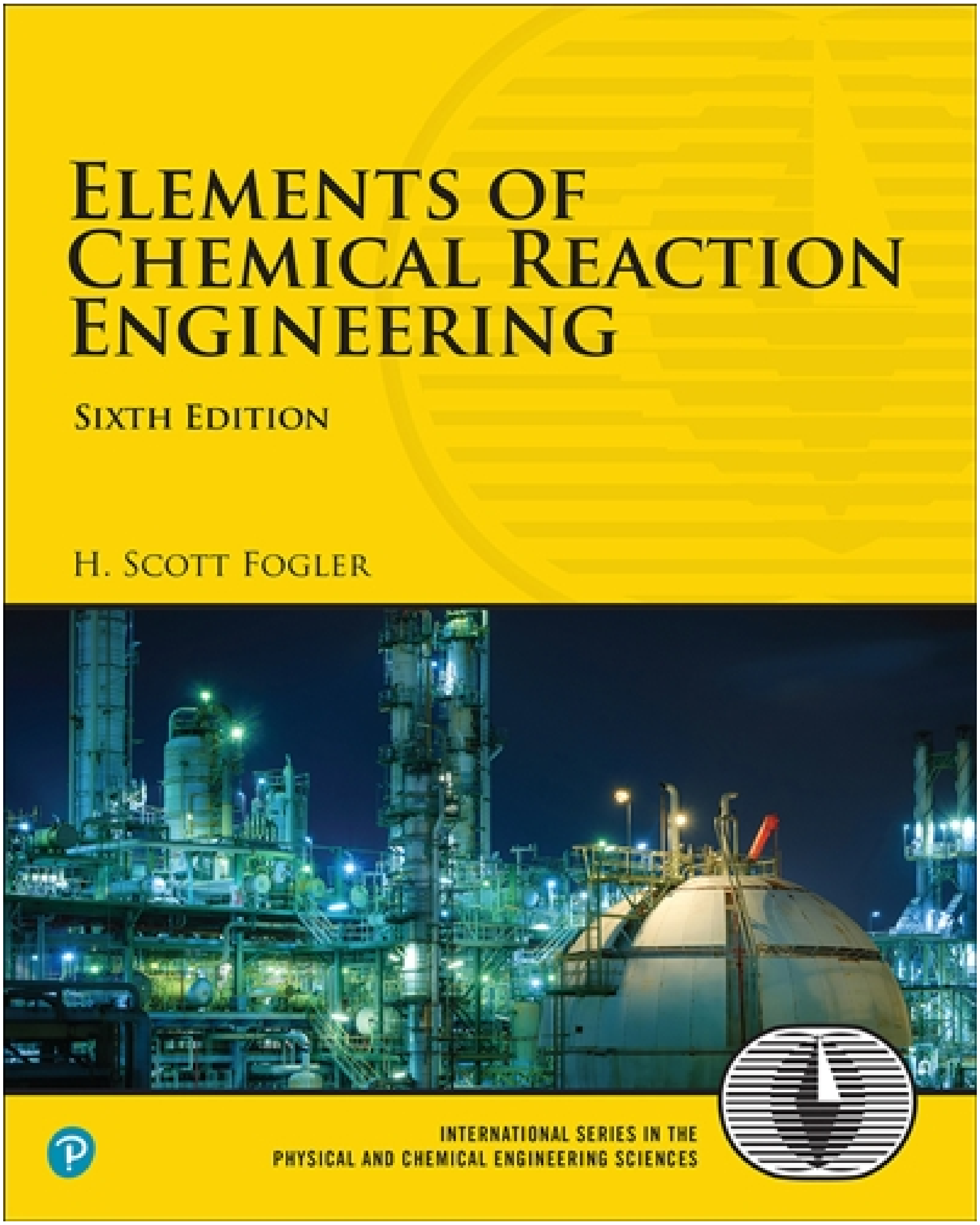
Solutions for Elements of Chemical Reaction Engineering 6th Edition by Fogler



Solutions

Solutions Manual for

Elements of Chemical Reaction Engineering

Sixth Edition

H. Scott Fogler
Ame and Catherine Vennema Professor of Chemical Engineering and
The Arthur F. Thurnau Professor at the University of Michigan,
Ann Arbor, Michigan

October, 2020

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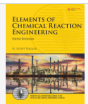
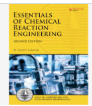
(2020)





Essentials of
Chemical Reaction Engineering
(2016)

Welcome to Chemical Reaction Engineering!

ENHANCED BY Google

Select Chapter

Let's Get Started

- Lecture Notes
- Software
- Undergraduate (ChE 344) Homepage
- Graduate (ChE 528) Homepage
- Asychronous Learning
- Additional Textbook Websites

Additional Resources

- SafeChemE Website
- Interactive Computer Games
- Web Modules
- Thoughts on Problem Solving
- FAQs, Typos, and Updates
- Fun YouTube Videos

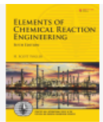
CLICK HERE TO ACCESS THE COMPLETE Solutions

INTERACTIVE COMPUTER GAMES (ICGs)

Elements of

Chemical Reaction Engineering

5th Edition



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Interactive Computer Games (ICGs)

The Interactive Computer Games (**ICGs**) listed below are contained on the *website below*. Game players can click on the Run from the website link to begin play each ICG title. Note that there will be a pause while the game is loaded from our servers. Alternately, one can use the Install to PC link to install each game on the PC. This installation will typically install an icon on the desktop. **Please take the default location for the installation files.** Detailed instructions for installing and using the ICGs are available.

As these interactive games are played, the player will be asked a number of questions related to the corresponding material in the textbook. The computer will keep track of all the correct answers and at the end of the game will display a coded ***performance number*** that reflects how well the player mastered the material in the text. Instructors will have a manual to decode the performance number.

Note: The Interactive Computer Games may **NOT** work on approximately 10% of Windows machines. We can't find a specific reason, so if it doesn't work, please try them on a different Windows computer.

Kinetics Challenge I (Install to PC, Installation Instructions)
Quiz Show
Introduction to Kinetics
Description of the Module
Objectives for Chapter One

Staging (Install to PC, Installation Instructions)
Reactor Sequencing Optimization
Description of the Module
Objectives for Chapter Two

Kinetics Challenge II (Install to PC, Installation Instructions)
Quiz Show
Stoichiometry and Rate Laws
Description of the Module
Objectives for Chapter Four

Murder Mystery(Install to PC, Installation Instructions)
CSTR Volume Algorithm
Description of the Module
Objectives for Chapter Five

Tic Tac Toe (Install to PC, Installation Instructions)
Isothermal Reactor Design: Ergun, Arrhenius, and Van't Hoff Equations
Description of the Module
Objectives for Chapter Six

Ecology A Wetlands Problem (Install to PC, Installation Instructions)
Collection and Analysis of Rate Date: Ecological Engineering
Description of the Module
Objectives for Chapter Seven

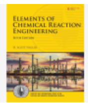
Great Race (Install to PC, Installation Instructions)
Multiple Reactions
Description of the Module
Objectives for Chapter Eight

Enzyme Man (Install to PC, Installation Instructions)
Enzyme Kinetics
Description of the Module
Objectives for Chapter Nine

Heterogeneous Catalysis (Install to PC, Installation Instructions)
Catalytic Rate Equations, Status: Alpha Release
Warning: This module is not fully tested. You may encounter abnormal behavior.
Description of the Module
Objectives for Chapter Ten

Heat Effects 1 (Install to PC,Installation Instructions)
Basketball Challenge
Mole and Energy Balances in a CSTR
Description of the Module
Objectives for Chapter Thirteen

Heat Effects 2 (Install to PC, Installation Instructions)
Effect of Parameter Variation on a PFR
Mole and Energy Balances in a PFR, Status: Alpha Release
Warning: This module is not fully tested. You may encounter abnormal behavior.
Description of the Module
Objectives for Chapter Thirteen



Interactive Computer Games (ICGs)

Kinetic Challenge 1

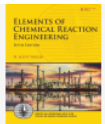
Kinetics Challenge 1 -- Quiz Show	
Concepts	Definitions of rates of reactions. Types of reactors. General mole balances for batch reactors, CSTR's and PFR's.
Time	29 minutes ± 10 minutes
Reference	Fogler: Chapter 1
Description	This game allows students to test their knowledge about general mole balance equations, reaction rate laws, and different types of reactions and reactors. Individual students will find themselves going head-to-head against computer opponents in an interactive game with timed responses. Twenty multiple-choice questions are selected from a pool of approximately 100 possible questions, so the game will be different every time. The questions fall under four main categories: mole balance, reactions, rate laws, and reactor types; and there are five difficulty levels within each category. Each correct answer will earn the student a given number of points; the more difficult the question, the higher the point values.

The student has 25 seconds to choose the correct answer. The module responds to the student's choice, either reinforcing the reasoning for a correct answer, or immediately clarifying a misunderstanding if an incorrect answer is entered. If no response is entered within the time limit, or if an incorrect response is entered, the points are lost, and one of the computer competitors tries to answer the question:

CLICK HERE TO ACCESS THE COMPLETE Solutions

LIVING EXAMPLE PROBLEMS (LEPs)

Elements of
Chemical Reaction Engineering
5th Edition



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Chapter 12: Steady-State Nonisothermal Reactor Design: Flow Reactors with Heat Exchange

Living Example Problems

The following examples can be accessed with Polymath™, MATLAB™, or Wolfram CDF Player™.

