ARIZONA STATE UNIVERSITY

GENERAL STUDIES COURSE PROPOSAL COVER FORM

Course information:

*Copy and paste **current** course information from Class Search/Course Catalog.*

College/School	Ira A. Fulton Schools of Engineering			Department	SEMTE		
Prefix	CHE	Number	384	Title	Numerical Methods for Chemical Engineers	Units:	3

Is this a cross-listed course? No If yes, please identify course(s)

Is this a shared course? No If so, list all academic units offering this course

*Note– For courses that are crosslisted and/or shared, a letter of support from the chair/director of **each** department that offers the course is required for **each** designation requested. By submitting this letter of support, the chair/director agrees to ensure that all faculty teaching the course are aware of the General Studies designation(s) and will teach the course in a manner that meets the criteria for each approved designation.*

Is this a permanent numbered course with topics? Yes

If yes, all topics under this permanent numbered course must be taught in a manner that meets the criteria for the approved designation(s). It is the responsibility of the chair/director to ensure that all faculty teaching the course are aware of the General Studies designation(s) and adhere to the above guidelines.

Chair/Director Initials: DN (Required)

Course description: **Study and application of numerical methods in solving problems commonly encountered in chemical engineering. Emphasis on chemical engineering applications using MATLAB and Excel. Roots, linear algebraic equations, matrices, curve fitting, differentiation, integration, ordinary and partial differential equations.**

Requested designation: Mathematical Studies-CS **Mandatory Review:** Yes

*Note- a **separate** proposal is required for each designation.*

Eligibility:

Permanent numbered courses must have completed the university's review and approval process.
For the rules governing approval of omnibus courses, contact Phyllis.Lucie@asu.edu.

Submission deadlines dates are as follow:

For Fall 2016 Effective Date: October 1, 2015 For Spring 2017 Effective Date: March 10, 2016

Area(s) proposed course will serve:

A single course may be proposed for more than one core or awareness area. A course may satisfy a core area requirement and more than one awareness area requirements concurrently, but may not satisfy requirements in two core areas simultaneously, even if approved for those areas. With departmental consent, an approved General Studies course may be counted toward both the General Studies requirement and the major program of study.

Checklists for general studies designations:

Complete and attach the appropriate checklist

- Literacy and Critical Inquiry core courses (L)
- Mathematics core courses (MA)
- Computer/statistics/quantitative applications core courses (CS)
- Humanities, Arts and Design core courses (HU)
- Social-Behavioral Sciences core courses (SB)
- Natural Sciences core courses (SQ/SG)
- Cultural Diversity in the United States courses (C)
- Global Awareness courses (G)
- Historical Awareness courses (H)

A complete proposal should include:

☒ Signed course proposal cover form
☒ Criteria checklist for General Studies designation(s) being requested
☒ Course catalog description
☒ Sample syllabus for the course
☒ Copy of table of contents from the textbook and list of required readings/books

It is respectfully requested that proposals are submitted electronically with all files compiled into one PDF.

Contact information:

Name: Jessica Caruthers E-mail: Jessica.caruthers@asu.edu Phone: 480-965-2335

Department Chair/Director approval: *(Required)*

Chair/Director name (Typed): David Nielsen Date: 10/13/16

Chair/Director (Signature): [signature]

Rev. 4/2015

Arizona State University Criteria Checklist for

MATHEMATICAL STUDIES [CS]

Rationale and Objectives

The **Mathematical Studies** requirement is intended to ensure that students have skill in basic mathematics, can use mathematical analysis in their chosen fields, and can understand how computers can make mathematical analysis more powerful and efficient. The **Mathematical Studies** requirement is completed by satisfying both the **Mathematics [MA]** requirement and the **Computer/Statistics/Quantitative Applications [CS]** requirement explained below.

The **Mathematics [MA]** requirement, which ensures the acquisition of essential skill in basic mathematics, requires the student to complete a course in College Mathematics, College Algebra, or Pre-calculus; or demonstrate a higher level of skill by completing a mathematics course for which a course in the above three categories is a prerequisite.

The **Computer/Statistics/Quantitative Applications [CS]** requirement, which ensures skill in real world problem solving and analysis, requires the student to complete a course that uses some combination of computers, statistics, and/or mathematics.* Computer usage is encouraged but not required in statistics and quantitative applications courses. At a minimum, such courses should include multiple demonstrations of how computers can be used to perform the analyses more efficiently.

*CS does *not* stand for computer science in this context; the "S" stands for statistics. Courses in computer science must meet the criteria stated for CS courses.

Revised April 2014

Proposer: Please complete the following section and attach appropriate documentation.

ASU--[CS] CRITERIA

A COMPUTER/STATISTICS/QUANTITATIVE APPLICATIONS [CS] COURSE MUST SATISFY ONE OF THE FOLLOWING CRITERIA: 1, 2, OR 3

YES	NO		Identify Documentation Submitted
		1. Computer applications*: courses must satisfy both **a** and **b**:	
☒	☐	**a.** Course involves the use of computer programming languages or software programs for quantitative analysis, algorithmic design, modeling, simulation, animation, or statistics.	CHE 384 Syllabus
		b. Course requires students to analyze and implement procedures that are applicable to at least one of the following problem domains **(check those applicable)**:	
☒	☐	i. Spreadsheet analysis, systems analysis and design, and decision support systems.	Quiz 4
☐	☒	ii. Graphic/artistic design using computers.	
☐	☒	iii. Music design using computer software.	
☒	☐	iv. Modeling, making extensive use of computer simulation.	Case study PPT CSTR-1
☒	☐	v. Statistics studies stressing the use of computer software.	HW-6 Prob. 14.1
☒	☐	vi. Algorithmic design and computational thinking.	Exam 1, Prob 1.

*The **computer applications** requirement **cannot** be satisfied by a course, the content of which is restricted primarily to word processing or report preparation skills, the study of the social impact of computers, or methodologies to select software packages for specific applications. Courses that emphasize the use of a computer software package are acceptable only if students are required to understand, at an appropriate level, the theoretical principles embodied in the operation of the software and are required to construct, test, and implement procedures that use the software to accomplish tasks in the applicable problem domains. Courses that involve the learning of a computer programming language are acceptable only if they also include a substantial introduction to applications to one of the listed problem domains.

