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Solutions for Chapter 1 – Mole Balances

P1-1.   This problem helps the student understand the course goals and objectives. Part (d) gives hints on how to solve problems when they get stuck.

P1-2.   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.   The results of this problem will appear in later chapters. Straight forward application of chapter 1 principles.

P1-10.   Straight forward modification of the mole balance. Assigned for those who emphasize bioreaction problems.

P1-11.   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 **P1-14**.

P1-12.   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.

P1-13.   Shows a bit of things to come in terms of reactor sizing. Can be rotated from year to year with **P1-6**.

P1-14. I **always** assign this problem so that the students will learn how to use POLYMATH/MATLAB before needing it for chemical reaction engineering problems.

P1-15 and **P1-16.**   Help develop critical thinking and analysis.

CDP1-A   Similar to problems 3, 4, and 10.

Summary

		Assigned	Alternates	Difficulty	Time (min)
●	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	1-13	SF	15
	P1-7	I		SF	15
●	P1-8	S		SF	15
	P1-9	S		SF	15
	P1-10	O		FSF	15
	P1-11	I		SF	1
	P1-12	O		FSF	30
	P1-13	O		SF	60
●	P1-14	AA		SF	60
	P1-15	O		--	30
	P1-16	O		FSF	15
	CDP1-A	AA		FSF	30

Assigned

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

<u>Alternates</u>

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.

<u>Time</u>

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

<u>Difficulty</u>

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 $\equiv$ 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

P1-1 Individualized solution.

P1-2

(b)   The negative rate of formation of a species indicates that its concentration is decreasing as the reaction proceeds ie. the species is being consumed in the course of the reaction.

  A positive number indicates production of the particular compound.

(c)   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 : $C_A = 0.1C_{A0}$, $k = 0.23 \text{ min}^{-1}$, $v_0 = 10 \text{dm}^3 \text{ min}^{-1}$

Substituting in the above equation we get:

$$V = \frac{C_{A0}v_0 - C_A v_0}{kC_A} = \frac{C_{A0}v_0(1-0.1)}{0.1kC_{A0}} = \frac{(10dm^3/\text{min})(0.9)}{(0.23\,\text{min}^{-1})(0.1)}$$

V = 391.304 m^3

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

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:

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

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

at $t = 0$, N_{AO} = 100 mol and $t = t$, N_A = (0.01)N_{AO}

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

$= \dfrac{1}{0.23} \ln(100)$ min

t = 20 min

P1-3 Individualized solution.

P1-4 Individualized solution.

P1-5 Individualized solution.

P1-6 Individualized solution

P1-7 (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- 7 (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.

P1-7(c)

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

- Steady state.

- No radial variation in properties of the system.

P1-7 (d)

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

- Steady state.

- No radial variation in properties of the system.

P1-7 (e)

For a reaction,

$$A \rightarrow B$$

- $-r_A$ is the number of moles of A reacting (disappearing) per unit time per unit volume [=] moles/ (dm^3.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 1-8

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 $r_j = \rho_b r_j^{`}$ and $W = V\rho_b$ where ρ_b is the bulk density of the bed.

$$\Rightarrow \qquad 0 = (F_{j0} - F_j) + \int r_j^{'}(\rho_b dV)$$
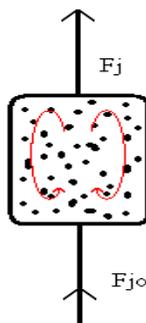
Hence the above equation becomes

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

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:

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

P1-9

Applying mole balance to Penicillin: Penicillin is produced in the cells stationary state (See Chapter 9), so there is no cell growth and the nutrients are used in making product.

Let's do part c first.

[Flowrate In (moles/time)] penicillin + [generation rate (moles/time)]penicillin − [Flowrate Out(moles/time)] penicillin = [rate of accumulation (moles/time)]penicillin

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

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

$$G_p = \int^{V} r_p .dV$$

Therefore,

$$\int^{V} r_p .dV - F_{p,out} = \frac{dNp}{dt}$$

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

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

And no variations

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

Or,

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

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.

P1-10

Given

$A = 2*10^{10} \, ft^2$ $T_{STP} = 491.69R$ $H = 2000 ft$

$V = 4*10^{13} \, ft^3$ T = 534.7° R   P$_O$ = 1atm

$R = 0.7302 \dfrac{atm \, ft^3}{lbmol \, R}$ y_A = 0.02 $C_S = 2.04*10^{-10} \dfrac{lbmol}{ft^3}$

$C = 4*10^5$ cars

F_S = CO in Santa Ana winds F_A = CO emission from autos

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

P1-10 (a)

Total number of lb moles gas in the system:

$$N = \frac{P_0 V}{RT}$$

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

P1-10 (b)

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

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

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

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

P1-10 (c)

Wind speed through corridor is v = 15mph

W = 20 miles

The volumetric flowrate in the corridor is

v_O = v.W.H = (15x5280)(20x5280)(2000) ft^3/hr = 1.673 x 10^{13} ft^3/hr

P1-10 (d)

