Solutions Manual for

Essentials of Chemical Reaction Engineering

Second Edition

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ISBN-13: 978-0-13-466396-8
ISBN-10: 0-13-466396-9

October 2017

Acknowledgments

The following students participated in the solutions to the end-of-chapter problems in the second edition of *Essentials of Chemical Reaction Engineering*:

Max Nori
Brian Vicente
Sombudda Ghosh
Nihat Gürman
Yongzhong Lui
Duc Ahn Nguyen
Vishal Chaudhary
Ravi Kapoor

Manosij Basu
Arpit Gupta
Sneh Shriyansh
Utkarsh Prasad
Darshan Shah
Anamika Singh
Sravya Jangareddy
Kaushik Nagaraj

Fan Zhang
Keyvan Edrisi
Richa Motwani
Prafful Bhansali
Maithri Venkat
Yimeng Lyu
Sheng Mark Zheng

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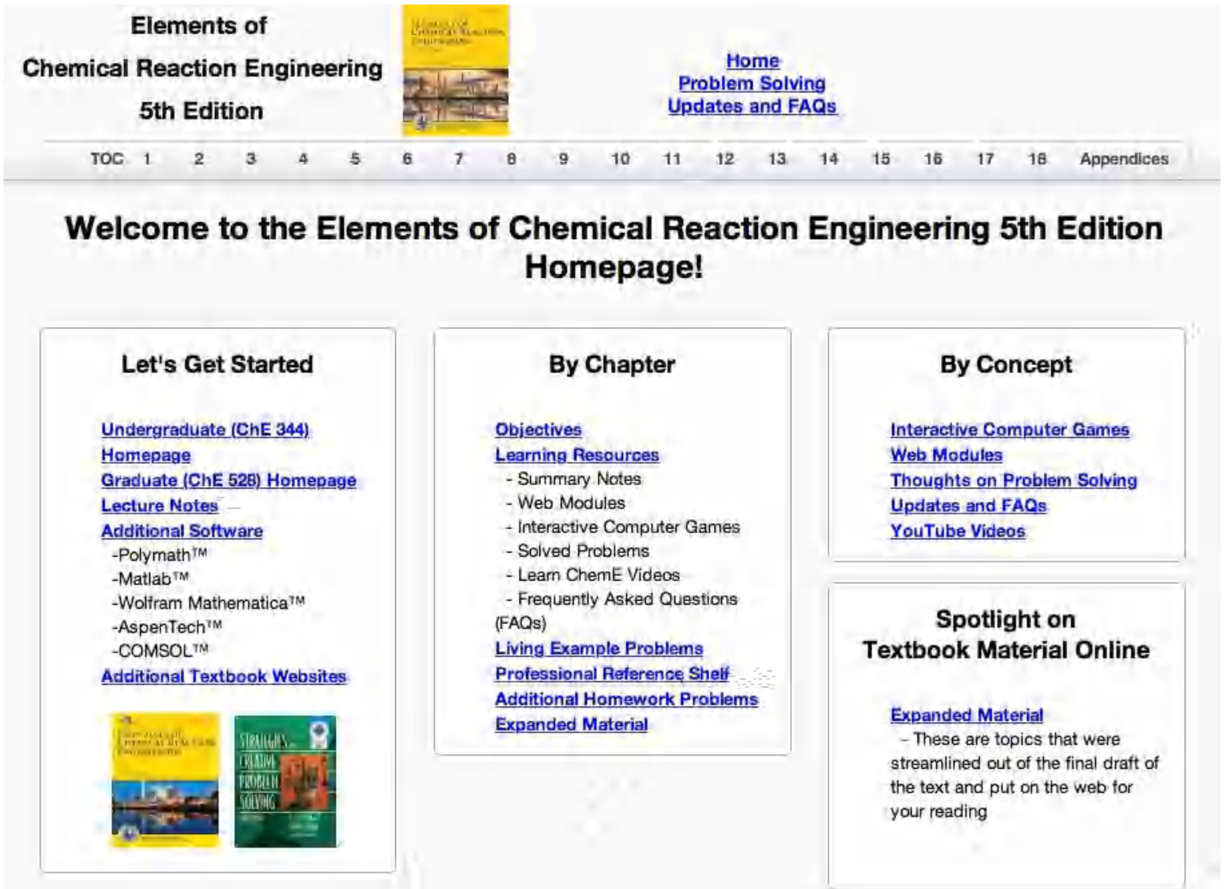

INTERACTIVE COMPUTER GAMES (ICGs)

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:

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

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

Note: 75% constitutes mastery.

KINETIC CHALLENGE II

CzBzzAzz

Score = 2.0 * AB.C
z = random numbers

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

Note: 75% constitutes mastery.

MURDER MYSTERY

zzAzz

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

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

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

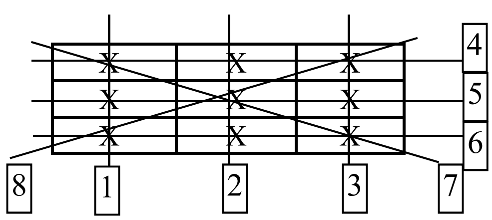
TIC TAC TOE

zDzCzBzA

Score = 4.0 * AB.C
z = random numbers

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

Configurations



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

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

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

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

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**12**5**4**8**2**9**13**

Final conversion = 2*AB.C conversion = 2*42.1 = 84.2
Final flow rate = 2*DE.F flow rate = 2*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 — 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 — C: Looked at review
did in the interaction: — 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

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%

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.

LIVING EXAMPLE PROBLEMS (LEPs)

Elements of
Chemical Reaction Engineering
5th Edition

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	--

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 2015
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, 5th edition, H. Scott Fogler
Web site: *www.umich.edu/~elements/5e*

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, Mole balances
Read:	Preface, Prerequisites, 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: P1-1_A, P1-6_B
In-Class Problem:	1
Study Problems:	P1-8_A

3) Wednesday, September 16

Topic:	Lecture 3 – Chapter 3, Rate laws
Read:	Chapter 2, Chapter 3
Hand In:	Problem Set 2: Define terms in the Arrhenius Equation, P2-2_A, Intro to Learncheme
In-Class Problem:	2 (*Hint:* Viewing the University of Alabama YouTube video "The Black Widow" noted in Problem P3-8_B 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: Define θ_i, θ_A, θ_B, and δ, P2-10_B, P3-5_A, P3-8_B, P3-11_B, P3-13_A

In-Class Problem: 3 - Bring i>clickers (tentative) - Test Run of System in 2166 Dow

Study Problems: P3-14_A

5) Wednesday, September 23

Topic: Lecture 5 – Chapter 4, Stoichiometry Flow Systems

Read: Chapter 4, Section 4.1

Hand In: Problem Set 4: Define ε, F_{T0}, C_{T0}, P4-2_A.

In-Class Problem: 4

Study Problems: P4-1_A parts (c) and (d)

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, P4-3_A, P4-4_B, P4-5_B.

In-Class Problem: 5

Study Problems: P4-10_C

7) Wednesday, September 30

Topic: Lecture 7 – Chapter 5, California Registration Exam Problem

Hand In: Problem Set 6: What are you asked to find P5-18_B? What is the Ergun Equation? P5-2_A.

In-Class Problem: 6

Study Problems: P5-1_B (a) and (b)

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: P5-3_A, P5-4_B, P5-5_A, P5-8_B, P5-13_B omit parts (j) and (k), P5-16_B (a).

In-Class Problem: 7 – Bring Laptops

Study Problems: P5-9_A, P5-10_B (a).

9) Wednesday, October 7

Topic: Lecture 9 – Chapter 6, Membrane Reactors

Read: Chapter 6

Hand In: Problem Set 8: P5-13_B part (j) and (k), P5-22_A.

