

Solutions for Chapter 1 – Mole Balances

Synopsis

General: The goal of these problems are to reinforce the definitions and provide an understanding of the mole balances of the different types of reactors. It lays the foundation for step 1 of the algorithm in Chapter 4.

- P1-1.** This problem helps the student understand the course goals and objectives.
- P1-2.** Part (d) gives hints on how to solve problems when they get stuck. Encourages students to get in the habit of writing down what they learned from each chapter. It also gives tips on problem solving.
- P1-3.** Helps the student understand critical thinking and creative thinking, which are two major goals of the course.
- P1-4.** Requires the student to at least look at the wide and wonderful resources available on the CD-ROM and the Web.
- P1-5.** The ICMs have been found to be a great motivation for this material.
- P1-6.** Uses Example 1-1 to calculate a CSTR volume. It is straight forward and gives the student an idea of things to come in terms of sizing reactors in chapter 4. An alternative to **P1-15**.
- P1-7.** Straight forward modification of Example 1-1.
- P1-8.** Helps the student review and member assumption for each design equation.
- P1-9 and P1-10.** The results of these problems will appear in later chapters. Straight forward application of chapter 1 principles.
- P1-11.** Straight forward modification of the mole balance. Assigned for those who emphasize bioreaction problems.
- P1-12.** Can be assigned to just be read and not necessarily to be worked. It will give students a flavor of the top selling chemicals and top chemical companies.
- P1-13.** Will be useful when the table is completed and the students can refer back to it in later chapters. Answers to this problem can be found on Professor Susan Montgomery's equipment module on the CD-ROM. See **P1-17**.

- P1-14.** Many students like this straight forward problem because they see how CRE principles can be applied to an everyday example. It is often assigned as an in-class problem where parts **(a)** through **(f)** are printed out from the web. Part **(g)** is usually omitted.
- P1-15.** Shows a bit of things to come in terms of reactor sizing. Can be rotated from year to year with **P1-6**.
- P1-16.** Open-ended problem.
- P1-17.** I **always** assign this problem so that the students will learn how to use POLYMATH/MaLab before needing it for chemical reaction engineering problems.
- P1-18.** Parts **(a)** and **(b)** are open-ended problem.
- P1-19 and P1-20.** Help develop critical thinking and analysis.
- CDP1-A** Similar to problems 3, 4, 11, and 12.
- CDP1-B** Points out difference in rate per unit liquid volume and rate per reactor volume.

Summary

	<u>Assigned</u>	<u>Alternates</u>	<u>Difficulty</u>	<u>Time (min)</u>
● P1-1	AA		SF	60
P1-2	I		SF	30
● P1-3	O		SF	30
P1-4	O		SF	30
P1-5	AA		SF	30
P1-6	AA	1-15	SF	15
P1-7	I		SF	15
● P1-8	S		SF	15
P1-9	S		SF	15
P1-10	S		SF	15
P1-11	O		FSF	15
P1-12	I	– Read Only	SF	30
P1-13	I		SF	1
P1-14	O		FSF	30
P1-15	O		SF	60
P1-16	S		SF	15
● P1-17	AA		SF	60
P1-18	S		SF	30
P1-19	O		--	30
P1-20	O		FSF	15

CDP1-A	AA	FSF	30
CDP1-B	I	FSF	30

Assigned

● = Always assigned, AA = Always assign one from the group of alternates,
O = Often, I = Infrequently, S = Seldom, G = Graduate level

Alternates

In problems that have a dot in conjunction with AA means that one of the problem, either the problem with a dot or any one of the alternates are always assigned.

Time

Approximate time in minutes it would take a B/B⁺ student to solve the problem.

Difficulty

SF = Straight forward reinforcement of principles (plug and chug)

FSF = Fairly straight forward (requires some manipulation of equations or an intermediate calculation).

IC = Intermediate calculation required

M = More difficult

OE = Some parts open-ended.

* Note the letter problems are found on the CD-ROM. For example A = CDP1-A.

Summary Table Ch-1

Review of Definitions and Assumptions	1,5,6,7,8,9
Introduction to the CD-ROM	1,2,3,4
Make a calculation	6
Open-ended	8,16

P1-1 Individualized solution.

P1-2 Individualized solution.

P1-3 Individualized solution.

P1-4 Individualized solution.

P1-5 Solution is in the decoding algorithm given with the modules.