Molar flowrate of CO into basin from Sant Ana wind.

$$F_S := v_0 \cdot C_S$$

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

   = 3.412 x 10^3 lbmol/hr

P1-10 (e)

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

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

P1-10 (f)

$t = 0$, $C_{co} = C_{coO}$

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

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

P1-10 (g)

Time for concentration to reach 8 ppm.

$$C_{CO0} = 2.04\times10^{-8}\frac{lbmol}{ft^3}, \quad C_{CO} = \frac{2.04}{4}\times10^{-8}\frac{lbmol}{ft^3}$$

From (f),

$$t = \frac{V}{v_o}\ln\left(\frac{F_A + F_S - v_O . C_{CO0}}{F_A + F_S - v_O . C_{CO}}\right)$$

$$= \frac{4\,ft^3}{1.673\times10^{13}\dfrac{ft^3}{hr}}\ln\left(\frac{6.7\times10^4\dfrac{lbmol}{hr} + 3.4\times10^3\dfrac{lbmol}{hr} - 1.673\times10^{13}\dfrac{ft^3}{hr}\times2.04\times10^{-8}\dfrac{lbmol}{ft^3}}{6.7\times10^4\dfrac{lbmol}{hr} + 3.4\times10^3\dfrac{lbmol}{hr} - 1.673\times10^{13}\dfrac{ft^3}{hr}\times0.51\times10^{-8}\dfrac{lbmol}{ft^3}}\right)$$

$t = 6.92$ hr

P1-10 (h)

(1) t_o = 0 t_f = 72 hrs

         C_{co} = 2.00E-10 lbmol/ft^3 a = 3.50E+04 lbmol/hr

         v_o = 1.67E+12 ft^3 /hr   b = 3.00E+04 lbmol/hr

         F_s = 341.23 lbmol/hr   V = 4.0E+13 ft^3

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

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

See Polymath program P1-10-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 (RKF45)

Differential equations as entered by the user

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

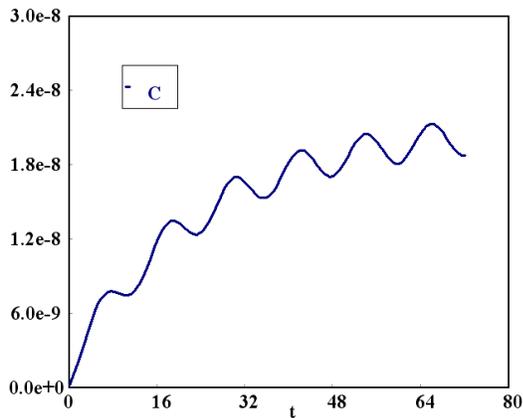Explicit equations as entered by the user

[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 $\qquad F_s = 0 \qquad\qquad a \ + \ b\sin\left(\pi\dfrac{t}{6}\right) \ - \ v_oC_{co} \ = \ V\dfrac{dC_{co}}{dt}$

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

See Polymath program P1-10-h-2.pol.

POLYMATH Results

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
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 (RKF45)

Differential equations as entered by the user
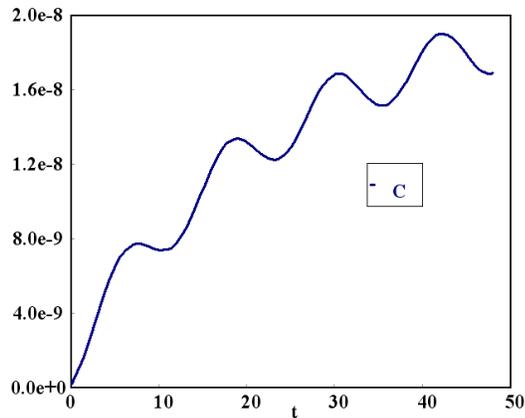
[1] d(C)/d(t) = (a+b*sin(3.14*t/6)-v0*C)/V

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 ➔ Increasing 'a' reduces the amplitude of ripples in graph. It reduces the effect of the sine function by adding to the baseline.

Changing b ➔ The amplitude of ripples is directly proportional to 'b'.

As b decreases amplitude decreases and graph becomes smooth.

Changing v_0 ➔ 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.

P1-11 (a)

$-r_A = k$ with k = 0.05 mol/h dm^3

CSTR: The general equation is

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

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

Substituting the values in the above equation we get,

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

→ **V = 99 dm³**

FR: The general equation is

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

Integrating the above equation we get

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

Hence **V = 99 dm³**

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

P1-11 (b)

- $r_A = kC_A$ with k = 0.0001 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 = 0.0001s⁻¹ = 0.0001 x 3600 hr⁻¹ = 0.36 hr⁻¹

$$\rightarrow V = \frac{(10 dm^3/hr)(0.5 mol/dm^3)(0.99)}{(0.36 hr^{-1})(0.01*0.5 mol/dm^3)}$$ => **V = 2750 dm³**