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 (a), P5-11_B, P6-4_B delete part (c), 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: LEP for Example 6-1, P6-2_B, P6-11_B omit part (c)
In-Class Problem: 10 – Bring Laptops to carry out Polymath Regression
Study Problems: P7-6_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: P7-7_A, P7-8_A.
In-Class Problem: 11
Study Problems P7-10_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) part (1) only, P8-1_A (b), P8-1_A (c) part (1) only, P8-2_B, P8-6_B, P8-7_C (a), (b) and (c)
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
In-Class Problem: 13 – Bring Laptops
Study Problems: P8-16_A

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 (b), P11-3_B, P11-4_A.
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: P12-3_B LEP
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:	P12-19_B, i>clicker questions handed out in class

21) Wednesday, November 18

Topic:	Lecture 20 – CSTR and Review for Exam II

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

23) Wednesday, November 25

Topic:	Lecture 22 – Multiple Steady States (MSS) Multiple Reactions with Heat Effects
Read:	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
Hand In:	Problem Set 18: P13-1_B (b) and (f), P13-8_B
In-Class Problem:	19 – Bring Laptops
Study Problems:	P13-4_B

25) Wednesday, December 2

Topic:	Lecture 24 –Catalysis Reactor Safety
Read:	Chapter 13, Sections 13.1 through 13.3, and 13.5
Hand In:	Problem Set 19: P10-2_A part (d), P10-4_B
In-Class Problem:	20
Study Problems:	P12-16_B

26) Monday, December 7

Topic:	Lecture 25 – Catalysis
Read:	Chapter 10, Sections 10.1 through 10.2.2
Hand In:	Problem Set 20: 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 21: $P9\text{-}4_A$, $P9\text{-}5_B$, $P9\text{-}9_B$, $P9\text{-}14_B$ $P9\text{-}19_A$
In-Class Problem:	22
Study Problems:	$P9\text{-}12_B$, $P9\text{-}16_B$, $P9\text{-}21_A$

28) FINAL EXAM

Solutions for Chapter 1 – Mole Balances

P1-1 (a) Example 1-3

(i) C_A decreases and C_B increases with an increase in k, and a decrease in v_0 for the same volume.

(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) Refer to the polymath report below

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

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

$V = 4*10^{13}\ ft^3$ $\quad T = 534.7^\circ R$ $\quad P_O = 1atm$

$R = 0.7302\dfrac{atm\,ft^3}{lbmol\,R}$ $\quad y_A = 0.02$ $\quad C_S = 2.04*10^{-10}\dfrac{lbmol}{ft^3}$ $\quad C = 4*10^5$ cars

F_S = CO in Santa Ana winds $\quad F_A$ = CO emission from autos $\quad v_A = 3000\dfrac{ft^3}{hr}$ 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.

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

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

$F_A = 6.685 \times 10^4$ 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 Sant 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.

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

From (f),

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

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

t = 6.92 hr

P1-2 (h)

(1)

t_o = 0 $\quad$ t_f = 72 hrs

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

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

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

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

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

See Polymath program P1-4-h-1.pol.

POLYMATH Results

Calculated values of the DEQ variables

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

ODE Report (RKF45)