P1-6

The general equation for a CSTR is:

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

Here r_A is the rate of a first order reaction given by:

$$r_A = -kC_A$$

Given : $C_A = 0.1C_{A0}$, $k = 0.23 \text{ min}^{-1}$, $v_0 = 10 \text{ dm}^3 \text{ min}^{-1}$, $F_A = 5.0 \text{ mol/hr}$

And we know that $F_A = C_A v_0$ and $F_{A0} = C_{A0} v_0$

$\Rightarrow C_{A0} = F_{A0} / v_0 = 0.5 \text{ mol/dm}^3$

Substituting in the above equation we get:

$$V = \frac{C_{A0}v_0 - C_A v_0}{kC_A} = \frac{(0.5 \text{ mol/dm}^3)(10 \text{ dm}^3/\text{min}) - 0.1(0.5 \text{ mol/dm}^3)(10 \text{ dm}^3/\text{min})}{(0.23 \text{ min}^{-1})(0.1(0.5 \text{ mol/dm}^3))}$$

$$V = 391.3 \text{ dm}^3$$

P1-7

$$t = \int_{N_{A0}}^{N_A} \frac{1}{-k \cdot N_A} dN_A$$

$$k = 0.23 \text{ min}^{-1}$$

From mole balance: $\frac{dN_A}{dt} = r_A \cdot V$

Rate law: $-r_A = k \cdot C_A$

$$-r_A = k \cdot \frac{N_A}{V}$$

Combine:

$$\frac{dN_A}{dt} = -k \cdot N_A$$

$$\tau = 0 \int_0^t 1 dt = -\left(\frac{1}{k}\right) \cdot \int_{N_{A0}}^{N_A} \frac{1}{N_A} dN_A$$

at $\tau = 0$, $N_{A0} = 100 \text{ mol}$ and $\tau = \tau$, $N_A = (0.01)N_{A0}$

$$\Rightarrow t = \frac{1}{k} \ln\left(\frac{N_{A0}}{N_A}\right)$$

$$= \frac{1}{0.23} \ln(100) \text{ min} \quad t = 20 \text{ min}$$

P1-8 (a)

The assumptions made in deriving the design equation of a batch reactor are:

- Closed system: no streams carrying mass enter or leave the system.
- Well mixed, no spatial variation in system properties
- Constant Volume or constant pressure.

P1-8 (b)

The assumptions made in deriving the design equation of CSTR, are:

- Steady state.
- No spatial variation in concentration, temperature, or reaction rate throughout the vessel.

P1-8 (c)

The assumptions made in deriving the design equation of PFR are:

- Steady state.
- No radial variation in properties of the system.

P1-8 (d)

The assumptions made in deriving the design equation of PBR are:

- Steady state.
- No radial variation in properties of the system.

P1-8 (e)

For a reaction,



$-r_A$ is the number of moles of A reacting (disappearing) per unit time per unit volume [=] moles/(dm³.s).

$-r_A'$ is the rate of disappearance of species A per unit mass (or area) of catalyst [=] moles/(time. mass of catalyst).

r_A' is the rate of formation (generation) of species A per unit mass (or area) of catalyst [=] moles/(time. mass catalyst).

$-r_A$ is an **intensive** property, that is, it is a function of concentration, temperature, pressure, and the type of catalyst (if any), and is defined at any **point** (location) within the system. It is independent of amount. On the other hand, an extensive property is obtained by summing up the properties of individual subsystems within the **total** system; in this sense, $-r_A$ is independent of the 'extent' of the system.

P 1-9

Rate of homogenous reaction r_A is defined as the mole of A formed per unit volume of the reactor per second. It is an Intensive property and the concentration, temperature and hence the rate varies with spatial coordinates.

r_A' on the other hand is defined as g mol of A reacted per gm. of the catalyst per second. Here mass of catalyst is the basis as this is what is important in catalyst reactions and not the reactor volume.

Applying general mole balance we get:

$$\frac{dN_j}{dt} = F_{j0} - F_j + \int r_j dV$$

No accumulation and no spatial variation implies

$$0 = F_{j0} - F_j + \int r_j dV$$

Also $r_j = Q_b r_j'$ and $W = VQ_b$ where Q_b is the bulk density of the bed.

$$\Rightarrow 0 = (F_{j0} - F_j) + \int r_j'(\rho_b dV)$$

Hence the above equation becomes

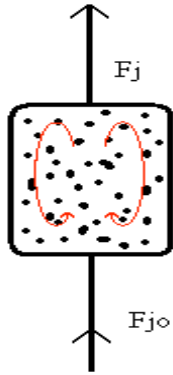
$$W = \frac{F_{j0} - F_j}{-r_j'}$$

We can also just apply the general mole balance as

$$\frac{dN_j}{dt} = (F_{j0} - F_j) + \int r_j'(dW)$$

Assuming no accumulation and no spatial variation in rate, we get the same form as above:

$$W = \frac{F_{j0} - F_j}{-r_j'}$$



P1-10

Mole balance on species j is:

$$F_{j0} - F_j + \int_0^V r_j dV = \frac{dN_j}{dt}$$

Let M_j = molecular wt. of species j

Then $F_{j0}M_j = w_{j0}$ = mass flow rate of j into reactor:

$$N_jM_j = m_j = \text{mass of species j in the reactor}$$

Multiplying the mole balance on species j by M_j

$$F_{j0}M_j - F_jM_j + M_j \int_0^V r_j dV = M_j \frac{dN_j}{dt}$$

Now M_j is constant:

$$F_{j0}M_j - F_jM_j + \int_0^V M_j r_j dV = \frac{d(M_j N_j)}{dt} = \frac{d(m_j)}{dt}$$

$$w_{j0} - w_j + \int_0^V M_j r_j dV = \frac{dm_j}{dt}$$

P1-11

Applying mole balance to Penicillin: Penicillin is produced in the cells stationary state (See Chapter 7), so there is no cell growth and the nutrients are used in making product.

