

***Elements of Chemical Reaction Engineering 7th
edition Fogler Solutions Manual***

SKU: 9780135337554-SOLUTIONS

Solutions Manual for
Elements of Chemical
Reaction Engineering
Seventh Edition

H. Scott Fogler

Ame and Catherine Vennema Professor of Chemical Engineering and
the Arthur F. Thurnau Professor

Bryan R. Goldsmith

Associate Professor of Chemical Engineering

Eranda Nikolla

Professor of Chemical Engineering

Nirala Singh

Associate Professor of Chemical Engineering

University of Michigan, Ann Arbor

May 2025



Pearson

Hoboken, New Jersey

The author and publisher have taken care in the preparation of this work but make no expressed or implied warranty of any kind and assume no responsibility for errors or omissions. No liability is assumed for incidental or consequential damages in connection with or arising out of the use of the information or programs contained herein.

Visit us on the Web: informit.com

Copyright © 2025 Pearson Education, Inc.

This work is protected by United States copyright laws and is provided solely for the use of instructors in teaching their courses and assessing student learning. Dissemination or sale of any part of this work (including on the World Wide Web) will destroy the integrity of the work and is not permitted. The work and materials from it should never be made available to students except by instructors using the accompanying text in their classes. All recipients of this work are expected to abide by these restrictions and to honor the intended pedagogical purposes and the needs of other instructors who rely on these materials.

ISBN-13: 978-0-13-534732-4

ISBN-10: 0-13-534732-7

Version 1, May 2025

Acknowledgment

The following students participated in the solutions to the end of chapter problems of the Elements of Chemical Reaction Engineering, editions 1 through 6:

Max Nori	Sneh Shriyansh	Maithri Venkat
Brian Vicente	Utkarsh Prasad	Yimeng Lyu
Sombudda Ghosh	Darshan Shah	Sheng Mark Zheng
Nihat Gürman	Anamika Singh	Mayur Tikmani
Yongzhong Lui	Sravya Jangareddy	Ayush Agarwal
Duc Ahn Nguyen	Fan Zhang	Vaibhav Jain
Vishal Chaudhary	Keyvan Edrisi	Devosmita Sen
Ravi Kapoor	Richa Motwani	Manjeet Singh
Manosij Basu	Prafful Bhansali	Jnana Sai Jagana
Arpit Gupta		

While many, many students contributed to the Elements of Chemical Reaction Engineering Solutions Manual, special mention is necessary to Mayur Tikmani who after graduating from IIT Guwahati spent 6 months in Ann Arbor working with Prof. Fogler, before he joined Reliance Industries Limited, to prepare all the Wolfram and Python LEPs.

Table of Contents

Screen Shot of Web Home Page	i
Screen Shot of Interactive Computer Games (ICGs)	ii
Screen Shot of Polymath Living Example Problems (LEPs)	iv
Algorithm to Decode ICGs.....	v
Sample Course Syllabus	ix
Solutions to Chapter 1 – Mole Balances	
Questions Q1-1 through Q1-12	
Problems P1-1 through P1-8	
Solutions to Chapter 2 – Conversion and Reactor Sizing	
Questions Q2-1 through Q2-6	
Problems P2-1 through P2-11	
Solutions to Chapter 3 – Rate Laws	
Questions Q3-1 through Q3-7	
Problems P3-1 through P3-16	
Solutions to Chapter 4 – Stoichiometry	
Questions Q4-1 through Q4-9	
Problems P4-1 through P4-13	
Solutions to Chapter 5 – Isothermal Reactor Design: Conversion	
Questions Q5-1 through Q5-13	
Problems P5-1 through P5-26	
Solutions to Chapter 6 – Isothermal Reactor Design: Moles and Molar Flow Rates	
Questions Q6-1 through Q6-7	
Problems P6-1 through P6-13	
Solutions to Chapter 7 – Collection and Analysis of Rate Data	
Questions Q7-1 through Q7-7	
Problems P7-1 through P7-12	
Solutions to Chapter 8 – Multiple Reactions	
Questions Q8-1 through Q8-5	
Problems P8-1 through P8-18	
Solutions to Chapter 9 – Reaction Mechanisms, Pathways, Bioreactions and Bioreactors	
Questions Q9-1 through Q9-4	
Problems P9-1 through P9-23	
Solutions to Chapter 10 – Catalysis and Catalytic Reactors	
Questions Q10-1 through Q10-9	
Problems P10-1 through P10-23	

