

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 five 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.

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

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

Problem 1

The liquid-phase reaction



$$r = k_{ACB}; \quad k = 2.68 \times 10^{15} (\text{liter/gmole-min}) \exp\left(\frac{-24,000 \text{ cal/gmole}}{RT}\right)$$

is conducted in an isothermal batch reactor at 308 K. The reactor is charged with 6 gmole/liter of A and 6 gmole/liter of B. A conversion of A equal to 90% is required.

The total production time includes the time to fill and drain the reactor (10 min), the time to clean the reactor (15 min), and the time to carry out the actual reaction.

It is desired to double the production of C. The fill/drain time and clean time cannot be changed. What new reactor condition do you recommend to realize the new production target?

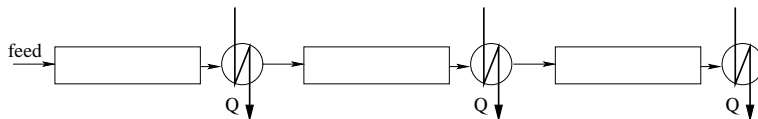


Figure 1: Plug flow reactor with temperature quenching zones.

Problem 2

Consider the following gas-phase reaction in a PFR



The rate constant has units of $\text{lbmoles}/(\text{hr}\cdot\text{ft}^3\cdot\text{atm}^2)$ and is

$$k_1 = 206000 \times \exp \frac{-27200}{RT}$$

where T is in degrees Rankine and R is in $\text{Btu}/(\text{lbmole}\cdot\text{R})$. The rate expression is

$$r_1 = k_1 \times P_A P_B$$

The feed is a 2:1 molar ratio of A to B and it enters at a feed rate of 0.51 lbmole/hr , 2 atm of pressure, and 392 °F (852 R). The heat of the exothermic reaction is

$$\Delta H_R = -85,000 \quad (\text{Btu}/\text{lbmole})$$

and the component heat capacities (A, B and C) are all

$$\tilde{C}_p = 70 \quad (\text{Btu}/\text{lbmole}\cdot\text{R})$$

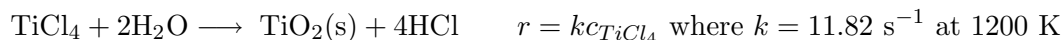
Assume ΔH_R and \tilde{C}_p are constant with temperature.

The reactor temperature must not be allowed to exceed 1,000 R and this is accomplished by operating the PFR adiabatically, quenching the reaction in a heat exchanger and then allowing it to continue in a subsequent section of the PFR. After each quenching step the temperature is 852 R. The reactor is shown schematically in Figure 1. If we assume the quenching is infinitely fast (*i.e.*, there is no reaction in the exchanger), will the conversion of B exceed the 85% production target at the end of the third adiabatic section?

Problem 3

[Adapted from M. E. Davis and R. J. Davis, Fundamentals of Chemical Reaction Engineering, McGraw Hill 2003.]

Titanium dioxide particles are produced in a gas-phase oxidation reaction of TiCl_4 vapor in a hydrocarbon flame. Assuming the reaction can be represented with



Note the product TiO_2 is a solid that gets entrained in the gas. If the reaction takes place in an isothermal PFR that operates at 1 atm, what is the reactor volume required to achieve 99% conversion of TiCl_4 . The feed enters at a total molar flowrate of 9.2 gmol/s and the feed has the following composition.

CO_2	8%
H_2O	8%
O_2	5%
TiCl_4	3%
N_2	remainder

Problem 4

The second order catalytic reaction



$$r = k \times C_A^2 \quad \text{gmoles/sec-gcat}$$

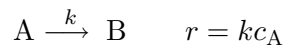
is carried out over a spherical catalyst pellet. The reactant and product are gases at the reaction conditions. A series of experiments was performed using 0.70-cm diameter catalyst beads. At 150 °C and 1 to 3 atm of pure A a plot of log rate versus log C_A was a straight line of slope 3/2. The table below lists additional information.

T (°C)	R_A (gmoles/sec-gmcat)	P_A (atm)
150	6.17×10^{-4}	1.0
200	2.37×10^{-3}	1.0

Estimate the value of W/N_{Af} required to achieve a conversion of A of 50% at 200 °C in a fixed bed reactor using the same catalyst but with a bead diameter of 1.00 cm. Pure A is fed to the reactor at a total pressure of 1 atm. Assume the diffusion coefficient is dominated by Knudsen diffusion and that it is constant.

Problem 5

A pulse input experiment was performed on a flow reactor. The effluent pulse data ($c_{\text{pulse}}(\theta)$) and the corresponding residence time distribution are tabulated below. Determine the effluent concentration of A for this reactor if $c_{Af} = 0.9$ gmole/liter and $k = 0.267 \text{ min}^{-1}$ for the following liquid-phase reaction



θ (min)	$c_{\text{pulse}}(\theta)$ ($\mu\text{mole/liter}$)	θ (min)	$c_{\text{pulse}}(\theta)$ ($\mu\text{mole/liter}$)	θ (min)	$c_{\text{pulse}}(\theta)$ ($\mu\text{mole/liter}$)
0	0.00	7	7.40	14	0.10
1	0.20	8	3.00	15	0.02
2	0.50	9	1.50	16	0.00
3	0.75	10	1.10		
4	2.10	11	0.80		
5	6.50	12	0.50		
6	8.90	13	0.20		

In general:

$$\bar{\theta} = \int_0^{\infty} \theta p(\theta) d\theta \quad \sigma^2 = \int_0^{\infty} (\theta - \bar{\theta})^2 p(\theta) d\theta$$

For segregated flow:

$$c_s(\theta) = \int_0^{\infty} p(\theta) c(\theta) d\theta$$

For CSTRs-in-series:

$$p(\theta) = \left(\frac{n}{\bar{\theta}}\right)^n \frac{\theta^{n-1}}{(n-1)!} \exp^{-n\theta/\bar{\theta}} \quad n = \frac{\bar{\theta}^2}{\sigma^2}$$

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

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

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

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)

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

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

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

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

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

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

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

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

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:

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

For heterogeneous reactions one must determine the rate per unit volume of pellet.

$$R_{jp} = \frac{1}{V_p} \int_{V_p} R_j dV = -\frac{S_p}{V_p} D_j \left. \frac{dc_j}{dr} \right|_{r=R_p}$$

The dimensionless steady-state concentration within a symmetrical pellet is found with

$$\nabla^2 \bar{c} + \left[\frac{a^2 |R_{js}|}{c_{js} D_j} \right] \bar{R} = 0 \quad \bar{R} = \frac{R_j}{R_{js}}$$

For a first-order reaction ($A \rightarrow B$) with a spherical pellet surface concentration of c_{As}

$$c_A = c_{As} \frac{R}{r} \times \frac{\sinh\left(\Phi\left(\frac{3r}{R}\right)\right)}{\sinh(3\Phi)}$$

$$R_{Ap} = \frac{1}{\Phi} \left[\frac{1}{\tanh 3\Phi} - \frac{1}{3\Phi} \right] \times (-k_1 c_{As})$$

$$\Phi = \frac{R}{3} \times \sqrt{\frac{k_1}{D_e}}$$

For some heterogeneous cases it is appropriate to use

$$\eta = \frac{R_j}{R_{js}}$$

$$\eta \approx \frac{1}{\Phi} \left[\frac{1}{\tanh 3\Phi} - \frac{1}{3\Phi} \right]$$

$$\Phi = \frac{V_p}{S_p} \left[\frac{n+1}{2} \times \frac{k_n c_s^{n-1}}{D_e} \right]^{0.5}$$

where

$$\tanh x = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$