Let's do part c first.

$$[\text{In flowrate (moles/time)}]_{\text{penicillin}} + [\text{generation rate (moles/time)}]_{\text{penicillin}} - [\text{Out flowrate (moles/time)}]_{\text{penicillin}} = [\text{rate of accumulation (moles/time)}]_{\text{penicillin}}$$

$$F_{p,\text{in}} + G_p - F_{p,\text{out}} = \frac{dNp}{dt}$$

$$F_{p,\text{in}} = 0 \dots\dots\dots (\text{because no penicillin inflow})$$

$$G_p = \int_0^V r_p \cdot dV$$

Therefore,

$$\int_0^V r_p \cdot dV - F_{p,\text{out}} = \frac{dNp}{dt}$$

Assuming steady state for the rate of production of penicillin in the cells stationary state,

$$\frac{dNp}{dt} = 0$$

And no variations

$$V = \frac{F_{p,\text{in}} - F_{p,\text{out}}}{-r_p}$$

Or,

$$V = \frac{F_{p,\text{out}}}{r_p}$$

Similarly, for Corn Steep Liquor with $F_C = 0$

$$V = \frac{F_{C0} - F_C}{-r_C} = \frac{F_{C0}}{-r_C}$$

Assume RNA concentration does not change in the stationary state and no RNA is generated or destroyed.

P1-12 (a)

Ranking of 10 most produced chemicals in 1995 and 2002 are listed in table below:

Rank 2002	Rank 1995	Chemical
1	1	H ₂ SO ₄
2	2	N ₂
3	4	C ₂ H ₄
4	3	O ₂
5	9	C ₃ H ₆
6	-	H ₂
7	6	NH ₃
8	10	Cl ₂
9	-	P ₂ O ₅
10	-	C ₂ H ₂ Cl ₂

→ Chemicals like H₂, P₂O₅, C₂H₂Cl₂ has come in top 10 chemicals and C₃H₆ has jumped to rank 5 now then rank 9 in 1995.

P1-12 (b)

Ranking of top 10 chemical companies in sales in year 2003 and 2002:

2003	2002	Company	Chemical Sales (\$ million 2003)
1	1	Dow Chemical	32632
2	2	DuPont	30249
3	3	ExxonMobil	20190
4	4	General Electric	8371
5	8	Chevron Phillips	7018
6	5	Huntsman Corp.	6990
7	6	PPG Industries	6606
8	7	Equistar Chemicals	6545
9	11	Air Products	6029
10	9	Eastman Chemicals	5800

Chemical and Engineering News may 17, 2004

→ We have Chevron Phillips which jumped to 5 rank in 2003 from 8th rank in 2002 and Air Products coming to 9th rank in 2003 from 11th in 2002.

→ Chemical sales of each company has increased compared to year 2002 from 9% (Eastman Chemical) to 28.2% (Chevron Phillips) but Huntsman Corp. has a decrease by 2.9%.

P1-12 (c)

Sulfuric acid is prime importance in manufacturing. It is used in some phase of the manufacture of nearly all industrial products. It is used in production of every other strong acid. Because of its large number of uses, it's the most produced chemical. Sulfuric acid uses are:

- It is consumed in production of fertilizers such as ammonium sulphate (NH₄)₂SO₄ and superphosphate (Ca(H₂PO₄)₂), which is formed when rock phosphate is treated with sulfuric acid.
- Used as dehydrating agent.
- Used in manufacturing of explosives, dyestuffs, other acids, parchment paper, glue, purification of petroleum and picking of metals.
- Used to remove oxides from iron and steel before galvanizing or electroplating.
- Used in non-ferrous metallurgy, in production of rayon and film.
- as laboratory reagent and etchant and in storage batteries.
- It is also general purpose food additive.

P1-12 (d)

Annual Production rate of ethylene for year 2002 is 5.21×10^{10} lb/year

Annual Production rate of benzene for year 2002 is 1.58×10^{10} lb/year

Annual Production rate of ethylene oxide for year 2002 is 7.6×10^9 lb/year

P1-12 (e)

Because the basic raw material 'coal and petroleum' for organic chemicals is very limited and their production is not increasing as production of raw material for inorganic chemicals.

