

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

N = Never assigned

E.g., means problem ● **P1-3_B** will be assigned every time I teach the course, problem **AA P1-8** means that this problem or one of the other problems with the prefix **AA** is always assigned for this chapter, Problem **I P1-2** will be infrequently assigned, Problem **O P1-6_B** will often be assigned, and Problem **S P3-16_B** is seldom assigned.

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.

- **Q1-1_A** (9 seconds) Questions Before Reading (**QBR**).
 - (a) John Falconer at the University of Colorado gives workshops on *Teaching* in which he points out that students have a better comprehension if they ask themselves a question before reading the text. The first question of each chapter, Q1, is just such a question.
 - (b) The students are asked, at a minimum read through the *Questions* to help put the chapter and their studies in perspective.
 - (c) I encourage using the i>Clicker questions.
- **Q1-2_A** (8-10 min) i>Clicker
- **Q1-5_A** (5-75 min) through **Q1-12_A**. To get a “feel” of the resources available, the students should spend a total of about 50-75 minutes on these questions.

Computer Simulations and Experiments (5-15 minutes per simulation)

These problems are interactive and are a minor paradigm shift in the way we use homework problems. Here the students are asked to explore the reaction and the reactor in which they occur to get an intuitive feel and understanding of the reactor system. This procedure is called **Inquiry Based Learning (IBL)**.

- **P1-1_A** (10-15 min) Good introduction to the use of Wolfram and Python.

Problems

- I **P1-2_B** (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.

- **P1-3_B** (45 min) I **always** assign this problem so that the students will learn how to use Polymath/MATLAB, Wolfram and Python before needing it for chemical reaction engineering problems. Most problems will use either Polymath or MATLAB to solve the end of chapter problems.
 - **P1-4_A** (30 min) The Interactive Computer Games (ICGs) have been found to be a great motivation for this material. This ICG will help student AIChE chapters prepare for the Jeopardy Competition at the Annual AIChE Meeting.
 - **P1-5_A** (10 min) Old Exam Question (OEQ) to reinforce the convention and stoichiometry in mole balances.
 - **P1-6_B** (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.
 - ! **P1-7_A** (30 min) Helps develop critical thinking and analysis.
 - AA P1-8_A** (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

Useful Links:

1. Click on the link given below to download Wolfram/python codes for Ch-1
<http://umich.edu/~elements/5e/01chap/obj.html#/>
 2. Click on the link given below to view Wolfram tutorial (for running Wolfram Codes)
http://umich.edu/~elements/5e/software/Wolfram_LEP_tutorial.pdf
 3. Click on the link given below to view Polymath tutorial (for running Polymath Codes)
http://umich.edu/~elements/5e/tutorials/Polymath_LEP_tutorial.pdf
-

Q1-1 Individualized solution.

Q1-2 Individualized solution.

Q1-3

For CSTR:

$$V = \frac{F_{A0} X_A}{-r_{A,exit}} = \frac{F_{A0} X_A}{k C_A} = \frac{v_0 C_{A0} X_A}{k C_{A0} (1 - X_A)} = \frac{v_0 X_A}{k (1 - X_A)} = \frac{10 * 0.9}{0.23 * (0.1)} = 391.3 \text{ dm}^3$$

Q1-4 Individualized solution.

Q1-5 Individualized solution

Q1-6 Individualized solution

Q1-7 (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

Q1-7 (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

Q1-7 (c)

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

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

Q1-7 (d)

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

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

Q1-7 (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.

Q1-8 Individualized solution.


Q1-9 Individualized solution.


Q1-10 Individualized solution.


Q1-11 Individualized solution.


Q1-12 Individualized solution.

P1-1 (a) Example 1-3

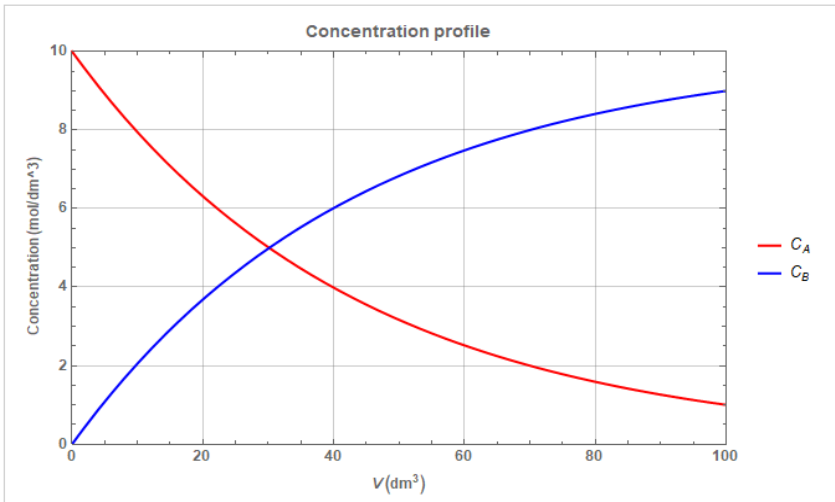
Rate constant, k (min⁻¹) 

