

(f) \dot{m}_c : $1 \leq \dot{m}_c \leq 1000$ g/s

$$\left[T_0 = 350 \text{ K}, \frac{U_a}{\rho_b} = 0.5 \frac{\text{cal}}{\text{kg} \cdot \text{s} \cdot \text{K}}, T_{a0} = 320 \text{ K}, F_{A0} = 5 \text{ mol/s}, \Theta_1 = 1 \right]$$

- (g) Repeat (e) and (f) for counter current coolant flow.
 (h) Determine the conversion in a 5,000 kg fluidized CSTR where $U_a = 500$ cal/s·K with $T_a = 320$ K and $\rho_b = 2$ kg/m³
 (i) Repeat (a), (b), and (d) if the reaction were endothermic with $K_c = 0.01$ at 303 and $\Delta H_{RX} = +20$ kcal/mol.
 (n) **Example 8-12. Instructions:** If you have not installed FEMLAB 3.1 ECRE, load the FEMLAB 3.1 ECRE CD-ROM and follow the installation instructions.

Double-click on the FEMLAB 3.1 ECRE icon on your desktop. In the Model Navigator, select model denoted "4-Non-Isothermal Reactor II" and press "Documentation". This will open your web browser and display the documentation of this specific model. You can also review the detailed documentation for the whole series of models listed on the left-hand side in the web browser window. Use chapter 2 in the online documentation to answer the questions below using the model "4-Non-Isothermal Reactor II". Select the Model Navigator and press "OK" to open the model.

(1) Why is the concentration of A near the wall lower than the concentration near the center? (2) Where in the reactor do you find the maximum and minimum reaction rates? Why? *Instructions:* Click the "Plot Parameters" button and select the "Surface" tab. Type "-rA" (replace "cA") in the "Expression" edit field to plot the absolute rate of consumption of A (moles m⁻³ s⁻¹). (3) Increase the activation energy of the reaction by 5%. How do the concentration profiles change? Decrease. *Instructions:* Select the "Constants" menu item in the "Options" menu. Multiply the value of "E" in the constants list by 1.05 (just type "*1.05" behind the existing value to increase or multiply by 0.95 to decrease). Press "Apply". Press the "Restart" button in the main toolbar (equal sign with an arrow on top). (4) Change the activation energy back to the original value. *Instructions:* Remove the factor "0.95" in the constant list and press "Apply". (5) Increase the thermal conductivity, k_e , by a factor of 10 and explain how this change affects the temperature profiles. At what radial position do you find the highest conversion? *Instructions:* Multiply the value of "ke" in the constants lists by 10. Press "Apply". Press "Restart". (6) Increase the coolant flow rate by a factor of 10 and explain how this change affects the conversion. (7) In two or three sentences, describe your findings when you varied the parameters (for all parts). (8) What would be your recommendation to maximize the average outlet conversion? (9) Review Figure E8-12.2 and explain why the temperature profile goes through a maximum and why the conversion profile goes through a maximum and a minimum. (10) See other problems in the web module.

- (o) **Example R8.2-1 Runaway Reactions.** Load the *Living Example Problem* on runaway trajectories. Vary some of the parameters, such as P_0 and T_0 along with the activation energy and heat of reaction. Write a paragraph describing what you found and what generalizations you can make.



P8-3A Load the Interactive Computer Module (ICM) from the CD-ROM. Run the module, and then record your performance number for the module, which indicates your mastery of the material. Your professor has the key to determine your performance number.

(a) ICM Heat Effects Basketball 1 Performance # _____.

(b) ICM Heat Effects Simulation 2 Performance # _____.

P8-4C The following is an excerpt from *The Morning News*, Wilmington, Delaware (August 3, 1977): "Investigators sift through the debris from blast in quest of the cause [that destroyed the new nitrous oxide plant]. A company spokesman said it appears more likely that the [fatal] blast was caused by another gas, ammonium nitrate—used to produce nitrous oxide." An 83% (wt) ammonium nitrate and 17% water solution is fed at 200°F to the CSTR operated at a temperature of about 510°F. Molten ammonium nitrate decomposes directly to produce gaseous nitrous oxide and steam. It is believed that pressure fluctuations were observed in the system and as a result the molten ammonium nitrate feed to the reactor may have been shut off approximately 4 min prior to the explosion. (a) Can you explain the cause of the blast? [Hint: See Problem P9-3 and Equation (8-75).] (b) If the feed rate to the reactor just before shutoff was 310 lb of solution per hour, what was the exact temperature in the reactor just prior to shutdown? (c) How would you start up or shut down and control such a reaction? (d) What do you learn when you apply the runaway reaction criteria?

Assume that at the time the feed to the CSTR stopped, there was 500 lb of ammonium nitrate in the reactor. The conversion in the reactor is believed to be virtually complete at about 99.99%.

Additional information (approximate but close to the real case):

$$\Delta H_{Rx}^{\circ} = -336 \text{ Btu/lb ammonium nitrate at } 500^{\circ}\text{F (constant)}$$

$$C_p = 0.38 \text{ Btu/lb ammonium nitrate} \cdot ^{\circ}\text{F}$$

$$C_p = 0.47 \text{ Btu/lb of steam} \cdot ^{\circ}\text{F}$$

$$-r_A V = k C_A V = k \frac{M}{V} V = k M (\text{lb/h})$$

where M is the mass of ammonium nitrate in the CSTR (lb) and k is given by the relationship below.

$T (^{\circ}\text{F})$	510	560
$k (\text{h}^{-1})$	0.307	2.912

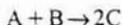
The enthalpies of water and steam are

$$H_w(200^{\circ}\text{F}) = 168 \text{ Btu/lb}$$

$$H_g(500^{\circ}\text{F}) = 1202 \text{ Btu/lb}$$

(e) Explore this problem and describe what you find. [For example, can you determine a form of $R(T)$ versus $G(T)$?] (f) Discuss what you believe to be the point of the problem. The idea for this problem originated from an article by Ben Horowitz.

