

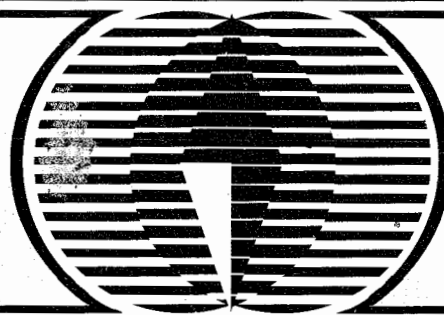


Brian Vicente / Max Nori / H. Scott Fogler

Solutions Manual for Elements of Chemical Reaction Engineering

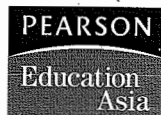
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$$\text{mole balance: } \frac{dC_A}{dt} = -kC_A \Rightarrow -k \int_0^t dt = \int_{C_{Ao}}^{C_A} \frac{dC_A}{C_A}$$

$$-kt = \ln\left(\frac{C_A}{C_{Ao}}\right), \text{ knowing } C_A = 0.01 C_{Ao} \text{ and our rate constant } (k = 0.1 \text{ min}^{-1}), \text{ we can solve}$$

$$\text{for the time of the reaction: } t = -\frac{1}{k} \ln(0.01) = \frac{4.61}{0.1 \text{ min}^{-1}} = 46.1 \text{ min}$$

CDP1-A (c)

Time for 2nd order reaction to consume 80% of A and final pressure (P) at $T = 127^\circ\text{C}$.

$$\text{rate law: } -r_A = kC_A^2$$

$$\text{mole balance: } \therefore \frac{dC_A}{dt} = -kC_A^2 \Rightarrow -k \int_0^t dt = \int_{C_{Ao}}^{C_A} \frac{dC_A}{C_A^2} \Rightarrow -kt = -\frac{1}{C_A} + \frac{1}{C_{Ao}}$$

We can solve for the time in terms of our rate constant ($k = 0.7$) and our initial

$$\text{concentration } (C_{Ao}): \quad -kt = -\frac{5}{C_{Ao}} + \frac{1}{C_{Ao}}$$

$$t = \frac{4}{kC_{Ao}} = \frac{4}{(0.7 \text{ dm}^3 / \text{mol min})(0.37 \text{ mol} / \text{dm}^3)} = 15.4 \text{ min. To determine}$$

the pressure of the reactor following this reaction, we will again use the ideal gas law.

First, we determine the number of moles in the reactor:

$$N_T = N_I + N_A + N_B + N_C = 0.25N_{To} + 0.2N_{Ao} + N_B + N_C$$

$$N_B = N_C = 0.8N_{Ao}$$

$$N_T = (0.25)N_{To} + (0.2 + 0.8 + 0.8)N_{Ao} = 0.25(97.6) + (1.8)(73.2) = 156.1 \text{ moles}$$

$$P = \frac{N_T RT}{V} = \frac{(156.1 \text{ mole}) \left(0.082 \frac{\text{dm}^3 \text{ atm}}{\text{mol K}} \right) (500 \text{ K})}{200 \text{ dm}^3} = 32 \text{ atm}$$

CDP1-B

Given: Liquid phase reaction in a foam reactor, $A \rightarrow B$

Consider a differential element, ΔV of the reactor:

By material balance

$$F_A - (F_A + \Delta F_A) = -r_A(1-e)\Delta V$$

PFR

Length of one segment = 23 ft

Length of entire reactor = (23 ft)(12)(11) = 3036 ft

D = 1 ft

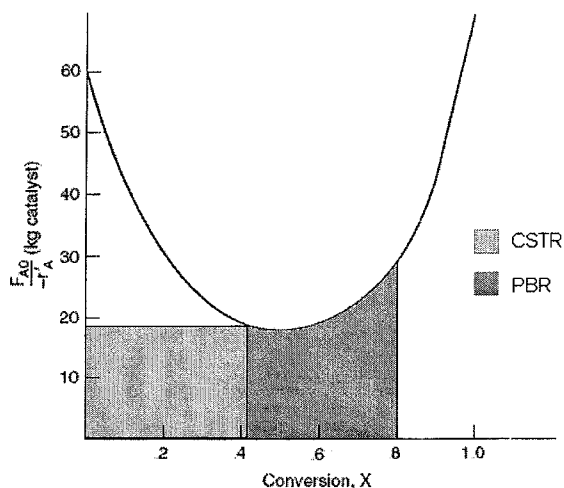
$V = \pi r^2 h = \pi (0.5 \text{ ft})^2 (3036 \text{ ft}) = 2384 \text{ ft}^3 = 67,507 \text{ L}$

Answers will vary slightly for each individual.