0.23 

Volumetric flowrate, v_0 (dm³/min) 

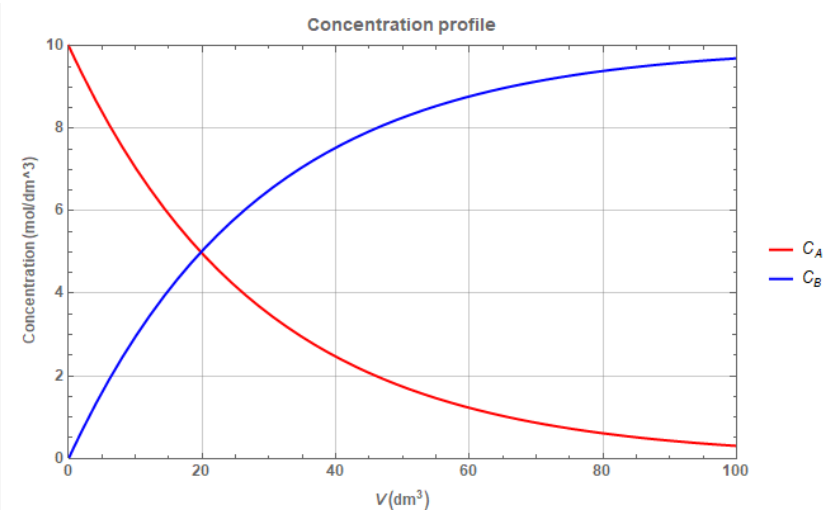
10 

profile Concentration Rate



The above graph represents initial C_A and C_B profiles for $k=0.23$ and $v_0 = 10$.

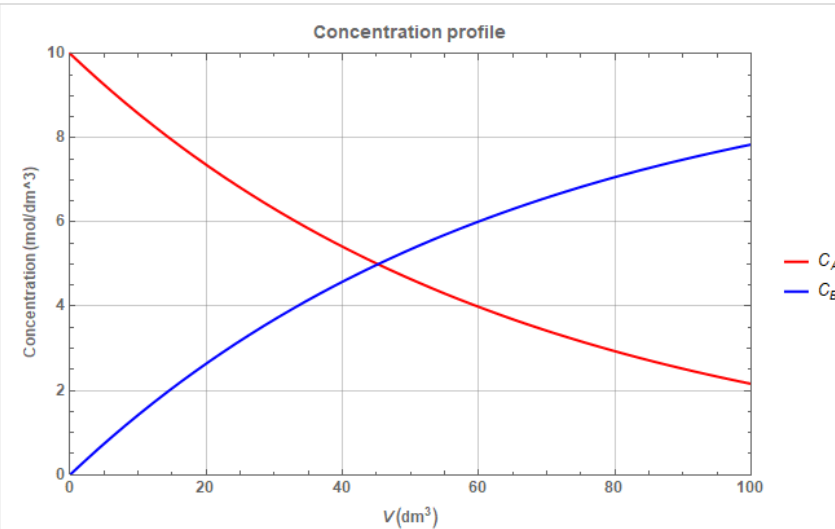
(i) With an increase in k (lets take $k = 0.35$) for same volume and v_0 , C_A decreases and C_B increases



Now lets make $k=0.23$ (initial value) and make an increase in v_0 (change from 10 to 15) for same volume.

We notice that now C_A increases and C_B decreases.

All of these graphs of concentration profiles are taken from Wolfram player by shifting the sliders.