P8-5_B The endothermic liquid-phase elementary reaction



proceeds, substantially, to completion in a single steam-jacketed, continuous-stirred reactor (Table P8-5). From the following data, calculate the steady-state reactor temperature:

Reactor volume: 125 gal

Steam jacket area: 10 ft²

Jacket steam: 150 psig (365.9°F saturation temperature)

Overall heat-transfer coefficient of jacket, U : 150 Btu/h · ft² · °F

Agitator shaft horsepower: 25 hp

Heat of reaction, $\Delta H_{R_x}^{\circ} = +20,000$ Btu/lb mol of A (independent of temperature)

TABLE P8-5

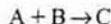
	Component		
	A	B	C
Feed (lbmol/hr)	10.0	10.0	0
Feed temperature (°F)	80	80	—
Specific heat (Btu/lb mol · °F)*	51.0	44.0	47.5
Molecular weight	128	94	222
Density (lb/ft ³)	63.0	67.2	65.0

*Independent of temperature.

(Ans: $T = 199^{\circ}\text{F}$)

(Courtesy of the California Board of Registration for Professional & Land Surveyors.)

P8-6_A The elementary irreversible organic liquid-phase reaction.



is carried out adiabatically in a flow reactor. An equal molar feed in A and B enters at 27°C, and the volumetric flow rate is 2 dm³/s and $C_{A0} = 0.1$ kmol/m³.

- Calculate the PFR and CSTR volumes necessary to achieve 85% conversion. What are the reasons for the differences?
- What is the maximum inlet temperature one could have so that the boiling point of the liquid (550 K) would not be exceeded even for complete conversion?
- Plot the conversion and temperature as a function of PFR volume (i.e., distance down the reactor).
- Calculate the conversion that can be achieved in one 500-dm³ CSTR and in two 250-dm³ CSTRs in series.
- Ask another question or suggest another calculation for this reaction.

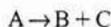
Additional information:

$$H_A^\circ(273) = -20 \text{ kcal/mol}, \quad H_B^\circ(273) = -15 \text{ kcal/mol}, \quad H_C^\circ(273) = -41 \text{ kcal/mol}$$

$$C_{p_A} = C_{p_B} = 15 \text{ cal/mol} \cdot \text{K} \quad C_{p_C} = 30 \text{ cal/mol} \cdot \text{K}$$

$$k = 0.01 \frac{\text{dm}^3}{\text{mol} \cdot \text{s}} \text{ at } 300 \text{ K} \quad E = 10,000 \text{ cal/mol}$$

- P8-7_B** Use the data and reaction in Problem 8-6 for the following exercises.
- Plot the conversion and temperature of the PFR profiles up to a reactor volume of 10 dm³ for the case when the reaction is reversible with $K_C = 10 \text{ m}^3/\text{kmol}$ at 450 K. Plot the equilibrium conversion profile.
 - Repeat (a) when a heat exchanger is added, $Ua = 20 \text{ cal/m}^3/\text{s/K}$, and the coolant temperature is constant at $T_a = 450 \text{ K}$.
 - Repeat (b) for a co-current heat exchanger for a coolant flow rate of 50 g/s and $C_{p_c} = 1 \text{ cal/g} \cdot \text{K}$, and in inlet coolant temperature of $T_{a0} = 450 \text{ K}$. Vary the coolant rate ($1 < \dot{m}_c < 1,000 \text{ g/s}$).
 - Repeat (c) for counter current coolant flow.
 - Compare your answers to (a) through (d) and describe what you find. What generalizations can you make?
 - Repeat (c) and (d) when the reaction is irreversible but endothermic with $\Delta H_{R_x} = 6,000 \text{ cal/mol}$.
 - Discuss the application of runaway criteria for the irreversible reaction occurring in a CSTR. What value of T_o would you recommend to prevent runaway if $\kappa = 3$ and $T_a = 450 \text{ K}$?
- P8-8_A** The elementary irreversible gas-phase reaction



is carried out adiabatically in a PFR packed with a catalyst. Pure A enters the reactor at a volumetric flow rate of 20 dm³/s at a pressure of 10 atm and a temperature of 450 K.

- Plot the conversion and temperature down the plug-flow reactor until an 80% conversion (if possible) is reached. (The maximum catalyst weight that can be packed into the PFR is 50 kg.) Assume that $\Delta P = 0.0$.
- What catalyst weight is necessary to achieve 80% conversion in a CSTR?
- Write a question that requires critical thinking and then explain why your question requires critical thinking. [Hint: See Preface Section B.2.]
- Now take the pressure drop into account in the PFR.

$$\frac{dP}{dW} = -\frac{\alpha}{2} \left(\frac{T}{T_0} \right) \frac{P_0}{(P/P_0)} (1 + \varepsilon X)$$

The reactor can be packed with one of two particle sizes. Choose one.

$$\alpha = 0.019/\text{kg cat. for particle diameter } D_1$$

$$\alpha = 0.0075/\text{kg cat. for particle diameter } D_2$$

Plot the temperature, conversion, and pressure along the length of the reactor. Vary the parameters α and P_0 to learn the ranges of values in which they dramatically affect the conversion.

Additional information:

$$C_{p_A} = 40 \text{ J/mol} \cdot \text{K} \quad C_{p_B} = 25 \text{ J/mol} \cdot \text{K} \quad C_{p_C} = 15 \text{ J/mol} \cdot \text{K}$$

$$H_A^\circ = -70 \text{ kJ/mol} \quad H_B^\circ = -50 \text{ kJ/mol} \quad H_C^\circ = -40 \text{ kJ/mol}$$

All heats of formation are referenced to 273 K.

$$k = 0.133 \exp \left[\frac{E}{R} \left(\frac{1}{450} - \frac{1}{T} \right) \right] \frac{\text{dm}^3}{\text{kg} \cdot \text{cat} \cdot \text{s}} \text{ with } E = 31.4 \text{ kJ/mol}$$

- P8-9_B** Use the data in Problem 8-8 for the case when heat is removed by a heat exchanger jacketing the reactor. The flow rate of coolant through the jacket is sufficiently high that the ambient exchanger temperature is constant at $T_a = 50^\circ\text{C}$.