P2-11 No solution necessary.

P2-12 (a)

The smallest amount of catalyst necessary to achieve 80 % conversion in a CSTR and PBR connected in series and containing equal amounts of catalyst can be calculated from the figure below.



The lightly shaded area on the left denotes the CSTR while the darker shaded area denotes the PBR. This figure shows that the smallest amount of catalyst is used when the CSTR is upstream of the PBR. See Polymath program P2-12.pol.

P2-12 (b)

Calculate the necessary amount of catalyst to reach 80 % conversion using a single CSTR by determining the area of the shaded region in the figure below.

Assume isothermal and constant pressure. Neglect the vapor pressure of $\text{Si}(s)$

$$\theta_B = 1 \text{ Stoichiometric feed}$$

δ only involves the changes in gas phase

$$\varepsilon = y_{AO} \delta = \frac{1}{2} \left(\frac{1}{3} + \frac{7}{3} - 1 - 1 \right)$$

$$\varepsilon = \frac{1}{2} \left(\frac{2}{3} \right) = \frac{1}{3}$$

$$C_{AO} = y_{AO} \frac{P_0}{R T_0} = \frac{1}{2} \left(\frac{2.0}{(0.0821)(1327)} \right) \quad C_{AO} = 0.0088 \text{ mol/dm}^3$$

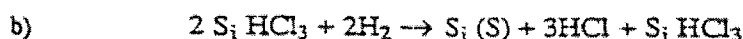
$$C_A = \frac{F_A}{v} = C_{AO} \frac{(1-X)}{(1+\varepsilon X)} = \frac{0.0088(1-X)}{1+X/3}$$

$$C_B = \frac{F_B}{v} = C_A \frac{(\theta_B - X)}{(1+\varepsilon X)} = \frac{0.0088(1-X)}{1+X/3}$$

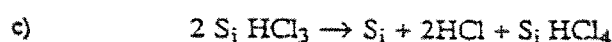
$$C_C = \frac{F_C}{v} = \frac{7}{3} \frac{F_{AO} X}{v_0(1+\varepsilon X)} = \frac{7}{3} C_{AO} \frac{X}{(1+\varepsilon X)} = 0.021 \frac{X}{(1+X/3)}$$

$$C_D = \frac{F_D}{v} = \frac{1}{3} \frac{F_{AO} X}{v_0(1+\varepsilon X)} = 0.0031 \frac{X}{1+X/3}$$

The solution to parts (b) and (c)



and



are similar to Part (a).

CDP3-H



$$T = 75^\circ\text{C} = 348 \text{ K}$$

$$P = 950 \text{ kPa} = 9.39 \text{ atm}$$

$$\text{Cl}_4 \text{ vapor pressure} = 95 \text{ kPa} = 0.94 \text{ atm} = P_v$$

- (d) By varying one parameter at a time we can see the effect of each:

Increasing the specific reaction rate causes changes in conversion, concentration, and molar flow rate to occur more quickly.

Lowering the transport coefficient (k_c) causes an increase in both C_B and F_B , which causes a decrease in conversion.

By raising the equilibrium constant (K_e), we cause a decrease in the molar flow rate of A and an increase in conversion.

- (e) A significant increase in temperature for an exothermic reaction would drive the reaction in the reverse. This would cause a decrease in X and C_B and an increase in the C_A .

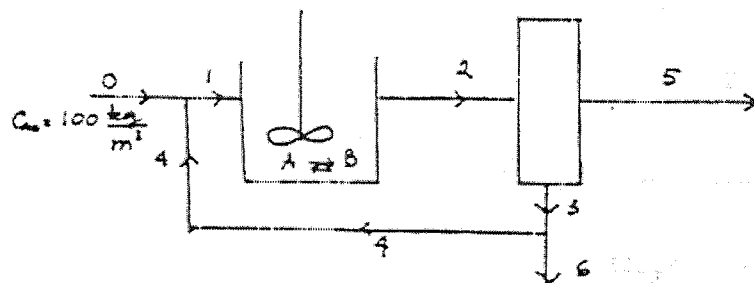
A significant decrease in temperature for an exothermic reaction would cause increase in the rate of the forward reaction. This would drive up X and C_B , while lowering C_A .

An increase in temperature would drive an endothermic reaction forward, raising X and C_B , while lowering C_A .