YES	NO		Identify Documentation Submitted
		2. Statistical applications: courses must satisfy **a**, **b**, and **c**.	
☒	☐	**a.** Course has a minimum mathematical prerequisite of College Mathematics, College Algebra, or Pre-calculus, or a course already approved as satisfying the MA requirement.	CHE 384 Syllabus
		b. The course must be focused principally on developing knowledge in statistical inference and include coverage of all of the following:	
☐	☒	i. Design of a statistical study.	
☒	☐	ii. Summarization and interpretation of data.	HW -6, Prob 14.1
☐	☒	iii. Methods of sampling.	
☐	☒	iv. Standard probability models.	
☐	☒	v. Statistical estimation	
☐	☒	vi. Hypothesis testing.	
☒	☐	vii. Regression or correlation analysis.	HW -6 , Prob 14.7
☒	☐	**c.** The course must include multiple demonstrations of how computers can be used to perform statistical analysis more efficiently, if use of computers to carry out the analysis is not required.	HW -6, Prob 15.3

YES	NO		Identify Documentation Submitted
		3. Quantitative applications: courses must satisfy **a, b, and c:**.	
☒	☐	**a.** Course has a minimum mathematical prerequisite of College Mathematics, College Algebra, or Pre-calculus, or a course already approved as satisfying the MA requirement.	CHE 384 Syllabus
		b. The course must be focused principally on the use of mathematical models in quantitative analysis and decision making. Examples of such models are:	
☒	☐	i. Linear programming.	Exam 2, Prob. 2
☐	☒	ii. Goal programming.	
☐	☒	iii. Integer programming.	
☐	☒	iv. Inventory models.	
☐	☒	v. Decision theory.	
☐	☒	vi. Simulation and Monte Carlo methods.	
☐	☒	vii. Other (explanation must be attached).	
☒	☐	**c.** The course must include multiple demonstrations of how computers can be used to perform the above applications more efficiently, if use of computers is not required by students.	Exam 2, Prob. 1 & 2

Course Prefix	Number	Title	General Studies Designation
CHE	384	Numerical Methods for Chemical Engineers	

Explain in detail which student activities correspond to the specific designation criteria. Please use the following organizer to explain how the criteria are being met.

Criteria (from checksheet)	How course meets spirit (contextualize specific examples in next column)	Please provide detailed evidence of how course meets criteria (i.e., where in syllabus)
Computer Applications	Using MS excel and MATLAB to solve numerical problems in CHE.	HW Assignments (10 sets), Average above 70% Quiz (10 sets), Average above 80% Exam (4), Average above 70% Lectures on Excel and MATLAB
Statistical Applications	Chapter 14 Linear Regression Chapter 15 Non-Linear Regression	HW 6, to be graded Quiz 4 (Average above 75%) Exam 3 (to be graded)
Quantitative Applications	Linear and Non-Linear Regression Excel Solver MATLAB Solver	Exam 2, Problem 2, Average above 86% Exam 2 (grades attached from spring 2016)

CHE 384: Numerical Methods for Chemical Engineers

School for Engineering of Matter, Transport and Energy, Arizona State University

Instructor

Dr. Shuguang Deng; Tel: 480-727-7238, e-mail: shuguang.deng@asu.edu
Office Hours: W 10:00-12:00, Office Location: Engineering Research Center 279

Course Description

Study and application of numerical methods in solving problems commonly encountered in chemical engineering. Emphasis on chemical engineering applications using MATLAB and Excel. Roots, linear algebraic equations, matrices, curve fitting, differentiation, integration, ordinary and partial differential equations.

Pre-requisites

Chemical Engineering BSE Student; MAT 274 or 275 with C or better; MAT 242, 342 or 343 with C or better; Pre- or corequisite(s): MAT 267 or 272 with C or better if completed.

Textbook

Steven C. Chapra, "Applied Numerical Methods with MATLAB® for Engineers and Scientists." 3rd edition, The McGraw-Hill Companies, Inc., ISBN 978-0-07-340110-2, (2012).

Course Objectives

- To study numerical analysis methods and their applications in solving chemical engineering problems
- To solve chemical engineering problems with numerical analysis techniques
- To learn the basics of MATLAB programing and to write simple MATLAB codes

Topics Covered

- MATLAB basics and programming
- Numerical solution of nonlinear equations
- Numerical solution of simultaneous linear algebraic equations
- Finite difference methods and interpolation
- Numerical differentiation and integration
- Linear and nonlinear regressions
- Numerical solution of ordinary differential equations
- Numerical solution of partial differential equations

Grading Policy

The semester score will be determined based on a set of evaluation methods, and the weights are: There will be ten homework assignments, ten quizzes, and four exams.

Homework	10%
Quiz	10%
Exam-1:	15%
Exam-2	20%
Exam-3	20%
Exam-4	25%

The semester grade will be determined according to following scale:
A: 90-100%; B: 80-89%; C: 70-79%; D: 60-69%; F: <60%

Course Outcomes for CHE 384

Course Outcome	ABET (a-k)	Level of Mastery
Students will be able to solve linear and non-linear equations using the bisection and Netwon's methods	a	Comprehension
Students will be able to solve a sets of linear equations with MATLAB or excel	a	Comprehension
Students will apply linear and non-linear regression techniques to correlate a set of experimental data	a	Comprehension
Students will apply numerical integration equations to solve relevant science and engineering problems	a	Comprehension
Students will be able to solve initial and boundary value problems of ordinary differential equations using Newton's and Runge-Kutta methods	a	Comprehension
Students will be able to solve selected chemical engineering problems by identifying the problems, formulating the governing equations, and solve the equations with the numerical methods learns in this course.	e	Comprehension
Students will be able to write simple MATLAB function m-files relevant to chemical engineering processes and execute the m-files in proper numerical method modules.	k	Comprehension

Mastery of Outcomes
Mastery of outcomes will be determined by student performance on selected exam and/or homework problems. Unless otherwise stated, a score of 70% will be required to demonstrate mastery. Students will be informed which problems are used to assess each outcome.

(a) An ability to apply knowledge of mathematics, science, and engineering
(e) An ability to identify, formulate, and solve engineering problems
(k) An ability to use the techniques, skills, and modern engineering tools necessary for engineering practic

CHE 384 Course Schedule

Session	Date	Topics	HW Due
1		Course Introduction/Chapter 1	
2		MATLAB Review	
3		Chapter 5 Bracketing Methods	
4		Chapter 6 Open Methods	HW-1
5		Chapter 8 Linear Algebra and Matrix	
6		Chapter 9 Gauss Elimination	
7		Chapter 10 LU Factorization	HW-2
8		Chapter 11 Matrix Inversion and Condition	
9		Exam -1 (Chapters 1 – 6)	
10		Chapter 12 Iterative Methods	HW-3
11		Chapter 14 Linear Regression	
12		Chapter 15 Non-linear Regression	HW-4
13		Chapter 17. Polynomial Interpolation (1)	
14		Chapter 17. Polynomial Interpolation (2)	HW-5
15		Exam -2 (Chapters 8-12)	
16		Chapter 18 Splines and Piecewise Interpolation (1)	HW-6
17		Chapter 18 Splines and Piecewise Interpolation (2)	
18		Chapter 19 Numerical Integration Formula (1)	
19		Chapter 19 Numerical Integration Formula (2)	HW-7
20		Chapter 20 Numerical Integration of Function	
21		Chapter 21 Numerical Differentiation	
22		Exam -3 (Chapters 14-18)	
23		Chapter 22 Initial-Value ODE (1)	HW-8
24		Chapter 22 Initial-Value ODEs (2)	
25		Chapter 23 Adaptive Methods and Stiff Systems	
26		Chapter 24 Boundary Value ODEs (1)	HW-9
27		Chapter 24 Boundary Value ODEs (2)	
28		Chapter 25 Partial Differential Equations (1)	
29		Chapter 25 Partial Differential Equations (2)	HW-10
30		Exam-4 (Chapter 19-24)	