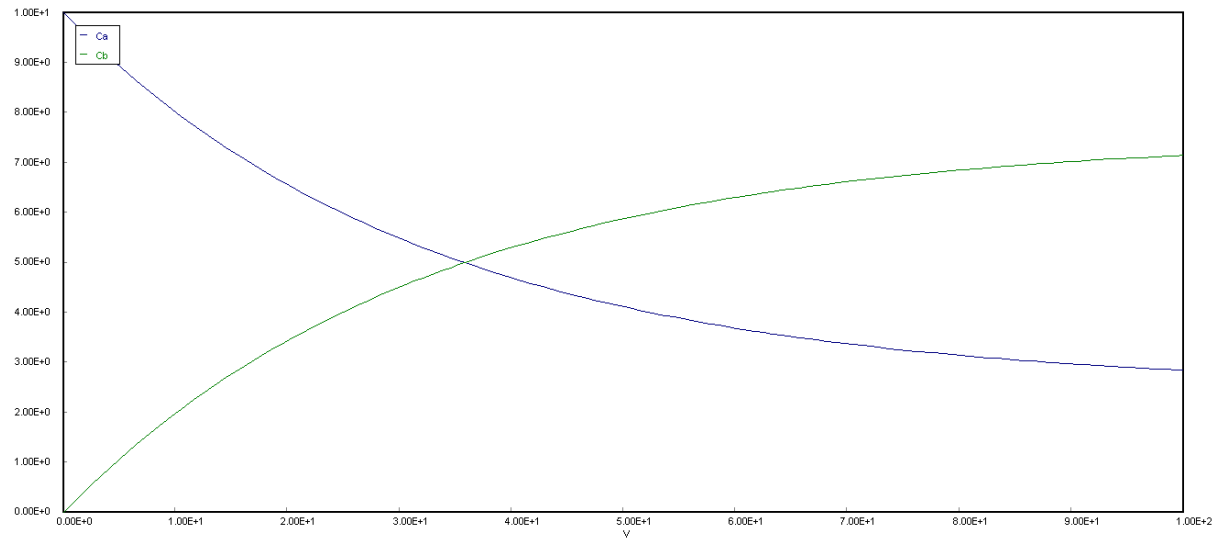
We can observe that varying rate constant has more effect on concentration profiles as compared to varying volumetric flow rate.

- (ii) C_A decreases and C_B increases with an increase in k and K_e , and a decrease in v_0 for the same volume.
- (iii) Individualized solution
- (iv) See the following polymath code:

Polymath Code:

```
d(Ca)/d(V) = ra / v0
d(Cb)/d(V) = rb / v0
k = 0.23
Ke=3
ra = -k * (Ca-Cb/Ke)
rb = -ra
v0 = 10
V(0)=0
V(f)=100
Ca(0)=10
Cb(0)=0
```

Output:



POLYMATH Report
Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	10.	2.849321	10.	2.849321
2	Cb	0	0	7.150679	7.150679
3	k	0.23	0.23	0.23	0.23
4	Ke	3.	3.	3.	3.
5	ra	-2.3	-2.3	-0.1071251	-0.1071251
6	rb	2.3	0.1071251	2.3	0.1071251
7	V	0	0	100.	100.
8	v0	10.	10.	10.	10.

Differential equations

- 1 $d(Ca)/d(V) = ra / v_0$
- 2 $d(Cb)/d(V) = rb / v_0$

Explicit equations

- 1 $k = 0.23$
- 2 $K_e = 3$
- 3 $r_a = -k \cdot (C_a - C_b/K_e)$
- 4 $r_b = -r_a$
- 5 $v_0 = 10$

P1-2

Given

$$\begin{aligned}
 A &= 2 \times 10^{10} \text{ ft}^2 & T_{STP} &= 491.69 R & H &= 2000 \text{ ft} \\
 V &= 4 \times 10^{13} \text{ ft}^3 & T &= 534.7^\circ R & P_0 &= 1 \text{ atm} \\
 R &= 0.7302 \frac{\text{atm} \cdot \text{ft}^3}{\text{lbmol} \cdot R} & y_A &= 0.02 & C_S &= 2.04 \times 10^{-10} \frac{\text{lbmol}}{\text{ft}^3} & C &= 4 \times 10^5 \text{ cars} \\
 F_S &= \text{CO in Santa Ana winds} & F_A &= \text{CO emission from autos} & v_A &= 3000 \frac{\text{ft}^3}{\text{hr}} \text{ per car at STP}
 \end{aligned}$$

P1-2 (a)

Total number of lb moles gas in the system:

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

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

P1-2 (b)

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

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

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

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

P1-2 (c)