(a) Plot the temperature and conversion profiles for a PBR with

$$\frac{Ua}{\rho_b} = 0.08 \frac{\text{J}}{\text{s} \cdot \text{kg cat} \cdot \text{K}}$$

where

ρ_b = bulk density of the catalyst (kg/m^3)

a = heat-exchange area per unit volume of reactor (m^2/m^3)

U = overall heat-transfer coefficient ($\text{J}/\text{s} \cdot \text{m}^2 \cdot \text{K}$)

How would the profiles change if Ua/ρ_b were increased by a factor of 3000?

- (b) Repeat part (a) for both co-current and counter current flow with $\dot{m}_c = 0.2 \text{ kg/s}$, $C_{p_c} = 5,000 \text{ J/kg K}$ and an entering coolant temperature of 50°C .
- (c) Find X and T for a "fluidized" CSTR [see margin] with 80 kg of catalyst.

$$UA = 500 \frac{\text{J}}{\text{s} \cdot \text{K}}, \quad \rho_b = 1 \text{ kg}/\text{m}^3$$

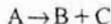
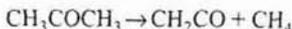
- (d) Repeat parts (a) and (b) for $W = 80.0 \text{ kg}$ assuming a reversible reaction with a reverse specific reaction rate of

$$k_r = 0.2 \exp \left[\frac{E_r}{R} \left(\frac{1}{450} - \frac{1}{T} \right) \right] \left(\frac{\text{dm}^6}{\text{kg cat} \cdot \text{mol} \cdot \text{s}} \right); \quad E_r = 51.4 \text{ kJ/mol}$$

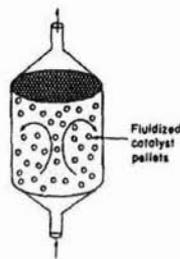
Vary the entering temperature, T_0 , and describe what you find.

- (e) Use or modify the data in this problem to suggest another question or calculation. Explain why your question requires either critical thinking or creative thinking. See Preface B.2 and B.3.

- P8-10_B** The irreversible endothermic vapor-phase reaction follows an elementary rate law



and is carried out adiabatically in a 500-dm^3 PFR. Species A is fed to the reactor at a rate of $10 \text{ mol}/\text{min}$ and a pressure of 2 atm. An inert stream is also fed



to the reactor at 2 atm, as shown in Figure P8-10. The entrance temperature of both streams is 1100 K.

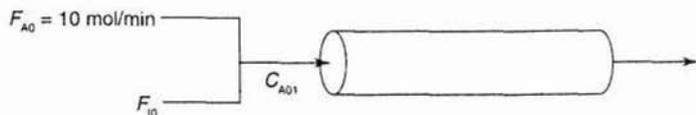


Figure P8-10 Adiabatic PFR with inerts.

- First derive an expression for C_{A01} as a function of C_{A0} and Θ_1 .
- Sketch the conversion and temperature profiles for the case when inerts are present. Using a dashed line, sketch the profiles when a moderate amount of inerts are added. Using a dotted line, sketch the profiles when a large amount of inerts are added. Sketch or plot the exit conversion as a function of Θ_1 . Qualitative sketches are fine.
- Is there a ratio of inerts to the entering molar flow rate of A (i.e., F_{I0}/F_{A0}) at which the conversion is at a maximum? Explain why "is" or "is not" a maximum.
- Repeat parts (b) and (c) for an exothermic reaction ($\Delta H_{rx} = -80$ kJ/mol).
- Repeat parts (b) and (c) for a second-order endothermic reaction.
- Repeat parts (b) and (c) for an exothermic reversible reaction ($K_c = 2$ dm³/mol at 1100 K).
- Repeat (b) through (f) when the total volumetric flow rate v_0 is held constant and the mole fractions are varied.
- Sketch or plot F_B for parts (d) through (g).

Additional information:

$$k = \exp(34.34 - 34,222/T) \text{ dm}^3/\text{mol} \cdot \text{min} \quad C_{P_i} = 200 \text{ J/mol} \cdot \text{K}$$

(T in degrees Kelvin)

$$C_{P_A} = 170 \text{ J/mol} \cdot \text{K}$$

$$C_{P_B} = 90 \text{ J/mol} \cdot \text{K}$$

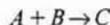
$$C_{P_C} = 80 \text{ J/mol} \cdot \text{K}$$

$$\Delta H_{rx} = 80,000 \text{ J/mol}$$

P8-11_C Derive the energy balance for a packed bed membrane reactor. Apply the balance to the reaction in Problem P8-8_B for the case when it is reversible with $K_c = 0.01$ mol/dm³ at 300 K. Species C diffuses out of the membrane.

- Plot the concentration profiles for different values of k_c when the reaction is carried out adiabatically.
- Repeat part (a) when the heat transfer coefficient is the same as that in P8-9(a). All other conditions are the same as those in Problem P8-9(a).

P8-12_B The liquid-phase reaction



follows an elementary rate law and takes place in a 1-m³ CSTR, to which the volumetric flow rate is 0.5 m³/min and the entering concentration of A is 1 mol/dm³. The reaction takes place isothermally at 300 K. For an equal molar feed of A and B, the conversion is 20%. When the reaction is carried out adiabatically, the exit temperature is 350 K and the conversion is 40%. The heat capacities of A, B, and C are 25, 35, and 60 kJ/mol · K, respectively. It is pro-



to add a second reactor of the same size downstream in series with the first CSTR. There is a heat exchanger attached to the second CSTR with $UA = 4.0 \text{ kJ/min} \cdot \text{K}$, and the coolant fluid enters and exits this reactor at virtually the same temperature the coolant feed enters 350 K .

