Synopsis for Chapter 1 – Mole Balances

Mole balances are the first building block of the chemical reaction engineering algorithm.
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 5.

Key to Nomenclature

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

E.g., AA P1-5 means that this problem or one of the other problems with the prefix AA is always assigned for this chapter and that Problem ●AA P1-2 will always be assigned as will ●AA P1-6.

Alternates: In problems that have a dot in conjunction with AA means that one of the problems, 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 student to solve the problem.

●AA P1-1. (30 min) This problem helps the student explore the example problems in this chapter. Part (a) shows an easier way to relate the rates of reaction between A, B, C and D. Part (b) is an excellent problem.

●AA P1-2. The Interactive Computer Games (ICGs) have been found to be a great motivation for this material.

●AA P1-3. (15 min) Old example problem to reinforce stoichiometry in mole balance.

S P1-4. (60 min) Problem reinforces wide range of applications of CRE and problem is given in the web module which can be accessed from the Web Home Page (*www.umich.edu/~elements*). 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 and given to the students in class. Part (g) is usually omitted.

AA P1-5. (30 min) A hint of things to come on sizing reactors. Fairly straight forward problem to make a calculation. 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.

AA P1-6. (45 min) I **always** assign this problem so that the students will learn how to use POLYMATH/MatLab before needing it for chemical reaction engineering problems.

I P1-7. (30 min) Helps develop critical thinking and analysis.

AA P1-8. (20 min) **Puzzle problem** to identify errors in the solution. Many students especially those who enjoy working Sudoku or crossword puzzles enjoy working these types of problems.

Solutions for Chapter 1 – Mole Balances

Q1-1 Individualized solution.

Q1-2 Individualized solution.

Q1-3 Individualized solution.

Q1-4(a) Individualized solution.

Q1-4 (b) The negative rate of formation of a species indicates that its concentration is decreasing as the reaction precedes i.e. the species is being consumed in the course of the reaction. A positive number indicates production of the particular compound.

Q1-5 (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.

Q1-5 (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.

Q1-5 (c)

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

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

Q1-5 (d)

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

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

Q1-5 (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.

Q1-6

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

$$0 = F_{j0} - F_j + r_j V$$

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

$$=> \quad 0 = (F_{j0} - F_j) + r_j' \rho_b V$$

Hence the above equation becomes

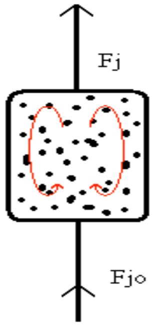
$$W = \frac{F_{j0} - F_j}{-r_j^{'}}$$

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:

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



P1-1 (a) Individualized Solution

P1-1(b)

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:

$$V = \frac{C_{A0}v_0 - C_Av_0}{kC_A} = \frac{C_{A0}v_0(1-0.1)}{0.1kC_{A0}} = \frac{(10\text{dm}^3/\text{min})(0.9)}{(0.23\text{min}^{-1})(0.1)}$$

***V* = 391.3 m^3**

P1-1(c)

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

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 $t = t$, $N_A = (0.01)N_{AO}$

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

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

t = 20 min

P1-2 Individualized solution.

P1-3

The correct answer is b.)

a.) Has the wrong sign for $-\int^V r_A dV$ and $-2\int^V r_A dV$. Should be $+\int^V r_A dV$ and $+2\int^V r_A dV$

b.) All are correct

c.) Wrong sign for F_c, should be $-F_c$.

d.) Wrong sign for $-\int^V r_C dV$, should be $+\int^V r_C dV$

P1-4

Given

$A = 2*10^{10}\, ft^2$

$T_{STP} = 491.69 R$

$H = 2000\, ft$

$V = 4*10^{13}\, ft^3$

T = 534.7 °R

P_O = 1atm

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

y_A = 0.02

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

C = $4*10^5$ cars

F_S = CO in Santa Ana winds

F_A = CO emission from autos

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

P1-4 (a)

Total number of lb moles gas in the system:

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

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

P1-4 (b)

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

$$F_A = y_A F_T = y_A \cdot v_A C_T \Big|_{STP}^{\bullet \text{ no. of cars}}$$

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

F_A = 6.685 x 10^4 lb mol/hr

P1-4 (c)

Wind speed through corridor is U = 15mph

W = 20 miles

The volumetric flowrate in the corridor is

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

P1-4 (d)

Molar flowrate of CO into basin from Sant Ana wind.

$$F_S := v_0 \cdot C_S$$

$= 1.673 \times 10^{13}\ \text{ft}^3/\text{hr} \times 2.04\times10^{-10}\ \text{lbmol/ft}^3$

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

P1-4 (e)

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

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

P1-4 (f)

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

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

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

P1-4 (g)

Time for concentration to reach 8 ppm.