Differential equations as entered by the user

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

Explicit equations as entered by the user

[1] v0 = 1.67*10^12

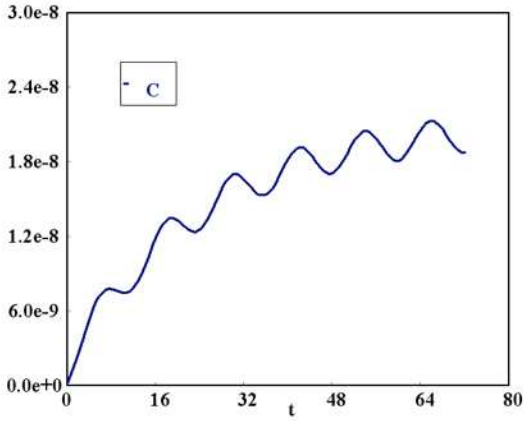
[2] a = 35000

[3] b = 30000

[4] F = 341.23

[5] V = 4*10^13

P1-2 (h) Continued



(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

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

POLYMATH Results

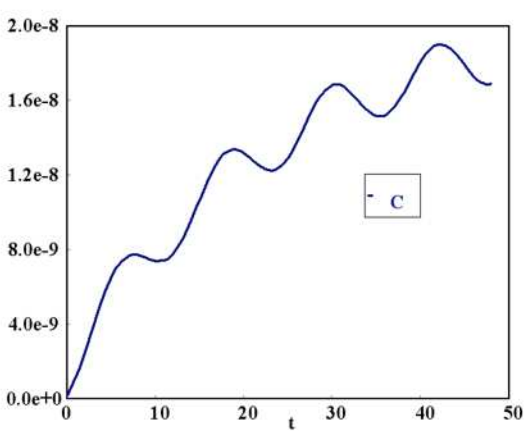
Calculated values of the DEQ variables

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

ODE Report (RKF45)

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

Explicit equations as entered by the user
[1] v0 = 1.67*10^12
[2] a = 35000
[3] b = 30000
[4] V = 4*10^13



P1-2 (h) Continued

(3)

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

Changing b → The amplitude of ripples is directly proportional to 'b'. As b decreases amplitude decreases and graph becomes smooth.

Changing v_0 → As the value of v_0 is increased the graph changes to a "shifted sin-curve". And as v_0 is decreased graph changes to a smooth increasing curve.

P1-3 (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 Polymath program P1-3-a.pol.

POLYMATH Results

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
T	0	0	500	500
X	500	2.9626929	519.40024	4.2199691
Y	200	1.1285722	4099.517	117.62928
k1	0.02	0.02	0.02	0.02
k2	4.0E-05	4.0E-05	4.0E-05	4.0E-05
k3	4.0E-04	4.0E-04	4.0E-04	4.0E-04
k4	0.04	0.04	0.04	0.04

ODE Report (RKF45)

Differential equations as entered by the user

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

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

Explicit equations as entered by the user

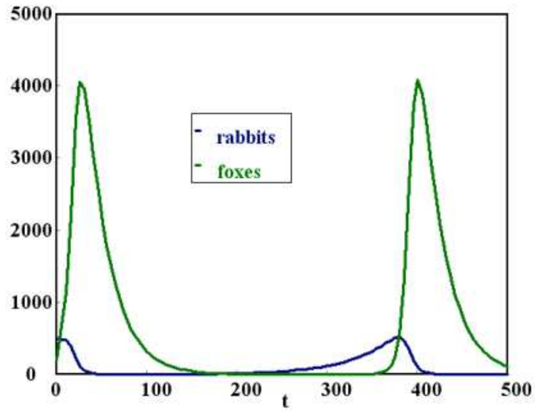
[1] k1 = 0.02

[2] k2 = 0.00004

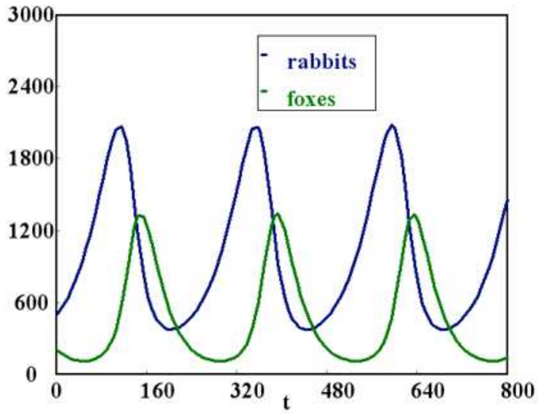
[3] k3 = 0.0004

[4] k4 = 0.04

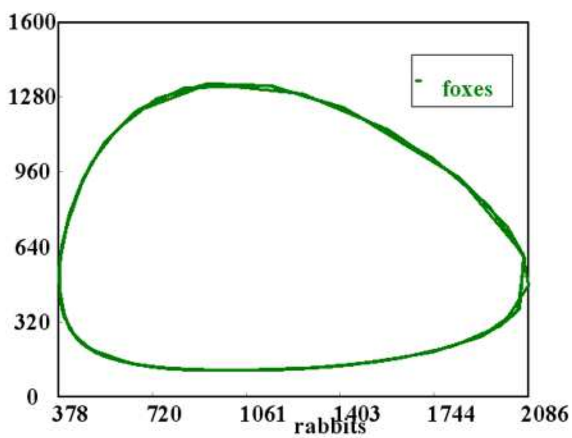
P1-3 (a) Continued



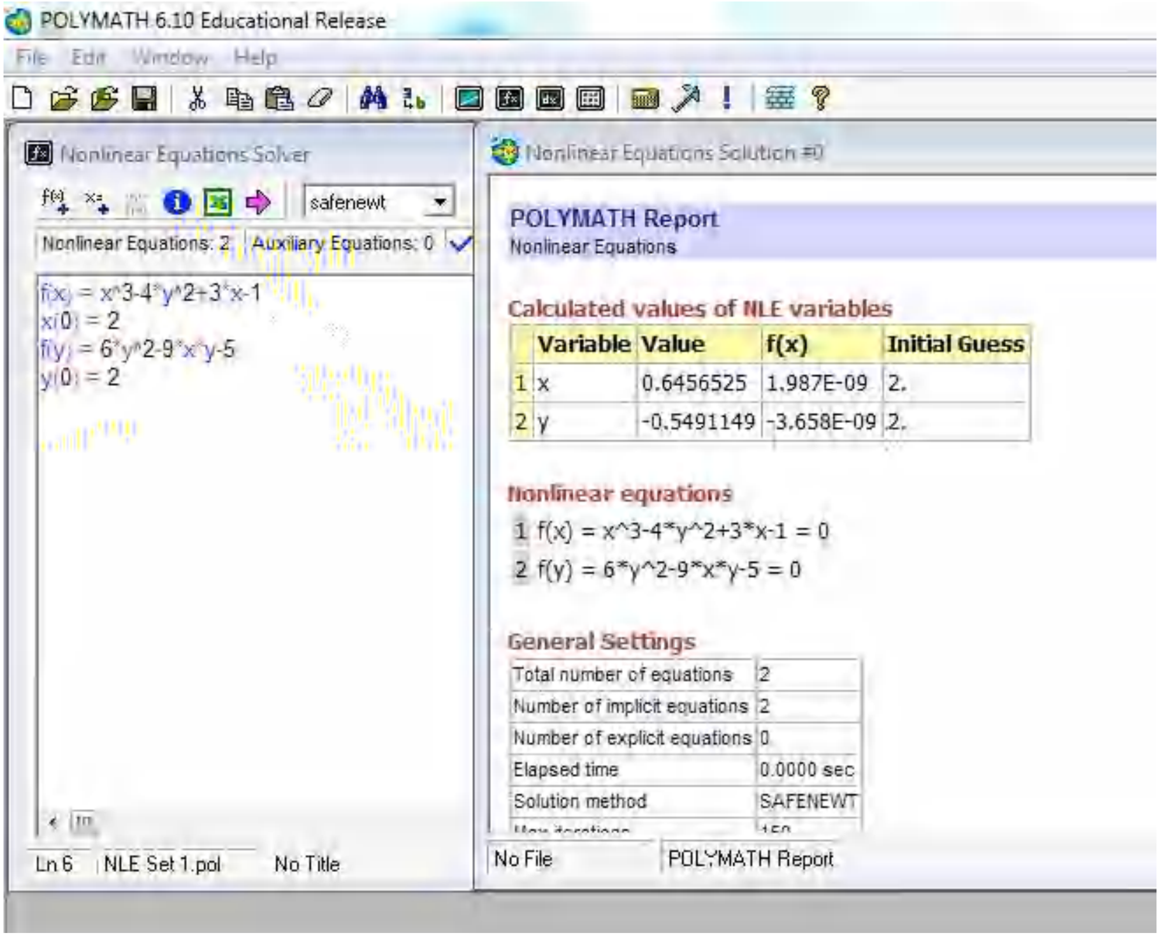
When, t_{final} = 800 and $k_3 = 0.00004/(day \times rabbits)$