HW-1	1.1, 1.3, 1.8, 1.11, 2.1, 2.5, 2.11, 2.13, 3.1, 3.18
HW-2	5.5, 5.8, 5.21, 6.1, 6.14, 6.22
HW-3	8.2, 8.3, 8.13, 9.2, 9.4, 9.6, 9.8
HW-4	10.3, 10.5, 10.12, 11.1, 11.3, 11.7
HW-5	12.1, 12.3, 12.4, 12.6
HW-6	14.1, 14.7, 14.12, 15.3, 15.10, 15.18
HW-7	17.2, 17.3, 18.1, 18.3
HW-8	19.4, 19.8, 19.15, 20.2, 20.3, 20.21, 21.9, 21.12
HW-9	22.1, 22.4, 23.5, 23.7
HW-10	24.1, 24.3, 24.11, 25.1, 25.2, 25.3

Absence Policies

Late submission is NOT accepted unless there is a justified excuse and may be subject to 10% penalty each day it is late. Make-up exams will NOT be considered except for extreme emergencies and an ASU excused absence such as religious observance (in accordance with ACD 304–04) and university-sanctioned events and activities (in accordance with ACD 304–02) with proof of justifications.

Policy regarding expected classroom behavior

Any student who arrives 15 min after the class starts is not allowed in class. Cell phones should be silenced and no cell phone usage is permitted during class time. No food or drinks during the class.

Academic Integrity Policy

Any incidence of cheating or plagiarism will be reported to the School Director and/or the Dean of Academic and Student Affairs for appropriate action which may include loss of credit for the course or the dismissal from the University. Examples of cheating or plagiarism include, but not limited to: copying homework from others, copying from Textbook solution manual, cheating during in-class exams, etc. Please note that while it is encouraged to collaborate with your classmates on the homework, your final submission should not be similar enough to raise a question of academic dishonesty. See the ASU Academic Integrity Policy at http://provost.asu.edu/academicintegrity for further details. Please also view and follow the expectations set forth in the Fulton Engineering Honor Code.

Policy Against Threatening Behavior

All incidents and allegations of violent or threatening conduct by an ASU student (whether on- or off-campus) must be reported to the ASU Police Department and the Office of the Dean of Students. The policy against threatening behavior, per the Student Services Manual, SSM 104–02, "Handling Disruptive, Threatening, or Violent Individuals on Campus" applies.

Disability Accommodations

Appropriate arrangements or accommodations including additional time or resources for taking exams can be arranged for disabled students. However, they must be registered with the Disability Resource Center (Disability-Q@asu.edu, 480- 965-1234), and they must submit to the instructor the appropriate documentation from the DRC for the request.

Drop/Withdraw Policy

ASU drop/withdraw policy can be found here.

TBD Fall 2017	Last day to register or drop/add without college approval
TBD Fall 2017	Course withdrawal deadline

The SEMTE's Advising Center is always available for those who have questions and seek advice regarding courses and programs.

CHE 384 Quiz – 4 (Due TBD)

Online Submission Only

Class ID:______________________

Name: ________________________ Score:____________

For the following non-linear equation system with initial guess $x_1=x_2=-5$:

$$f_1 = 2x_1 - x_2 - e^{-x_1} = 0$$

$$f_2 = -x_1 + 2x_2 - e^{-x_2} = 0$$

1. Solve the above system with excel Solver. **(20 points)**
2. Solve the above system with Newton's method. **(20 points)**
3. Check your solution with MATALB fsolve. **(20 points)**

Solution Key

1. Excel solver method

excel solver solution of non-linear equations

x_1	0.56714329
x_2	0.56714329
f_1	1.73614E-11
f_2	1.73614E-11
Sumsq	6.0284E-22

2. The Newton's method

For the Newton's method, we need to define the Jacobian matrix as follows:

$$J = \begin{bmatrix} \frac{\partial f1}{\partial x1} & \frac{\partial f1}{\partial x2} \\ \frac{\partial f2}{\partial x1} & \frac{\partial f2}{\partial x2} \end{bmatrix} = \begin{bmatrix} 3 + e^{-x1} & -1 \\ -1 & 2 + e^{-x2} \end{bmatrix}$$

```
function [J, F]=quiz4Jacobian(x)
J=[2+exp(-x(1)) -1;-1 2+exp(-x(2))];
   F=[2*x(1)-x(2)-exp(-x(1));-x(1)+2*x(2)-exp(-x(2))];
end
```

```
>> [x, f, ea, iter]=newtmult(@quiz4Jacobian, [-5; -5])

x =

   0.567143290409781
   0.567143290409781


f =

   1.0e-06 *
  -0.196480471559290
  -0.196480471559290


ea =

    2.210639195271743e-05

iter =

    4
```

3. MATLAB fsolve method

```
function f=quiz4func(x)
f=[2*x(1)-x(2)-exp(-x(1));...
    -x(1)+2*x(2)-exp(-x(2))];
end
```

```
>> x=fsolve(@quiz4func,[-5 -5])

>> x =

    0.567143165036970   0.567143165036970
```

Exam 1 CHE 384 (Numerical Methods for Chemical Engineers)

School for Engineering of Matter, Transport and Energy, Arizona State University

Date: TBD

Solution Key

Name: ____________________ Score:__________

Class ID:__________________

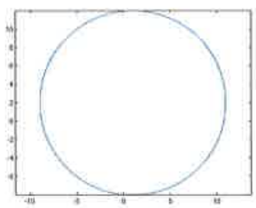
1. Create a function M-file to draw a circle with the center at (x_0, y_0) of (1, 2) and radius (r) of 10. (Hint: you can draw the circle in a X-Y coordinate with $x = x_0 + r * \sin(\theta)$; $y = y_0 + r * \cos(\theta)$, $0 \le \theta \le 2\pi$). You need to submit the function M-file, command of running the M-function and the expected output of the M-function operation. If you create the circle without using an function M-file, you will lose at least 10 points. **(15 points)**

```
function []=circdrwf(x0,y0,r)
t=0:0.001:2*pi;
x=x0+r*cos(t);
y=y0+r*sin(t);
plot(x,y)
axis('equal')
end
```

+10

>> circdrwf(1, 2, 10);

+3



+2

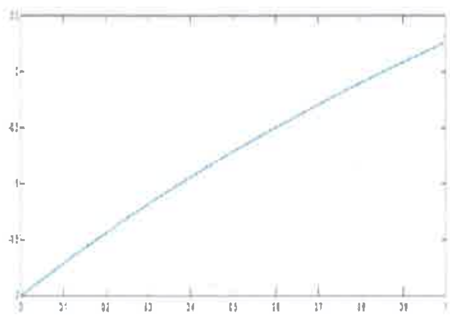
2. Solve the following equation with different methods and show the iteration equations and the first four calculation steps.

$$x = 2e^{-x}$$

a. Use MATLAB to plot f(x) for x within [0 1], and submit the output of the figure. **(5 points)**

In this solution f(x) = x-2*exp(-x)=0 is used. If f(x)= 2*exp(-x)-x=0 is used in your solution, the plot will be different.