Living Example Problem	Polymath™ Code	Matlab Code	Wolfram CDF Code	AspenTech ™
Example 12-1 Isomerization of Normal Butane with Heat Exchanger	a) Co-current: LEP-12-1a.pol b) Countercurrent: LEP-12-1b.pol c) Constant T_a: LEP-12-1c.pol d) Adiabatic: LEP-12-1d.pol	a) Co-current: LEP-12-1a.zip b) Countercurrent: LEP-12-1b.zip c) Constant T_a: LEP-12-1c.zip d) Adiabatic: LEP-12-1d.zip	a) Co-current: LEP-12-1a.cdf b) Countercurrent: LEP-12-1b.cdf c) Constant T_a: LEP-12-1c.cdf d) Adiabatic: LEP-12-1d.cdf	--
Example 12-2 Production of Acetic Anhydride	a) Adiabatic: LEP-12-2a.pol b) Constant T_a: LEP-12-2b.pol c) Co-current LEP-12-2c.pol d) Countercurrent: LEP-12-2d.pol	a) Adiabatic: LEP-12-2a.zip b) Constant T_a: LEP-12-2b.zip c) Co-current: LEP-12-2c.zip d) Countercurrent: LEP-12-2d.zip	a) Adiabatic: LEP-12-2a.cdf b) Constant T_a: LEP-12-2b.cdf c) Co-current: LEP-12-2c.cdf d) Countercurrent: LEP-12-2d.cdf	a) Adiabatic: Tutorial, ASPEN Backup File b) Constant Heat Exchange: Tutorial, ASPEN Backup File
Example 12-3 Production of Propylene Glycol in an Adiabatic CSTR	--	--	LEP-12-3.cdf	--
Example 12-4 CSTR with a Cooling Coil	LEP-12-4.pol	LEP-12-4.zip	LEP-12-4.cdf	--
Example 12-5 Parallel Reaction in a PFR with Heat Effects	LEP-12-5.pol	LEP-12-5.zip	LEP-12-5.cdf	--
Example 12-6 Multiple Reactions in a CSTR	LEP-12-6.pol Alternative Solution: LEP-12-6a.pol	LEP-12-6.zip	LEP-12-6.cdf	--
Example 12-7 Complex Reactions	a) Co-current: LEP-12-7a.pol b) Countercurrent: LEP-12-7b.pol c) Constant T_a:LEP-12-7c.pol d) Adiabatic: LEP-12-7d.pol	a) Co-current: LEP-12-7a.zip b) Countercurrent: LEP-12-7b.zip c) Constant T_a:LEP-12-7c.zip d) Adiabatic: LEP-12-7d.zip	a) Co-current: LEP-12-7a.cdf b) Countercurrent: LEP-12-7b.cdf c) Constant T_a:LEP-12-7c.cdf d) Adiabatic: LEP-12-7d.cdf	--
Example R12-1 Industrial Oxidation of SO_2	LEP-RE12-1.pol	LEP-RE12-1.zip	--	--
Example 12-T12-3 PBR with Variable Coolant Temperature	LEP-T12-3.pol	LEP-T12-3.zip	LEP-T12-3.cdf	--
Example Lecture 19 A=B Adiabatic	Adiabatic A=B.pol	---	Adiabatic A=B.cdf	--

Updates and the ordering of POLYMATH software along with additional educational materials can be found on https://www.polymath-software.com/

Wolfram and Python can be downloaded and installed on your computer free of charge

ALGORITHM TO DECODE ICGs

**** CONFIDENTIAL ****

UNIVERSITY OF MICHIGAN
INTERACTIVE COMPUTER MODULES FOR CHEMICAL ENGINEERING
CHEMICAL REACTION ENGINEERING MODULES

H. Scott Fogler, Project Director

M. Nihat Gürmen, Project Manager (2002-2004)
Susan Montgomery, Project Manager (1991-1993)

Department of Chemical Engineering
University of Michigan
Ann Arbor, MI 48109-2136

INTERPRETATION OF PERFORMANCE NUMBERS

Students should record their Performance Number for each program, along with the name of the program, and turn it in to the instructor. The Performance Number for each program is decoded as described in the following pages.

The official site for the distribution of the modules is
http://www.engin.umich.edu/~cre/icm

Please report problems to icm.support@umich.edu.

****** CONFIDENTIAL ******

ICMs with Windows® interface

Module **Format** **Interpretation** **Example**

KINETIC CHALLENGE I

CzBzzAzz

Score = 1.5 * AB.C
z = random numbers

Note: 75% constitutes mastery.

Perf. No. = **7**5**2**41**6**92
Score = 1.5*(62.7) = 94 %

KINETIC CHALLENGE II

CzBzzAzz

Score = 2.0 * AB.C
z = random numbers
Note: 75% constitutes mastery.

Perf. No. = **0**3**7**76**4**67
Score = 2.0*(47.0) = 94 %

MURDER MYSTERY

zzAzz

A even: Killer and victim correctly identified
A odd: Killer and victim not identified
z = random numbers

Note: An even number for the middle digit constitutes mastery.

Perf. No. = 50**7**32
Score: No credit

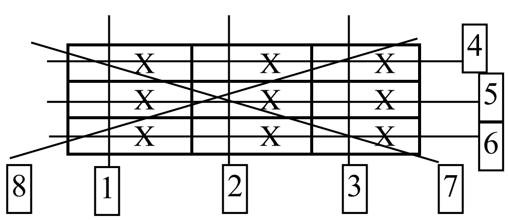
TIC TAC TOE

zDzCzBzA

Score = 4.0 * AB.C
z = random numbers

Configurations

Perf. No. = 77803581
Score = 4*(15.0) = 60
configuration 7 completed



Note: Student receives 20 points for every square answered correctly.
A score of 60 is needed for mastery of this module.

GREAT RACE

zzzCzABz

Score = 6.0 * AB.C
z = random numbers

Note: A score of 40 is needed for mastery of this module.

Perf. No. = 77738078
Score = 6*(07.3) = 44

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ECOLOGY

AzBCzaaD **z = random numbers**
a = random characters

A gives info on r^2 value of the student's linearized plot
A=Y if r^2 >= 0.9
A=A if 0.9 > r^2 >= 0.8
A=X if 0.8 > r^2 >= 0.7
A=F if 0.7 > r^2
A=Q if Wetland Analysis/Simulator portion has not been completed

B gives info on alpha
B=1 to 4 => student's alpha < (simulator's alpha ± 0.5)
B=5 to 9 => student's alpha > (simulator's alpha ± 0.5)
B=X if Wetland Analysis/Simulator portion has not been completed

C indicates number of data points deactivated during analysis
C=number of deactivated data points if at least 1 point has been deactivated
C=a randomly generated letter from A to Y if 0 points deactivated
C=Z if Wetland Analysis/Simulator portion has not been completed

D gives info on solution method used by student
D=1 if polynomial regression was used
D=2 if differential formulas were used
D=3 if graphical differentiation was used
D=4 to 9 if Wetland Analysis/Simulator portion has not been completed

Perf No. = A7213DF2

1) A => 0.9 > r^2 >= 0.8
2) 2 => student's alpha < (simulator's alpha ± 0.5)
3) 1 => one data point was deactivated
4) 2 => differential formulas were used

STAGING

zCBzAFzED **z = random numbers**

Perf. No. = 2**1**2**5**4**8**2**9**1**3**

Final conversion = 2*AB.C
Final flow rate = 2*DE.F

conversion = 2*42.1 = 84.2
flow rate = 2*31.2 = 62.4

Please make a pass/fail criterion based on these values.

****** CONFIDENTIAL ******

ICMs with Dos® interface

Module	Format	Interpretation	Example
HETCAT			
	zzABzCD	A=2,3,5,7: interaction done	Perf. No. = 80**27**4**35**
		B=2,3,5,7: intro done	A: Worked on interaction
		C=2,3,5,7: review done	B: Looked at intro
		D denotes how much they did in the interaction:	C: Looked at review
			D: found parameter values, didn't find mechanism
		D<2	Not done
		2 < D:5 4	Dependences
		4 < D:5 6	Parameter values
		6<D	Mechanism
		z = random numbers	

Note: Performance number given only if student goes through the interaction portion of the module

Module	Format	Interpretation	Example
HEATFX1			
	zzAzz	A even: score > 85 %	Perf. No. = 53**6**07
		z = random numbers	Score > 85 %

Note: Student told they have achieved mastery if their score is greater than 85%

Module	Format	Interpretation	Example
HEATFX2			
	zzzAzz	A even: completed interaction	Perf. No. = 407**5**82
		z = random numbers	Interaction not completed

Note: Performance number given only if student goes through the interaction portion of the module.

SAMPLE COURSE SYLLABUS

ChE 344: CHEMICAL REACTION ENGINEERING

Fundamentals of chemical reaction engineering. Rate laws, kinetics, and mechanisms of homogeneous and heterogeneous reactions. Analysis of rate data, multiple reactions, heat effects, bioreactors. Design of industrial reactors.