Solutions to Chapter 11 – Nonisothermal Reactor Design: The Steady-State Energy Balance and Adiabatic PFR Applications

Questions Q11-1 through Q11-14

Problems P11-1 through P11-10

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

Questions Q12-1 through Q12-6

Problems P12-1 through P12-27

Solutions to Chapter 13 – Unsteady State Nonisothermal Reactor Design

Questions Q13-1 through Q13-5

Problems P13-1 through P13-11

Solutions to Chapter 14 – Mass Transfer Limitations in Reacting Systems

Questions Q14-1 through Q14-8

Problems P14-1 through P14-17

Solutions to Chapter 15 – Diffusion and Reaction

Questions Q15-1 through Q15-8

Problems P15-1 through P15-17

Solutions to Chapter 16 – Residence Time Distributions of Chemical Reactors

Questions Q16-1 through Q16-5

Problems P16-1 through P16-13

Solutions to Chapter 17 – Predicting Conversion Directly from the Residence Time Distribution

Questions Q17-1 through Q17-4

Problems P17-1 through P17-18

Solutions to Chapter 18 – Models for Nonideal Reactors

Questions Q18-1 through Q18-6

Problems P18-1 through P18-20

Solutions to Chapter 19 – Electrochemical Reactor Design

Questions Q19-1 through Q19-8

Problems P19-1 through P19-11

WEB HOME PAGE

Elements of Chemical Reaction Engineering

7th edition

TOC Preface 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 Appendices

Let's Get Started

Lecture Notes

Software

Undergraduate (ChE 344) Homepage

Graduate (ChE 528) Homepage

Asynchronous Learning

Additional Textbook Websites

Additional Resources

SafeChemE Website

Interactive Computer Games

Web Modules

Thoughts on Problem Solving

FAQs

Fun YouTube Videos

Updates and Typos

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 *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](#))

Out2Show

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](#))

Out2Show

Stoichiometry and Rate Laws

[Description of the Module](#)

Objectives for [Chapter Four](#)

Order 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 Data: 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](#)



INTERACTIVE COMPUTER GAMES (ICGs)

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 $\pm$ 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:



Kinetics Challenge I

FINAL SCORES

Bob:	300
Arrhenius:	1187
Nigel:	-1500

It looks like Arrhenius won the game. Well, goody for him.

PERFORMANCE

Module Performance:	49
(75 points needed for mastery)	
Performance number:	76288337

Continue

LIVING EXAMPLE PROBLEMS (LEPs)

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	--

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

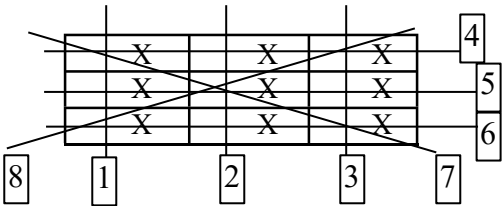
©2005
Regents of the University of Michigan
- All Rights Reserved -

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.

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

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. = <u>75241692</u> Score = $1.5*(62.7) = 94 \%$
KINETIC CHALLENGE II			
	CzBzzAzz	Score = $2.0 * AB.C$ z = random numbers Note: 75% constitutes mastery.	Perf. No. = <u>03776467</u> 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. = <u>50732</u> Score: No credit
TIC TAC TOE			
	zDzCzBzA	Score = $4.0 * AB.C$ z = random numbers Configurations	Perf. No. = <u>77803581</u> 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. = <u>77738078</u> Score = $6*(07.3) = 44$

