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 4.
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 CSTR with a first-order, liquid-phase reaction

$$\mathrm{A} \longrightarrow \mathrm{B}, \qquad r = kc_A \tag{1}$$

operates at the conditions shown below

Parameter	Value	Units
T_f	325	°K
c_{Af}	3.0	$kmol/m^3$
Q_f	100×10^{-6}	m^3/s
ΔH_R	-2.09×10^8	J/kmol
$\hat{C}_p$	4.19×10^3	J/kg °K
ρ	10^3	kg/m^3
V_R	18×10^{-3}	m^3
k	$4.48 \times 10^6 \ \exp(-7550/T)$	s^{-1}; T in °K

Find the steady-state operating temperature.

Problem 2

[This problem was adapted from Laidler, *Chemical Kinetics.*] Consider the reaction of H_2 and I_2 to form HI.

$$H_2 + I_2 \longrightarrow 2HI$$

Two mechanisms have been proposed for this reaction; H, I and H_2I are reaction intermediates.

Mechanism 1

$$I_2 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2I \qquad \text{(fast)}$$

$$I + H_2 \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} H_2I \qquad \text{(fast)}$$

$$H_2I + I \overset{k_3}{\longrightarrow} 2HI \qquad \text{(slow)}$$

Mechanism 2

$$I_2 \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} 2I$$

$$I + H_2 \overset{k_5}{\longrightarrow} HI + H$$

$$H + I_2 \overset{k_6}{\longrightarrow} HI + I$$

In Mechanism 2 we do not specify if reactions are fast or slow, or equilibrated.

Develop rate expressions for the rate of formation of HI, R_{HI}, in terms of the stable molecules (H_2, I_2, HI) for both Mechanism 1 and Mechanism 2. In your derivations list the assumptions you are making for each mechanism separately.

Problem 3

The gas-phase oxidation of o-xylene to phthalic anhydride

$$\text{o-xylene } + 3\text{O}_2 \longrightarrow \text{phthalic anhydride } + 3\text{H}_2\text{O}$$

is highly exothermic. The feed consists of o-xylene mixed with air (assumed to be a mixture of nitrogen and oxygen). The reaction is carried out in PFR tube bundles with molten salt circulating as the heat transfer fluid; the molten salt temperature is constant at T_a. The reaction rate is given by

$$r = kc_{\text{oxylene}}$$

Assume you have polynomial representations for the molar heat capacities for each component, $C_{pj} = A_j + B_jT^2 + C_jT^3 + D_jT^4$, the heats of formation at 298 K, H^o_{fj}, and the value for the heat transfer coefficient, U^o corresponding to a reactor diameter, D_t. For a given feed mole fraction of o-xylene of $y_{\text{oxylene,f}}$, feed temperature of T_f, and inlet molar flow rate, N_{feed}, develop the equations you need to predict the temperature within the reactor. Define all the terms and discuss how you would solve these 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

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

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

Continuous Stirred Tank Reactor (constant phase)

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

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

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

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

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

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

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

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

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:

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