Prerequisite: ChE 330, ChE 342

Fall
Lectures: M,W 8:40 (Sharp) to 10:30 (not so sharp) – Room: 1013 Dow

Instructor:
Professor H. Scott Fogler
3168 Dow, 763-1361, sfogler@umich.edu
Office Hours: M,W 10:30a to 11:30a
Course assistants include: Instructional aids, tutor, proctors, and graders

Text Required
Elements of Chemical Reaction Engineering, 6th edition, H. Scott Fogler
Web sites: Chemical Reaction Engineering, *http://www.umich.edu/~elements/6e/index.html*
Process Safety Across the Chemical Engineering Curriculum, *http://umich.edu/~safeche/*

Recommended Reading List
- *Problem Solving in Chemical and Biochemical Engineering with POLYMATH, Excel, and MATLAB*, 2nd Edition 2008, Cutlip & Shacham
- *The Elements of Style*, Strunk and White
- *Strategies for Creative Problem Solving*, 3rd Edition 2014, Fogler, LeBlanc & Rizzo (for OEP's)

<u>Schedule</u>
Note - all ICGs (Interactive Computer Games) are Individual

1) Wednesday, September 9

Topic:	Lecture 1 – Chapter 1, Introduction, POLYMATH, MATLAB, Wolfram and Polymath, Mole balances Intro to LearnChemE – view one LearnChemE video of your choice
Read:	Introduction, Appendix B
In-Class Problem:	No In-Class Problem

2) Monday, September 14

Topic:	Lecture 2 – Chapter 2, Design equations, Levenspiel plots, Reactor staging
Read:	Chapter 1, P1-9$_A$, Appendix A, from the Web Chapter 2, Sections 2.1, 2.2, and 2.3
Hand In:	Problem Set 1: Q1-1$_A$, Q1-2$_A$ Do five i>clicker questions, P1-1$_A$ only use Wolfram or Python, P1-3$_B$, P1-5$_A$, Q2-1$_A$, Q2-2$_A$
In-Class Problem:	1
Study Problems:	P1-6$_A$ (a) and (c), P1-8$_A$ Note: Study problems have found their way many times on exams

3) Wednesday, September 16

Topic:	Lecture 3 – Chapter 3, Rate laws
Read:	Chapter 2, Chapter 3
Hand In:	Problem Set 2: P2-2$_A$ (a), (d) and (g), Q3-1$_A$, Q3-2$_A$ Do five i>clicker questions.
In-Class Problem:	2, P3-9$_B$ (*Hint:* Viewing the University of Alabama YouTube video "The Black Widow" may help you with today's in class problem)
Study Problems:	P2-7$_A$

4) Monday, September 21

Topic:	Lecture 4 – Chapter 4, Stoichiometry Batch Systems
Read:	Chapter 4 Section 4.1
Hand In:	Problem Set 3: P2-10$_B$, P3-6$_A$, P3-12$_B$, P3-14$_A$, Q4-1$_A$, Q4-2$_A$ Do five i>clicker questions
In-Class Problem:	3 - Bring i>clickers (tentative)
Study Problems:	P3-15$_A$

5) Wednesday, September 23

Topic:	Lecture 5 – Chapter 4, Stoichiometry Flow Systems
Read:	Chapter 4, Section 4.1
Hand In:	Problem Set 4: P4-2$_A$ (ICG)
In-Class Problem:	4
Study Problems:	Q4-3$_A$, Q4-4$_B$, Q4-5$_B$, Q4-6$_A$, Q4-9$_A$

6) Monday, September 28

Topic:	Lecture 6 – Chapter 5, Isothermal reactor design
Read:	Chapter 5, Chapter 5 Summary Notes on the Web site
Hand In:	Problem Set 5: P4-1$_A$ (a) and (b) only use Wolfram or Python, P4-3$_A$, P4-4$_B$, P4-5$_B$
In-Class Problem:	5
Study Problems:	P4-9$_B$, P4-10$_B$, P4-13$_C$

7) Wednesday, September 30

Topic:	Lecture 7 – Chapter 5, California Registration Exam Problem
Hand In:	Problem Set 6: Q5-1$_A$, Q5-2$_A$ Do five i>clicker questions, Q5-10$_A$, Q5-11$_A$, Q5-12$_A$, Q5-13$_A$; P5-2$_A$, What are you asked to find P5-18$_B$? What is the Ergun Equation?
In-Class Problem:	6
Study Problems:	P5-1$_B$ (a) only use Wolfram or Python

8) Monday, October 5

Topic:	Lecture 8 – Chapter 5, Pressure drop
Read:	Chapter 5, Sections 5.4 and 5.5
Hand In:	Problem Set 7: P5-1$_A$ (b), (c) only use Wolfram or Python, P5-3$_A$, P5-4$_B$, P5-5$_A$, P5-8$_B$, P5-13$_B$, P5-16$_B$
In-Class Problem:	7 – Bring Laptops
Study Problems:	P5-9$_A$, P5-10$_B$

9) Wednesday, October 7

Topic:	Lecture 9 – Chapter 6, Membrane Reactors
Read:	Chapter 6
Hand In:	Problem Set 8: P5-22$_A$, Q6-1$_A$, Q6-2$_A$ Do five i>clicker questions
In-Class Problem:	8 – Bring Laptops
Study Problems:	P5-21$_B$

10) Monday, October 12

Topic:	Lecture 10 – Chapter 6, Semibatch Reactors
Read:	Chapter 6
Hand In:	Problem Set 9: P5-1$_A$ (d), (e) and (f) only use Wolfram or Python, P5-11$_B$, P6-4$_B$, P6-5$_B$
In-Class Problem:	9 – Bring Laptops to carry out Polymath ODE Solver
Study Problems:	P6-7$_B$

11) Wednesday, October 14

Topic:	Lecture 11 – Chapter 7, Analysis of Rate Data/Chapter 9, Pseudo Steady State
Read:	Chapter 7, Chapter 9, Section 9.1 and the cobra web module
Hand In:	Problem Set 10: P6-1$_B$ (a) and (b) only use Wolfram or Python, P6-2$_B$ (ICG), P6-11$_B$ omit part (c), Q7-1$_A$, Q7-2$_A$ Do five i>clicker questions
In-Class Problem:	10 – Bring Laptops to carry out Polymath Regression
Study Problems:	P7-7$_B$

12) Monday, October 19

Topic:	*No Classes – Fall Study Break*

13) Wednesday, October 21

Topic:	Lecture 12 – Chapter 8, Multiple Reactions
Read:	Chapter 8, Sections 8.1, 8.2, 8.3 and 8.4
Hand In:	Problem Set 11: P7-6$_A$, P7-9$_A$, Q8-1$_A$, Q8-2$_A$ Do five i>clicker questions
In-Class Problem:	11
Study Problems	P7-11$_A$

14) Monday, October 26

Topic:	Lecture 13 – EXAM I – Covers Chapters 1 through 7 Closed book, web, notes, in-class problems and home problems

15) Wednesday, October 28

Topic:	Lecture 14 – Chapter 8: Multiple Reactions
Read:	Chapter 8, Sections 8.5, 8.6, 8.7 and 8.8
In-Class Problem:	12 – Bring Laptops
Hand In:	Problem Set 12: P8-1$_A$ (a), (b) and (c) only use Wolfram or Python, P8-2$_B$ (ICG), P8-5$_B$, P8-6$_B$, P8-7$_C$ (a), (b) and (c), P8-16$_B$ (a) and (b)
Study Problems	P8-10$_B$

16) Monday, November 2

Topic:	Lecture 15 – Derivation of Energy Balance
Read:	Chapter 11, Sections 11.1, 11.2 and 11.3
Hand In:	Problem Set 13: P8-12$_B$ Comprehensive Problem, Q11-1$_A$ Do five i>clicker questions, Q11-7$_A$, Q11-13$_A$
In-Class Problem:	13 – Bring Laptops
Study Problems:	P8-17$_B$

17) Wednesday, November 4

Topic:	Lecture 16 – Chapter 11: Adiabatic Equilibrium Conversion and Reactor Staging
Read:	Finish Reading Chapter 11, Equilibrium conversion appendix
In-Class Problem:	14
Study Problems	P11-6$_B$

18) Monday, November 9

Topic:	Lecture 17 – Heat Exchange, Adiabatic Reactors ICPs
Read:	Chapter 12, Sections 12.1 through 12.2
Hand In:	Problem Set 14: P11-1$_A$ (a), (b) and (d) only use Wolfram or Python, P11-3$_B$, P11-4$_A$, Q12-1$_A$, Q12-2$_A$ Do five i>clicker questions
In-Class Problem:	15
Study Problem:	P12-6$_A$

19) Wednesday, November 11
Topic: Lecture 18 – Trends in Conversion and Temperature Profiles
Applications of the Energy Balance to PFRs
Read: Chapter 12, Section 12.3 and 12.4
Hand In: Problem Set 15: P12-1 $_B$ (a), (b) and (c) LEP only use Wolfram or Python
In-Class Problem: 16 – Bring Laptops

20) Monday, November 16
Topic: Lecture 19 – Multiple Reactions with Heat Effects
This topic is a major goal of this course, to carry out calculations for non-isothermal multiple reactions
Applications of the Energy Balance to PFRs
Hand In: Problem Set 16: P12-4$_A$ (a) and (b), P12-14$_B$, P12-17$_B$, P12-21$_B$
In-Class Problem: 17 – Bring Laptops
Study Problem: P12-20$_B$, i>clicker questions handed out in class

21) Wednesday, November 18
Topic: Lecture 20 – CSTR and Review for Exam II
Study Problem: P12-5$_C$

22) Monday, November 23
Topic: Lecture 21 – EXAM II – Chapters 8, 11 and 12
Book and notecard are the only materials allowed
Hand In: Problem Set 17: P12-26$_C$ Term Comprehensive Problem

