} , and T_0 (assume absolute). The reactor has a volume, V , and outlet conditions of \dot{V} , C_A , and T .
- (a) Starting from a mass balance, derive an implicit equation for C_A as a function of C_{A_0} , V , \dot{V} , E_a , and T . Compare your results with the explicit result for the $n = 1$ case: $C_A = \frac{C_{A_0}}{1 + \frac{V}{\dot{V}}(k_0 e^{-E_a/RT})}$
- (b) Starting from the 1st Law, derive an equation for C_A^n as a function of T_0 , T , V , \dot{V} , E_a , \dot{Q} , and the enthalpy of reaction, $\Delta\hat{H}_r^\circ$. Compare your results with the result for the $n = 1$ case:
- $$C_A = \frac{\dot{Q}}{(\Delta\hat{H}_r^\circ)Vk_0 e^{-E_a/RT}} + \frac{\rho C_p \dot{V}(T_0 - T)}{(\Delta\hat{H}_r^\circ)Vk_0 e^{-E_a/RT}}$$
- (c) Again starting from the 1st Law, by making the substitution $rV = \dot{V}C_{A_0}f_A$, derive an expression for f_A as a function of T_0 , T , \dot{V} , \dot{Q} , $\Delta\hat{H}_r^\circ$, and C_{A_0} . It should be a linear function of T
7. The following set of experimental data was obtained from an adiabatic pilot-scale CSTR for the first-order reaction $A \rightarrow R$, $\Delta\hat{H}_r^\circ = -80 \text{ kJ/mol}$. The reactor

has a volume of 250 liters. The feed had an initial concentration of 3.00 kmol/m³, a density of 1000 kg/m³, a heat capacity of 4000 J/kg K, and a temperature of 300 K. Determine the activation energy of the reaction.

Table 3:

$\dot{V} \frac{\text{m}^3}{\text{s}}$	$T \text{ (K)}$
0.200	307.32
0.180	308.61
0.160	310.50
0.140	313.65
0.120	320.34
0.100	334.97
0.080	344.49
0.060	350.10
0.040	354.13
0.020	357.33
0.010	358.72
0.001	359.88

8. This problem examines the determination of the operating point of a mixed reactor by graphical means.
- Take the 1st-order expression in part (a) of Problem 6 and derive an explicit expression for the fractional conversion of A, f_A , as a function of the other parameters. A plot of f_A vs. T is a sigmoidal (s-shaped) curve.
 - A plot of f_A vs. T for the expression you derived in part (c) of Problem 6 is a straight line. What two parameters control the intercept but don't affect the slope?
 - The operating point of a mixed reactor is where the functions in parts (a) and (b) intercept. Plot the two functions for $k_0 = 1.50 \times 10^{10} \text{ s}^{-1}$,
 $E_a = 82 \text{ kJ/mol}$, $\rho = 1000 \text{ kg/m}^3$, $C_p = 4184 \text{ J/kg}$, $\Delta \hat{H}_r^\circ = -82 \text{ kJ/mol}$,

$V = 0.100 \text{ m}^3$, $\dot{V} = 0.00100 \text{ m}^3/\text{s}$, $C_{A_0} = 5 \text{ mol/lit}$, $\dot{Q} = 0$, and $T_0 = 29^\circ\text{C}$. How many operating points are there? Which ones are stable? Why?

- (d) Holding $\dot{Q} = 0$, what are the maximum and minimum T_0 's for which there are more than one operating point?
- (e) Holding $T_0 = 29^\circ\text{C}$, what are the maximum and minimum \dot{Q} 's for which there are more than one operating point?