

Instructions

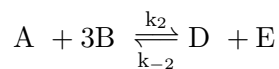
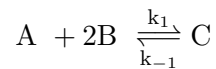
1. Write your name at the top of each answer sheet and on the front page of the exam questions.
2. Start each problem at the top of a new page.
3. The exam consists of three equally weighted problems.
4. Useful integrals and equations are listed beginning on page 3.
5. Return the exam questions or you will receive a grade of zero.

$$R = 82.06 \text{ cm}^3\text{-atm/gmole-K}; R = 1.987 \text{ cal/gmole-K}$$

$$\text{The van't Hoff relation is } \frac{\partial \ln K}{\partial T} = \frac{\Delta H^\circ}{RT^2}$$

Problem 1

The following gas phase reactions are conducted in a closed system and are at equilibrium. The reactor is maintained at a constant pressure of $P = 5 \text{ atm}$. The volume is allowed to change to keep the pressure constant. The reactor is charged with one mole of A ($n_{A_0} = 1.0 \text{ mol}$) and three moles of B ($n_{B_0} = 3 \text{ mol}$). Determine the reaction temperature if the equilibrium moles of C and D are $n_C = 0.0147 \text{ mol}$ and $n_D = 0.926 \text{ mol}$. You can assume the heats of reaction are constant.

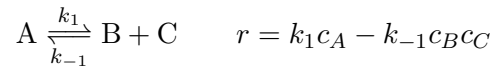


The Gibbs free energies of formation from the elements and the heats of formation from the elements for the components at 700 K are

	ΔG_f^{700} (cal/gmol)	ΔH_f^{700} (cal/gmol)
A	-41,530	-26,410
B	0	0
C	-44,840	-50,880
D	-3,060	-20,400
E	-49,920	-58,710

Problem 2

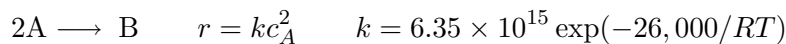
Consider the reversible liquid-phase reaction



that will be conducted in an isothermal batch reactor. If the initial concentrations are $c_{A0} = 6.5$ gmol/liter, $c_{B0} = c_{C0} = 0$ gmol/liter, determine the time to realize 90% conversion of A at a temperature of 328 K. At 328 K, $k_1 = 3.8 \times 10^{-3} \text{ sec}^{-1}$ and $k_{-1} = 0.3 \times 10^{-4} \text{ l/gmol-sec}$. Further, at 328K a conversion of 90% is attainable. Assume constant density.

Problem 3

Consider the liquid-phase reaction



where the units on k are liter/gmol-min, T is in degrees Kelvin and $R = 1.987 \text{ cal/gmol-K}$. This reaction will be conducted in a 1000-liter steady-state CSTR. The reactor is operated isothermally at 358 K and you may assume constant density. The inlet stream has a volumetric flow rate of $Q_f = 100$ liter/min and the concentration of A in the feed is $c_{Af} = 5$ gmol/liter. As the new engineer on the site your boss has asked you to rationalize how it is possible that more of the A is reacting than should be, and to offer a possible solution. Having just completed ChE 372 that year you just know you will be able to solve this problem.

You provide a qualitative answer and to back it up perform some calculations. Produce the calculations for Parts (1) and (2).

1. You suspect the reaction is continuing in the exit pipe from the reactor and you decide to model it as a CSTR with a residence time that is 5.0 % the residence time of the reactor. By how much does the conversion of A increase with this second reactor?
2. You boldly tell the boss all that needs to be done is to cool the pipe by 25 degrees and the increased conversion will be acceptable. Ok then show her how much less the overall conversion will be if you lower the temperature of this exit pipe by 25 K (*i.e.*, the second CSTR is now 25 K cooler).

Design Equations

Batch Reactor

$$\frac{d(V_R c_j)}{dt} = \sum_i^{n_{rxns}} \nu_{ij} r_i V_R$$

$$\frac{dT}{dt} = \frac{UA(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri} V_R}{V_R \sum_j^{n_{components}} c_j C_{pj}}$$

Plug Flow Reactor

$$\frac{d(Qc_j)}{dV} = \sum_i^{n_{rxns}} \nu_{ij} r_i$$

$$\frac{dT}{dV} = \frac{\frac{2}{R}U(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri}}{Q \sum_j^{n_{components}} c_j C_{pj}}$$

Stirred Tank Reactor

$$\frac{d(V_R c_j)}{dt} = Q_f c_{jf} - Q c_j + \sum_i^{n_{rxns}} \nu_{ij} r_i V_R$$

$$\frac{dT}{dt} = \frac{UA(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri} V_R + Q_f \sum_j^{n_{components}} c_{jf} (H_{jf} - H_j)}{V_R \sum_j^{n_{components}} c_j C_{pj}}$$

Continuous Stirred Tank Reactor (constant phase)

$$0 = Q_f c_{jf} - Q c_j + \sum_i^{n_{rxns}} \nu_{ij} r_i V_R$$

$$0 = UA(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri} V_R + \sum_j^{n_{components}} Q_f c_{jf} \int_T^{T_f} C_{pj} dT$$

Useful Integrals

$$\int \frac{1}{a+bx} dx = \frac{1}{b} \ln(a+bx)$$

$$\int (a+bx)^n dx = \frac{(a+bx)^{n+1}}{(n+1)b} \quad ; n \neq -1$$

$$\int \frac{dx}{(a+bx)(a'+b'x)} = \frac{1}{ab' - a'b} \ln \left(\frac{a'+b'x}{a+bx} \right)$$

$$\int \frac{a+bx}{a'+b'x} dx = \frac{bx}{b'} + \frac{ab' - a'b}{b'^2} \ln(a'+b'x)$$

$$\int \frac{(a+bx)^m}{(a'+b'x)^n} dx = \frac{-1}{(n-1)b'} \left[\frac{(a+bx)^m}{(a'+b'x)^{n-1}} - mb \int \frac{(a+bx)^{m-1}}{(a'+b'x)^{n-1}} dx \right]$$

$$\int x^m (a+bx)^n dx = \frac{x^{m+1} (a+bx)^n}{m+n+1} + \frac{an}{m+n+1} \int x^m (a+bx)^{n-1} dx$$

Simpson's three-eighth's rule for numerical integration:

$$\int_{X_0}^{X_3} f(X) dX = \frac{3h}{8} [f(X_0) + 3f(X_1) + 3f(X_2) + f(X_3)]$$

where:

$$h = \frac{X_3 - X_0}{3} \quad X_1 = X_0 + h \quad X_2 = X_0 + 2h$$

Integration of $N + 1$ points, where N is even:

$$\int_{X_0}^{X_N} f(X) dX = \frac{h}{3} [f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \dots + 4f_{(N-1)} + f_N]$$

where:

$$h = \frac{X_N - X_0}{N}$$