23) Wednesday, November 25
Topic: Lecture 22 – Multiple Steady States (MSS)
Multiple Reactions with Heat Effects
Hand In: Problem Set 18: P12-1$_B$ (e), (f) and (g) only use Wolfram or Python, Q13-1$_A$, Q13-2 $_A$ Do five i>clicker questions
Read: Chapter 12, Sections 12.6 and 12.7
In-Class Problem: 18 – Bring a Ruler/Straight Edge
Study Problems: P13-4$_B$

24) Monday, November 30
Topic: Lecture 23 – Safety (CSI)
Read: Chapter 13, Sections 13.1 through 13.3
Hand In: Problem Set 19: P13-1$_B$ (b) and (f) only use Wolfram or Python, P13-9$_B$
In-Class Problem: 19 – Bring Laptops
Study Problems: P13-2$_B$

25) Wednesday, December 2
Topic: Lecture 24 –Catalysis Reactor Safety
Read: Chapter 13, Section 13.5
Hand In: Problem Set 20: Q10-1$_A$, Q10-2 $_A$ Do five i>clicker questions, P10-2$_A$ (ICG – only do the review – extra credit if you do the game), P10-4$_B$
In-Class Problem: 20
Study Problems: P12-16$_B$, P13-11$_B$

26) Monday, December 7

Topic:	Lecture 25 – Catalysis
Read:	Chapter 10, Sections 10.1 through 10.2.2
Hand In:	Problem Set 21: P10-3_A, P10-8_B, P10-10_B
In-Class Problem:	21
Study Problems:	P10-7_B, P10-9_B

27) Wednesday, December 9

Topic:	Lecture 23 – PSSH and Enzyme
Read	Chapter 9
Hand In:	Problem Set 22: Q9-1_A, Q9-2_A Do five i>clicker questions, P9-2_A (ICG), P9-5_B parts (b) and (c), P9-9_B, P9-14_B P9-20_A
In-Class Problem:	22
Study Problems:	P9-12_B, P9-17_B, P9-23_A

28) FINAL EXAM

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.

O **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.

I **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:

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

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

$$A \rightarrow B$$

- $-r_A$ 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.

Q1-8 Individualized solution.

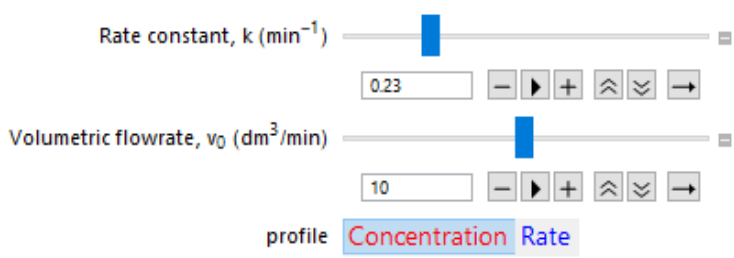
Q1-9 Individualized solution.

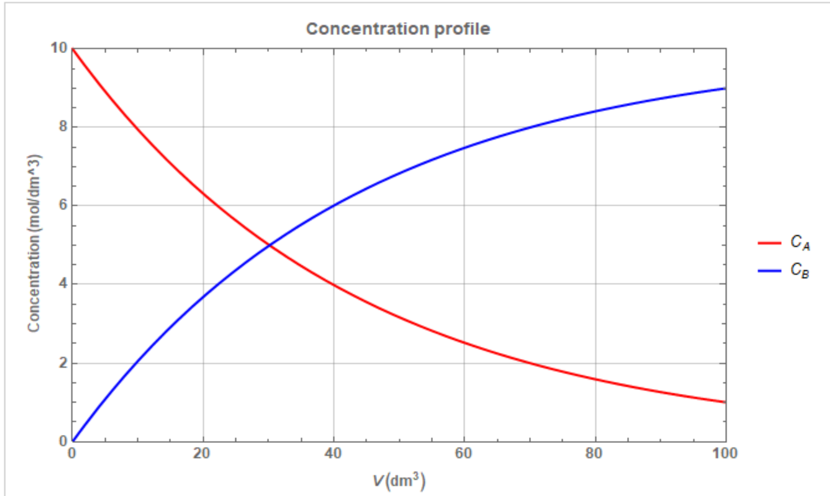
Q1-10 Individualized solution.

Q1-11 Individualized solution**.**

Q1-12 Individualized solution.

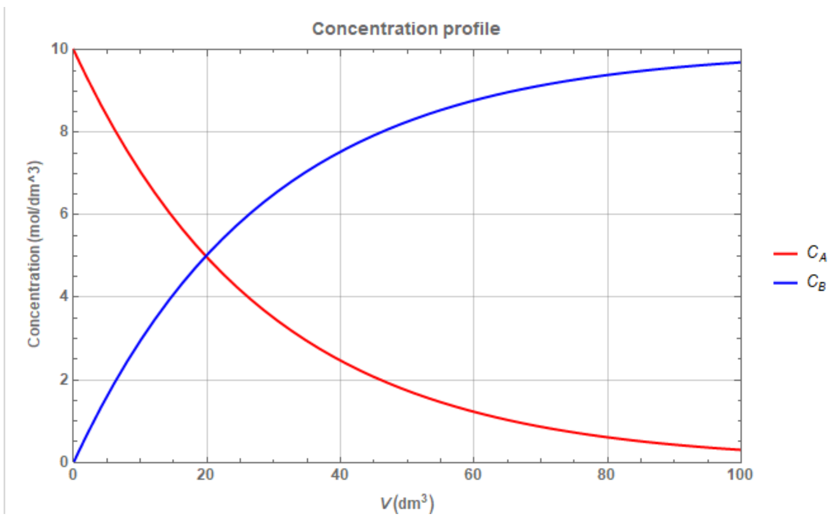
P1-1 (a) Example 1-3





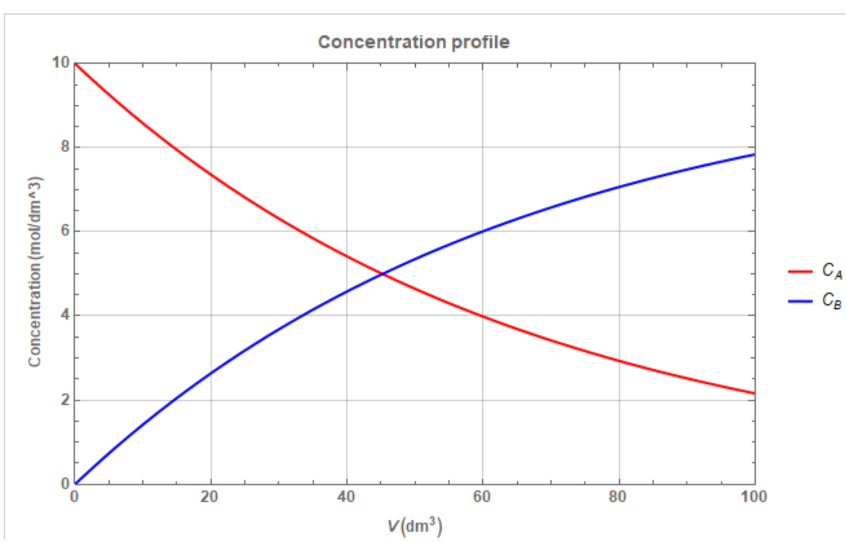
The above graph represents intial Ca and Cb profiles for k=0.23 and v_0 = 10.

(i) With an increase in k (lets take k =0.35) for same volume and v_0 , Ca decreases and Cb 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 Ca increases and Cb 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.

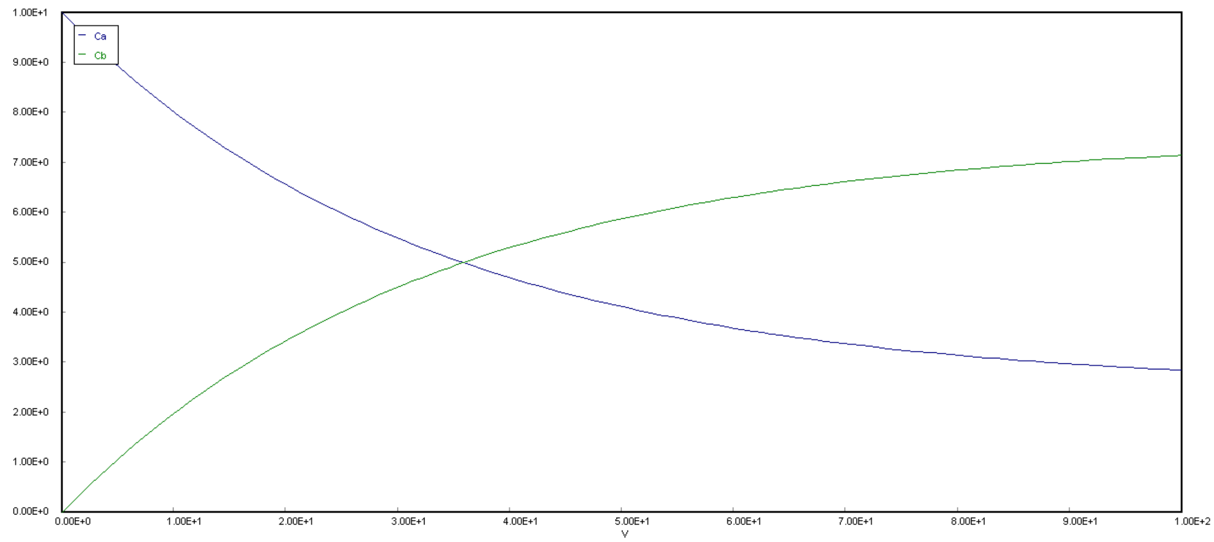
(iii) Individualized solution

(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 / v0

2 d(Cb)/d(V) = rb / v0

Explicit equations

1 k = 0.23
2 Ke = 3
3 ra = -k * (Ca-Cb/Ke)
4 rb = -ra
5 v0 = 10

P1-2
Given

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

$V = 4*10^{13} ft^3$ T = 534.7 $^\circ$ 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

P1-2 (a)
Total number of lb moles gas in the system:

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

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

P1-2 (b)
Molar flowrate of CO into L.A. Basin by cars.