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

From (f),

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

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

t = 6.92 hr

P1-4 (h)

(1) $t_o = 0$ $\quad$ $t_f = 72$ hrs

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

$v_o = 1.67\text{E+}12\ \text{ft}^3/\text{hr}$ $\quad$ b = 3.00E+04 lbmol/hr

$F_s = 341.23$ lbmol/hr $\quad$ $V = 4.0\text{E+}13\ \text{ft}^3$

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

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

P1-4 (h) continued

See Polymath program P1-4-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
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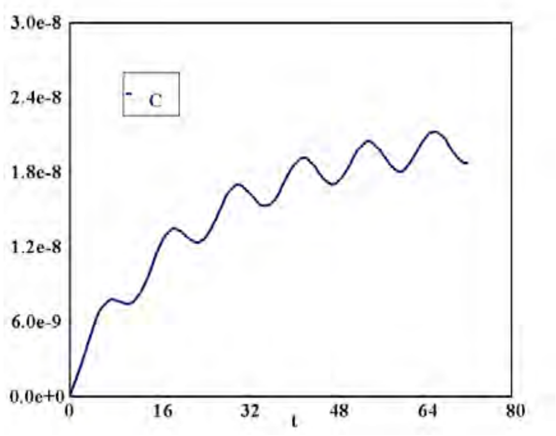


(2) t_f = 48 hrs $F_s = 0$ $a + b\sin\left(\pi\frac{t}{6}\right) - v_oC_{co} = V\frac{dC_{co}}{dt}$

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

See Polymath program P1-4-h-2.pol.

POLYMATH Results

Calculated values of the DEQ variables

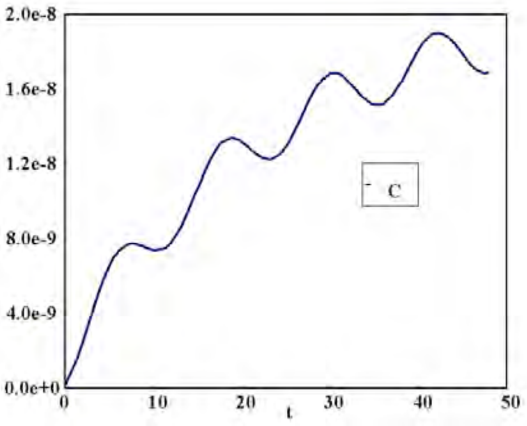
Variable	initial value	minimal value	maximal value	final value
T	0	0	72	72
C	2.0E-10	2.0E-10	2.134E-08	1.877E-08
v0	1.67E+12	1.67E+12	1.67E+12	1.67E+12
a	3.5E+04	3.5E+04	3.5E+04	3.5E+04
b	3.0E+04	3.0E+04	3.0E+04	3.0E+04
F	341.23	341.23	341.23	341.23
V	4.0E+13	4.0E+13	4.0E+13	4.0E+13

P1-4 (h) continued

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.

P1-5 (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 dm^3**

PFR: 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

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

Hence **V = 99 dm^3**

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

P1-5 (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}

$$\rightarrow V = \frac{(10dm^3/hr)(0.5mol/dm^3)(0.99)}{(0.36hr^{-1})(0.01*0.5mol/dm^3)}$$ => **V = 2750 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 = 0.0001s^{-1} = 0.0001 x 3600 hr^{-1}= 0.36 hr^{-1}

Substituting the values in above equation we get **V = 127.9 dm^3**

P1-5 (c)

- r_A = kC_A^2 with k = 300 dm^3/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

$$V = \frac{(10dm^3/hr)(0.5mol/dm^3)(0.99)}{(300dm^3/mol.hr)(0.01*0.5mol/dm^3)^2}$$ => **V = 660 dm^3**

PFR:

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

Integrating

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

$$=> V=\frac{10dm^3/hr}{300dm^3/mol.hr}\left(\frac{1}{0.01C_{A0}}-\frac{1}{C_{A0}}\right) \quad = \mathbf{6.6\ dm^3}$$

P1-5 (d)

$C_A = .001C_{A0}$

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

Constant Volume $V=V_0$

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

Zero order:

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

First order:

$$t=\frac{1}{k}\ln\left(\frac{C_{A0}}{C_A}\right)=\frac{1}{0.0001}\ln\left(\frac{1}{.001}\right)=69078s=19.19h$$

Second order:

$$t=\frac{1}{k}\left[\frac{1}{C_A}-\frac{1}{C_{A0}}\right]=\frac{1}{300}\left[\frac{1}{0.5\cdot 0.001}-\frac{1}{0.5}\right]=6.66h$$

P1-6 (a)

Initial number of rabbits, x(0) = 500

Initial number of foxes, y(0) = 200

Number of days = 500

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

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

Given,

$k_1=0.02day^{-1}$

$k_2=0.00004/(day\times foxes)$

$k_3=0.0004/(day\times rabbits)$

$k_4=0.04day^{-1}$

See Polymath program P1-6-a.pol.

POLYMATH Results

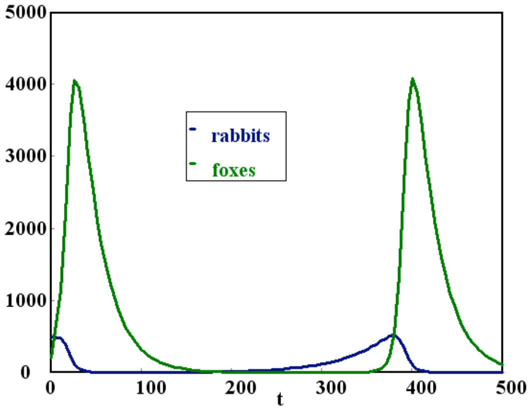
Calculated values of the DEQ variables

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

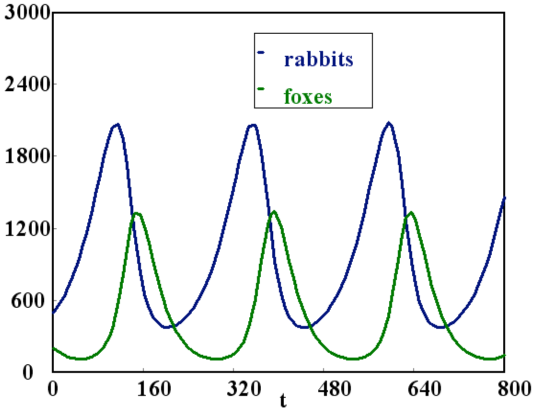
ODE Report (RKF45)

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)

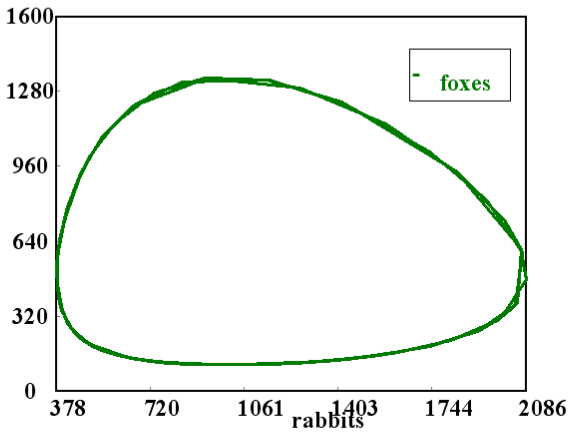
Explicit equations as entered by the user
[1] k1 = 0.02
[2] k2 = 0.00004
[3] k3 = 0.0004
[4] k4 = 0.04