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

$W = 20 \text{ miles}$

The volumetric flowrate in the corridor is

$$v_0 = U \cdot W \cdot H = (15 \times 5280)(20 \times 5280)(2000) \text{ ft}^3/\text{hr} = 1.673 \times 10^{13} \text{ ft}^3/\text{hr}$$

P1-2 (d)

Molar flowrate of CO into basin from Santa Ana wind.

$$\begin{aligned}
 F_S &:= v_0 \cdot C_S \\
 &= 1.673 \times 10^{13} \text{ ft}^3/\text{hr} \times 2.04 \times 10^{-10} \text{ lbmol}/\text{ft}^3 \\
 &= 3.412 \times 10^3 \text{ lbmol/hr}
 \end{aligned}$$

P1-2 (e)

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

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

P1-2 (f)

$t = 0, C_{CO} = C_{CO0}$

$$\int_0^t dt = V \int_{C_{CO0}}^{C_{CO}} \frac{dC_{CO}}{F_A + F_S - v_o C_{CO}}$$

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

P1-2 (g)

Time for concentration to reach 8 ppm.

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

From (f),

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

$$= \frac{4 \text{ ft}^3}{1.673 \times 10^{13} \frac{\text{ft}^3}{\text{hr}}} \ln \left(\frac{6.7 \times 10^4 \frac{\text{lbmol}}{\text{hr}} + 3.4 \times 10^3 \frac{\text{lbmol}}{\text{hr}} - 1.673 \times 10^{13} \frac{\text{ft}^3}{\text{hr}} \times 2.04 \times 10^{-8} \frac{\text{lbmol}}{\text{ft}^3}}{6.7 \times 10^4 \frac{\text{lbmol}}{\text{hr}} + 3.4 \times 10^3 \frac{\text{lbmol}}{\text{hr}} - 1.673 \times 10^{13} \frac{\text{ft}^3}{\text{hr}} \times 0.51 \times 10^{-8} \frac{\text{lbmol}}{\text{ft}^3}} \right)$$

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

P1-2 (h)

(1)

$$t_o = 0$$

$$t_f = 72 \text{ hrs}$$

$$C_{CO} = 2.00\text{E-}10 \text{ lbmol/ft}^3$$

$$a = 3.50\text{E+}04 \text{ lbmol/hr}$$

$$v_o = 1.67\text{E+}12 \text{ ft}^3/\text{hr}$$

$$b = 3.00\text{E+}04 \text{ lbmol/hr}$$

$$F_s = 341.23 \text{ lbmol/hr}$$

$$V = 4.0\text{E+}13 \text{ ft}^3$$

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

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

See the following polymath code:

Polymath Code:
v0 = 1.67*10^12
A= 35000
B = 30000
F = 341.23
V = 4*10^13
d(C)/d(t) = (A+B*sin(3.14*t/6)+F-v0*C)/V
C(0)=2.0e-10
t(0)=0
t(f)=72

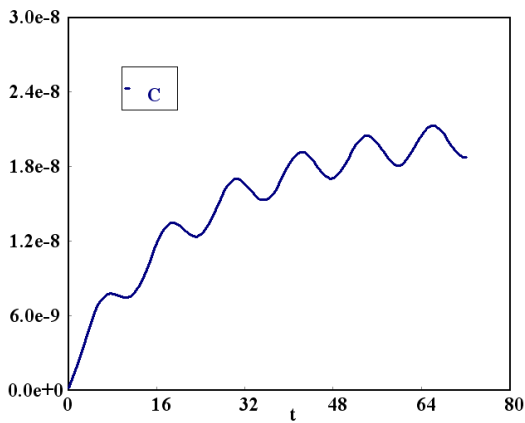
Output:
POLYMATH Report
Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	A	3.5E+04	3.5E+04	3.5E+04	3.5E+04
2	B	3.0E+04	3.0E+04	3.0E+04	3.0E+04
3	C	2.0E-10	2.0E-10	2.134E-08	1.877E-08
4	F	341.23	341.23	341.23	341.23
5	t	0	0	72.	72.
6	V	4.0E+13	4.0E+13	4.0E+13	4.0E+13
7	v0	1.67E+12	1.67E+12	1.67E+12	1.67E+12

Differential equations
1 d(C)/d(t) = (A+B*sin(3.14*t/6)+F-v0*C)/V

Explicit equations
1 v0 = 1.67*10^12
2 A = 35000
3 B = 30000
4 F = 341.23
5 V = 4*10^13