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

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

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

P1-2 (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 = 1.673×10^{13} ft^3/hr

P1-2 (d)
Molar flowrate of CO into basin from Santa Ana wind.

$$F_S := v_0 \cdot C_S$$

= 1.673×10^{13} ft^3/hr $\times 2.04 \times 10^{-10}$ lbmol/ft^3
= 3.412×10^3lbmol/hr

P1-2 (e)

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

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

P1-2 (f)

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

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

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

P1-2 (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

P1-2 (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 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

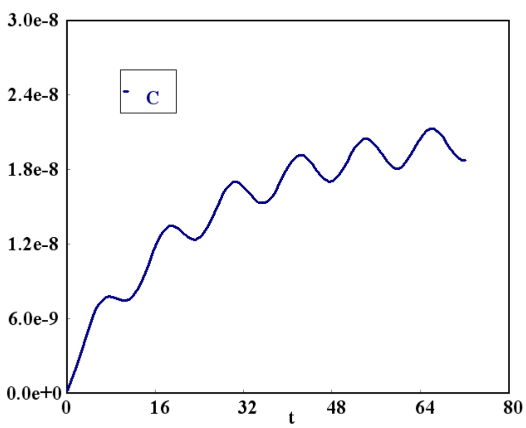
1 v0 = 1.67*10^12

2 A = 35000

3 B = 30000

4 F = 341.23

5 V = 4*10^13



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

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

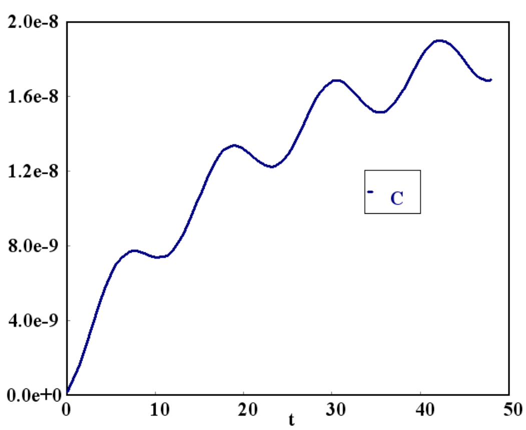
1 v0 = 1.67*10^12

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 ➔ 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.

P1-3 (a)

Initial number of rabbits, x(0) = 500
Initial number of foxes, y(0) = 200
Number of days = 500

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

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

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 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) = (k1*x)-(k2*x*y)
2	d(y)/d(t) = (k3*x*y)-(k4*y)

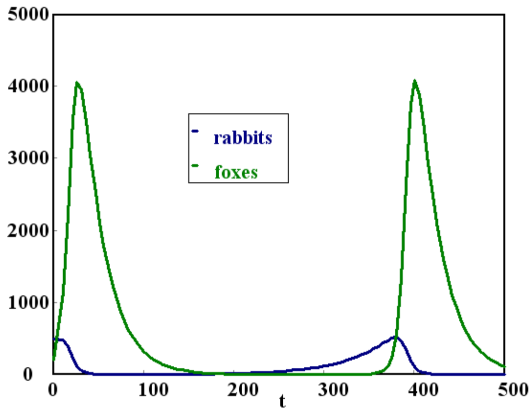
Explicit equations

1 k1 = 0.02

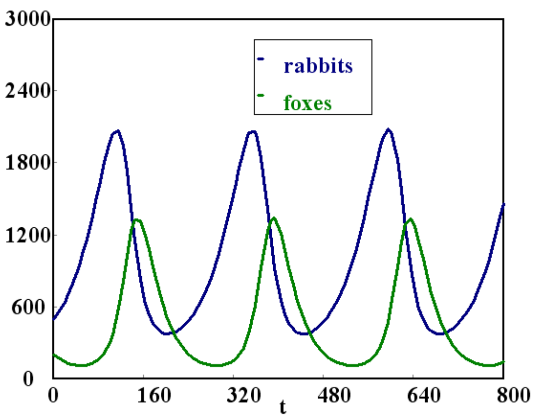
2 k2 = 0.00004

3 k3 = 0.0004

4 k4 = 0.04



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



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

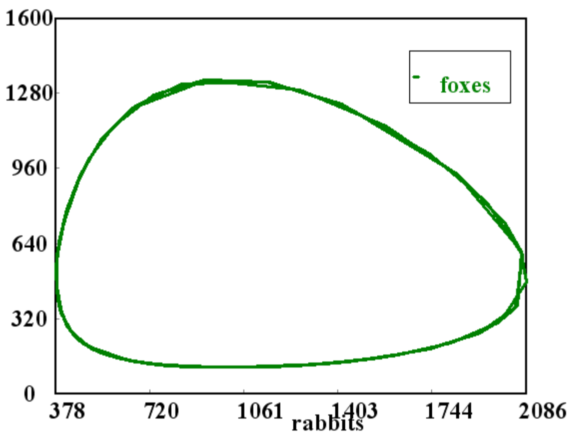
1 d(x)/d(t) = (k1*x)-(k2*x*y)

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

Explicit equations

1 k1 = 0.02
2 k2 = 0.00004
3 k3 = 0.00004
4 k4 = 0.04

Plotting rabbits vs. foxes

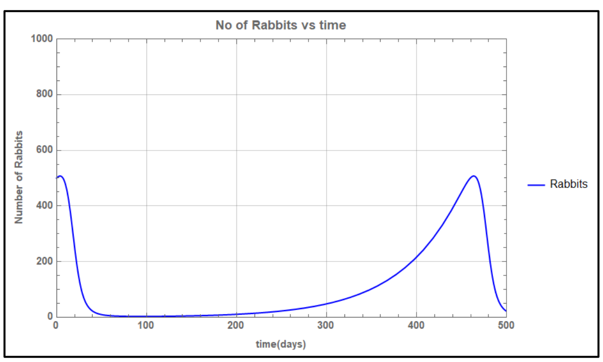


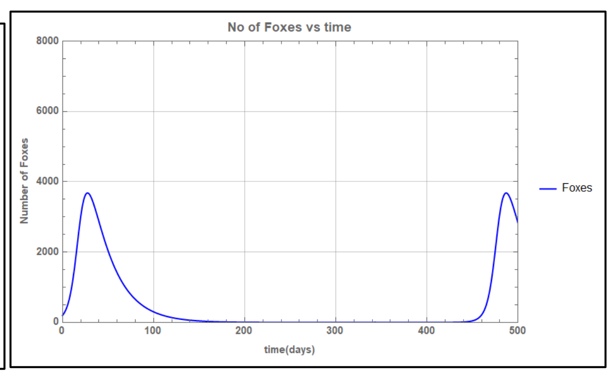
P1-3 (b)

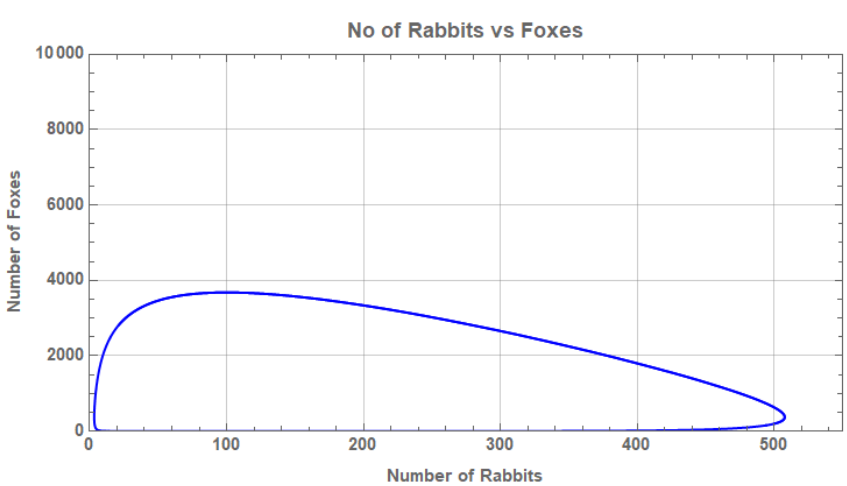
By increasing k_4 and decreasing k_2, foxes verses rabbits plot tends to become circular

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

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

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

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

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

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

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

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

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

P1-6 (c)

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

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

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

PFR:

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

Integrating

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

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

P1-6 (d)

$C_A = 0.001C_{A0}$

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

Constant Volume $V=V_0$

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

Zero order:

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

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:

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

P1-7 Enrico Fermi Problem

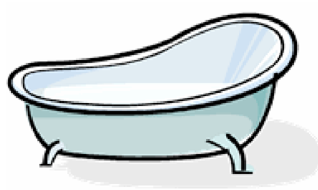
P1-7 (a) Population of Chicago = 4,000,000
Size of Households = 4
Number of Households = 1,000,000
Fraction of Households that own a piano = 1/5
Number of Pianos = 200,000
Number of Tunes/year per Piano = 1
Number of Tunes Needed Per Year = 200,000
Tunes per day = 2

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

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

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 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:

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

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

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

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

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

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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**).