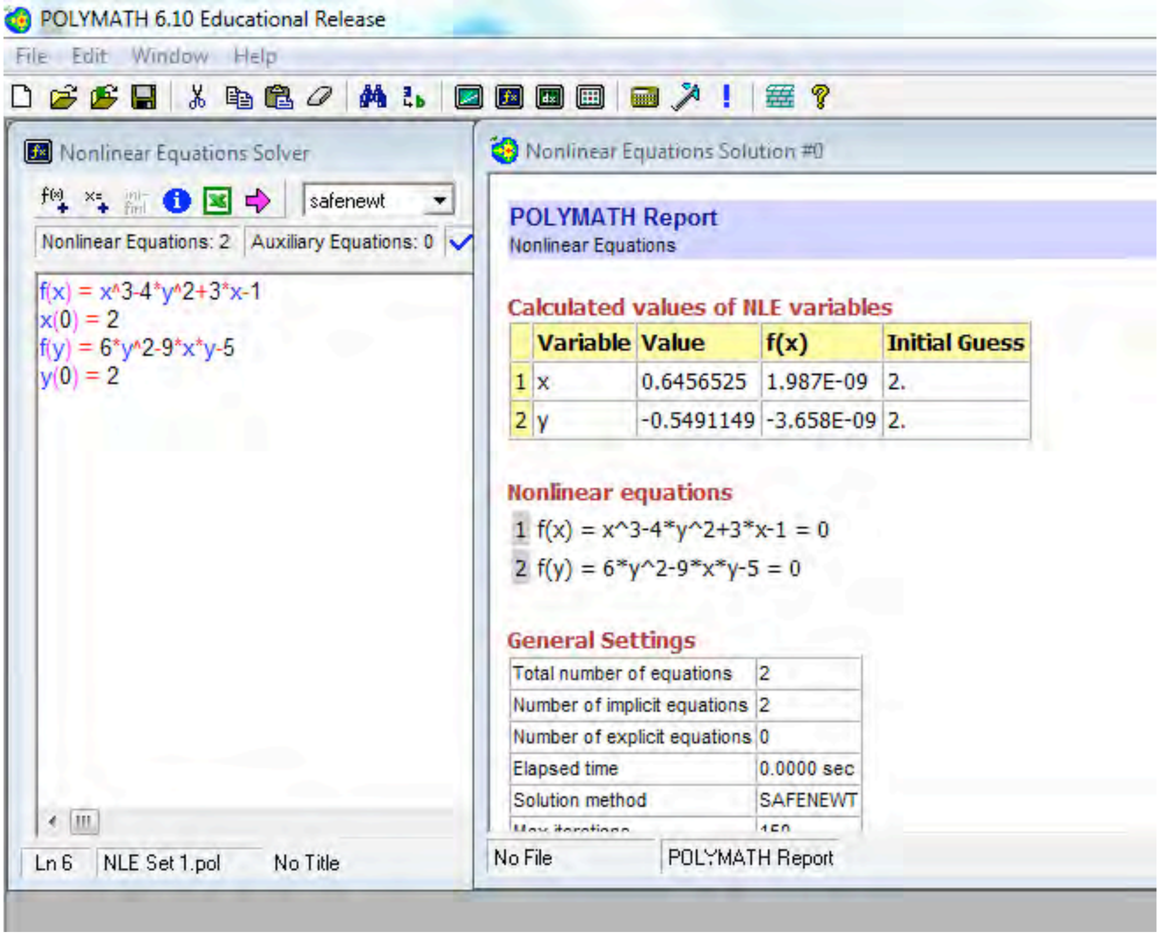
When, $t_{final} = 800$ and $k_3 = 0.00004/(day \times rabbits)$



Plotting rabbits vs. foxes



P1-6 (b)



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f(x) = x^3-4*y^2+3*x-1
x(0) = 2
f(y) = 6*y^2-9*x*y-5
y(0) = 2
```

POLYMATH Report
Nonlinear Equations

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	x	0.6456525	1.987E-09	2.
2	y	-0.5491149	-3.658E-09	2.

Nonlinear equations

1 f(x) = x^3-4*y^2+3*x-1 = 0

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

General Settings

Total number of equations	2
Number of implicit equations	2
Number of explicit equations	0
Elapsed time	0.0000 sec
Solution method	SAFENEWT

P1-7 Enrico Fermi Problem

P1-7(a) Population of Chicago = 4,000,000
Size of Households = 4
Number of Households = 1,000,000
Fraction of Households that own a piano = 1/5
Number of Pianos = 200,000

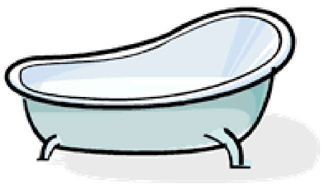
Number of Tunes/year per Piano = 1
Number of Tunes Needed Per Year = 200,000
Tunes per day = 2

Tunes per year per tuner = $\frac{250\,days}{yr} \times \frac{2}{day}$ = 500/yr/tuner

$$\frac{200{,}000\,tunes}{yr} \times \frac{1}{500\,tunes\,/\,yr\,/\,tuner} = \text{ 400 Tuners}$$

P1-7(b) Assume that each student eats 2 slices of pizza per week.
Also, assume that it is a 14” pizza, with 8 pieces.
Hence, the area of 1 slice of pizza = 19.242 inch^2 = 0.012414 m^2
Thus, a population of 20000, over a span of 4 months, eats
20000 * 2 slices * 4 months * 4 weeks/month = 640000 slices of pizza, with a total area of 640000 * 0.012414 m^2 = 7945 m^2 of pizza in the fall semester.

P1-7(c) Assume you drink 1L/day
Assume you live 75 years*365days/year = 27375 days
1L/day*27375 days = 27375 L drank in life
Bathtub dimensions: 1m*0.7m*0.5m = 0.35m^3 = 350L/tub
Bathtubs drunk = 27375L*1tub/350L = 78 tubs



P1-7(d) Jean Valjean, Les Misérables.

P1-8

Mole Balance:

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

Rate Law :

$$-r_A = kC_A^2$$

Combine:

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

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

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

$$V = \frac{(6-0.3)\frac{mol}{s}}{(0.03\frac{dm^3}{mol.s})(0.1\frac{mol}{dm^3})^2} = 1900dm^3$$

The incorrect part is in step 6, where the initial concentration has been used instead of the exit concentration.