P1-13

Type	Characteristics	Phases	Usage	Advantage	Disadvantage
Batch	All the reactants fed into the reactor. During reaction nothing is added or removed. Easy heating or cooling.	1. Liquid phase 2. Gas phase 3. Liquid Solid	1. Small scale pdn. 2. Used for lab experimentation. 3. Pharmaceuticals 4. Fermentation	1. High Conversion per unit volume. 2. Flexibility of using for multiple reactions. 3. Easy to clean	1. High Operating cost. 2. Variable product quality.
CSTR	Continuous flow of reactants and products. Uniform composition throughout.	1. Liquid phase 2. Gas – liquid 3. Solid - liquid	1. Used when agitation required. 2. Series Configuration possible for different configuration streams	1. Continuous Operation. 2. Good Temperature Control 3. Two phase reactions possible. 4. Good Control 5. Simplicity of construction. 6. Low operating cost 7. Easy to clean	1. Lowest conversion per unit volume. 2. By passing possible with poor agitation. 3. High power Input reqd.
PFR	One long reactor or number of CSTR's in series. No radial variations. Conc. changes along the length.	1. Primarily gas Phase	1. Large Scale pdn. 2. Fast reactions 3. Homogenous reactions 4. Heterogeneous reactions 5. Continuous pdn.	1. High conversion per unit volume 2. Easy to maintain (No moving parts) 3. low operating cost 4. continuous operation	1. Undesired thermal gradient. 2. Poor temperature control 3. Shutdown and cleaning expensive.

PBR	Tubular reactor that is packed with solid catalyst particles.	1. Gas Phase (Solid Catalyst) 2. Gas – solid reactions.	1. Used primarily in the heterogeneous gas phase reaction with solid catalyst e.g Fischer tropsch synthesis.	1. High conversion per unit mass of catalyst 2. low operating cost 3. Continuous operation	1. Undesired thermal gradient. 2. Poor temperature control 3. Channeling 4. Cleaning expensive.
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P1-14

Given

$$A = 2 \times 10^{10} \text{ ft}^2$$

$$T_{STP} = 491.69 R$$

$$H = 2000 \text{ ft}$$

$$V = 4 \times 10^{13} \text{ ft}^3$$

$$T = 534.7^\circ R$$

$$P_0 = 1 \text{ atm}$$

$$R = 0.7302 \frac{\text{atm} \cdot \text{ft}^3}{\text{lbmol} \cdot R}$$

$$y_A = 0.02$$

$$C_S = 2.04 \times 10^{-10} \frac{\text{lbmol}}{\text{ft}^3}$$

$$C = 4 \times 10^5 \text{ cars}$$

F_S = CO in Santa Ana wind

F_A = CO emission from autos

$$v_A = 3000 \frac{\text{ft}^3}{\text{hr}} \text{ per car at STP}$$

P1-14 (a)

Total number of lb moles gas in the system:

$$N := \frac{P_0 \cdot V}{R \cdot T}$$

$$N = \frac{1 \text{ atm} \times (4 \times 10^{13} \text{ ft}^3)}{\left(0.73 \frac{\text{atm} \cdot \text{ft}^3}{\text{lbmol} \cdot R}\right) \times 534.69 R} = 1.025 \times 10^{11} \text{ lb mol}$$

P1-14 (b)

Molar flowrate of CO into L.A. Basin by cars.

$$F_A = y_A F_T = y_A \cdot \frac{v_A C P_0}{R T_{STP}}$$

$$F_T = \frac{3000 \text{ ft}^3}{\text{hr car}} \times \frac{1 \text{ lbmol}}{359 \text{ ft}^3} \times 400000 \text{ cars} \quad (\text{See appendix B})$$

$$F_A = 6.685 \times 10^4 \text{ lb mol/hr}$$

P1-14 (c)

Wind speed through corridor is $v = 15 \text{ mph}$

$W = 20 \text{ miles}$

The volumetric flowrate in the corridor is

$$v_o = v \cdot W \cdot H = (15 \times 5280)(20 \times 5280)(2000) \text{ ft}^3/\text{hr} \\ = 1.673 \times 10^{13} \text{ ft}^3/\text{hr}$$

P1-14 (d)

Molar flowrate of CO into basin from Sant Ana wind.

$$F_S := v_o C_S$$

$$= 1.673 \times 10^{13} \text{ ft}^3/\text{hr} \times 2.04 \times 10^{-10} \text{ lbmol}/\text{ft}^3$$

$$F_S = 3.412 \times 10^3 \text{ lbmol}/\text{hr}$$

P1-14 (e)

$$\text{Rate of emission of CO by cars} + \text{Rate of CO by Wind} - \text{Rate of removal of CO} = \frac{dN_{CO}}{dt}$$

$$F_A + F_S - v_o C_{co} = V \frac{dC_{co}}{dt} \quad (V = \text{constant}, N_{co} = C_{co} V)$$

P1-14 (f)

$$t = 0, \quad C_{co} = C_{co0}$$

$$\int_0^t dt = V \int_{C_{co0}}^{C_{co}} \frac{dC_{co}}{F_A + F_S - v_o C_{co}}$$

$$t = \frac{V}{v_o} \ln \left(\frac{F_A + F_S - v_o C_{co0}}{F_A + F_S - v_o C_{co}} \right)$$

P1-14 (g)

Time for concentration to reach 8 ppm.

$$C_{CO0} = 2.04 \times 10^{-8} \frac{\text{lbmol}}{\text{ft}^3}, \quad C_{CO} = \frac{2.04}{4} \times 10^{-8} \frac{\text{lbmol}}{\text{ft}^3}$$