O **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.

O **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.

I **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

O **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.

O **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.

O **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$_C$**.

I **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 dm^3= 400/1000 m^3 =0.4 m^3

For 10% conversion,

$$t = (100/0.4) \int_0^{10} \frac{dX}{-r_A}$$

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

Using trapezoidal rule,

Area= 0.5*(2.22+2.7)*0.1= 0.246

Thus, time= 250*0.246 = 61.5 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_{AO} is cut in half.

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

Therefore, volume of CSTR in example 2-1,

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

If the flow rate is doubled,

$F_2 = 2F_{AO}$ and C_{AO} will remain same,

Volume of CSTR in example 2-1,

$V_2 = F_2X/-r_A = 12.8\ m^3$

For Example, 2-2,

If flow rate is cut to half,

V= 0.5*2.165 m^3 =1.083 m^3

If flow rate is doubled,

V=2*2.165= 4.33 m^3

For Example, 2-3,

If flow rate is cut to half,

VCSTR= 0.5*6.4 m^3 =3.2 m^3

VPFR= 0.5*2.165 m^3 =1.08 m^3

If flow rate is doubled,

VCSTR= 2*6.4 m^3 =12.8 m^3

VPFR=2*2.165= 4.33 m^3

In a 4.5 m^3 PFR,

We need to find the value of X at which area under the curve of (Fao/-rA) and X is 4.5

From Figure E2-2.1 it can be seen that 80% conversion is achieved in 2.165 m3. Since data is only available till X=0.8, it is expected that with 4.5 m3, conversion achieved would be near to 100 %

In a 4.5 m^3 CSTR,

$$4.5 = \frac{F_{A0} * X}{-r_A}$$

So, we need to find a value of ($F_{A0}/-r_A$) and X which when multiplied gives 4.5

We can see that it is achieved at approximately 74 % conversion at which ($F_{A0}/-r_A$) is 6.1

P2-2 (c)

$$V = \frac{F_{A0} * X}{-r_A}$$

So, we need to find a value of ($F_{A0}/-r_A$) and X which when multiplied gives 2.5

We can see that it is achieved at approximately 63.5 % conversion at which ($F_{A0}/-r_A$) is 3.9

P2-2 (d)

Conversion achieved in a 2.4 m^3 CSTR is 62.5 %. Now we add a 1 m^3 PFR volume to it.

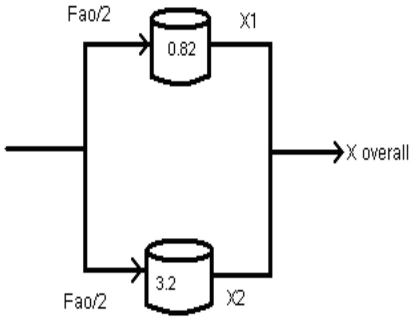
We need to find X at which area under the curve of (Fao/-rA) and X is 1. The starting point is X=0.625.

So, by trial and error, using trapezoidal rule, we find at 80 % conversion, below equation is satisfied

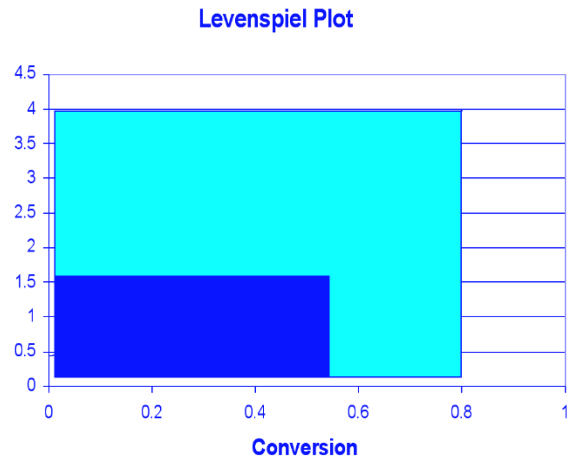
1= 0.5 (8+3.7)*(0.8-0.625)

So, Conversion achieved is 80 %.

P2-2 (e) Example 2-4



x



Now, F_{AO} = 0.4/2 = 0.2 mol/s,

Table: Divide each term $\frac{F_{A0}}{-r_A}$ in Table 2-3 by 2.

X	0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{AO}/-r_{A]}(m^3)$	0.445	0.545	0.665	1.025	1.77	2.53	4

Reactor 1

$V_1 = 0.82 m^3$

$V = (F_{AO}/-r_A)X$

$$0.82 = \left(\frac{F_{A0}}{-r_A}\right)_{X_1}(X_1)$$

Reactor 2

$V_2 = 3.2\ m^3$

$$3.2 = \left(\frac{F_{A0}}{-r_A}\right)_{X_2}(X_2)$$

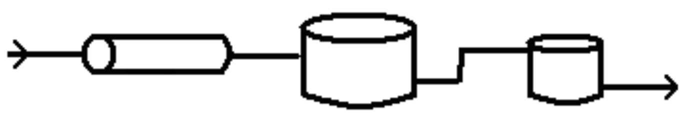
By trial and error, we get:

$X_1 = 0.546$ and $X_2 = 0.8$

Overall conversion $X_{Overall} = (1/2)X_1 + (1/2)X_2 = (0.546+0.8)/2 = 0.673$

P2-2 (f) Example 2-5

(1) The worst arrangement is to put the PFR first, followed by the larger CSTR and finally the smaller CSTR.



Conversion	Original Reactor Volumes	Worst Arrangement
$X_1 = 0.20$	$V_1 = 0.188$ (CSTR)	$V_1 = 0.23$ (PFR)
$X_2 = 0.60$	$V_2 = 0.38$ (PFR)	$V_2 = 0.53$ (CSTR)
$X_3 = 0.65$	$V_3 = 0.10$ (CSTR)	$V_3 = 0.10$ (CSTR)

For PFR,

$X_1 = 0.2$

$$V_1 = \int_0^{X_1}\left(\frac{F_{AO}}{-r_A}\right)dX$$

Using trapezoidal rule,

$X_O = 0$, $X_1 = 0.2$

$$V_1 = \frac{1}{2}\frac{(X_1 - X_0)(f(X_0) + f(X_1))}{-r_A}$$
= 0.2(1.28+0.94)/2
= 0.222 m^3

For CSTR,

At $X_2 = 0.6 \frac{F_{A0}}{-r_A} = 1.32\ m^3$, $V_2 = \frac{F_{A0}}{-r_A}(X_2 - X_1) = 1.32(0.6 - 0.2) = 0.53\ m^3$

For 2nd CSTR,

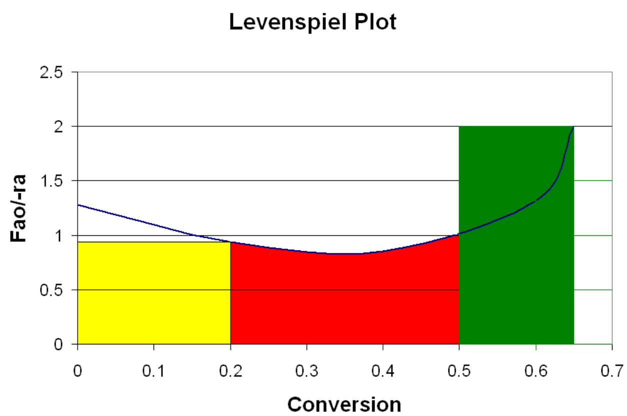
At $X_3 = 0.65, \frac{F_{A0}}{-r_A} = 2\ m^3$, $V_3 = \frac{F_{A0}}{-r_A}(X_3 - X_2) = 2\ m^3(0.65 - 0.6) = 0.1\ m^3$

(2) For first CSTR,
At X=0.2,

$\frac{F_{A0}}{-r_A} = 0.94\,\text{m}^3$; $V_1 = (0.94\ m^3)(0.2) = 0.188\ m^3$

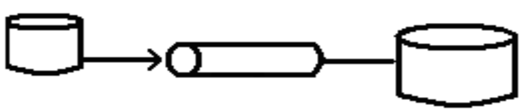
From previous example; V_1 (volume of first CSTR) = 0.188 m^3
Also, the next reactor is PFR, Its volume is calculated as follows

$$V_2 = \int_{0.2}^{0.5} \left(\frac{F_{AO}}{-r_A}\right) dX$$
$$= 0.247 m^3$$



For next CSTR,

$X_3 = 0.65$, $\frac{F_{AO}}{-rA} = 2m^3$, $V_3 = \frac{F_{AO}(X_3 - X_2)}{-rA} = .3m^3$



(3) Now the sequence of the reactors remain unchanged.