Plotting rabbits vs. foxes



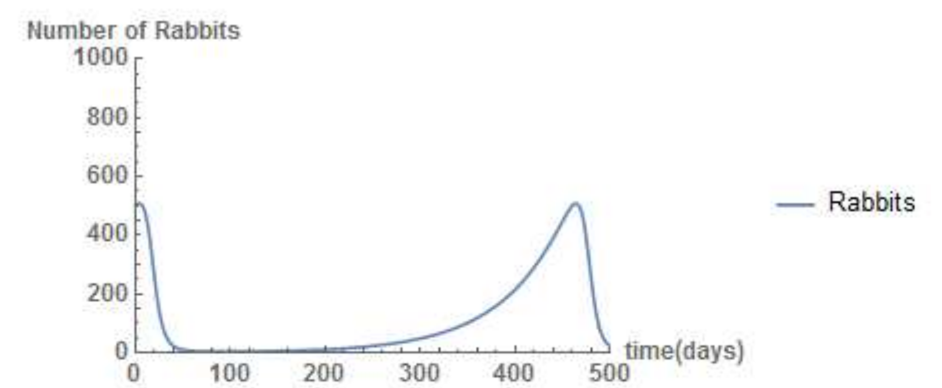
P1-3 (b)



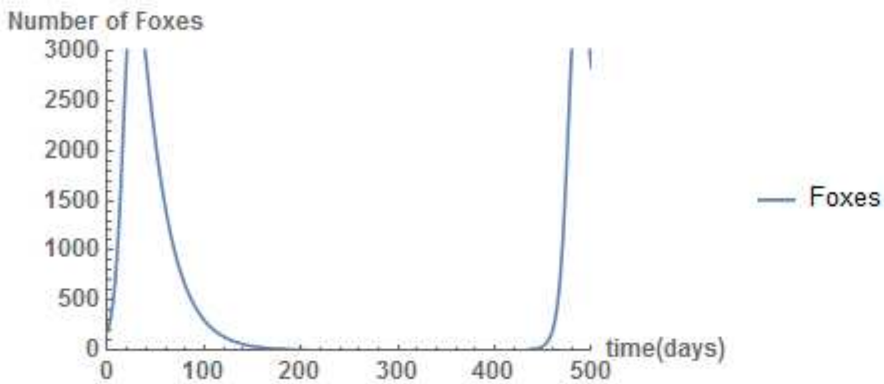
P1-3 (c)

We would have to change k2 and k4 for the plot to become a circle from an oval.

P1-3 (d)



P1-3 (d) Continued



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

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

Integrating the above equation we get

P1-6 (a) Continued

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

Hence **V = 99 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 $k = 0.0001\ s^{-1}$

CSTR:

We have already derived that

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

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

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

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

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

P1-6 (c)

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

CSTR:

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

Substituting all the values we get

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

PFR:

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

P1-6 (c) Continued

Integrating

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

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

P1-6 (d)

$C_A = 0.001C_{A0}$

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

Constant Volume $V=V_0$

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

Zero order:

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

First order:

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

Second order:

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

P1-7 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 Tuners