- What is the rate of heat removal necessary for isothermal operation?
- What is the conversion exiting the second reactor?
- What would be the conversion if the second CSTR were replaced with a 1-m^3 PFR with $Ua = 10 \text{ kJ/m}^3 \cdot \text{min}$ and $T_a = 300 \text{ K}$?
- A chemist suggests that at temperatures above 380 K the reverse reaction cannot be neglected. From thermodynamics, we know that at 350 K , $K_c = 2 \text{ dm}^3/\text{mol}$. What conversion can be achieved if the entering temperature to the PFR in part (b) is 350 K ?
- Write an in-depth question that extends this problem and involves critical thinking, and explain why it involves critical thinking.
- Repeat part (c) assuming the reaction takes place entirely in the gas phase (same constants for reaction) with $C_{T0} = 0.2 \text{ mol/dm}^3$.

P8-13_A The reaction



is carried out adiabatically in a series of staged packed-bed reactors with interstage cooling. The lowest temperature to which the reactant stream may be cooled is 27°C . The feed is equal molar in A and B and the catalyst weight in each reactor is sufficient to achieve 99.9% of the equilibrium conversion. The feed enters at 27°C and the reaction is carried out adiabatically. If four reactors and three coolers are available, what conversion may be achieved?

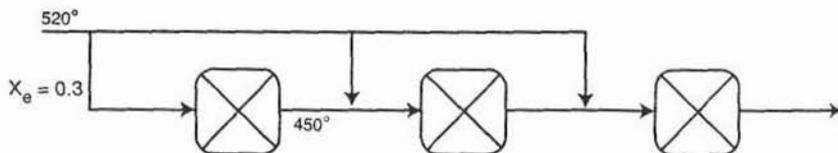
Additional information:

$$\Delta H_{R_{xx}} = -30,000 \text{ cal/mol A} \quad C_{P_A} = C_{P_B} = C_{P_C} = C_{P_D} = 25 \text{ cal/g mol} \cdot \text{K}$$

$$K_e(50^\circ\text{C}) = 500,000 \quad F_{A0} = 10 \text{ mol A/min}$$

First prepare a plot of equilibrium conversion as a function of temperature. [Partial ans.: $T = 360 \text{ K}$, $X_e = 0.984$; $T = 520 \text{ K}$, $X_e = 0.09$; $T = 540 \text{ K}$, $X_e = 0.057$]

P8-14_A Figure 8-8 shows the temperature-conversion trajectory for a train of reactors with interstage heating. Now consider replacing the interstage heating with injection of the feed stream in three equal portions as shown here:

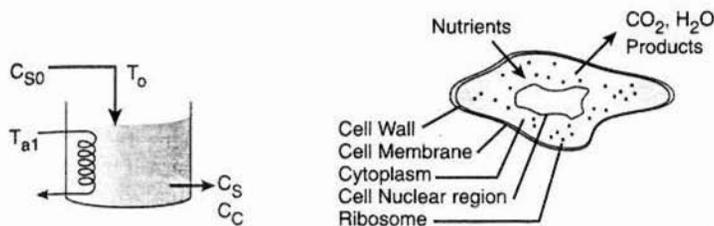


Sketch the temperature-conversion trajectories for (a) an endothermic reaction with entering temperatures as shown, and (b) an exothermic reaction with the temperatures to and from the first reactor reversed, i.e., $T_0 = 450^\circ\text{C}$.

P8-15 The biomass reaction



is carried out in a 6 dm^3 chemostat with a heat exchanger.



The volumetric flow rate is $1 \text{ dm}^3/\text{h}$, the entering substrate concentration and temperature are 100 g/dm^3 and 280 K , respectively. The temperature dependence of the growth rate follows that given by Aibe et al., Equation (7-63)

$$r_g = \mu C_C$$

and

$$-r_S = r_g / Y_{CS}$$

$$\mu(T) = \mu(310 \text{ K}) \Gamma = \mu_{1\max} \left[\frac{0.0038 \cdot T \cdot \exp[21.6 - 6700/T]}{1 + \exp[153 - 48000/T]} \right] \frac{C_S}{K_m + C_S} \quad (\text{P8-16.1})$$

- Plot $G(T)$ and $R(T)$ for both adiabatic and non-adiabatic operation assuming a very large coolant rate (i.e., $\dot{Q} = UA(T_a - T)$ with $A = 1.1 \text{ m}^2$ and $T_a = 290 \text{ K}$).
- What is the heat exchanger area that should be used to maximize the exiting cell concentration for an entering temperature of 288 K ? Cooling water is available at 290 K and up to a maximum flow rate of 1 kg/minute .
- Identify any multiple steady states and discuss them in light of what you learned in this chapter. *Hint:* Plot T_s vs. T_0 from Part (a).
- Vary T_0 , \dot{m}_c , and T_a and describe what you find.

Additional Information:

$$Y_{CS} = 0.8 \text{ g cell/g substrate}$$

$$K_S = 5.0 \text{ g/dm}^3$$

$$\mu_{1\max} = 0.5 \text{ h}^{-1} \text{ (note } \mu = \mu_{\max} \text{ at } 310 \text{ K)}$$

$$C_{P_S} = \text{Heat capacity of substrate solution including all cells} = 74 \text{ J/g/K}$$

$$m_s = \text{Mass of substrate solution in chemostat} = 6.0 \text{ kg}$$

$$\Delta H_{\text{Rx}} = -20,000 \text{ J/g cells}$$

$$U = 50,000 \text{ J/h/Km}^2$$

$$C_{P_c} = \text{Heat capacity of cooling water } 74 \text{ J/g/K}$$

$$\dot{m}_c = \text{coolant flow rate (up to } 60,000 \text{ kg/h)}$$

$$\rho_S = \text{solution density} = 1 \text{ kg/dm}^3$$

$$\dot{Q} = \dot{m}_c \dot{C}_{P_c} [T - T_a] \left[1 - e^{-\frac{UA}{\dot{m}_c \dot{C}_{P_c}}} \right]$$

P8-16_B The first-order irreversible exothermic liquid-phase reaction

is to be carried out in a jacketed CSTR. Species A and an inert I are fed to the reactor in equimolar amounts. The molar feed rate of A is 80 mol/min.