But all reactors have same volume.
First CSTR remains unchanged
$V_{cstr} = .1 = (F_{A0}/-r_A)*X_1$
⇨ X_1 = .088

Now
For PFR:

$$V = \int_{0.088}^{X_2} \left(\frac{F_{AO}}{-r_A}\right) dX$$

By estimation using the Levenspiel plot
X_2 = .183

For CSTR,

$$V_{CSTR2} = \frac{F_{AO}\left(X_3 - X_2\right)}{-rA} = 0.1m^3$$

=> X_3 = .316

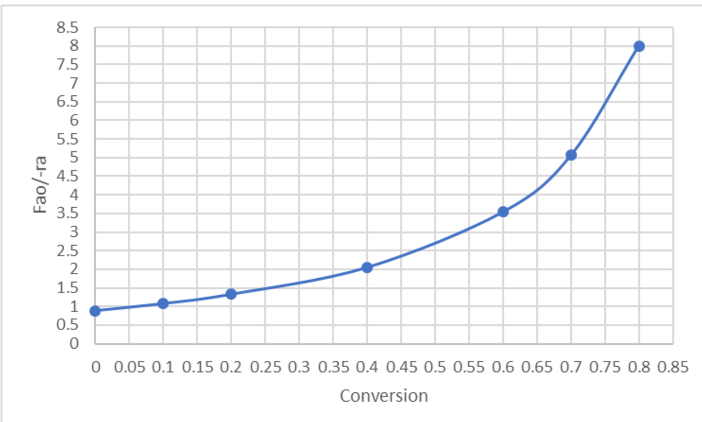
P2-2 (g)

Residence time, τ is given as 2 sec

Since, $\tau = \frac{V}{v_0}$

$$v_0 = \frac{3}{2} = 1.5\frac{m^3}{s} = 75\ m^3/min$$

P2-3



X	0	0.1	0.2	0.4	0.6	0.7	0.8
$F_{AO}/-r_A$ (m^3)	0.89	1.08	1.33	2.05	3.54	5.06	8.0

V = 1 m^3

P2-3 (a) Two CSTRs in series

For first CSTR,

V = ($F_{Ao}/-r_{AX1}$) X

So, we have to find a value of ($F_{Ao}/-r_{AX1}$) and X in such a way that on multiplication it gives 1

So at ($F_{Ao}/-r_{AX1}$) = 2.3, X= 0.435

=> X1 = 0.435

For second CSTR,

V = ($F_{Ao}/-r_{AX2}$) ($X_2 - X_1$)

Again, by trial and error, we have to find a condition which satisfy

1=($F_{Ao}/-r_{AX2}$)*(X_2-0.435)

=> X2 = 0.66

P2-3 (b)

Two PFRs in series

$$V = \int_0^{X_1}\left(\frac{F_{Ao}}{-r_A}\right)dX + \int_{X_1}^{X_2}\left(\frac{F_{Ao}}{-r_A}\right)dX$$

For X_1, we need to find area under the curve such that area =1. We can use trapezoidal rule to estimate the conversion taking two points at a time to get

$X_1 = 0.565$ $X_2 = 0.775$

P2-3 (c)

Two CSTRs in parallel with the feed, F_{AO}, divided equally between two reactors. $F_{ANEW}/-r_{AX1} = 0.5F_{AO}/-r_{AX1}$

$V = (0.5F_{AO}/-r_{AX1})\ X_1$

$2=(F_{Ao}/-r_{AX1})\ X$

Solving in similar manner as part a, we get, $X_{out} = 0.585$

P2-3 (d)

Two PFRs in parallel with the feed equally divided between the two reactors.

$F_{ANEW}/-r_{AX1} = 0.5F_{AO}/-r_{AX1}$

So, similar to part b, the area under the curve must be 2 in this case i.e. V=2

$$V = \int_0^{X_1} \left(\frac{F_{Ao}}{-r_A} \right) dX$$

$X_{out} = 0.775$

P2-3 (e)

A PFR followed by a CSTR,

$X_{PFR} = 0.565$ (using part(b))

$V = (F_{Ao}/-r_{A\text{-}XCSTR})\ (X_{CSTR} - X_{PFR})$

Now, $1=(F_{Ao}/-r_{A\text{-}XCSTR})\ (X_{CSTR} - 0.565)$

By looking at graph we get, $X_{CSTR} = 0.732$

P2-3 (f)

A CSTR followed by a PFR,

$X_{CSTR} = 0.435$ (using part(a))

$$V = \int_{X_{CSTR}}^{X_{PFR}} \frac{F_{AO}}{-r_A} dX$$

1= Area under the curve (with starting point as 0.435)

By calculating area, we get $X_{PFR} = 0.71$

P2-3 (g)

A 1 m^3 PFR followed by two 0.5 m^3 CSTRs,

For PFR,

$X_{PFR} = 0.565$ (using part(b))

$CSTR_1$: $V = (F_{Ao}/-r_{A\text{-}XCSTR})\ (X_{CSTR} - X_{PFR}) = 0.5\ m^3$

$X_{CSTR} = 0.673$

$CSTR_2$: $V = (F_{Ao}/-r_{A\text{-}XCSTR2})\ (X_{CSTR2} - X_{CSTR1}) = 0.5\ m^3$

$X_{CSTR2} = 0.75$

Two PFR in parallel or series was a better option as exit conversion was higher

P2-3 (h)

A CSTR and a PFR are in parallel with flow equally divided

Since the flow is divided equally between the two reactors, the overall conversion is the average of the CSTR conversion (part C) and the PFR conversion (part D)

X_o = (0.585 + 0.775) / 2 = 0.68

P2-4

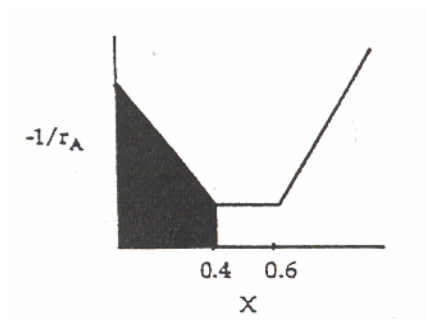
Exothermic reaction: A → B + C

X	r(mol/dm^3.min)	1/-r(dm^3.min/mol)
0	1	1
0.20	1.67	0.6
0.40	5	0.2
0.45	5	0.2
0.50	5	0.2
0.60	5	0.2
0.80	1.25	0.8
0.90	0.91	1.1

P2-4 (a) For a batch reactor,

To solve this problem, first plot $1/-r_A$ vs. X from the chart above.

$$t = NA0\int_0^X \frac{dX}{-r_A V}$$



NA0=400 moles

V=400 dm3

t=(400 /400)*(area under the curve)

For X=0.4, area under curve is

=0.4*0.2+0.5*0.4*0.8=0.24 dm3.min/mol, thus

t= 0.24 mins

Similarly,

For X=0.8, area under curve is

=0.4*0.2+0.5*0.4*0.8+0.2*0.2+0.2*0.2+0.5*0.2*0.6= 0.38 dm3.min/mol, thus

t= 0.38 mins

P2-4 (b)

Use mole balance as given below.

CSTR:

Mole balance: $V_{CSTR} = \frac{F_{A0}X}{-r_A} = \frac{(300 mol/\min)(0.4)}{(5 mol/dm^3.\min)}$ =>

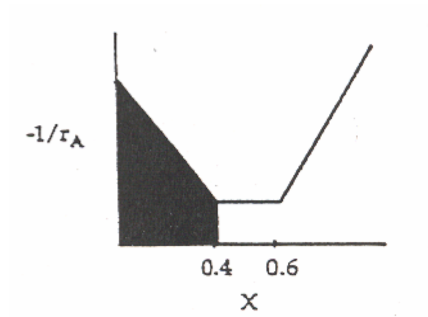
=>V_{CSTR} = 24 dm^3

PFR:

Mole balance: $V_{PFR} = F_{A0}\int_0^X \frac{dX}{-r_A}$

= 300(area under the curve)

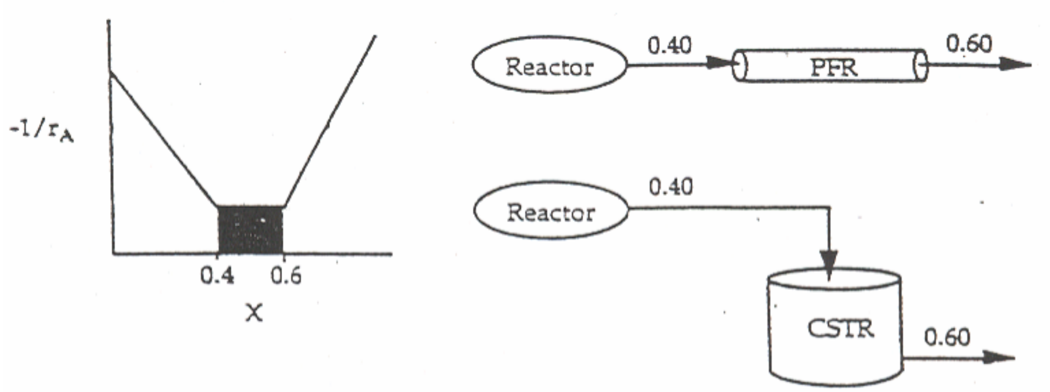
V_{PFR} = 72 dm^3



P2-4 (c)

For a feed stream that enters the reaction with a previous conversion of 0.40 and leaves at any conversion up to 0.60, the volumes of the PFR and CSTR will be identical because of the rate is constant over this conversion range.

$$V_{PFR} = \int_{.4}^{.6} \frac{F_{A0}}{-r_A} dX = \frac{F_{A0}}{-r_A} \int_{.4}^{.6} dX = \frac{F_{A0}}{-r_A} X\Big|_{.4}^{.6}$$



P2-4 (d)

V_{CSTR} = 105 dm^3

Mole balance: $V_{CSTR} = \frac{F_{A0}X}{-r_A}$

$$\frac{X}{-r_A} = \frac{105dm^3}{300mol/\min} = 0.35dm^3 \min/mol$$

Use trial and error to find maximum conversion.

At X = 0.70, 1/–r_A = 0.5, and X/–r_A = 0.35 dm3.min/mol

Maximum conversion = 0.70

P2-4 (e)

From part (a) we know that X_1 = 0.40.