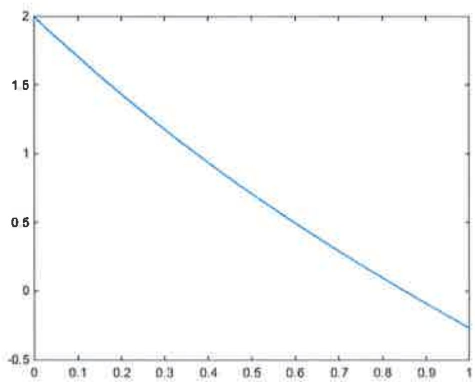
```
fplot(@(x)x-2*exp(-x), [0 1])
```



+5

Or

```
fplot(@(x)2*exp(-x)-x, [0 1])
```



+5

b. Bisection with a bracket of [0, 1]; **(15 points)**

$x_r = (x_l+x_u)/2$ $\boxed{+5}$

In this solution f(x) = x-2*exp(-x) is used. If f(x)= 2*exp(-x)-x is used, the f(x) values will be slightly different.

Step	x_l	x_u	x_r	$f(x_l)$	$f(x_u)$	$f(x_r)$
1	0.0000	1.0000	0.5000	-2.0000	0.2642	-0.7131
2	0.5000	1.0000	0.7500	-0.7131	0.2642	-0.1947
3	0.7500	1.0000	0.8750	-0.1947	0.2642	0.0413
4	0.7500	0.8750	0.8125	-0.1947	0.0413	-0.0750

$\boxed{+10}$

c. False position with a bracket of [0, 1]; **(15 points)**

$x_r = x_u - f(x_u)*(x_l-x_u)/[f(x_l)-f(x_u)]$ $\boxed{+5}$

In this solution f(x) = x-2*exp(-x) is used. If f(x)= 2*exp(-x)-x is used, the f(x) values will be slightly different.

Step	x_l	x_u	x_r	$f(x_l)$	$f(x_u)$	$f(x_r)$
1	0.0000	1.0000	0.8833	-2.0000	0.2642	0.0565
2	0.0000	0.8833	0.8590	-2.0000	0.0565	0.0119
3	0.0000	0.8590	0.8540	-2.0000	0.0119	0.0025
4	0.0000	0.8540	0.8529	-2.0000	0.0025	0.0005

$\boxed{+10}$

d. Fixed point iteration, $x_0 = 0$; **(15 points)**

$G(x) = 2e^{-x}$ $\boxed{+5}$

$x_{i+1} = 2*\exp(-x_i)$

In this solution f(x) = x-2*exp(-x) is used. If f(x)= 2*exp(-x)-x is used, the f(x) values will be slightly different.

Step	x	G(x)	f(x)
1	0.0000	2.0000	-2.0000
2	2.0000	0.2707	1.7293
3	0.2707	1.5257	-1.2551
4	1.5257	0.4349	1.0908

$\boxed{+10}$

e. Newton-Raphson with $x_0 = 0$; **(15 points)**

$$x_{i+1} = x_i - f(x_i)/f'(x_i) = x_i - \frac{x_i - 2e^{-x_i}}{1+2e^{-x_i}}$$

+7

In this solution f(x) = x-2*exp(-x) is used. If f(x)= 2*exp(-x)-x is used, the f(x) values will be slightly different.

Step	x	f(x)	f'(x)
1	0.0000	-2.0000	3.0000
2	0.6667	-0.3602	2.0268
3	0.8444	-0.0153	1.8597
4	0.8526	0.0000	1.8526

+8

f. Secant method with $x_1 = 0$, $x_2 = 1$; **(15 points)**

$$x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})} = x_i - \frac{(x_i - 2e^{-x_i})(x_i - x_{i-1})}{(x_i - 2e^{-x_i}) - (x_{i-1} - 2e^{-x_{i-1}})}$$

+7

In this solution f(x) = x-2*exp(-x) is used. If f(x)= 2*exp(-x)-x is used, the f(x) values will be slightly different.

Step	x	f(x)	Δf(x)
1	0.0000	-2.0000	
2	1.0000	0.2642	2.2642
3	0.8833	0.0565	-0.2078
4	0.8516	-0.0019	-0.0584
5	0.8526	0.0000	0.0019

+8

g. Use MATLAB function fzero to verify your answer; **(5 points)**

```
fzero (@(x)x-2*exp(-x), 0, 1)
```

+4

```
ans =

  0.8526
```

+1

Exam 2 CHE 384 (Numerical Methods for Chemical Engineers)

School for Engineering of Matter, Transport and Energy, Arizona State University

Date: TBD

Solution Key

1. For the following linear equation system

$10\,X_1 + 2X_2 - X_3 = 27$
$-3X_1 - 6X_2 + 2X_3 = 61.5$
$X_1 + X_2 + 5X_3 = -21.5$

1) Express the linear equation system in the matrix form **(10 points)**

[A] [X] = [b]

2) Solve the above system with Gauss elimination method and show the upper triangular matrix before the back substitution step. It is required to show the elimination and back substitution steps in a matrix form. **(25 points)**

[A] [X] = [b]

3) Solve the above system using Gauss-Seidel iterative method, write the iterative equations and show the values of [X] in the first two steps. **(25 points)**

a. $X_1^{i+1} =$
b. $X_2^{i+1} =$
c. $X_3^{i+1} =$

Iterative Step	X_1	X_2	X_3
0	3	10	4
1			
2			

2. Solve the following non-linear equation system with one of the methods discussed in our lecture (successive substitution, excel solver, Newton-Raphson or MATLAB fsolve). If you use successive substitution, you need to show at least two steps of calculations. If excel solver is applied, copy all the excel formula to the answer sheet. If you use Newton-Raphson or MATLAB fsolve, you need to write the function m-file and the command for solving the equations. In all cases, the final solution must be clearly shown in the answer sheet. **(40 points)**

$$f_1 = 3x_1 - 2x_2 - e^{-3x_1} = 0$$
$$f_2 = -2x_1 + 3x_2 - e^{-3x_2} = 0$$

Solution Key

1.1 $\begin{bmatrix}10 & 2 & -1\\ -3 & -6 & 2\\ 1 & 1 & 5\end{bmatrix}\begin{bmatrix}X_1\\ X_2\\ X_3\end{bmatrix} = \begin{bmatrix}27\\ 61.5\\ -21.5\end{bmatrix}$, A= $\begin{bmatrix}10 & 2 & -1\\ -3 & -6 & 2\\ 1 & 1 & 5\end{bmatrix}$, X = $\begin{bmatrix}X_1\\ X_2\\ X_3\end{bmatrix}$; b = $\begin{bmatrix}27\\ 61.5\\ -21.5\end{bmatrix}$ +10