- What is the reactor temperature for a feed temperature of 450 K?
- Plot the reactor temperature as a function of the feed temperature.
- To what inlet temperature must the fluid be preheated for the reactor to operate at a high conversion? What are the corresponding temperature and conversion of the fluid in the CSTR at this inlet temperature?
- Suppose that the fluid is now heated 5°C above the temperature in part (c) and then cooled 20°C, where it remains. What will be the conversion?
- What is the inlet extinction temperature for this reaction system? (Ans.: $T_0 = 87^\circ\text{C}$.)

Additional information:

Heat capacity of the inert: 30 cal/g mol·°C $\tau = 100$ min

Heat capacity of A and B: 20 cal/g mol·°C $\Delta H_{\text{Rx}} = -7500$ cal/mol

UA : 8000 cal/min·°C $k = 6.6 \times 10^{-3} \text{ min}^{-1}$ at 350 K

Ambient temperature, T_a : 300 K $E = 40,000$ cal/mol·K

P8-17_C The zero-order exothermic liquid-phase reaction

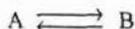
is carried out at 85°C in a jacketed 0.2-m³ CSTR. The coolant temperature in the reactor is 32°F. The heat-transfer coefficient is 120 W/m²·K. Determine the critical value of the heat-transfer area below which the reactor will run away and explode [*Chem. Eng.*, 91(10), 54 (1984)].

Additional information:

$$k = 1.127 \text{ kmol/m}^3 \cdot \text{min at } 40^\circ\text{C}$$

$$k = 1.421 \text{ kmol/m}^3 \cdot \text{min at } 50^\circ\text{C}$$

The heat capacity of the solution is 4 J/°C/g. The solution density is 0.90 kg/dm³. The heat of reaction is -500 J/g. The feed temperature is 40°C and the feed rate is 90 kg/min. MW of A = 90 g/mol.

P8-18_B The elementary reversible liquid-phase reaction

takes place in a CSTR with a heat exchanger. Pure A enters the reactor.

- Derive an expression (or set of expressions) to calculate $G(T)$ as a function of heat of reaction, equilibrium constant, temperature, and so on. Show a sample calculation for $G(T)$ at $T = 400$ K.
- What are the steady-state temperatures? (Ans.: 310, 377, 418 K.)
- Which steady states are locally stable?
- What is the conversion corresponding to the upper steady state?
- Vary the ambient temperature T_a and make a plot of the reactor temperature as a function of T_a , identifying the ignition and extinction temperatures.

- (f) If the heat exchanger in the reactor suddenly fails (i.e., $UA = 0$), what would be the conversion and the reactor temperature when the new steady state is reached? (*Ans.*: 431 K)
- (g) What heat exchanger product, UA , will give the maximum conversion?
- (h) Write a question that requires critical thinking and then explain why that question requires critical thinking. [*Hint*: See Preface Section B.2.]
- (i) What is the adiabatic blowout flow rate, v_0 ?
- (j) Suppose that you want to operate at the lower steady state. What parameter values would you suggest to prevent runaway?

Additional information:

$$UA = 3600 \text{ cal/min} \cdot \text{K} \quad E/R = 20,000 \text{ K}$$

$$C_{pA} = C_{pB} = 40 \text{ cal/mol} \cdot \text{K} \quad V = 10 \text{ dm}^3$$

$$\Delta H_{Rx} = -80,000 \text{ cal/mol A} \quad v_0 = 1 \text{ dm}^3/\text{min}$$

$$K_{eq} = 100 \text{ at } 400 \text{ K} \quad F_{A0} = 10 \text{ mol/min}$$

$$k = 1 \text{ min}^{-1} \text{ at } 400 \text{ K}$$

$$\text{Ambient temperature, } T_a = 37^\circ\text{C} \quad \text{Feed temperature, } T_0 = 37^\circ\text{C}$$

P8-19c The first-order irreversible liquid-phase reaction



is to be carried out in a jacketed CSTR. Pure A is fed to the reactor at a rate of 0.5 g mol/min. The heat-generation curve for this reaction and reactor system

$$G(T) = \frac{-\Delta H_{Rx}^0}{1 + 1/(\tau k)}$$

is shown in Figure P8-19.

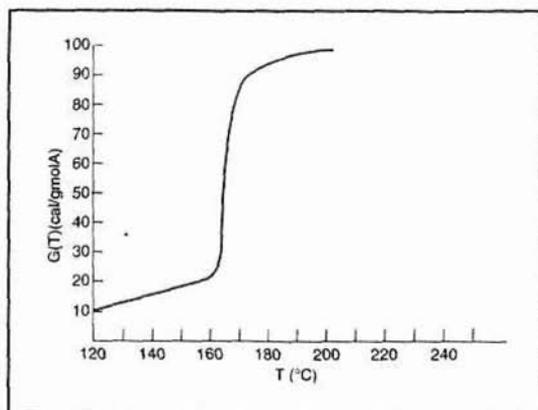
- (a) To what inlet temperature must the fluid be preheated for the reactor to operate at a high conversion? (*Ans.*: $T_0 \geq 214^\circ\text{C}$.)
- (b) What is the corresponding temperature of the fluid in the CSTR at that inlet temperature? (*Ans.*: $T_s = 164^\circ\text{C}$, 184°C .)
- (c) Suppose that the fluid is now heated 5°C above the temperature in part (b) and then cooled 10°C , where it remains. What will be the conversion? (*Ans.*: $X = 0.9$.)
- (d) What is the extinction temperature for this reaction system? (*Ans.*: $T_0 = 200^\circ\text{C}$.)
- (e) Write a question that requires critical thinking and then explain why that question requires critical thinking. [*Hint*: See Preface Section B.2.]