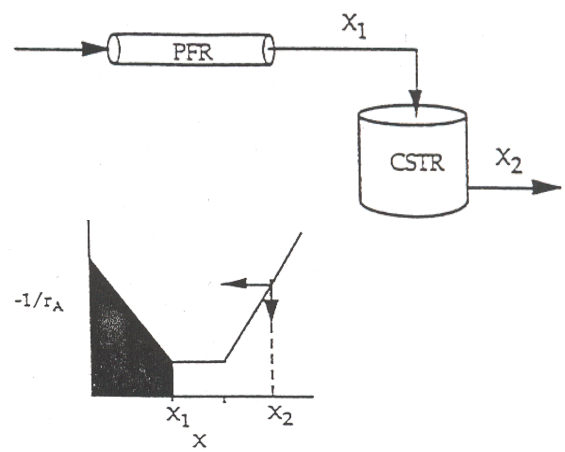
Use trial and error to find X_2.

Mole balance: $V = \frac{F_{A0}(X_2 - X_1)}{-r_A|_{X_2}}$

Rearranging, we get $\frac{X_2 - 0.40}{-r_A|_{X_2}} = \frac{V}{F_{A0}} = 0.008$

At X_2 = 0.64, $\frac{X_2 - 0.40}{-r_A|_{X_2}} = 0.008$

Conversion = 0.64



P2-4 (f)

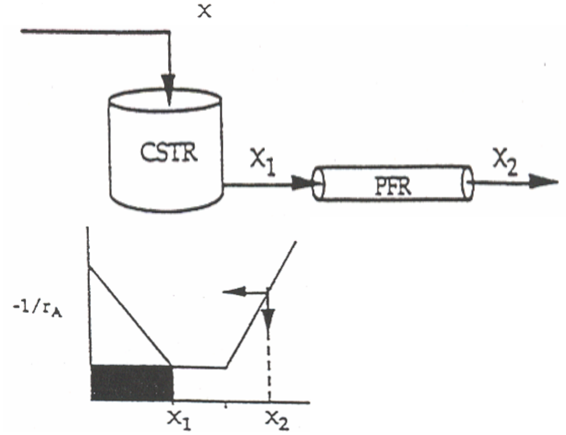
From part (a), we know that X_1 = 0.40. Use trial and error to find X_2.

Mole balance: $V_{PFR} = 72 = F_{A0} \int_{0.40}^{X_2} \frac{dX}{-r_A} = 300 \int_{0.40}^{X_2} \frac{dX}{-r_A}$

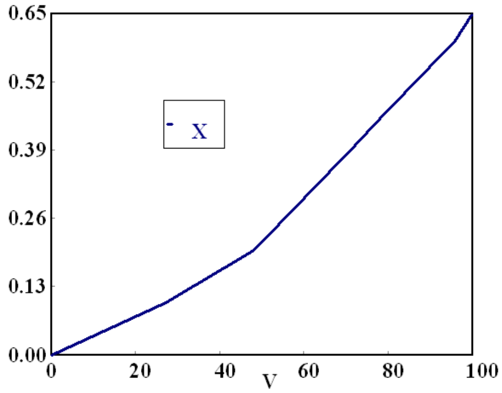
At X_2 = 0.908, V = 300 x (area under the curve)

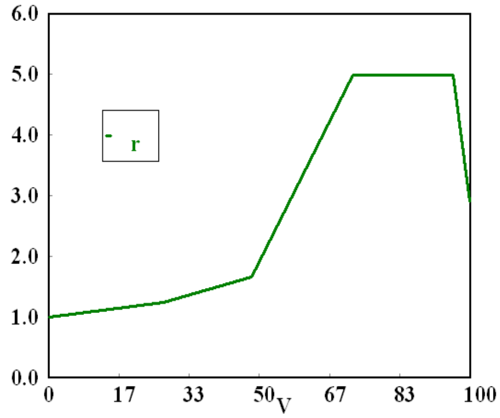
=> V = 300(0.24) = 72dm^3

Conversion = 0.908.



P2-4 (g)





P2-5

We must first find a CSTR up to X = 0.2 to minimize the volume, and hence the cost of reactor.
We can either use a CSTR or a PFR for X = 0.2 to X = 0.6 since the rate is independent of X in that range.
A PFR for X > 0.6 is preferable since it will reduce the volume required and the cost.
Let's calculate the volumes for the different cases.

i) X = 0 to X = 0.2
Volume for CSTR = 20*0.2 = 4 dm^3
Volume for PFR = 0.5*(50+20)*0.2 = 7 dm^3

ii) X = 0.2 to X = 0.6
Volume for CSTR = Volume for PFR = 0.4*20 = 8 dm^3

iii) X > 0.6

Volume for PFR < Volume for CSTR; for the same conversion.
Hence a PFR would minimize the cost.
First, we use the 4 dm^3 CSTR worth $2000. Conversion at this stage = 0.2
After this, we have $8000, and we see that the PFR minimizes the cost (So, we can have more conversion with the same money)
Hence, we can use a 12 dm^3 PFR followed by a 4 dm^3 PFR, totally worth $8000, which will give the highest conversion.
The first 8 dm^3 of PFR would give conversion up to 0.6, and the rest (16 – 8) dm^3 = 8 dm^3 would give the conversion of:

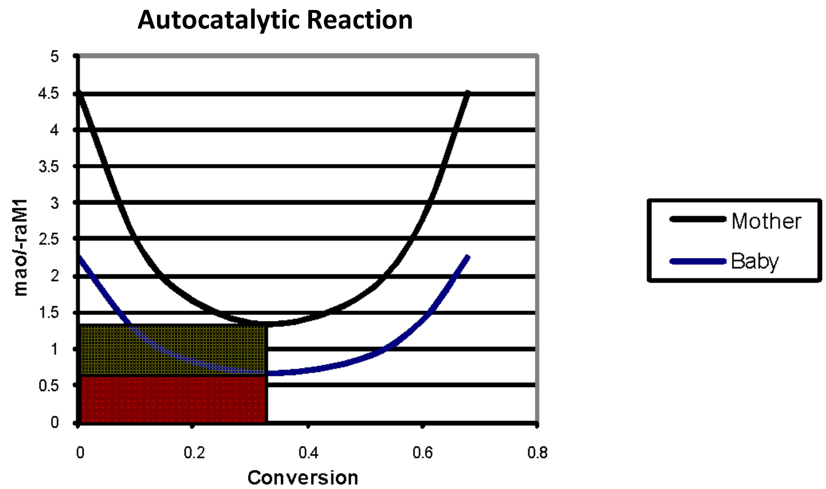
$$8 = \int_{0.6}^{X} \frac{F_{A0}}{-r_A} dX = \frac{1}{2}(20 + 200X - 100)(X - 0.6)$$

Therefore, X = 0.8
Final conversion = 0.8

P2-6 (a) Individualized Solution

P2-6 (b)

1) In order to find the age of the baby hippo, we need to know the volume of the stomach. The metabolic rate, $-r_A$, is the same for mother and baby, so if the baby hippo eats one half of what the mother eats then Fao (baby) = ½ Fao (mother). The Levenspiel Plot is shown:



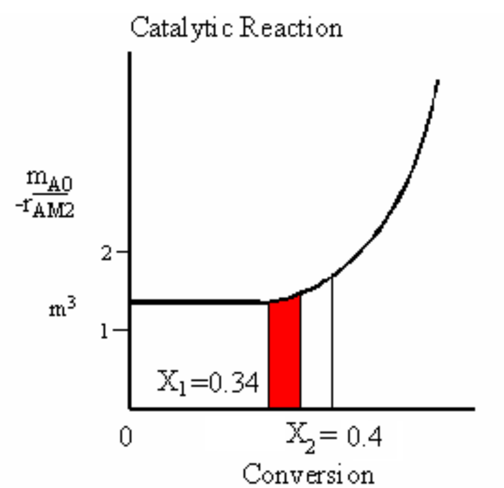
$$V_{baby} = \frac{FaoX}{-r_A} = \frac{1.36}{2} * 0.34 = 0.23 m^3$$

Since the volume of the stomach is proportional to the age of the baby hippo, and the volume of the baby's stomach is half of an adult, then the baby hippo is half the age of a full grown hippo.

$$Age = \frac{4.5\ years}{2} = 2.25\ years$$

P2-6 (b)

2) If Vmax and m_{ao} are both one half of the mother's then



$$\frac{m_{Ao}}{-r_{AM2}} = \frac{\left(\frac{1}{2} m_{A0_{mother}}\right)}{-r_{AM2}}$$

and since

$$-r_{AM2} = \frac{v_{max} C_A}{K_M + C_A} \text{ then}$$

$$-r_{AM2_{baby}} = \frac{\frac{1}{2} v_{max} C_A}{K_M + C_A} = -\frac{1}{2} r_{AM2_{mother}}$$

$$\left(\frac{m_{Ao}}{-r_{AM2}}\right)_{baby} = \left(\frac{\frac{1}{2} m_{Ao}}{-\frac{1}{2} r_{AM2}}\right)_{mother} = \left(\frac{m_{Ao}}{-r_{AM2}}\right)_{mother}$$

$\frac{m_{Ao}}{-r_{AM2}}$ will be identical for both the baby and mother.

Assuming that like the stomach the intestine volume is proportional to age then the volume of the intestine would be 0.75 m^3 and the final conversion would be 0.40

P2-6 (c)

$V_{stomach} = 0.2\ m^3$

From the web module we see that if a polynomial is fit to the autocatalytic reaction we get: