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 5.
5. Return the exam questions or you will receive a grade of zero.

R = 82.06 cm^3-atm/gmole-K; R = 1.987 cal/gmole-K

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

Problem 1

The gas phase reaction

$$2\text{A} \longrightarrow \text{B} + \text{C} \qquad r = kc_A$$

will be conducted in an adiabatic PFR. The feed enters as 650 K and the reactor contents cannot exceed 800 K. This is prevented by injecting a cold, inert gas into the reactor at that location where the temperature reaches 800 K. Figure **??** illustrates the arrangement. After the quench the reaction continues in the adiabatic PFR and now the mixture also contains the inert material. This reactor operates at a constant pressure of 1 atm. The table below contains the reactor and reaction parameters.

Parameter	Value	Units
T_f	650	K
P	1	atm
Q_f	8×10^4	cm^3/sec
k_o	9.5×10^{10}	sec^{-1}
E_A	29,000	cal/gmol
ΔH_R	-38,000	cal/gmol
$\overline{C}_{pA}$	70	cal/gmol-K
$\overline{C}_{pB}$	70	cal/gmol-K
$\overline{C}_{pC}$	70	cal/gmol-K
$\overline{C}_{pI}$	45	cal/gmol-K
T_I	475	K

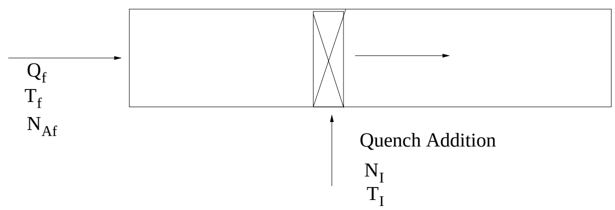

Figure 1: Schematic of the PFR with quench

Make several assumptions. First, assume the thermodynamic parameters do not change with temperature. Second, assume the quench stream is added infinitely fast, that the mixing of this stream with the reactor contents occurs infinitely fast, and that the quench is adiabatic *i.e.,* no heat is lost or gained by the surroundings during the quench and no reaction takes place in this zone in the reactor.

(a) If the reactor contents are to be cooled to 700 K, what volumetric flow rate of inert (pure gas at 1 atm and 475 K) is required?

(b) Will a second quench to keep the temperature from exceeding 800 K be required before the conversion of A reaches 95%? Justify your answer with suitable calculations.

Problem 2

Part A List the assumptions that are used in developing the material and energy balances for a plug flow reactor.

Part B List the assumptions that are used in developing the material and energy balances for a CSTR.

Part C Consider the following first order liquid-phase reaction

$$\mathrm{A} \longrightarrow \mathrm{B} \qquad r = kc_A \qquad k = 1.05 \times 10^{-3}\ \mathrm{sec}^{-1}$$

If a PFR operating with a feed concentration of $c_{Af} = 0.045$ gmol/cm^3 and a residence time of $\tau = 1,800$ sec is considered the reference case. What is the minimum number of identical CSTRs operating in series, with the same total residence time (volume) as the PFR, required to come within 10% of the performance of the PFR (*i.e.* $(c_{A,\mathrm{cstr}} - c_{A,\mathrm{pfr}})/c_{A,\mathrm{pfr}} = 0.10$)? What is the minimum number of CSTRs in series required to come within 20%? Does your answer make sense? Explain it.

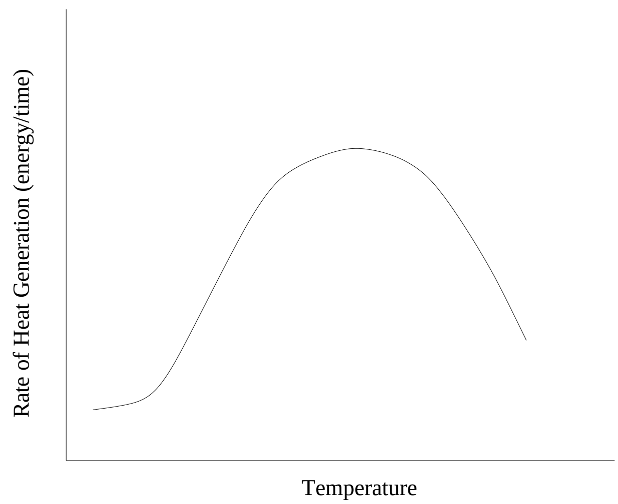

Figure 2: Rate of heat generation versus reactor temperature

Problem 3

Part A In constructing a van Heerden diagram for the following reaction A $\rightleftharpoons$ B in a CSTR you would find the generation curve has the shape illustrated in Figure **??**. Using equations to support your answer discuss why the curve for Q_{gen} is not the familiar S-curve illustrated in the text.

Part B Consider the following set of reactions in a CSTR. The feed consists of pure A at 350 K. You are to maximize the production of D. Would you operate this reactor adiabatically or nonadiabatically? Explain your answer with enough detail that we are convinced you are not guessing.

		k_o (sec^{-1})	E_a (cal/gmol)	ΔH_R (cal/gmol)
$A \xrightarrow{k_1} B$	$r_1 = k_1 c_A$	8.25×10^5	12,500	-15,000
$B \xrightarrow{k_2} C$	$r_2 = k_2 c_B$	4.27×10^9	19,700	-17,000
$B \xrightarrow{k_3} D + E$	$r_3 = k_3 c_B$	2.28×10^7	15,300	-13,000

Part C The following liquid-phase reaction will take place in a CSTR

$$A + B \longrightarrow C \qquad r = kc_A$$

The feed enters at 75 °F, a total volumetric flow of $Q_f = 226.34$ ft^3/hr, and consists of a mixture of A and B having molar flow rates of $N_{Af} = 35$ lbmol/hr and $N_{Bf} = 500$ lbmol/hr. The remaining process parameters are listed in the table below. You may assume the thermodynamic properties are constant with temperature. This reactor has an upper stable operating temperature at 798 R. What is the rate of heat removal that will give this operating condition?

Variable	Value	Units
$\overline{C}_{pA}$	35	Btu/lbmol-R
$\overline{C}_{pB}$	18	Btu/lbmol-R
$\overline{C}_{pC}$	46	Btu/lbmol-R
ΔH_R	-226,000	Btu/lbmol
V_R	50	ft^3
k	$9.0 \times 10^{12} \exp(-19,628/T)$	hr^{-1}; T in Rankine

Batch Reactor

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

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

Plug Flow Reactor

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

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

Stirred Tank Reactor

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

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

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

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

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

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

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

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

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

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

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

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

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

where:

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

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

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

where:

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