(2) $t_f = 48 \text{ hrs}$ $F_s = 0$ $a + b \sin\left(\pi \frac{t}{6}\right) - v_o C_{co} = V \frac{dC_{co}}{dt}$
Now solving this equation using POLYMATH we get plot between C_{co} vs t

Polymath Code:

```
v0 = 1.67*10^12
A = 35000
B = 30000
F = 341.23
V = 4*10^13
d(C)/d(t) = (A+B*sin(3.14*t/6)+F-v0*C)/V
C(0)=2.0e-10
t(0)=0
t(f)=48
```

Output:

POLYMATH Report
Ordinary Differential Equations

Calculated values of DEQ variables

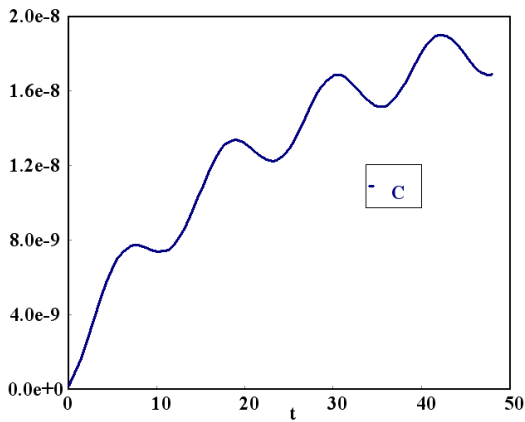
	Variable	Initial value	Minimal value	Maximal value	Final value
1	A	3.5E+04	3.5E+04	3.5E+04	3.5E+04
2	B	3.0E+04	3.0E+04	3.0E+04	3.0E+04
3	C	2.0E-10	2.0E-10	1.921E-08	1.71E-08
4	F	341.23	341.23	341.23	341.23
5	t	0	0	48.	48.
6	V	4.0E+13	4.0E+13	4.0E+13	4.0E+13
7	v0	1.67E+12	1.67E+12	1.67E+12	1.67E+12

Differential equations

1 $d(C)/d(t) = (A+B*\sin(3.14*t/6)+F-v0*C)/V$

Explicit equations

- 1 $v0 = 1.67*10^{12}$
- 2 $A = 35000$
- 3 $B = 30000$
- 4 $F = 341.23$
- 5 $V = 4*10^{13}$



P1-2 (i)

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 $b \rightarrow$ 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.

P1-3 (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,

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

See the following polymath code:

Polymath Code:

```
d(x)/d(t) = (k1*x)-(k2*x*y)
d(y)/d(t) = (k3*x*y)-(k4*y)
k1 = 0.02
k2 = 0.00004
k3 = 0.0004
k4 = 0.04
t(0)=0
t(f)=500
x(0)=500
y(0)=200
```

Output:

POLYMATH Report
Ordinary Differential Equations

Calculated values of DEQ variables

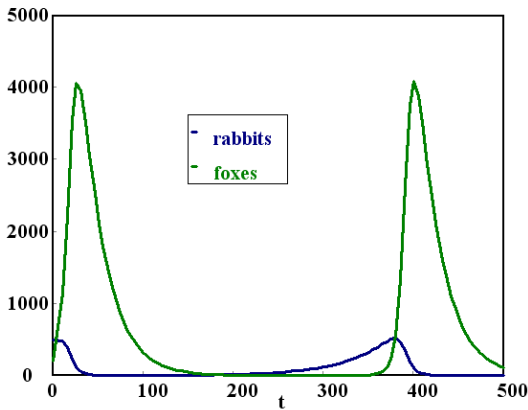
	Variable	Initial value	Minimal value	Maximal value	Final value
1	k1	0.02	0.02	0.02	0.02
2	k2	4.0E-05	4.0E-05	4.0E-05	4.0E-05
3	k3	0.0004	0.0004	0.0004	0.0004
4	k4	0.04	0.04	0.04	0.04
5	t	0	0	500.	500.
6	x	500.	2.962693	519.4002	4.219969
7	y	200.	1.128572	4099.517	117.6293