ECOLOGY

AzBCzaaD

z = random numbers
a = random characters

A gives info on r^2 value of the student's linearized plot
 A=Y if $r^2 \geq 0.9$
 A=A if $0.9 > r^2 \geq 0.8$
 A=X if $0.8 > r^2 \geq 0.7$
 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 $\pm$ 0.5)
 B=5 to 9 => student's alpha > (simulator's alpha $\pm$ 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 => $0.9 > r^2 \geq 0.8$
 2) 2 => student's alpha < (simulator's alpha $\pm$ 0.5)
 3) 1 => one data point was deactivated
 4) 2 => differential formulas were used

STAGING

zCBzAFzED

z = random numbers

Perf. No. = 2125482913

Final conversion = $2 \cdot AB.C$
 Final flow rate = $2 \cdot DE.F$

conversion = $2 \cdot 42.1 = 84.2$
 flow rate = $2 \cdot 31.2 = 62.4$

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

ICMs with Dos® interface

Module	Format	Interpretation	Example
HETCAT	zzABzCD	A=2,3,5,7: interaction done B=2,3,5,7: intro done C=2,3,5,7: review done D denotes how much they did in the interaction: D<2 2 < D:5 4 4 < D:5 6 6<D z = random numbers	Perf. No. = 80 <u>27435</u> A: Worked on interaction B: Looked at intro C: Looked at review D: found parameter values, didn't find mechanism Not done Dependences Parameter values Mechanism
		Note: Performance number given only if student goes through the interaction portion of the module	
HEATFX1	zzAzz	A even: score > 85 % z = random numbers	Perf. No. = 53 <u>607</u> Score > 85 %
		Note: Student told they have achieved mastery if their score is greater than 85%	
HEATFX2	zzzAzz	A even: completed interaction z = random numbers	Perf. No. = 407 <u>582</u> 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 Bryan R. Goldsmith

3168 Dow, bgoldsm@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, 7th edition, H. Scott Fogler

Web sites: Chemical Reaction Engineering, <http://www.umich.edu/~elements/7e/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)

Schedule

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

Page intentionally blank

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

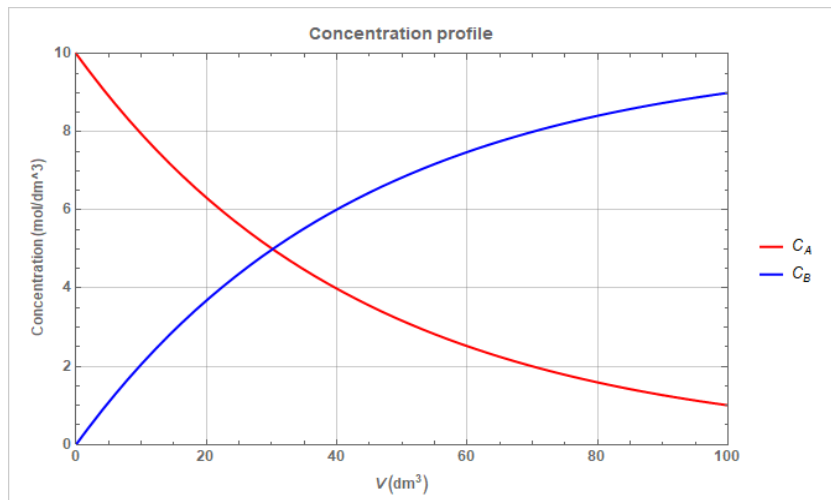
Rate constant, k (min⁻¹) 

0.23 

Volumetric flowrate, v_0 (dm³/min) 