Additional information:

Heat of reaction (constant): -100 cal/g mol A

Heat capacity of A and B: $2 \text{ cal/g mol} \cdot ^\circ\text{C}$

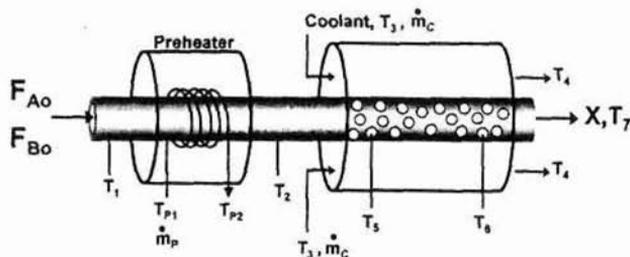
UA : $1 \text{ cal/min} \cdot ^\circ\text{C}$, Ambient temperature, T_a : 100°C

Figure P8-19 $G(T)$ curve.

P8-20_c Troubleshooting. The following reactor system is used to carry out the reversible catalytic reaction



The feed is equal molar in A and B at a temperature T_1 of 300 K.



Troubleshoot the reaction system to deduce the problems for an exothermic and an endothermic reaction. Next, suggest measures to correct the problem. You can change \dot{m}_p , \dot{m}_c , and F_{A0} along with T_2 and T_3 .

Troubleshoot what temperatures are normal and what are different and what the distinction is. Explain your reasoning in each of the cases below.

(a) Exothermic reaction. The expected conversion and the exit temperature are $X = 0.75$ and $T = 400$ K. Unfortunately, here is what was found in six different cases.

Case 1 at the exit $X = 0.01$, $T_7 = 305$ K

Case 2 at the exit $X = 0.10$, $T_7 = 550$ K

Case 3 at the exit $X = 0.20$, $T_7 = 350$ K

Case 4 at the exit $X = 0.5$, $T_7 = 450$ K

Case 5 at the exit $X = 0.01$, $T_7 = 400$ K

Case 6 at the exit $X = 0.3$, $T_7 = 500$ K

- (b) Endothermic reaction. The expected conversion and the exit temperature are $X = 0.75$ and $T_7 = 350$ K. Here is what was found.

Case 1 at the exit $X = 0.4$, $T_7 = 320$ K

Case 2 at the exit $X = 0.02$, $T_7 = 349$ K

Case 3 at the exit $X = 0.002$, $T_7 = 298$ K

Case 4 at the exit $X = 0.2$, $T_7 = 350$ K



P8-21

If you have not installed FEMLAB 3.1 ECRE, load the FEMLAB 3.1 CD-ROM and follow the installation instructions.

- (a) Before running the program, sketch the radial temperature profile down a PFR for (1) an exothermic reaction for a PFR with a cooling jacket and (2) an endothermic reaction for a PFR with a heating jacket.
- (b) Run the FEMLAB 3.1 ECRE program and compare with your results in (a). Double-click on the FEMLAB 3.1 ECRE icon on your desktop. In the Model Navigator, select the model denoted "3-Non-Isothermal I" and press OK. You can use this model to compare your results in (1) and (2) above. You can select "Documentation" in the "Help" menu in order to review the instructions for this model and other models in FEMLAB ECRE.

Change the velocity profile from laminar parabolic to plug flow. Select "Scalar Expressions" in the "Expression" menu item in the "Options" menu. Change the expression for u_z (the velocity) to " u_0 " (replace the expression " $2 \cdot u_0 \cdot (1 - (r/R_a)^2)$ ", which describes the parabolic velocity profile). Press "Apply".

You can now continue to vary the input data and change the exothermic reaction to an endothermic one. (Hint: Select the "Constants" menu item in the "Options" menu. Do not forget " T_{a0} " the jacket temperature at the end of the list). Write a paragraph describing your findings.

- (c) The thermal conductivity in the reactor, denoted "ke" in Figure E8-12.1, is the molecular thermal conductivity for the solution. In a plug flow reactor, the flow is turbulent. In such a reactor, the apparent thermal conductivity is substantially larger than the molecular thermal conductivity of the fluid. Vary the value of the thermal conductivity "ke" to learn its influence on the temperature and concentration profile in the reactor.
- (d) In turbulent flow, the apparent diffusivity is substantially larger than the molecular diffusivity. Increase the molecular diffusivity in the PFR to reflect turbulent conditions and study the influence on the temperature and concentration profiles. Here you can go to the extremes. Find something interesting to turn in to your instructor. See other problems in the web module.
- (e) See other problems in the web module.

P8-22_c A reaction is to be carried out in the packed-bed reactor shown in Figure P8-22.

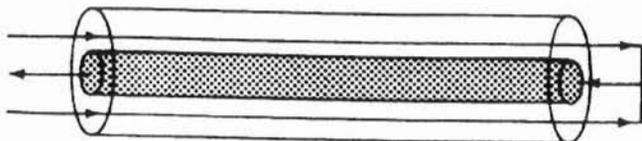
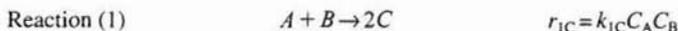


Figure P8-22

The reactants enter in the annular space between an outer insulated tube and an inner tube containing the catalyst. No reaction takes place in the annular region. Heat transfer between the gas in this packed-bed reactor and the gas flowing counter currently in the annular space occurs along the length of the reactor. The overall heat-transfer coefficient is $5 \text{ W/m}^2 \cdot \text{K}$. Plot the conversion and temperature as a function of reactor length for the data given in

- (a) Problem P8-6.
 (b) Problem P8-9(d).

P8-23_B The irreversible liquid-phase reactions



are carried out in a PFR with heat exchange. The following temperature profile was obtained for the reaction and the coolant stream.