[A] [X] = [b]

1.2 $\left\{\begin{array}{ccc|c}10 & 2 & -1 & 27\\ -3 & -6 & 2 & 61.5\\ 1 & 1 & 5 & -21.5\end{array}\right\}$ time the first row by 3/10 and add it to the second row →

$\left\{\begin{array}{ccc|c}10 & 2 & -1 & 27\\ 0 & -5.4 & 1.7 & 69.6\\ 1 & 1 & 5 & -21.5\end{array}\right\}$ time the first row by -1/10 and add it to the third row → +5

$\left\{\begin{array}{ccc|c}10 & 2 & -1 & 27\\ 0 & -5.4 & 1.7 & 69.6\\ 0 & 0.8 & 5.1 & -24.2\end{array}\right\}$ time the second row by 4/27 and add it to the third row +5

$\rightarrow\left\{\begin{array}{ccc|c}10 & 2 & -1 & 27\\ 0 & -5.4 & 1.7 & 69.6\\ 0 & 0 & 5.3519 & -13.8889\end{array}\right\}$ +5

The upper triangle can be obtained by MATALB "lu (A)" command.

[L U] = lu(A)

```
[L U]=lu(A)

L =
   1.0000        0        0
  -0.3000   1.0000        0
   0.1000  -0.1481   1.0000

U =
  10.0000   2.0000  -1.0000
        0  -5.4000   1.7000
        0        0   5.3519
```

The upper triangle matrix U is exactly the same as the upper triangle matrix that was obtained after the Gauss elimination.

The upper triangle can be written in the equation form as:

$$10X_1 + 2X_2 - X_3 = 27$$
$$-5.4X_2 + 1.7X_3 = 69.6$$
$$5.3519X_3 = -13.8889$$

+5

Solve $X_3 = -2.5952$; substitute to the second equation to get $X_2 = -13.7059$, then solve $X_1 =$ 5.1817

$$\begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = \begin{bmatrix} 5.1817 \\ -13.7059 \\ -2.5952 \end{bmatrix}$$

+5

This solution can be confirmed by MATLAB command: X = inv(A)*b = $\begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = \begin{bmatrix} 5.1817 \\ -13.7059 \\ -2.5952 \end{bmatrix}$

```
A =
   10    2   -1
   -3   -6    2
    1    1    5
b =
  27.0000
  61.5000
 -21.5000
X=inv(A)*b
X =
   5.1817
 -13.7059
  -2.5952
```

1.3.

$$X_1^{i+1} = \frac{27 - 2X_2^i + X_3^i}{10}$$
$$X_2^{i+1} = \frac{61.5 + 3X_1^{i+1} - 2X_3^i}{-6}$$
$$X_3^{i+1} = \frac{-21.5 - X_1^{i+1} - X_2^{i+1}}{5}$$

+10

Iterative Step	X_1	X_2	X_3
0	3	10	4
1	1.1000	-9.4667	-2.6267
2	4.3307	-13.2909	-2.5080

+15

The above iteration can be carried out by excel spreadsheet.

i	X_1	X_2	X_3
0	3	10	4
1	1.1000	-9.4667	-2.6267
2	4.3307	-13.2909	-2.5080
3	5.1074	-13.6397	-2.5935
4	5.1686	-13.6988	-2.5940
5	5.1804	-13.7048	-2.5951
6	5.1815	-13.7058	-2.5951
7	5.1816	-13.7059	-2.5952
8	5.1817	-13.7059	-2.5952
9	5.1817	-13.7059	-2.5952
10	5.1817	-13.7059	-2.5952

2. (1) Successive substitution, rewrite the equation as:

$$x_1 = (2x_2 + e^{-3x_1})/3$$
$$x_2 = (2x_1 + e^{-3x_2})/3$$

+10

or:

Step 1. Assume x1_0=x2_0=0

x1_1 =(2(0)+exp(3*0))/3=1/3
x2_1 = (2(0)+exp(3*0))/3=1/3

+15

Step 2
x1_2= [2(1/3)+exp(-3*(1/3))]/3 = 0.344849
x2_2= [2(1/3)+exp(-3*(1/3))]/3 = 0.344849

+15

These calculations can be carried out in excel or MATLAB very easily, the solutions are x1=0.3500, x2=0.3500.

(2). For the Newton's method, we need to define the Jacobian matrix as follows:

$$J = \begin{bmatrix} \frac{\partial f1}{\partial x1} & \frac{\partial f1}{\partial x2} \\ \frac{\partial f2}{\partial x1} & \frac{\partial f2}{\partial x2} \end{bmatrix} = \begin{bmatrix} 3 + 3e^{-3x1} & -2 \\ -2 & 3 + 3e^{-3x2} \end{bmatrix}$$

+10

```
function [J, F]=exam2Jacobian(x)
J=[3+3*exp(-3*x(1)) -2;-2 3+3*exp(-3*x(2))];
   F=[3*x(1)-2*x(2)-exp(-3*x(1));-2*x(1)+3*x(2)-exp(-3*x(2))];
end
```

+20

```
>> [x, f, ea, iter]=newtmult(@exam2Jacobian, [0; 0])

x =

    0.3500
    0.3500


f =

   1.0e-08 *

  -0.3783
  -0.3783


ea =

   5.2725e-07


iter =

     5
```

+5

+5

(3). Excel solver

excel solver solution of non-linear equations

x_1 (C3)	0.349969632	+10
x_2 (C4)	0.349969632	
f_1 (=3*C3-2*C4-EXP(-3*C3))	3.09007E-10	+10
f_2 (=-2*C3+3*C4-EXP(-3*C4))	3.09007E-10	
Sumsq (=C5^2+C6^2)	1.90971E-19	+20

If the excel codes are not given and you did not obtain the correct solution, 30 points will be deducted.