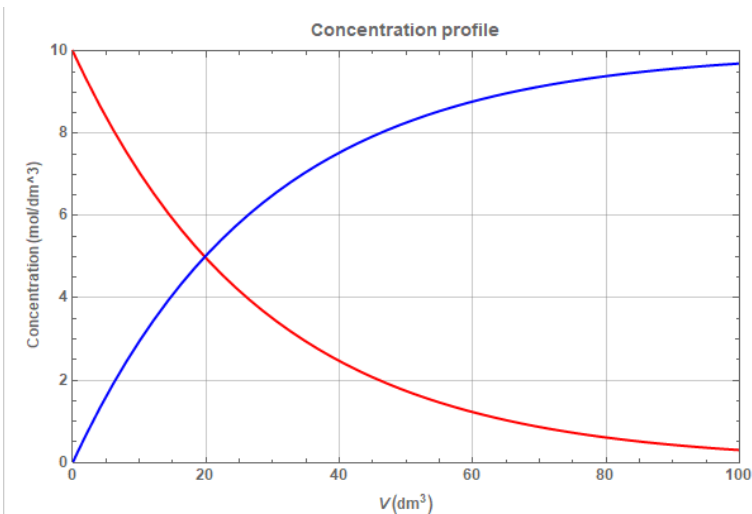
10 

profile Concentration Rate



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

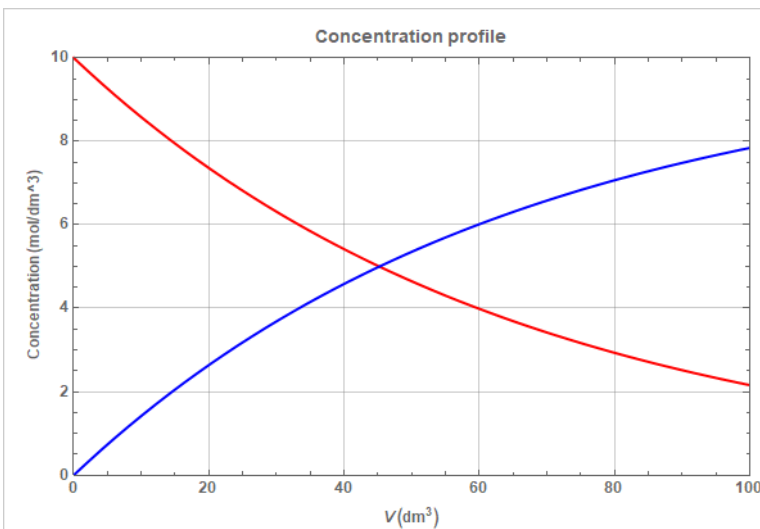
(i) With an increase in k (lets take $k=0.35$) for same volume and v_0 , C_A decreases and C_B increases



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:

$$d(C_A)/d(V) = r_a / v_0$$

$$d(C_B)/d(V) = r_b / v_0$$

$$k = 0.23$$

$$K_e = 3$$

$$r_a = -k * (C_A - C_B / K_e)$$

$$r_b = -r_a$$

$$v_0 = 10$$

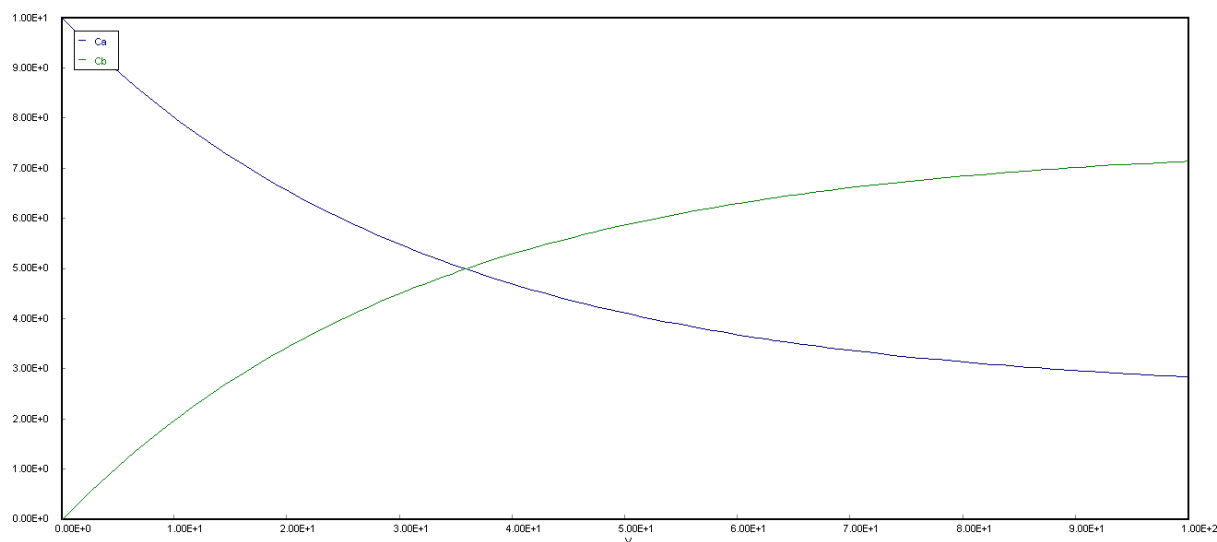
$$V(0) = 0$$

$$V(f) = 100$$

$$C_A(0) = 10$$

$$C_B(0) = 0$$

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 $d(C_A)/d(V) = r_a / v_0$

2 $d(C_B)/d(V) = r_b / v_0$

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

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

P1-2 (a)

Total number of lb moles gas in the system:

$$N = \frac{P_0 V}{RT}$$
$$N = \frac{1 \text{ atm} \times (4 \times 10^{13} \text{ ft}^3)}{0.73 \frac{\text{atm} \cdot \text{ft}^3}{\text{lbmol} \cdot \text{R}} \times 534.69 \text{ R}} = 1.025 \times 10^{11} \text{ lb mol}$$

P1-2 (b)

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

$$F_A = y_A F_T = y_A \cdot v_A C_T \left|_{\text{STP}} \cdot \text{no. of cars}\right.$$
$$F_T = \frac{3000 \text{ ft}^3}{\text{hr car}} \times \frac{1 \text{ lbmol}}{359 \text{ ft}^3} \times 400000 \text{ cars} \quad (\text{See appendix B})$$
$$F_A = 6.685 \times 10^4 \text{ lb mol/hr}$$

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.

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

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)

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

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

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

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),

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

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

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

P1-2 (h)

(1) $t_o = 0$ $t_f = 72 \text{ hrs}$

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

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

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

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

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

See the following polymath code:

Polymath Code:

$$v0 = 1.67 \times 10^{12}$$

$$A = 35000$$

$$B = 30000$$

$$F = 341.23$$

$$V = 4 \times 10^{13}$$

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

$$C(0) = 2.0 \times 10^{-10}$$

$$t(0) = 0$$

$$t(f) = 72$$

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

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

Explicit equations

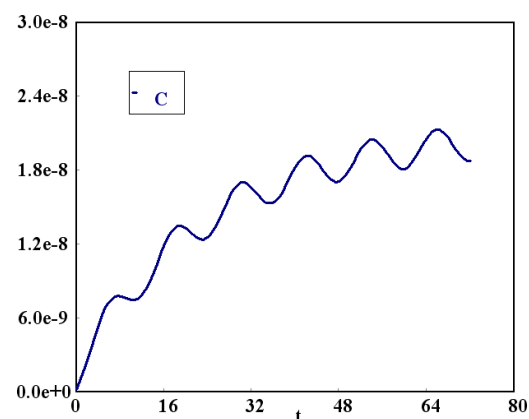
$$1 \quad v0 = 1.67 \times 10^{12}$$

$$2 \quad A = 35000$$

$$3 \quad B = 30000$$

$$4 \quad F = 341.23$$

$$5 \quad V = 4 \times 10^{13}$$



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

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

Polymath Code:

$$v0 = 1.67 \times 10^{12}$$

$$A = 35000$$

$$B = 30000$$

$$F = 341.23$$

$$V = 4 \times 10^{13}$$

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

$$C(0) = 2.0 \times 10^{-10}$$

$$t(0) = 0$$

$$t(f) = 48$$

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

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

Explicit equations

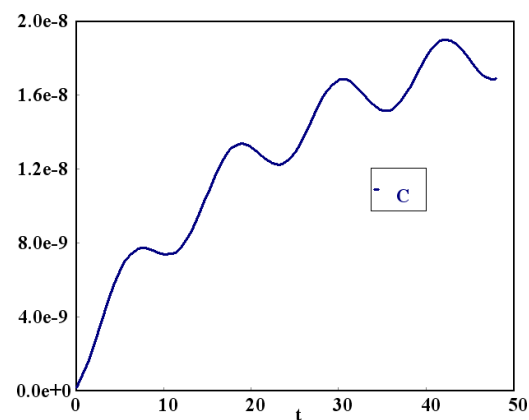
$$1 \quad v0 = 1.67 \times 10^{12}$$

$$2 \quad A = 35000$$

$$3 \quad B = 30000$$

$$4 \quad F = 341.23$$

$$5 \quad V = 4 \times 10^{13}$$

**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

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

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

Given,

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

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

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

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

See 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

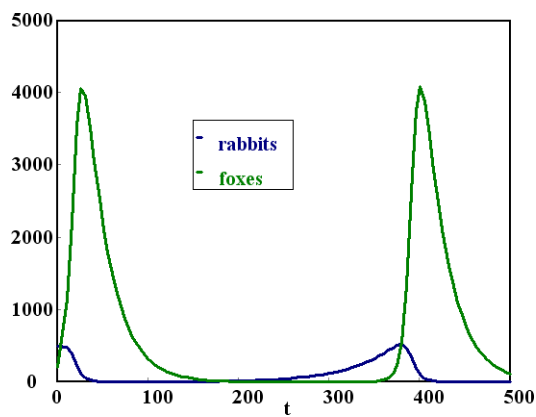
Differential equations

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

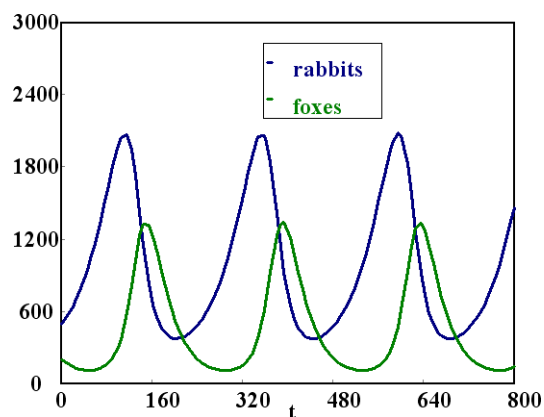
$$2 \quad d(y)/d(t) = (k3*x*y)-(k4*y)$$

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

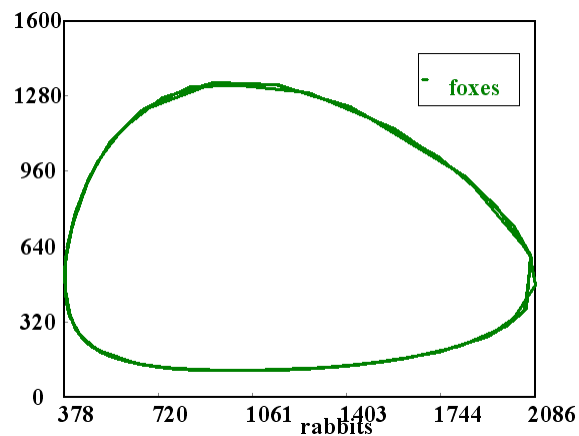
Differential equations

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

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

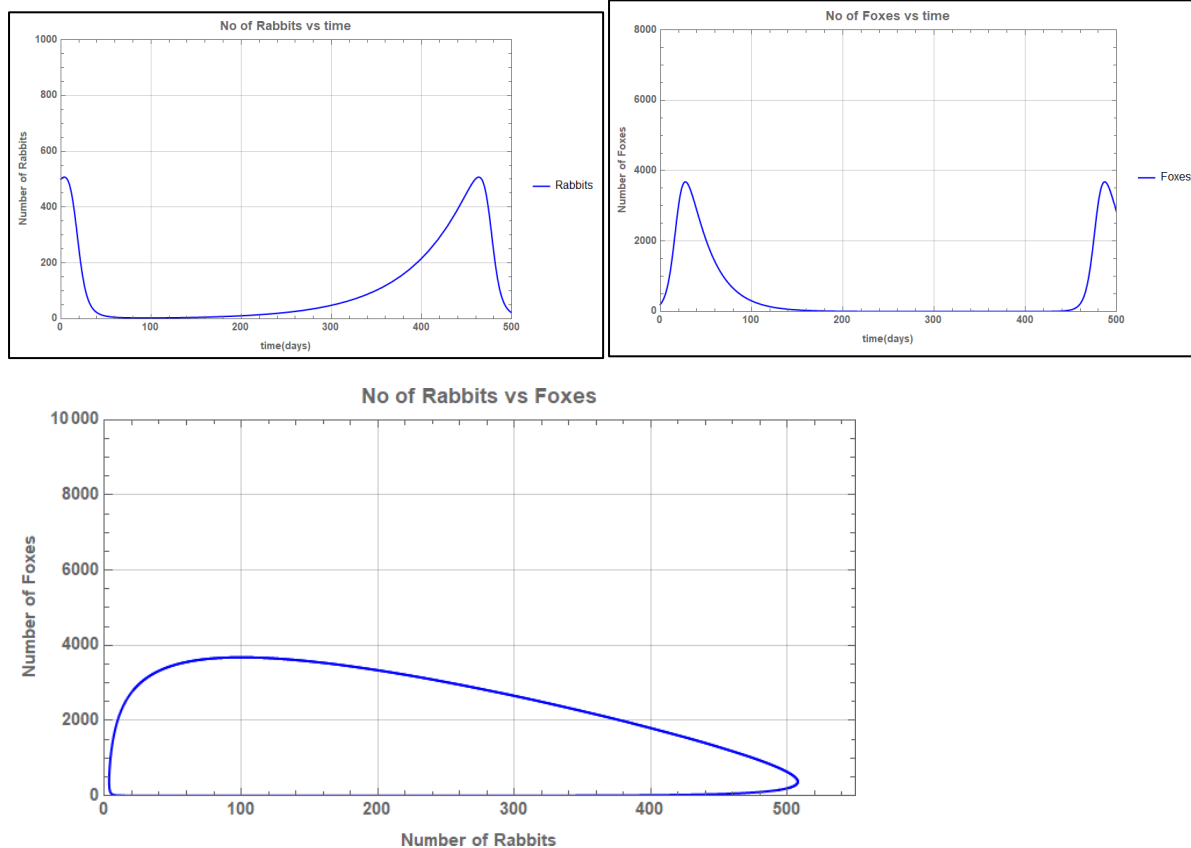


P1-3 (b)

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.
	y	3.797028	1.72E-12	2.

Nonlinear equations

$$1 \quad f(x) = (x^3)y - 4y^2 + 3x - 1 = 0$$

$$2 \quad f(y) = 6y^2 - 9xy - 5 = 0$$

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)

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

CSTR: The general equation is

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

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

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

Substituting the values in the above equation we get,

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

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