From (f),

$$t = \frac{V}{v_o} \ln \left(\frac{F_A + F_S - v_o C_{CO0}}{F_A + F_S - v_o C_{CO}} \right) \\ = \frac{4 \text{ ft}^3}{1.673 \times 10^{13} \frac{\text{ft}^3}{\text{hr}}} \ln \left(\frac{6.7 \times 10^4 \frac{\text{lbmol}}{\text{hr}} + 3.4 \times 10^3 \frac{\text{lbmol}}{\text{hr}} - 1.673 \times 10^{13} \frac{\text{ft}^3}{\text{hr}} \times 2.04 \times 10^{-8} \frac{\text{lbmol}}{\text{ft}^3}}{6.7 \times 10^4 \frac{\text{lbmol}}{\text{hr}} + 3.4 \times 10^3 \frac{\text{lbmol}}{\text{hr}} - 1.673 \times 10^{13} \frac{\text{ft}^3}{\text{hr}} \times 0.51 \times 10^{-8} \frac{\text{lbmol}}{\text{ft}^3}} \right)$$

$$t = 6.92 \text{ hr}$$

P1-14 (h)

(1) $t_o = 0$ $t_f = 72$ hrs
 $C_{co} = 2.00E-10$ lbmol/ft³ $a = 3.50E+04$ lbmol/hr
 $v_o = 1.67E+12$ ft³/hr $b = 3.00E+04$ lbmol/hr
 $F_s = 341.23$ lbmol/hr $V = 4.0E+13$ ft³

$$a + b \sin\left(\pi \frac{t}{6}\right) + F_s - v_o C_{co} = V \frac{dC_{co}}{dt}$$

Now solving this equation using POLYMATH we get plot between C_{co} vs t

See Polymath program [P1-14-h-1.pol](#).

POLYMATH Results

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
t	0	0	72	72
C	2.0E-10	2.0E-10	2.134E-08	1.877E-08
v0	1.67E+12	1.67E+12	1.67E+12	1.67E+12
a	3.5E+04	3.5E+04	3.5E+04	3.5E+04
b	3.0E+04	3.0E+04	3.0E+04	3.0E+04
F	341.23	341.23	341.23	341.23
V	4.0E+13	4.0E+13	4.0E+13	4.0E+13

ODE Report (RK45)

Differential equations as entered by the user

[1] $d(C)/d(t) = (a+b*\sin(3.14*t/6)+F-v0*C)/V$

Explicit equations as entered by the user

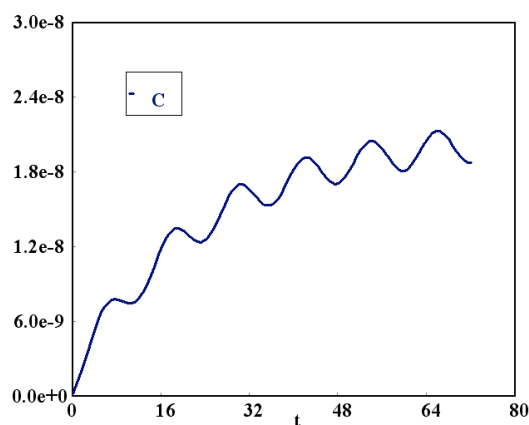
[1] $v0 = 1.67*10^{12}$

[2] $a = 35000$

[3] $b = 30000$

[4] $F = 341.23$

[5] $V = 4*10^{13}$



(2) $t_f = 48$ hrs $F_s = 0$ $a + b \sin\left(\pi \frac{t}{6}\right) - v_o C_{co} = V \frac{dC_{co}}{dt}$

Now solving this equation using POLYMATH we get plot between C_{co} vs t

See Polymath program **P1-14-h-2.pol**.

POLYMATH Results

Calculated values of the DEQ variables

<u>Variable</u>	<u>initial value</u>	<u>minimal value</u>	<u>maximal value</u>	<u>final value</u>
t	0	0	48	48
C	2.0E-10	2.0E-10	1.904E-08	1.693E-08
v0	1.67E+12	1.67E+12	1.67E+12	1.67E+12
a	3.5E+04	3.5E+04	3.5E+04	3.5E+04
b	3.0E+04	3.0E+04	3.0E+04	3.0E+04
V	4.0E+13	4.0E+13	4.0E+13	4.0E+13

ODE Report (RK45)

Differential equations as entered by the user

[1] $d(C)/d(t) = (a+b*\sin(3.14*t/6)-v0*C)/V$

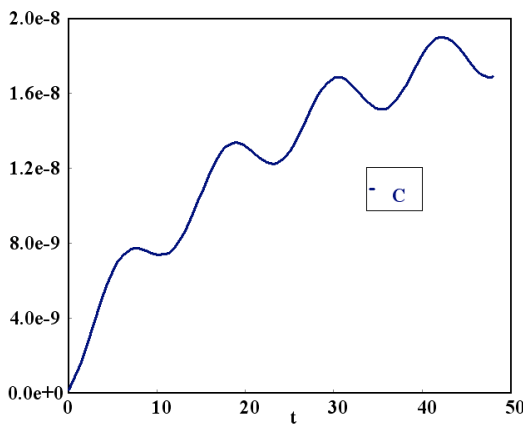
Explicit equations as entered by the user

[1] $v0 = 1.67*10^{12}$

[2] $a = 35000$

[3] $b = 30000$

[4] $V = 4*10^{13}$



(3)

Changing $a \rightarrow$ Increasing 'a' reduces the amplitude of ripples in graph. It reduces the effect of the sine function by adding to the baseline.

