

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.

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

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

Problem 1

The liquid-phase parallel reactions



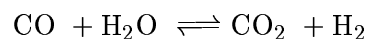
are to be carried out in a steady state CSTR. The feed enters at 83°C and consists of pure A at a concentration of $c_{Af} = 5 \text{ mol/liter}$.

Variable	Value	Units
ρQ	93,000	g/min
ΔH_{R1}	-4,200	cal/mol
ΔH_{R2}	-2,000	cal/mol
V_R	100	liter
Q_f	100	liter/min
T_a	50	°C
C_{pf}	0.22	cal/g-K
U	0.65	cal/min-cm ² -K
A	15,400	cm ²
k_1	$3.16 \times 10^{14} \exp(-12,500/T)$	min ⁻¹ ; T in K
k_2	$2.52 \times 10^9 \exp(-8,500/T)$	min ⁻¹ ; T in K

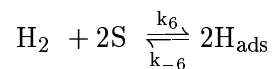
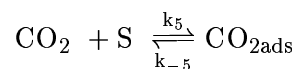
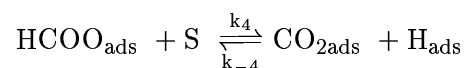
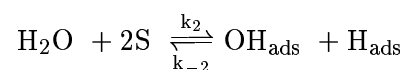
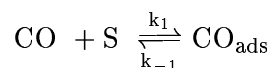
Find the operating temperature for this reactor and the concentration of A (c_A) in the effluent stream. You may assume constant density.

Problem 2

Hydrogen is produced in the heterogeneously-catalyzed water-gas shift reaction

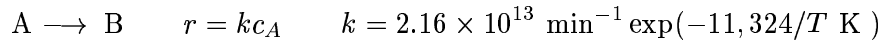


Several mechanism have been proposed for this reaction based on the catalyst used. One such mechanism proposed for copper-zinc oxide involves a surface formate formation (HCOO^-). For our purposes here assume the formate formation reaction, r_3 , is the rate limiting step and all the other reactions are at equilibrium. Develop a rate expression for the rate of CO_2 formation in terms of gas phase concentrations of stable molecules.



Problem 3

The following liquid-phase reaction will be conducted in a batch reactor



The initial conditions and selected processes conditions are listed below.

Item	Value	Units
V_R	1,000	liter
ΔH_R	-40,000	cal/gmol
\hat{C}_p	0.65	cal/g-K
ρ	1.1×10^3	g/liter
T_o	318	K
c_{Ao}	1.25	gmol/liter

Part (a) List the equations that are needed to determine the how the dependent variables change in the batch reactor if it is operated adiabatically. Put a numerical value in for each term, *i.e.*, no symbols for variables that have a value. Tell how you would solve this problem.

Part (b) Sketch the temperature profile on the blank figure provided on the next page, remove the page and include it along with your solution. Be sure to write your name on the page. I am not interested in the exact solution to this problem so there is no need to put a scale on the x-axis for time. I do want you to put scale on the y-axis and I want you to show the maximum temperature (*i.e.*, write down the numerical value) that will be realized in the adiabatic batch reactor. Be sure to label this the adiabatic curve.

Part (c) What would the temperature profile look like and would it be qualitatively and quantitatively different from the curve sketched for Part (b) if the mechanical agitation effectively added heat to the reactor at a constant rate of 4×10^4 cal/min? Sketch the curve for Part (c) on the same diagram and be sure we can tell which curve corresponds to Part (b) and which curve corresponds to Part (c).

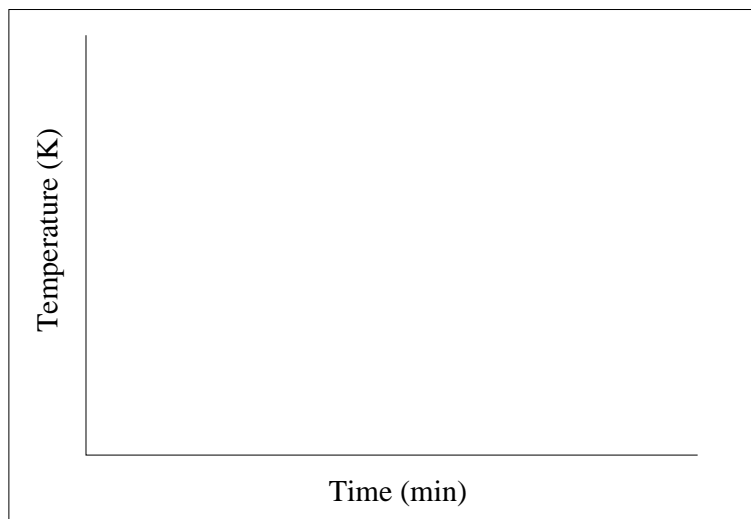


Figure 1: Temperature change with time in the batch reactor.

NAME:

Design 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

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

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

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

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

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

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

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

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

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

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:

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