Differential equations

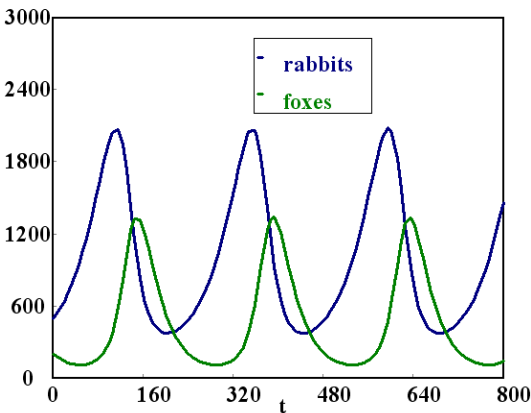
- 1 $d(x)/d(t) = (k_1*x)-(k_2*x*y)$
- 2 $d(y)/d(t) = (k_3*x*y)-(k_4*y)$

Explicit equations

- 1 $k_1 = 0.02$
- 2 $k_2 = 0.00004$
- 3 $k_3 = 0.0004$
- 4 $k_4 = 0.04$



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



POLYMATH Report

Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	k1	0.02	0.02	0.02	0.02
2	k2	4.0E-05	4.0E-05	4.0E-05	4.0E-05
3	k3	4.0E-05	4.0E-05	4.0E-05	4.0E-05
4	k4	0.04	0.04	0.04	0.04
5	t	0	0	800.	800.
6	x	500.	377.9769	2086.088	1467.831
7	y	200.	114.6959	1341.876	143.6569

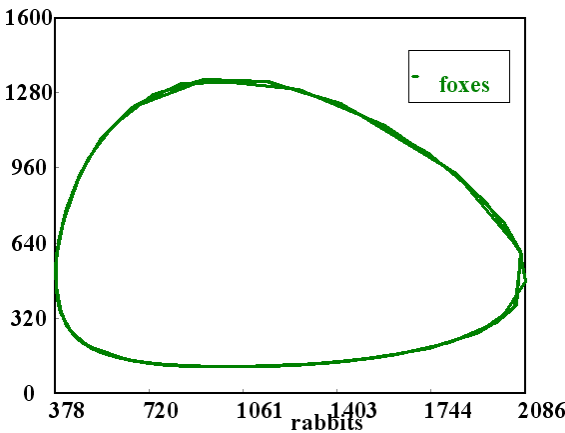
Differential equations

- 1 $d(x)/d(t) = (k_1 * x) - (k_2 * x * y)$
- 2 $d(y)/d(t) = (k_3 * x * y) - (k_4 * y)$