Changing $b \rightarrow$ The amplitude of ripples is directly proportional to 'b'.
As b decreases amplitude decreases and graph becomes smooth.

Changing $v_0 \rightarrow$ As the value of v_0 is increased the graph changes to a "shifted sin-curve". And as v_0 is decreased graph changes to a smooth increasing curve.

P1-15 (a)

$$-r_A = k \text{ with } k = 0.05 \text{ mol/h dm}^3$$

CSTR: The general equation is

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

Here $C_A = 0.01 C_{A0}$, $v_0 = 10 \text{ dm}^3/\text{min}$, $F_A = 5.0 \text{ mol/hr}$

Also we know that $F_A = C_A v_0$ and $F_{A0} = C_{A0} v_0$, $C_{A0} = F_{A0}/v_0 = 0.5 \text{ mol/dm}^3$

Substituting the values in the above equation we get,

$$V = \frac{C_{A0}v_0 - C_A v_0}{k} = \frac{(0.5)10 - 0.01(0.5)10}{0.05}$$

$$\rightarrow V = 99 \text{ dm}^3$$

PFR: The general equation is

$$\frac{dF_A}{dV} = r_A = k, \text{ Now } F_A = C_A v_0 \text{ and } F_{A0} = C_{A0} v_0 \Rightarrow \frac{dC_A v_0}{dV} = -k$$

Integrating the above equation we get

$$\frac{v_0}{k} \int_{C_{A0}}^{C_A} dC_A = \int_0^V dV \Rightarrow V = \frac{v_0}{k} (C_{A0} - C_A)$$

Hence $V = 99 \text{ dm}^3$

Volume of PFR is same as the volume for a CSTR since the rate is constant and independent of concentration.

P1-15 (b)

- $r_A = kC_A$ with $k = 0.0001 \text{ s}^{-1}$

CSTR:

We have already derived that

$$V = \frac{C_{A0}v_0 - C_A v_0}{-r_A} = \frac{v_0 C_{A0} (1 - 0.01)}{kC_A}$$

$$k = 0.0001 \text{ s}^{-1} = 0.0001 \times 3600 \text{ hr}^{-1} = 0.36 \text{ hr}^{-1}$$

$$\rightarrow V = \frac{(10 \text{ dm}^3 / \text{hr})(0.5 \text{ mol} / \text{dm}^3)(0.99)}{(0.36 \text{ hr}^{-1})(0.01 * 0.5 \text{ mol} / \text{dm}^3)} \Rightarrow V = 2750 \text{ dm}^3$$

PFR:

From above we already know that for a PFR

$$\frac{dC_A v_0}{dV} = r_A = kC_A$$

Integrating

$$\frac{v_0}{k} \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = - \int_0^V dV$$

$$\frac{v_0}{k} \ln \frac{C_{A0}}{C_A} = V$$

Again $k = 0.0001 \text{ s}^{-1} = 0.0001 \times 3600 \text{ hr}^{-1} = 0.36 \text{ hr}^{-1}$

Substituting the values in above equation we get

$$V = 127.9 \text{ dm}^3$$

P1-15 (c)

$$-r_A = kC_A^2 \text{ with } k = 3 \text{ dm}^3/\text{mol.hr}$$

CSTR:

$$V = \frac{C_{A0}v_0 - C_A v_0}{-r_A} = \frac{v_0 C_{A0}(1 - 0.01)}{kC_A^2}$$

Substituting all the values we get

$$V = \frac{(10 \text{ dm}^3/\text{hr})(0.5 \text{ mol/dm}^3)(0.99)}{(3 \text{ dm}^3/\text{hr})(0.01 * 0.5 \text{ mol/dm}^3)^2} \Rightarrow V = 66000 \text{ dm}^3$$

PFR:

$$\frac{dC_A v_0}{dV} = r_A = kC_A^2$$

Integrating

$$\frac{v_0}{k} \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A^2} = - \int_0^V dV \Rightarrow \frac{v_0}{k} \left(\frac{1}{C_A} - \frac{1}{C_{A0}} \right) = V$$

$$\Rightarrow V = \frac{10 \text{ dm}^3/\text{hr}}{3 \text{ dm}^3/\text{mol.hr}} \left(\frac{1}{0.01 C_{A0}} - \frac{1}{C_{A0}} \right) = 660 \text{ dm}^3$$