(4). fsolve

```
function f=exam2func(x)
f=[3*x(1)-2*x(2)-exp(-3*x(1));...
    -2*x(1)+3*x(2)-exp(-3*x(2))];
end
```

+25

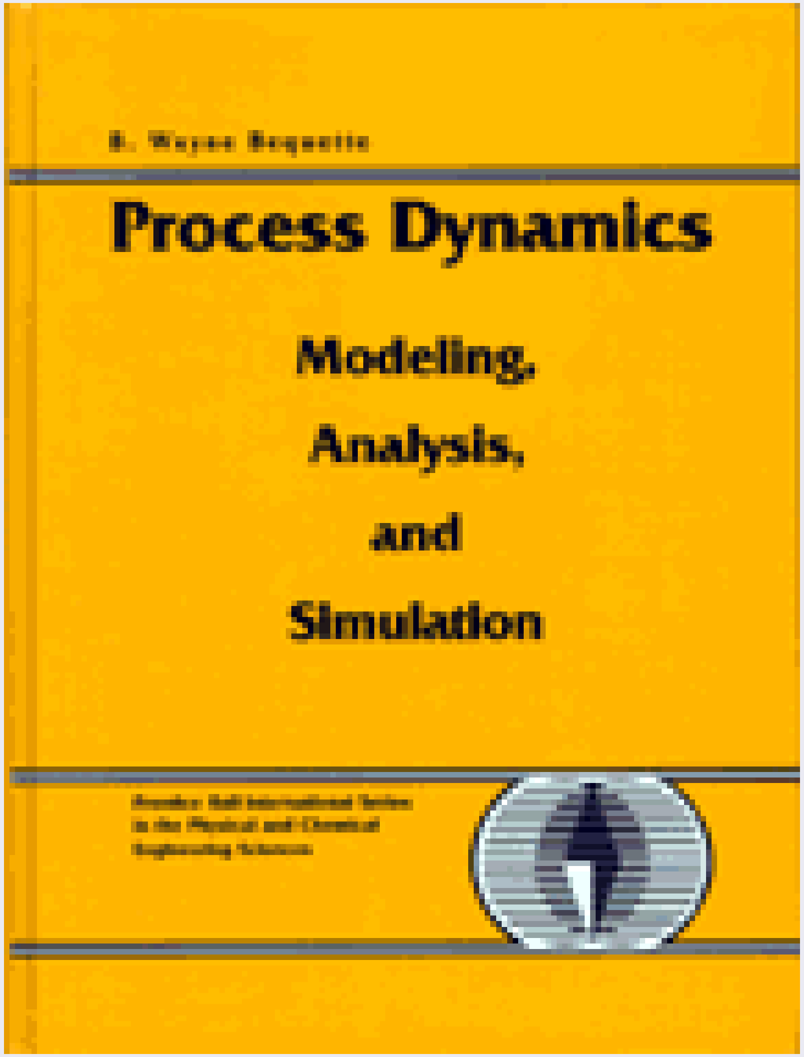
\>> x=fsolve(@exam2func,[0 0]) +10

\>> x =

0.3500 0.3500 +5

ID	Last Na	First Na	G	%	T	H1	H2	H3	H4	H5	E1	E2	Q-1	Q-2	Q-3	Q-4	Grades
1	[redacted]	[redacted]	A	97%	2,728	95	54		58	40	1,044	1,377	60	60	60		A
2	[redacted]	[redacted]	C	78%	2,200	88	59		58	40	660	1,235	60	60	58		C
3	[redacted]	[redacted]	C	70%	1,966	58	43		58	40	543	1,164	60	60	58		C
4	[redacted]	[redacted]	D	63%	1,756	98	59		58	40	490	951	60	60	58		D
5	[redacted]	[redacted]	C	76%	2,119	95	59		0	34	522	1,349	60	0	60		C
6	[redacted]	[redacted]	D	60%	1,674	93	55		58	40	565	809	54	60	54		D
7	[redacted]	[redacted]	D	68%	1,919	93	53		58	25	575	1,065	50	60	56		D
8	[redacted]	[redacted]	D	62%	1,732	92	55		58	40	394	1,093		60	53		D
9	[redacted]	[redacted]	F	36%	1,011	100	0		0	0	357	554	0	0	36		F
10	[redacted]	[redacted]	D	64%	1,782	85	55		27	22	623	923	47	60			D
11	[redacted]	[redacted]	A	90%	2,528	94	55		58	38	831	1,392	60	60	56		A
12	[redacted]	[redacted]	A	97%	2,730	94	50		58	36	1,012	1,420	60	60	56		A
13	[redacted]	[redacted]	D	68%	1,904	94	48		52	36	479	1,136	59	0	59		D
14	[redacted]	[redacted]	B	84%	2,370	76	53		58	28	1,044	1,051	60	59	56		B
15	[redacted]	[redacted]	F	47%	1,328	82	42		42	26	373	710	53	55	60		F
16	[redacted]	[redacted]	A	99%	2,769	98	53		58	36	1,044	1,420	60	60	60		A
17	[redacted]	[redacted]	B	80%	2,231	100	58		43	25	841	1,164	0	0	60		B
18	[redacted]	[redacted]	D	69%	1,937	98	53		58	36	682	951	59	60	36		D
19	[redacted]	[redacted]	B	82%	2,294	98	53		58	40	735	1,250	60	60	60		B
20	[redacted]	[redacted]	C	70%	1,957	99	53		52	32	575	1,093	53	60	60		C
21	[redacted]	[redacted]	C	70%	1,958	98	58		54	38	351	1,349	10	52	53		C
22	[redacted]	[redacted]	D	68%	1,921	99	53		58	32	724	895	60	60	60		D
23	[redacted]	[redacted]	C	78%	2,183	93	55		58	40	607	1,292	38	60	54		C
24	[redacted]	[redacted]	A	93%	2,616	88	55		58	40	895	1,420	60	60	60		A
25	[redacted]	[redacted]	B	82%	2,304	0			0	0	895	1,349	60	60	46		B
26	[redacted]	[redacted]	A	91%	2,545	95	50		58	0	905	1,377	60	55	60		A
27	[redacted]	[redacted]	F	59%	1,654	77	56		45	3	703	710	60	60	56		F
28	[redacted]	[redacted]	F	41%	1,142	87	15		53	32	895		60	0	50		F
29	[redacted]	[redacted]	C	71%	1,994	95	53		53	36	746	951	60	60	47		C
30	[redacted]	[redacted]	A	91%	2,555	85	60		51	40	873	1,392	54	60	54		A
31	[redacted]	[redacted]	C	77%	2,158	98	59		60	38	565	1,278	60	50	60		C
32	[redacted]	[redacted]	A	92%	2,578	95	54		58	40	959	1,321	51	60	60		A
33	[redacted]	[redacted]	A	92%	2,588	94	60		58	30	937	1,349	60	60	59		A
34	[redacted]	[redacted]	A	95%	2,676	90	46		47	23	990	1,420	60	60	58		A
35	[redacted]	[redacted]	F	57%	1,604	28	42		30	4	650	795	55	0	43		F
36	[redacted]	[redacted]	B	83%	2,321	82			0	0	905	1,278	56	0			B
37	[redacted]	[redacted]	B	81%	2,268	92	40		58	13	799	1,207	59	60	35		B
38	[redacted]	[redacted]	B	81%	2,266	60			0	40	767	1,349	50	60	60		B
39	[redacted]	[redacted]	D	69%	1,928	82	53		0	0	799	994			54		D
40	[redacted]	[redacted]	B	85%	2,388	56	27		55	28	884	1,278	60	60	56		B
41	[redacted]	[redacted]	B	86%	2,399	31	22		57	24	884	1,321	60	60	56		B
42	[redacted]	[redacted]	A	93%	2,597	95	55		55	32	1,022	1,278	60	0	50		A
44	[redacted]	[redacted]	F	37%	1,044	78			0	0	0	966		0	59		F
45	[redacted]	[redacted]	B	87%	2,434	88	52		54	36	724	1,420	60	55	51		B
46	[redacted]	[redacted]	C	79%	2,210	85	57		60	34	554	1,420		60	60		C
47	[redacted]	[redacted]	B	86%	2,426	80	54		58	40	714	1,420	60	60	58		B

