

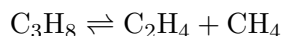
Instructions

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 (34 points) The thermal cracking of propane is one route to the generation of ethylene.

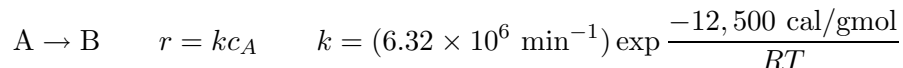


The reaction is operated close to the equilibrium limit. Heats of formation from the elements and Gibbs free energies of formation from the elements are known at 700 K and provided in the table below. Presently the process operates isothermally at 700 K and a total pressure of 25 psia. The feed to the tubular reactor is pure propane. You need to increase the production of ethylene and are given two choices: 1) change the pressure by up to a factor of 4 while holding the temperature at 700 K, or 2) change the temperature by up to 75 K while holding the pressure constant at 25 psia. You can decrease or increase the process condition anywhere within the allowed range.

	ΔG_f^{700} (kcal/mol)	ΔH_f^{700} (kcal/mol)
C_3H_8	22.94	-29.48
C_2H_4	22.68	10.15
CH_4	-3.06	-20.40

- (A) Compute the equilibrium mole fraction of ethylene at the base case of pure propane fed, a temperature of 700 K and a total pressure of 25 psia.
- (B) If you change the pressure, what is the maximum percentage increase in the ethylene mole fraction relative to the base case?
- (C) If you change the temperature, what is the maximum percentage increase in the ethylene mole fraction relative to the base case?
- (D) Which change would you advocate and why?

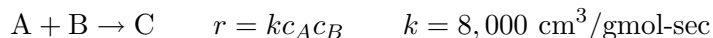
Problem 2 (33 points) The liquid-phase reaction



will be conducted in three isothermal, equal volume CSTRs-in-series that are operating at steady state. The feed consists of pure A at a concentration of $c_{Af} = 1$ gmol/lit and a temperature of 50 °C. Your former co-worker was asked to size the units so that a conversion of 90% of A would be realized across the cascade of reactors. The design calculations were performed and the units have been installed. Unfortunately, the conversion is much less than needed.

You have been told to fix the problem, and a meeting with the Plant Manager is scheduled in two hours at which you will make your recommendations. Upon reviewing the calculations of your co-worker, you notice that an equal conversion of 30 % was used in each reactor. What possible solution or solutions can you recommend? Justify any recommendation(s) with quantitative values.

Problem 3 (33 points) The gas-phase reaction



will be conducted in an isothermal ($T = 475$ K), constant pressure ($P = 2.5$ atm) PFR. The feed consists of an equimolar mixture of A and B in an inert diluent, with the following molar feed ratios A:B:Inert of 1:1:2. The total volumetric feed rate is $Q_f = 12,500 \text{ cm}^3/\text{sec}$. What volume is required for the conversion of A to equal 90% (*i.e.*, $x_A = 0.9$)?

Batch Reactor

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

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

Plug Flow Reactor

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

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

Stirred Tank Reactor

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

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

Continuous Stirred Tank Reactor at Steady-state (constant phase)

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

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

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

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

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

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

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

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

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:

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