P1-15 (d)

$$C_A = .001 C_{A0}$$

$$t = \int_{N_A}^{N_{A0}} \frac{dN}{-r_A V}$$

Constant Volume $V = V_0$

$$t = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A}$$

Zero order:

$$t = \frac{1}{k} [C_{A0} - 0.001 C_{A0}] = \frac{.999 C_{A0}}{0.05} = 9.99 h$$

First order:

$$t = \frac{1}{k} \ln \left(\frac{C_{A0}}{C_A} \right) = \frac{1}{0.001} \ln \left(\frac{1}{.001} \right) = 6908 s$$

Second order:

$$t = \frac{1}{k} \left[\frac{1}{C_A} - \frac{1}{C_{A0}} \right] = \frac{1}{3} \left[\frac{1}{0.0005} - \frac{1}{0.5} \right] = 666 h$$

P1-16 Individualized Solution

P1-17 (a)

Initial number of rabbits, $x(0) = 500$

Initial number of foxes, $y(0) = 200$

Number of days = 500

$$\frac{dx}{dt} = k_1x - k_2xy \dots\dots\dots(1)$$

$$\frac{dy}{dt} = k_3xy - k_4y \dots\dots\dots(2)$$

Given,

$$k_1 = 0.02 \text{ day}^{-1}$$

$$k_2 = 0.00004 / (\text{day} \times \text{foxes})$$

$$k_3 = 0.0004 / (\text{day} \times \text{rabbits})$$

$$k_4 = 0.04 \text{ day}^{-1}$$

See Polymath program **P1-17-a.pol**.

POLYMATH Results

Calculated values of the DEQ variables

<u>Variable</u>	<u>initial value</u>	<u>minimal value</u>	<u>maximal value</u>	<u>final value</u>
t	0	0	500	500
x	500	2.9626929	519.40024	4.2199691
y	200	1.1285722	4099.517	117.62928
k1	0.02	0.02	0.02	0.02
k2	4.0E-05	4.0E-05	4.0E-05	4.0E-05
k3	4.0E-04	4.0E-04	4.0E-04	4.0E-04
k4	0.04	0.04	0.04	0.04

ODE Report (RK45)

Differential equations as entered by the user

[1] $d(x)/d(t) = (k1*x)-(k2*x*y)$

[2] $d(y)/d(t) = (k3*x*y)-(k4*y)$

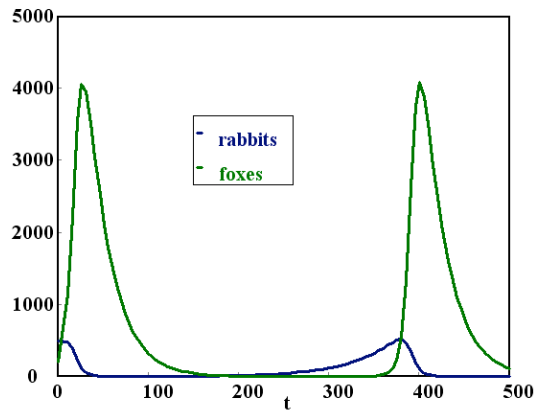
Explicit equations as entered by the user

[1] $k1 = 0.02$

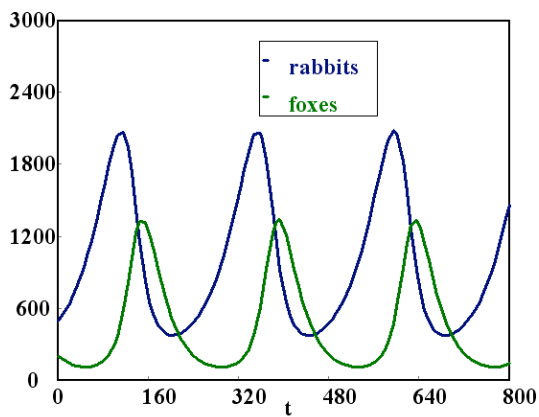
[2] $k2 = 0.00004$

[3] $k3 = 0.0004$

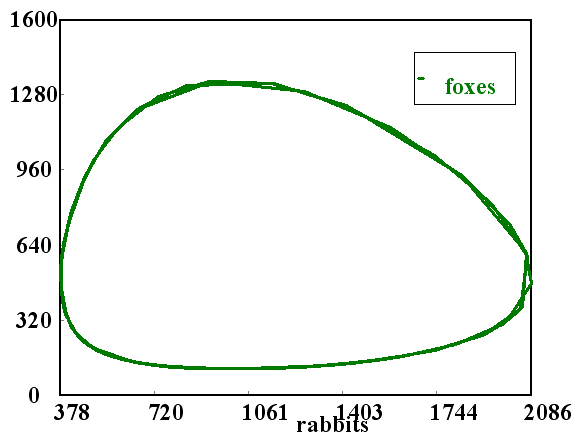
[4] $k4 = 0.04$



When, $t_{\text{final}} = 800$ and $k_3 = 0.00004 / (\text{day} \times \text{rabbits})$



Plotting rabbits Vs. foxes



P1-17 (b)

POLYMATH Results

See Polymath program [P1-17-b.pol](#).