48	[redacted]	D	66%	1,864	62	50		0	23	490	1,179	60	0	47	D
49	[redacted]	B	85%	2,389	95	57		55	34	767	1,321	60	60	51	B
50	[redacted]	A	94%	2,629	82	60		43	24	1,044	1,321	55	60	56	A
51	[redacted]	B	89%	2,505	93	52		45	36	884	1,349	46	60	60	B
52	[redacted]	C	77%	2,160	28	32		55	14	852	1,179		0	18	C
53	[redacted]	C	78%	2,181	67			0	0	735	1,349	30	60	26	C
54	[redacted]	A	99%	2,777	98	60		55	40	1,044	1,420	60	60	58	A
55	[redacted]	B	86%	2,424	92	51		55	40	777	1,349	60	60	60	B
56	[redacted]	A	91%	2,564	95	57		58	40	948	1,306	60	60	52	A
57	[redacted]	C	72%	2,022	0	48		0	0	788	1,136	50	60		C
58	[redacted]	B	88%	2,477	46	44		53	30	895	1,349	60	60	60	B
59	[redacted]	A	95%	2,656	88	55		58	38	937	1,420	60	60	60	A
60	[redacted]	C	79%	2,215	80	48		23	40	746	1,278		0	0	C
61	[redacted]	A	90%	2,529	91	52		38	36	841	1,420	51	60	60	A
62	[redacted]	C	78%	2,186	91	57		51	16	564	1,349	58	60	60	C
63	[redacted]	C	73%	2,034	41	52		0	0	682	1,221	38	60		C
64	[redacted]	B	84%	2,357	0	59		50	40	1,044	1,164		0		B
65	[redacted]	A	97%	2,712	91	60		58	40	1,054	1,349	60	60	60	A
66	[redacted]	A	96%	2,700	88	40		52	18	1,022	1,420	60	60	54	A
67	[redacted]	F	27%	754	0	54		47	0	596	0	57	60	49	F
68	[redacted]	B	88%	2,473	97	52		55	36	852	1,321	60	55	60	B
69	[redacted]	A	99%	2,781	84	58		58	36	1,065	1,420	60	60	60	A
70	[redacted]	A	92%	2,585	99	59		57	34	927	1,349	60	60	60	A
71	[redacted]	D	68%	1,898	84	35		57	32	639	994	57	60	48	D
72	[redacted]	A	95%	2,676	88	60		54	40	959	1,420	55	60	60	A
73	[redacted]	A	90%	2,519	89	53		53	32	911	1,321	60	60	42	A
74	[redacted]	A	93%	2,605	27	48		52	36	1,033	1,349	60	45	59	A
75	[redacted]	A	90%	2,525	63	48		40	24	1,001	1,349		0	58	A
76	[redacted]	A	95%	2,675	100	60		58	40	937	1,420	60	60	60	A
77	[redacted]	F	6%	162	62	34		8	0	0		58	60	52	F
78	[redacted]	F	55%	1,539	48	58		53	38	362	923	57	60	40	F
79	[redacted]	B	84%	2,370	73	40		53	32	905	1,207	60	60	60	B
80	[redacted]	B	80%	2,243	95	58		55	40	799	1,136	60	60	51	B
81	[redacted]	A	94%	2,626	78	54		58	40	916	1,420	60	60	58	A
82	[redacted]	A	93%	2,603	97	53		60	40	948	1,349	56	60	56	A
83	[redacted]	C	74%	2,071	42			52	18	692	1,207	60	48	58	C
84	[redacted]	A	92%	2,587	83	25		58	0	1,012	1,349	60	60	60	A
85	[redacted]	A	90%	2,537	96	56		58	36	841	1,392	58	60	50	A
86	[redacted]	B	87%	2,446	87	50		53	28	852	1,321	55	48	34	B
87	[redacted]	A	99%	2,775	96	60		60	35	1,044	1,420	60	60	56	A
88	[redacted]	A	98%	2,755	87	54		58	32	1,044	1,420	60	60	60	A
	Total		100%	2,805	100	60		60	40	1,065	1,420	60	60	60	
	Average		79%	2,228	79	51		46	28	780	1,225	55	49	54	
										73%	86%				



Non-linear Equations

Diabatic CSTR

Steady-State Solutions

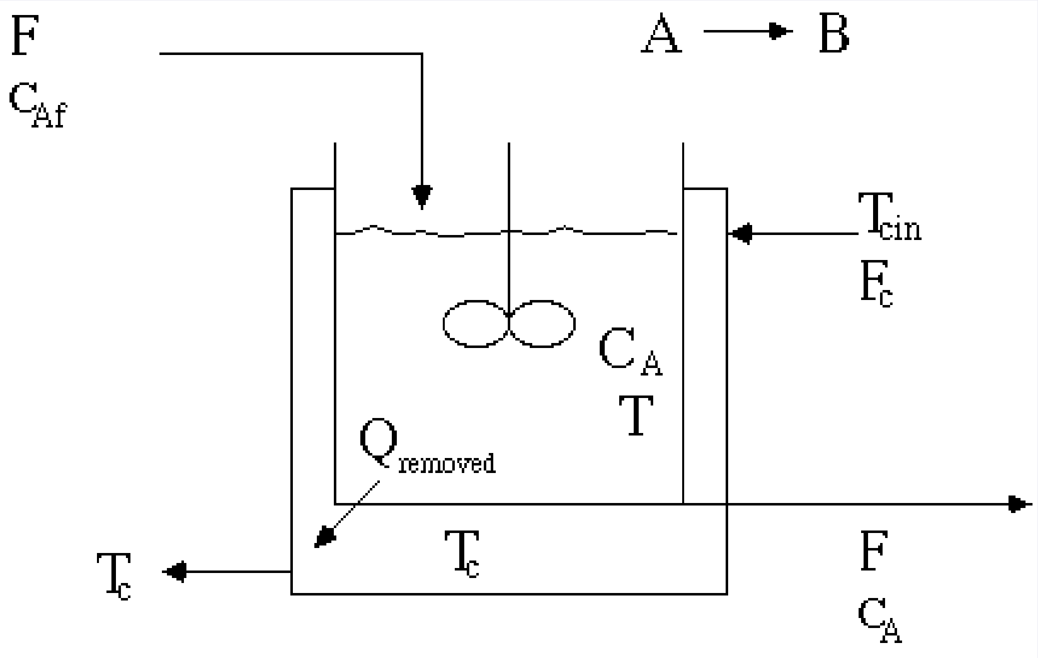
B. Wayne Bequette; Professor of Chemical and Biological Engineering, Rensselaer Polytechnic Institute

Background

The most important unit operation in a chemical process is generally a chemical reactor. Chemical reactions are either exothermic (release energy) or endothermic (require energy input) and therefore require that energy either be removed or added to the reactor for a constant temperature to be maintained. Exothermic reactions are the most interesting systems to study because of potential safety problems (rapid increases in temperature, sometimes called "ignition" behavior) and the possibility of exotic behavior such as multiple steady-states (for the same value of the input variable there may be several possible values of the output variable).