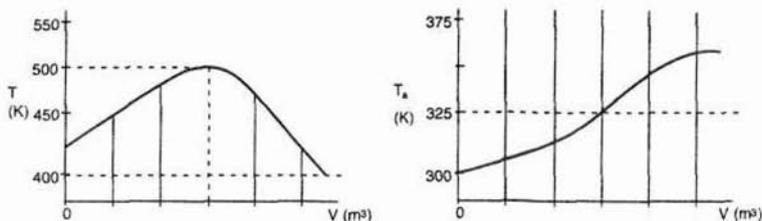


Figure P8-23

The concentrations of A, B, C, and D were measured at the point down the reactor where the liquid temperature, T , reached a maximum, and they were found to be $C_A = 0.1$, $C_B = 0.2$, $C_C = 0.5$, and $C_D = 1.5$ all in mol/dm^3 . The product of the overall heat-transfer coefficient and the heat-exchanger area per unit volume, Ua , is $10 \text{ cal/s} \cdot \text{dm}^3 \cdot \text{K}$. The feed is equal molar in A and B, and the entering molar flow rate of A is 10 mol/s . What is the activation energy for Reaction (1)? $E = ? \text{ cal/mol}$.

Additional Information

$$C_{p_A} = C_{p_B} = C_{p_C} = 30 \text{ cal/mol/K}$$

$$C_{p_D} = 90 \text{ cal/mol/K}, \quad C_{p_1} = 100 \text{ cal/mol/K}$$

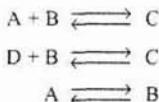
$$\Delta H_{R_{x1A}} = +50,000 \text{ cal/molA}$$

$$k_{1C} = 0.043 \frac{\text{dm}^3}{\text{mol} \cdot \text{s}} \text{ at } 400 \text{ K}$$

$$\Delta H_{R_{x2B}} = +5000 \text{ cal/molB}$$

$$k_{2D} = 0.4 \frac{\text{dm}^3}{\text{mol} \cdot \text{s}} e^{5000 \text{ K} \left[\frac{1}{500} - \frac{1}{T} \right]}$$

- P8-24** (*Comprehensive Term Problem*) T-Amyl Methyl Ether (TAME) is an oxygenated additive for green gasolines. Besides its use as an octane enhancer, it improves the combustion of gasoline and reduces the CO and HC (and, to a smaller extent, the NO_x) automobile exhaust emissions. Due to the environmental concerns related to those emissions, this and other ethers (MTBE, ETBE, TAEE) have been lately studied intensively. TAME is currently catalytically produced in the liquid phase by the reaction of methanol (MeOH) and isoamylenes 2-methyl-1-butene (2M1B) and 2-methyl-2-butene (2M2B). There are three simultaneous equilibrium reactions in the formation and splitting of TAME (the two etherification reactions and the isomerization between isoamylenes):



These reactions are to be carried out in a plug-flow reactor and a membrane reactor in which MeOH is fed uniformly through the sides. For isothermal operation:

- (a) Plot the concentration profiles for a 10-m^3 PFR.
 (b) Vary the entering temperature, T_0 , and plot the exit concentrations as a function of T_0 .

For a reactor with heat exchange ($U = 10 \text{ J} \cdot \text{m}^{-2} \cdot \text{s}^{-1} \text{ K}^{-1}$):

- (c) Plot the temperature and concentration profiles for an entering temperature of 353 K.
 (d) Repeat (a) through (c) for a membrane reactor.

Additional information:

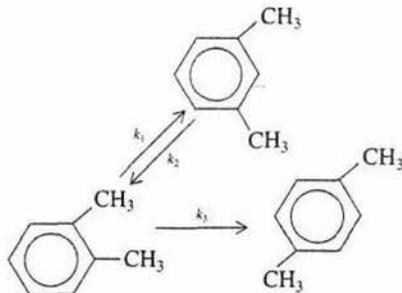
The data for this problem is found at the end of the Additional Homework Problems for Chapter 8 on the CD-ROM and on the web. [Problem by M. M. Vilarenho Ferreira, J. M. Loureiro, and D. R. Frias, University of Porto, Portugal.]



Homework Problems

- P8-25_C** (*Multiple reactions with heat effects*) Xylene has three major isomers: *m*-xylene, *o*-xylene, and *p*-xylene. When *o*-xylene is passed over a Crystalline catalyst, the following elementary reactions are observed:

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for Problem
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The feed to the reactor is equal molar in both *m*-xylene and *o*-xylene (species A and B). For a total feed rate of 2 mol/min and the reaction conditions

below, plot the temperature and the molar flow rates of each species as a function of catalyst weight up to a weight of 100 kg.

- Find the lowest concentration of *o*-xylene achieved in the reactor.
- Find the highest concentration of *m*-xylene achieved in the reactor.
- Find the maximum concentration of *o*-xylene in the reactor.
- Repeat parts (a) to (c) for a pure feed of *o*-xylene.
- Vary some of the system parameters and describe what you learn.
- What do you believe to be the point of this problem?

*Additional information:*¹¹

All heat capacities are virtually the same at 100 J/mol·K.

$$C_{T0} = 2 \text{ mol/dm}^3$$

$$\Delta H_{R_{X10}} = -1800 \text{ J/mol } o\text{-xylene}^{11}$$

$$\Delta H_{R_{X30}} = -1100 \text{ J/mol } o\text{-xylene}$$

$$k_1 = 0.5 \exp[2(1 - 320/T)] \text{ dm}^3/\text{kg cat} \cdot \text{min}$$

$$k_2 = k_1/K_C$$

$$k_3 = 0.005 \exp\{[4.6(1 - (460/T))]\} \text{ dm}^3/\text{kg cat} \cdot \text{min}$$

$$K_C = 10 \exp[4.8(430/T - 1.5)]$$

$$T_0 = 330 \text{ K}$$

$$T_a = 500 \text{ K}$$

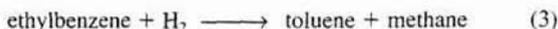
$$Ua/\rho_b = 16 \text{ J/kg cat} \cdot \text{min} \cdot ^\circ\text{C}$$

$$W = 100 \text{ kg}$$

P8-26_C (*Comprehensive Problem on multiple reactions with heat effects*) Styrene can be produced from ethylbenzene by the following reaction:



However, several irreversible side reactions also occur:



[J. Snyder and B. Subramaniam, *Chem. Eng. Sci.*, 49, 5585 (1994)]. Ethylbenzene is fed at a rate of 0.00344 kmol/s to a 10.0-m³ PFR (PBR) along with inert steam at a total pressure of 2.4 atm. The steam/ethylbenzene molar ratio is initially [i.e., parts (a) to (c)] 14.5:1 but can be varied. Given the following data, find the exiting molar flow rates of styrene, benzene, and toluene along with $\dot{S}_{S/BT}$ for the following inlet temperatures when the reactor is operated adiabatically.