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 = 0.0001s⁻¹ = 0.0001 x 3600 hr⁻¹ = 0.36 hr⁻¹

Substituing the values in above equation we get **V = 127.9 dm³**

P1-11 (c)

- $r_A = kC_A^2$ with k = 3 dm³/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

$$V = \frac{(10dm^3/hr)(0.5mol/dm^3)(0.99)}{(3dm^3/hr)(0.01*0.5mol/dm^3)^2} \quad => \text{**V = 66000 dm³**}$$

PFR:

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

Integrating

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

$$=> V = \frac{10dm^3/hr}{3dm^3/mol.hr}(\frac{1}{0.01C_{A0}} - \frac{1}{C_{A0}}) = \text{**660 dm³**}$$

P1-11 (d)

$C_A = .001C_{A0}$

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

Constant Volume V=V₀

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

Zero order:

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

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:

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

P1-12 (a)

Initial number of rabbits, x(0) = 500

Initial number of foxes, y(0) = 200

Number of days = 500

$$\frac{dx}{dt} = k_1 x - k_2 xy \quad \text{.................................(1)}$$

$$\frac{dy}{dt} = k_3 xy - k_4 y \quad \text{.................................(2)}$$

Given,

$$k_1 = 0.02\,day^{-1}$$
$$k_2 = 0.00004/(day \times foxes)$$
$$k_3 = 0.0004/(day \times rabbits)$$
$$k_4 = 0.04\,day^{-1}$$

See Polymath program P1-12-a.pol.

POLYMATH Results

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
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 (RKF45)

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)
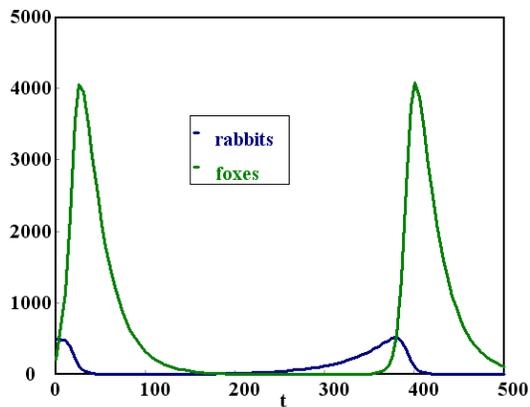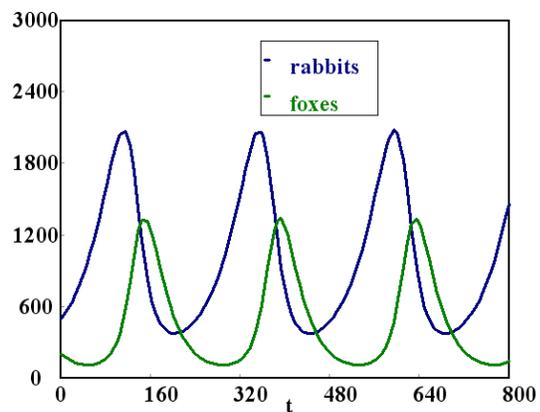
Explicit equations as entered by the user

[1] k1 = 0.02

[2] k2 = 0.00004

[3] k3 = 0.0004

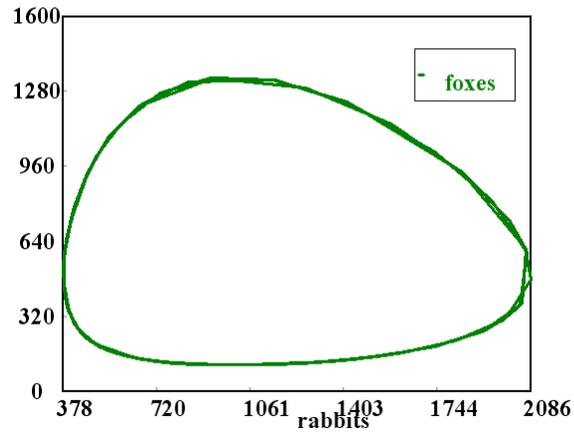[4] k4 = 0.04

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

Plotting rabbits Vs. foxes

P1-12 (b)

POLYMATH Results

See Polymath program P1-12-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^3*y-4*y^2+3*x-1 = 0

[2] f(y) = 6*y^2-9*x*y-5 = 0

P1-13 Enrico Fermi Problem – no definite solution

P1-14

Mole Balance:

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

Rate Law :

$$-r_A = kC_A^2$$

Combine:

$$V = \frac{F_{A0} - F_A}{kC_A^2}$$

$$F_{A0} = v_0 C_A = 3\frac{dm^3}{s} \cdot \frac{2molA}{dm^3} = \frac{6molA}{s}$$

$$F_A = v_0 C_A = 3\frac{dm^3}{s} \cdot \frac{0.1molA}{dm^3} = \frac{0.3molA}{s}$$

$$V = \frac{(6-0.3)\dfrac{mol}{s}}{(0.03\dfrac{dm^3}{mol.s})(0.1\dfrac{mol}{dm^3})^2} = 19,000dm^3$$