Explicit equations

- 1 $k_1 = 0.02$
- 2 $k_2 = 0.00004$
- 3 $k_3 = 0.00004$
- 4 $k_4 = 0.04$

Plotting rabbits vs. foxes

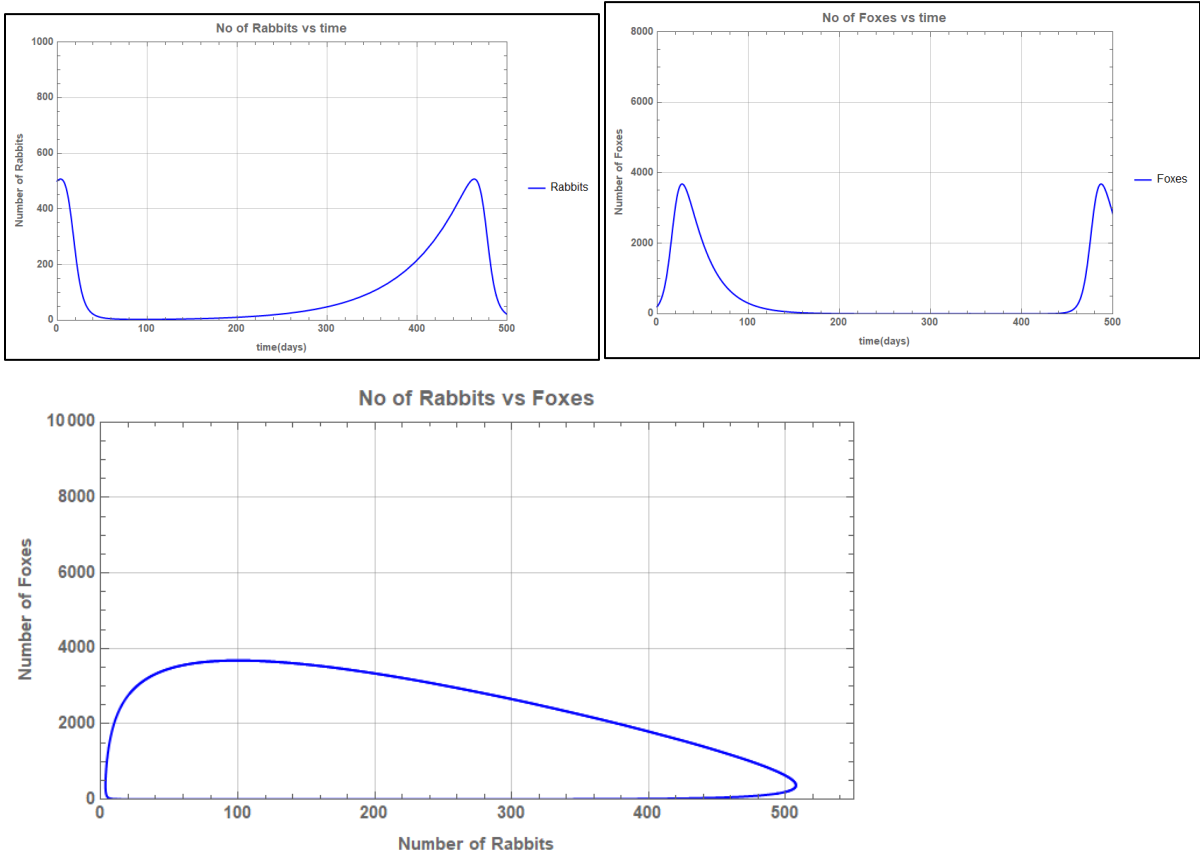


P1-3 (b)

By increasing k_4 and decreasing k_2 , foxes versus rabbits plot tends to become circular

P1-3 (c)

Below are the graphs when death rate is taken in to account



P1-3 (d)

To solve the system of equation, we can use Polymath Nonlinear Equation Solver

Polymath Code:

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

Polymath Output:

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	x	2.385039	2.53E-11	2.
2	y	3.797028	1.72E-12	2.

Nonlinear equations

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

P1-4 Individualized solution

P1-5

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 $+\int^V r_C dV$
-

P1-6 (a)

$-r_A = k$ 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 dm³**

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

P1-6 (b)

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

CSTR:

We have already derived that

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

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

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

PFR:

From above we already know that for a PFR

$$\frac{dC_A v_0}{dV} = r_A = -k C_A$$

Integrating

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

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

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

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

P1-6 (c)

$-r_A = kC_A^2$ with $k = 300 \text{ dm}^3 / \text{mol} \cdot \text{hr}$

CSTR:

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

Substituting all the values we get

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

PFR:

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

Integrating

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

$$\Rightarrow V = \frac{10 \text{ dm}^3 / \text{hr}}{300 \text{ dm}^3 / \text{mol} \cdot \text{hr}} \left(\frac{1}{0.01 C_{A0}} - \frac{1}{C_{A0}} \right) = 6.6 \text{ dm}^3$$

P1-6 (d)

$$C_A = 0.001 C_{A0}$$

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

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:

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

Second order:

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

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

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

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

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 = $19.242 \text{ inch}^2 = 0.012414 \text{ m}^2$

Thus, a population of 20000, over a span of 4 months, eats

$20000 * 2 \text{ slices} * 4 \text{ months} * 4 \text{ weeks/month} = 640000 \text{ slices of pizza}$, with a total area of
 $640000 * 0.012414 \text{ m}^2 = 7945 \text{ m}^2$ of pizza in the fall semester.

P1-7(c) Assume you drink 1L/day

Assume you live $75 \text{ years} * 365 \text{ days/year} = 27375 \text{ days}$

$1\text{L/day} * 27375 \text{ days} = 27375 \text{ L drunk in life}$

Bathtub dimensions: $1\text{m} * 0.7\text{m} * 0.5\text{m} = 0.35\text{m}^3 = 350\text{L/tub}$

Bathtubs drunk = $27375\text{L} * 1\text{tub}/350\text{L} = 78 \text{ tubs}$



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:

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

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

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

$$V = \frac{(6 - 0.3) \frac{\text{mol}}{\text{s}}}{(0.03 \frac{\text{dm}^3}{\text{mol.s}})(0.1 \frac{\text{mol}}{\text{dm}^3})^2} = 19000 \text{ dm}^3$$

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

Page intentionally blank

Synopsis for Chapter 2 – Conversion and Reactor Sizing

General: The overall goal of these problems is to help the student realize that if they have $-r_A = f(X)$ they can “design” or size a large number of reaction systems. It sets the stage for the algorithm developed in Chapter 5.

