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

Problem 1

An adiabatic PFR will be used for the gas phase reaction

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{D} + \mathrm{E} \qquad r = kP_\mathrm{A}P_\mathrm{B} \qquad k = 200{,}000\exp(-14{,}000/T)$$

The units for the rate are lbmoles/hr-ft^3, P_j is in atm and T is in °R. The feed enters at 500 °F and 2 atm total pressure. The inlet molar feed rate of B is $N_{\mathrm{B}f} = 0.17$ lbmole/hr. The feed only contains A and B. The heat of reaction is $\Delta H_r = -58{,}000$ Btu/lbmole and the molar average heat capacity of the fluid phase is $\tilde{C}_p = 95$ Btu/lbmole-R. You may assume ΔH_r and $\tilde{C}_p$ remain constant.

(a) Determine the maximum reactor temperature if the feed consists of a 4:1 molar mixture of A:B (i.e., the molar flow rate of A is 4 times the molar flow rate of B).

(b) Determine the maximum possible reactor temperature if the inlet flow of B is held fixed at 0.17 lbmole/hr.

Problem 2

The liquid-phase reaction

$$\text{A} \longrightarrow \text{B} \qquad r = kc_A \qquad k = k_o \exp(-E_a/RT)$$

is to be carried out in a nonisothermal, nonadiabatic CSTR. The feed contains pure A at 45 °C and 5 gmoles/liter. The total mass feed rate is m_t. Other system parameters are listed below.

Item	value	units
V_R	1000	liter
Q_f	100	liter/min
m_t	93,200	g/min
k_o	3.16×10^{14}	min^{-1}
E_a	24,837	cal/gmole
T_a	35	°C
ΔH_R	-3,700	cal/gmole
C_p	0.22	cal/g-K
U	0.45	cal/min-cm^2-K
A	18,000	cm^2

(a) Determine the reactor temperature and concentration of A for an operating condition that leads to a conversion of A ($x_A \geq 0.85$). Note: The reactor will operate to give a conversion that is greater than or equal to 0.85 and you are to determine what this operating condition is.

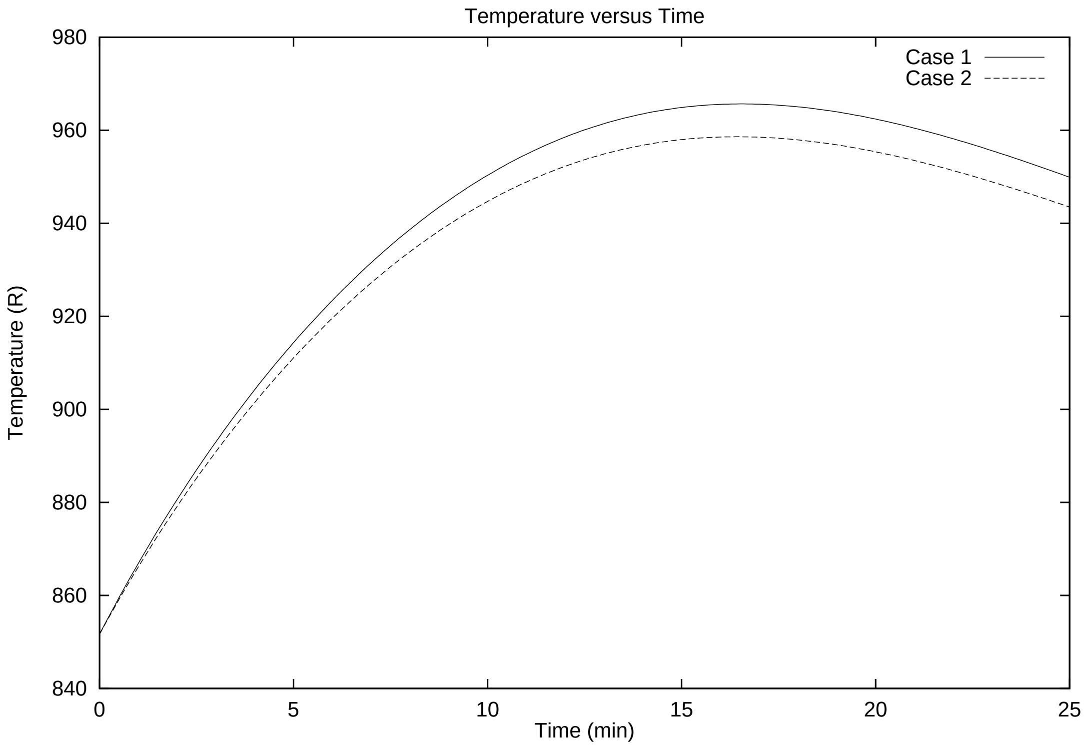

Figure 1: Temperature change with time in the batch reactor for two different mixers.

Problem 3

Part 1 - 20 points. A batch reactor is to be used for a liquid-phase reaction.

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C} + \mathrm{D} \tag{1}$$

This reaction is exothermic and the reactor is operated nonisothermally and nonadiabatically. Heat is removed through a cooling coil immersed in the reactor and the wall of the cooling coil is at a constant temperature. The fluids for this reaction are quite viscous and the motor used to drive the mixing impeller burned up. A new motor was purchased that delivered more power. Figure 1 shows the temperature history for two cases. One of these cases corresponds to the lower power mixing motor and the other case corresponds to the higher power mixing motor.

(a) Identify which case (Case 1 or Case 2) corresponds to the temperature history for the new, higher power motor.

(b) Explain your answer to Part a. In particular why do the temperature histories have similar shapes and why are the temperature maxima different.

Part 2 - 14 points. Use the following reactions

$$\mathrm{Cl_2} + \mathrm{C_3H_6} \xrightarrow{k_1} \mathrm{C_3H_5Cl} + \mathrm{HCl}$$
$$\mathrm{Cl_2} + \mathrm{C_3H_6} \xrightarrow{k_2} \mathrm{C_3H_6Cl_2}$$

to develop the proof that

$$\sum_{i=1}^{n_{\mathrm{rxns}}} \Delta H_{Ri} r_i = \sum_{j=1}^{n_{\mathrm{components}}} R_j H_j$$

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)

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

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

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

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

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

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

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

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

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:

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