

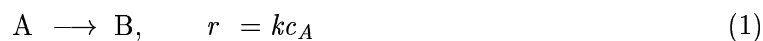
Instructions

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.

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

**Problem 1**

An adiabatic CSTR with a first-order, liquid-phase reaction



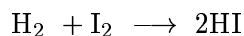
operates at the conditions shown below

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

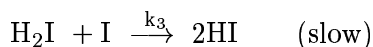
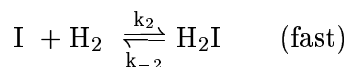
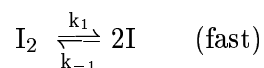
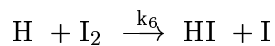
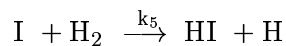
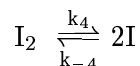
Find the steady-state operating temperature.

**Problem 2**

[This problem was adapted from Laidler, *Chemical Kinetics*.] Consider the reaction of  $\text{H}_2$  and  $\text{I}_2$  to form  $\text{HI}$ .



Two mechanisms have been proposed for this reaction;  $\text{H}$ ,  $\text{I}$  and  $\text{H}_2\text{I}$  are reaction intermediates.

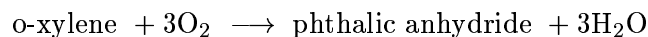
**Mechanism 1****Mechanism 2**

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

Develop rate expressions for the rate of formation of  $\text{HI}$ ,  $R_{\text{HI}}$ , in terms of the stable molecules ( $\text{H}_2$ ,  $\text{I}_2$ ,  $\text{HI}$ ) 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



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

$$r = kc_{\text{o-xylene}}$$

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,  $H_{fj}^o$ , 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  $y_{\text{o-xylene},f}$ , 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.

## Design Equations

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### 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

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

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

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

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

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

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

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:

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