PFR: The general equation is

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

Integrating the above equation, we get

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

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

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

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

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

PFR:

From above we already know that for a PFR

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

Integrating

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

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

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

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:

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

Substituting all the values we get

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

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:

$$t = \frac{1}{k} \left(C_{A0} - 0.001 C_{A0} \right) \lambda = \frac{.999 C_{A0}}{0.05} = 9.99 h$$

First order:

$$t = \frac{1}{k} \ln \left(\frac{C_{A0}}{C_A} \right) = \frac{1}{0.0001} \ln \left(\frac{1}{0.001} \right) = 69078 s = 19.19 h$$

Second order:

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

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

$$\begin{aligned}\text{Tunes per year per tuner} &= \frac{250 \text{ days}}{\text{yr}} \times \frac{2}{\text{day}} = 500/\text{yr}/\text{tuner} \\ \frac{200,000 \text{ tunes}}{\text{yr}} \times \frac{1}{500 \text{ tunes} / \text{yr} / \text{tuner}} &= 400 \text{ Tuners}\end{aligned}$$

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.

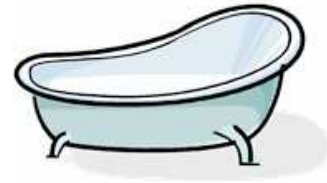
P1-7(c) Assume you drink 1L/day

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:

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

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

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

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

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

Page intentionally blank