A decrease in temperature would cause an increase in the reverse reaction for an endothermic reaction. This would raise C_A , and lower both X and C_B .

CDP4-M No solution

CDP4-N



$$A_3 = \frac{.25}{\exp\left(\frac{-30000}{1.98(300)}\right)} = 1.798e21$$

Now we use a mole balance on species A

$$V = \frac{F_{A0} - F_A}{-r_A}$$

$$V = \frac{v(C_{A0} - C_A)}{-r_A}$$

$$\tau = \frac{C_{A0} - C_A}{-r_A} = \frac{C_{A0} - C_A}{k_1 C_A^{0.5} + k_2 C_A + k_3 C_A^2}$$

A mole balance on the other species gives us:

$$F_i = vC_i = r_i V$$

$$C_i = \tau r_i$$

Using these equations we can make a Polymath program and by varying the temperature, we can find a maximum value for C_B at $T = 306$ K. At this temperature the selectivity is only 5.9. This may result in too much of X and Y, but we know that the optimal temperature is not above 306 K. The optimal temperature will depend on the price of B and the cost of removing X and Y, but without actual data, we can only state for certain that the optimal temperature will be equal to or less than 306 K.

See Polymath program P6-6-f.pol.

POLYMATH Results

NLE Solution

| Variable | Value | f(x) | Ini Guess |
|----------|-----------|-----------|-----------|
| Ca | 0.0170239 | 3.663E-10 | 0.05 |
| T | 306 | | |
| R | 1.987 | | |
| k1 | 0.0077215 | | |
| k2 | 0.4168076 | | |
| Cao | 0.1 | | |
| Cb | 0.070957 | | |
| k3 | 0.6707505 | | |
| tau | 10 | | |
| Cx | 0.0100747 | | |
| Cy | 0.0019439 | | |
| Sbxy | 5.9039386 | | |

NLE Report (safenewt)

Nonlinear equations

[1] $f(Ca) = (Cao - Ca) / (k_1 Ca^{0.5} + k_2 Ca + k_3 Ca^2) - 10 = 0$

Explicit equations

[1] $T = 306$

[2] $R = 1.987$

[3] $k_1 = 1.49e12 \cdot \exp(-20000/R/T)$

[4] $k_2 = 5790000 \cdot \exp(-10000/R/T)$

[5] $Cao = .1$

Equations:

$$d(cm)/d(t) = rm$$

$$d(ch)/d(t) = rh$$

$$d(cx)/d(t) = rx$$

$$d(cme)/d(t) = rme$$

$$d(ct)/d(t) = rt$$

$$d(cb)/d(t) = rb$$

$$rm = -55.2 * cm * ch^{.5}$$

$$rb = 11.2 * ct * ch^{.5}$$

$$rx = -rm - 30.2 * cx * ch^{.5}$$

$$rt = 30.2 * cx * ch^{.5} - rb$$

$$rh = rm - 30.2 * cx * ch^{.5} - rb$$

$$rme = -rm + 30.2 * cx * ch^{.5} + rb$$

$$t_0 = 0, \quad t_f = 0.51$$

Initial value

0.0105

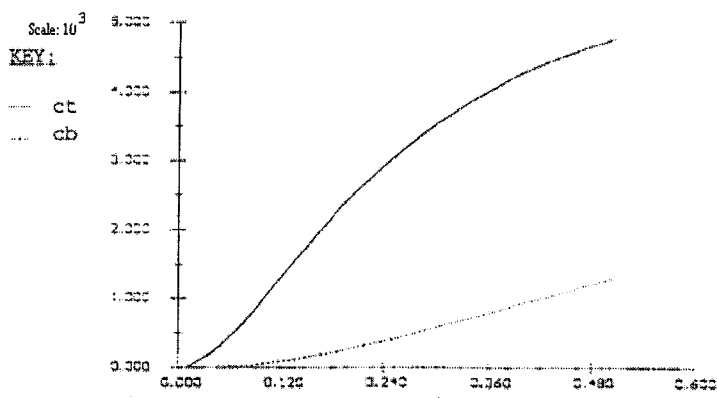
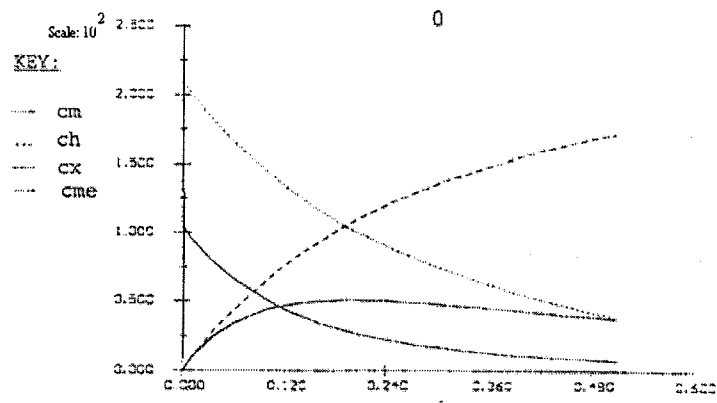
0.021

0

0

0

0



| Variable | Initial value | Maximum value | Minimum value | Final value |
|----------|---------------|---------------|---------------|-------------|
| t | 0 | 0.51 | 0 | 0.51 |
| cm | 0.0105 | 0.0105 | 0.000699836 | 0.000699836 |
| ch | 0.021 | 0.021 | 0.00381847 | 0.00381847 |
| cx | 0 | 0.00506614 | 0 | 0.00372332 |
| cme | 0 | 0.0171815 | 0 | 0.0171815 |
| ct | 0 | 0.00477233 | 0 | 0.00477233 |
| cb | 0 | 0.00130452 | 0 | 0.00130452 |
| rm | -0.083992 | -0.00238715 | -0.083992 | -0.00238715 |
| rb | 0 | 0.00352127 | 0 | 0.00330288 |
| rx | 0.083992 | 0.083992 | -0.00523484 | -0.0045612 |
| rt | 0 | 0.0146868 | 0 | 0.00364547 |
| rh | -0.083992 | -0.0126384 | -0.083992 | -0.0126384 |
| rme | 0.083992 | 0.083992 | 0.0126384 | 0.0126384 |

The maximum concentration of xylene occurs at $\tau = 0.19$ h.

The first time period covers the simple batch culture, when glucose and dissolved oxygen are being consumed for cell growth.

METHOD Stiff

STARTTIME = 0

STOPTIME = 3.4

DT = 0.02

INIT G = 100

INIT X = 1.0

INIT O = 7.5

INIT P = 0

mumax = 1.2

KG = 1.0

KO = 1.0

Yxs = 0.5

Yps = 0.3

q = 1000

kLa = 1000

alpha = 0

SATG = G/(KG+G)

SATO = O/(KO+O)

SATP = 1.0 - (P/10)

mux = mumax * SATG*SATO*SATP*X

d/dt(X) = mux

d/dt(G) = - mux/Yxs

d/dt(O) = kLa*(7.5 - O) - q*mux

d/dt(P) = alpha*mux

The numerical simulation results shown below identifies the time at which the dissolved oxygen concentration falls below the critical value of 0.5 mg/liter, triggering the formation of the by-product acetic acid.

From the simulation results, we find that the dissolved oxygen concentration falls below the critical values of 0.5 mg/l at the batch culture time of 3.64 hours. At that time, the glucose concentration has fallen to 67.1 g/l and cell mass concentration has growth to 17.45 g/l. The by-product acetic acid concentration remains zero through the early batch culture, as the dissolved oxygen concentration is above the critical level throughout this time. In the program above, the parameter alpha is set to zero to ensure that no acetic acid is produced.

$$\frac{dX}{dW} = \frac{-r_A}{F_{A0}}$$

$$-r_A = kC_A$$

$$C_A = C_{A0} \frac{1-X}{1+X} \frac{T_0}{T} y$$

$$\frac{dy}{dW} = \frac{-\alpha}{2y}$$

$$\frac{dT}{dW} = \frac{U(r) \frac{2h}{\rho} (T_A - T) + (-r_A)(-\Delta H_R)}{F_{A0} C_{pA}}$$

$$U = U(r_0) \left(\frac{r_0}{r} \right)^5 \left(\frac{T}{T_0} \right)^5$$

Since h and ρ are unknown, we will assume that they are both equal to one.
We will also assume that r varies as W^5 varies.

so:

$$\frac{dT}{dW} = \frac{U(r)(T_A - T) + (-r_A)(-\Delta H_R)}{F_{A0} C_{pA}}$$

$$U = U(r_0) \left(\frac{W_0^5}{W} \right)^5 \left(\frac{T}{T_0} \right)^5$$

See Polymath program P8-30.b.pol.

POLYMATH Results

Calculated values of the DEQ variables

| Variable | initial value | minimal value | maximal value | final value |
|----------|---------------|---------------|---------------|-------------|
| W | 0 | 0 | 50 | 50 |
| Y | 1 | 0.8062258 | 1 | 0.8062258 |
| X | 0 | 0 | 0.7845538 | 0.7845538 |
| T | 450 | 450 | 756.08452 | 756.08452 |
| Fao | 5 | 5 | 5 | 5 |
| alpha | 0.007 | 0.007 | 0.007 | 0.007 |
| Ta | 300 | 300 | 300 | 300 |
| dHr1 | -2.0E+04 | -2.0E+04 | -2.0E+04 | -2.0E+04 |
| Wo | 0.01 | 0.01 | 0.01 | 0.01 |
| To | 450 | 450 | 450 | 450 |
| E | 3.14E+04 | 3.14E+04 | 3.14E+04 | 3.14E+04 |
| R | 8.314 | 8.314 | 8.314 | 8.314 |
| Cao | 0.2498645 | 0.2498645 | 0.2498645 | 0.2498645 |
| X1 | 0 | 0 | 784.55376 | 784.55376 |
| y1 | 1000 | 806.22577 | 1000 | 806.22577 |
| U | 5.0E+04 | 0.9244844 | 5.0E+04 | 0.9244844 |
| k | 1 | 1 | 29.893648 | 29.893648 |

- [15] $C_{ao} = 0$
[16] $C_{po} = 0$
[17] $C_{co} = 2000$
[18] $C_{oo} = 0$

P13-15 (c)

The selectivities are reported in the following table:

| SMM_{PFR} | XMM_{CSTR} | Xsm_{PFR} | Xsm_{CSTR} |
|-------------|--------------|-------------|--------------|
| 4.83 | 0.99 | 4.174 | 0.92 |

P13-15 (d)

Normal Distribution with $\tau = 5 \text{ min}$ and $\sigma = 3 \text{ min}$

$$E(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(t-\tau)^2}{2\sigma^2}\right] = \frac{1}{3\sqrt{2\pi}} \exp\left[-\frac{(t-5)^2}{2\cdot 3^2}\right]$$

Segregation Model

See Polymath program P13-15-d-1.pol

POLYMATH Results

Calculated values of the DEQ variables

| Variable | initial value | minimal value | maximal value | final value |
|----------|---------------|---------------|---------------|-------------|
| t | 0 | 0 | 2 | 2 |
| ca | 0 | 0 | 171.75027 | 171.75027 |
| cp | 0 | 0 | 52.879376 | 52.879376 |
| cc | 2000 | 1991.2989 | 2000 | 1991.2989 |
| cabar | 0 | 0 | 11.116671 | 11.116671 |
| cpbar | 0 | 0 | 3.2689487 | 3.2689487 |
| ccbar | 0 | 0 | 221.39065 | 221.39065 |
| co | 0 | 0 | 7.0306771 | 7.0306771 |
| cobar | 0 | 0 | 0.3200147 | 0.3200147 |
| k1 | 0.012 | 0.012 | 0.012 | 0.012 |
| k2 | 0.046 | 0.046 | 0.046 | 0.046 |
| k3 | 0.02 | 0.02 | 0.02 | 0.02 |
| k4 | 0.034 | 0.034 | 0.034 | 0.034 |
| k5 | 0.04 | 0.04 | 0.04 | 0.04 |
| rc | 0 | -8.5350648 | 0 | -8.5350648 |
| ra | 92 | 79.947816 | 92 | 79.947816 |
| rp | 24 | 24 | 28.677508 | 28.677508 |
| sigma | 3 | 3 | 3 | 3 |
| ro | 0 | 0 | 6.8700107 | 6.8700107 |
| tau | 5 | 5 | 5 | 5 |
| Spo | 2.4E+08 | 4.1743032 | 2.4E+08 | 4.1743032 |
| E1 | 10 | 10 | 10 | 10 |
| E | 0.0331675 | 0.0331675 | 0.0806774 | 0.0806774 |

ODE Report (RK45)

Differential equations as entered by the user

- [1] $d(ca)/d(t) = ra$
[2] $d(cp)/d(t) = rp$
[3] $d(cc)/d(t) = rc$
[4] $d(cabar)/d(t) = ca \cdot E$
[5] $d(cpbar)/d(t) = cp \cdot E$
[6] $d(ccbar)/d(t) = cc \cdot E$
[7] $d(co)/d(t) = ro$
[8] $d(cobar)/d(t) = co \cdot E$