- $T_0 = 800 \text{ K}$
- $T_0 = 930 \text{ K}$
- $T_0 = 1100 \text{ K}$



¹¹ Obtained from inviscid pericosity measurements.

- (d) Find the ideal inlet temperature for the production of styrene for a steam/ethylbenzene ratio of 58:1. (*Hint*: Plot the molar flow rate of styrene versus T_0 . Explain why your curve looks the way it does.)
- (e) Find the ideal steam/ethylbenzene ratio for the production of styrene at 900 K. [*Hint*: See part (d).]
- (f) It is proposed to add a counter current heat exchanger with $Ua = 100 \text{ kJ/min/K}$ where T_o is virtually constant at 1000 K. For an entering stream to ethylbenzene ratio of 2, what would you suggest as an entering temperature? Plot the molar flow rates and $\dot{S}_{St/BT}$.
- (g) What do you believe to be the points of this problem?
- (h) Ask another question or suggest another calculation that can be made for this problem.

Additional information:

Heat capacities

Methane	68 J/mol·K	Styrene	273 J/mol·K
Ethylene	90 J/mol·K	Ethylbenzene	299 J/mol·K
Benzene	201 J/mol·K	Hydrogen	30 J/mol·K
Toluene	249 J/mol·K	Steam	40 J/mol·K

$$\rho = 2137 \text{ kg/m}^3 \text{ of pellet}$$

$$\phi = 0.4$$

$$\Delta H_{R_{x1EB}} = 118,000 \text{ kJ/kmol ethylbenzene}$$

$$\Delta H_{R_{x2EB}} = 105,200 \text{ kJ/kmol ethylbenzene}$$

$$\Delta H_{R_{x3EB}} = -53,900 \text{ kJ/kmol ethylbenzene}$$

$$K_{p1} = \exp \left\{ b_1 + \frac{b_2}{T} + b_3 \ln(T) + [(b_4 T + b_5) T + b_6] T \right\} \text{ atm}$$

$$b_1 = -17.34 \qquad b_4 = -2.314 \times 10^{-10}$$

$$b_2 = -1.302 \times 10^4 \qquad b_5 = 1.302 \times 10^{-6}$$

$$b_3 = 5.051 \qquad b_6 = -4.931 \times 10^{-3}$$

The kinetic rate laws for the formation of styrene (St), benzene (B), and toluene (T), respectively, are as follows. (EB = ethylbenzene)

$$r_{1St} = \rho(1 - \phi) \exp \left(-0.08539 - \frac{10,925}{T} \right) \left(P_{EB} - \frac{P_{St} P_{H_2}}{K_{p1}} \right) \quad (\text{kmol/m}^3 \cdot \text{s})$$

$$r_{2B} = \rho(1 - \phi) \exp \left(13.2392 - \frac{25,000}{T} \right) (P_{EB}) \quad (\text{kmol/m}^3 \cdot \text{s})$$

$$r_{3T} = \rho(1 - \phi) \exp \left(0.2961 - \frac{11,000}{T} \right) (P_{EB} P_{H_2}) \quad (\text{kmol/m}^3 \cdot \text{s})$$

The temperature T is in kelvin.

- P8-27_B** Compare the profiles in Figure E8-3.1, E8-4.1, E8-5.1, E8-5.3, E8-5.4, 8-10, E8-10.1, and E8-10.2.
- If you were to classify the profiles into groups, what would they be? What are the common characteristics of each group?
 - What are the similarities and differences in the profiles in the various groups and in the various figures?
 - Describe why Figure E8-5.3 and Figure E8-3.1 look the way they do. What are the similarities and differences? Describe qualitatively how they would change if inerts were added.
 - Repeat (c) for Figure E8-10.1 and for Figure E8-10.2.

TAME



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• **CD-ROM Complete Data Set**

P8-24_C The TAME data set is given on the CD-ROM. This problem is a very comprehensive problem; perhaps can be used as a term (semester) problem.

• **Good Alternative Problems on CD-ROM Similar to Above Problems**

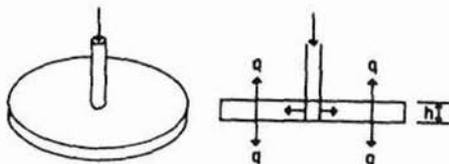
P8-28_B Industrial data for the reaction



are given. You are asked to make PFR calculations similar to those in Problems P8-6_B to P8-9_B. [3rd Ed. P8-9_B]

P8-29_B Reactor staging with interstage cooling. Similar to P8-13_B, but shorter because X_c versus T is given. [3rd Ed. P8-15_B]

P8-30_B Use the data in Problems P8-6 and P8-8 to carry out reactions in a radial flow reactor. [3rd Ed. P8-18_A]



P8-31_B The reactions



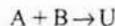
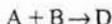
are carried out in a CSTR with a heat exchanger. [3rd Ed. P8-28_J]

P8-32_B Elementary irreversible reaction



is carried out in a PFR with heat exchange and pressure drop. [3rd Ed., P8-12]

P8-33_B Liquid-phase reactions



in a CSTR. Maximize D . [3rd Ed. P8-31]