See Chapter 1 Synopsis for nomenclature guide to problem assignments.

Questions

- **Q2-1_A** (4 seconds) Questions Before Reading (**QBR**).
- **Q2-2_A** (20 min) Secondly, I also encourage going through the i>Clicker questions **AFTER** the students have completed all the reading and homework associated with this chapter.
- **Q2-4_A** (20-25 min) Firstly, I encourage students to take the Solomon/Felder Inventory of Learning Styles test (<https://www.engr.ncsu.edu/stem-resources/legacy-site/learning-styles/>) and then use Appendix I.2 to see how they can best use the text and interactive web materials.
- **Q2-5_A** (15 min) If a student did not visit the University of Colorado’s LearnChemE site in Chapter 1, I recommend they view one or two screencasts now.
- ! **Q2-6_A** (7 min) NFPA. Now is also the time to visit the tutorials of the Safety Website (<http://umich.edu/~safeche/>) to become acquainted with the wealth of safety resources available on the safety website.

Interactive Computer Games (ICG)

- **P2-1_A** (20-25 min) Because this interactive game has so many choices of reactions to maximize the conversion, the time to play the game is a little longer than other ICGs.

Problems

- **P2-2_A** (45 min) Helps the student explore the example problems in this chapter. Parts (d) and (e) take a little longer than the other parts.
- **P2-3_B** (35 min) Reinforces use of the Levenspiel plots.
- AA **P2-4_B** (40 min) Requires the student to construct a Levenspiel plot. Alternative to problems **P2-5_B**, **P2-7_B**, and **P2-10_C**.
- AA **P2-5_B** (30 min) This problem is a reasonably challenging trial and error problem that reinforces Levenspiel’s plots and reactor staging.
- **P2-6_B** (45 min) Novel application of Levenspiel plots from an article in CEE by Professor Alice Gast formerly at Massachusetts Institute of Technology, now President of Imperial College, London.
- AA **P2-7_B** (30 min) Straight forward problem alternative to problems **P2-4_B** and **P2-10_C**. The answer gives ridiculously large reactor volume. The point is to encourage the student to question their numerical answers. Alternative to **P2-4_B**, **P2-5_B** and **P2-10_C**.
- ! **P2-8_A** (30 min) Helps the students get a feel of real reactor sizes.
- **P2-9_D** (2 min) Great motivating problem. Students from all universities around the world remember this problem long after the course is over.

AA P2-10_c (45 min) Alternative problem to **P2-4_B**, **P2-5_B**, and **P2-7_B**.

- **P2-11_B** (45 min) This problem is a departure from the other problems in this chapter **because it is a batch reactor**.
-

Solutions for Chapter 2 – Conversion and Reactor Sizing

Q2-1 Individualized solution.

Q2-2 Individualized solution.

Q2-3 Individualized solution.

Q2-4 Individualized solution.

Q2-5 Individualized solution.

Q2-6 Individualized solution.

P2-1 The key for decoding the algorithm to arrive at a numerical score for the Interaction Computer Games (ICGs) is given at the front of this Solutions Manual.

P2-2 (a) For a batch reactor,

$$t = N_{A0} \int_0^X \frac{dX}{-r_A V}$$

$$400 \text{ dm}^3 = 400/1000 \text{ m}^3 = 0.4 \text{ m}^3$$

For 10% conversion,

$$t = (100/0.4) \int_0^{0.1} \frac{dX}{-r_A}$$

The area under the curve of $1/-r_A$ vs X needs to be found out till $X=0.1$

Using trapezoidal rule,

$$\text{Area} = 0.5 \cdot (2.22 + 2.7) \cdot 0.1 = 0.246$$

$$\text{Thus, time} = 250 \cdot 0.246 = 61.5 \text{ s}$$

To find BR times for $X=0.5$ and $X=0.8$, apply Simpson's rule and find time in similar way as described above

P2-2 (b) Example 2-1 through 2-3

For Example, 2-1

If flow rate F_{A0} is cut in half.

$v_1 = v/2$, $F_1 = F_{A0}/2$ and C_{A0} will remain same.

Therefore, volume of CSTR in example 2-1,

$$V_1 = \frac{F_1 X}{-r_A} = \frac{1}{2} \frac{F_{A0} X}{-r_A} = \frac{1}{2} 6.4 = 3.2$$