POLYMATH Results

NLES Solution

Variable	Value	f (x)	Ini Guess
x	2.3850387	2.53E-11	2
y	3.7970279	1.72E-12	2

NLES Report (safenewt)

Nonlinear equations

[1] $f(x) = x^3y - 4y^2 + 3x - 1 = 0$

[2] $f(y) = 6y^2 - 9xy - 5 = 0$

P1-18 (a)

No preheating of the benzene feed will diminish the rate of reaction and thus lesser conversions will be achieved.

P1-18 (b)

An interpolation can be done on the logarithmic scale to find the desired values from the given data.

Now we can interpolate to get the cost at 6000 gallons and 15000 gallons

Cost of 6000 gal reactor = 1.905×10^5 \$

Cost of 15000 gal reactor = 5.623×10^5 \$

P1-18 (c)

We are given C_A is 0.1% of initial concentration

$$\rightarrow C_A = 0.001C_{A0}$$

Also from Example 1.3,

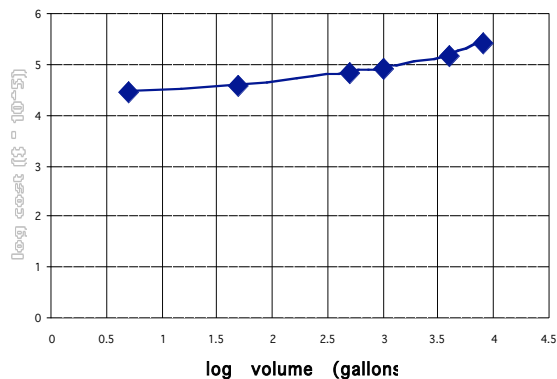
$$V = \frac{v_0}{k} \ln\left(\frac{C_{A0}}{C_A}\right)$$

Substituting $v_0 = 10 \text{ dm}^3/\text{min}$ and $k = 0.23 \text{ min}^{-1}$ we get

$$V = 300 \text{ dm}^3$$

which is three times the volume of reactor used in Example 1-3.

Cost vs Volume of reactor (log - log plot)



P1-18 (d) Safety of Plant.

P1-19 Enrico Fermi Problem – no definite solution

P1-20 Enrico Fermi Problem – no definite solution

P1-21 Individualized solution.

CDP1-A (a)

How many moles of A are in the reactor initially? What is the initial concentration of A?

If we assume ideal gas behavior, then calculating the moles of A initially present in the reactor is quite simple. We insert our variables into the ideal gas equation:

$$n = \frac{PV}{RT} = \frac{(20\text{atm})(200\text{dm}^3)}{\left(8.3145 \frac{\text{kJPa} \cdot \text{dm}^3}{\text{molK}}\right)(500)} \left(\frac{101.33\text{kPa}}{1\text{atm}}\right) = 97.5\text{moles}$$

Knowing the mole fraction of A (y_{A0}) is 75%, we multiply the total number of moles (N_{T0}) by the y_A :

$$\text{moles A} = N_{A0} = 0.75 \times 97.5 = 73.1$$

The initial concentration of A (C_{A0}) is just the moles of A divided by the volume:

$$C_{A0} = \frac{\text{moles}}{\text{volume}} = \frac{N_{A0}}{V} = \frac{73.1\text{moles}}{200\text{dm}^3} = 0.37\text{moles} / \text{dm}^3$$

CDP1-A (b)

Time (t) for a 1st order reaction to consume 99% of A.

$$r_A = \frac{dC_A}{dt}$$

Our first order rate law is:

$$-r_A = kC_A$$

$$\text{mole balance: } \frac{dC_A}{dt} = -kC_A \Rightarrow -k \int_0^t dt = \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A}$$

$$-kt = \ln\left(\frac{C_A}{C_{A0}}\right), \text{ knowing } C_A=0.01 C_{A0} \text{ and our rate constant (k=0.1 min}^{-1}\text{), we can solve}$$

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

CDP1-A (c)

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

rate law:

$$-r_A = kC_A^2$$

$$\text{mole balance: } \therefore \frac{dC_A}{dt} = -kC_A^2 \Rightarrow -k \int_0^t dt = \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A^2} \Rightarrow -kt = -\frac{1}{C_A} + \frac{1}{C_{A0}}$$

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

$$\text{concentration (C}_{A0}\text{): } -kt = -\frac{1}{C_A} + \frac{1}{C_{A0}}$$

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

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

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

Where, $(1-e)\Delta V$ = fraction of reactor element which is liquid.

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

$$\frac{dF_A}{dV} = r_A(1-e)$$

Must relate $(-r_A)$ to F_A ,

where, F_A is the total (gas + liquid) molar flow rate of A.

$-r_A$ = rate of reaction (g mol A per cubic cm. of liquid per sec.); e = volume fraction of gas; F_A = molar flow rate of A (g mol/sec.); V = volume of reactor