Background

In this module we consider a perfectly mixed, continuously stirred tank reactor (CSTR), shown in Figure 1. The case of a single, first-order exothermic irreversible reaction, A --> B. We will show that very interesting behavior that can arise in such a simple system.



The Modeling Equations

$$\frac{dV\rho}{dt} = F_{in}\rho_{in}\text{-}F_{out}\rho$$

$$\frac{dV\rho}{dt} = 0 \qquad F_{in}\rho_{in}{=}F_{out}\rho \qquad F_{in}{=}F_{out} = F \qquad \frac{dV}{dt} = 0$$

$$\frac{dVC_A}{dt} = FC_{Af}\text{-}FC_A - rV$$

$$\frac{d\left(V\rho c_p(T-T_{ref})\right)}{dt} = F\rho c_p(T_f - T_{ref})\text{-}F\rho c_p(T - T_{ref}) + (-\Delta H)Vr - UA(T - T_j)$$

The Modeling Equations

$$f_1(C_A, T) = \frac{dC_A}{dt} = \frac{F}{V}(C_{Af}\text{-}C_A) - r$$

$$f_2(C_A, T) = \frac{dT}{dt} = \frac{F}{V}(T_f\text{-}T) + \left(\frac{-\Delta H}{\rho c_p}\right) r - \frac{UA}{V\rho c_p}\left(T - T_j\right)$$

$$r = r_0 \exp\left(\frac{-\Delta E}{RT}\right) C_A$$

Steady State Solutions

$dC_A/dt = 0$ and $dT/dt = 0$

$$\boxed{f_1(C_A, T) = \frac{dC_A}{dt} = \frac{F}{V}(C_{Af} - C_A) - r_0 \exp\left(\frac{-\Delta E}{RT}\right) C_A = 0}$$

$$\boxed{f_2(C_A, T) = \frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right) r_0 \exp\left(\frac{-\Delta E}{RT}\right) C_A - \frac{UA}{V\rho c_p}\left(T - T_j\right) = 0}$$

Reactor Parameters

Parameter	case 1	case 2	case 3
F/V, hr^{-1}	1	1	1
k_0, hr^{-1}	14,825*3600	9,703*3600	18,194*3600
$(-\Delta H)$, kcal/kgmol	5215	5960	8195
E, kcal/kgmol	11,843	11,843	11,843
ρc_p, kcal/(m^3°C)	500	500	500
T_f, °C	25	25	25
C_{Af}, kgmol/m^3	10	10	10
UA/V, kcal/(m^3°C hr)	250	150	750
T_j, °C	25	25	25

MATALB M-Function Files

fsolve (An MATLAB built-in solver for solving systems of nonlinear equations of several variables)

X = fsolve(FUN,X0,OPTIONS)

You need to input an M-function file(FUN) to define the systems of equations and a vector of initial guesses X0.

MATALB M-Function Files

cstr_ss.m (an M-function for defining the two equations (mass and energy balance), which was developed by Prof. Bequette of RPI.) The M-file is uploaded to ChE394 course Blackboard.

CSTR_PAR.m (An M-file for saving the CSTR reactor parameters as a script file).

MATALB M-Function Files

```
function f = cstr_ss(x)
%
% 2-state diabatic CSTR model
% Use fsolve to find steady-state concentration and temperature
%
% The call statement from the command window is:
%
%   x = fsolve('cstr_ss',x0);
%
% where x is the solution vector (x = [conc;temp])
% and x0 is an initial guess vector
%
% define the following global parameter so that values
% can be entered in the command window
%     global CSTR_PAR
% parameters (case 2)
% CSTR_PAR(1):  frequency factor (9703*3600)
% CSTR_PAR(2):  heat of reaction (5960)
% CSTR_PAR(3):  activation energy (11843)
% CSTR_PAR(4):  density*heat cap. (500)
% CSTR_PAR(5):  heat trans coeff * area (150)
```

Solutions & Interpretation

Case 2 values are shown in the function code. There are three possible solutions depending on the initial guesses for the states. Before calling fsolve, we need to define CSTR_PAR as global variables.

Guess 1 - *High concentration (low conversion), Low temperature*. Here we consider an initial guess of $C_A = 9$ and T = 300 K.

```
x = fsolve('cstr_ss', [9; 300]);
x =
8.5636
311.1710
```

so the steady-state solution for guess 1 is $\begin{bmatrix} C_{AS} \\ T_S \end{bmatrix} = \begin{bmatrix} 8.5636 \\ 311.2 \end{bmatrix}$

, which is high concentration (low conversion) and low temperature.

Solutions & Interpretation

Guess 2 - *Intermediate concentration and temperature.*

Here we consider an initial guess of C_A = 5 and T = 350 K.

```
x = fsolve('cstr_ss', [5; 350]);
x =
5.5179
339.0971
```

so the steady-state solution for guess 2 is

$$\begin{bmatrix} C_{AS} \\ T_S \end{bmatrix} = \begin{bmatrix} 5.5179 \\ 339.1 \end{bmatrix}.$$

Solutions & Interpretation

Guess 3 - *Low concentration and high temperature.* Here we consider an initial guess of C_A = 1 and T = 450 K.

```
x = fsolve('cstr_ss', [1; 450]);
x =
2.3589
368.0629
```

so the steady-state solution for guess 3 is

$$\begin{bmatrix} C_{AS} \\ T_S \end{bmatrix} = \begin{bmatrix} 2.3589 \\ 368.1 \end{bmatrix}.$$

Solutions & Interpretation

Guess and Solution	Guess 1	Guess 2	Guess 3
$x_0(1)$, C_A guessed	9	5	1
$x_0(2)$, T guessed	300	350	450
$x(1)$, C_A solution	8.564	5.518	2.359
$x(2)$, T solution	311.2	339.1	368.1

14.6 CASE STUDY continued

best-fit line follows a Gaussian distribution, and that the standard deviation is the same at every value of the dependent variable. These assumptions are rarely true after transforming data.

As a consequence of the last conclusion, some analysts suggest that rather than using linear transformations, nonlinear regression should be employed to fit curvilinear data. In this approach, a best-fit curve is developed that directly minimizes the untransformed residuals. We will describe how this is done in Chap. 15.

PROBLEMS

14.1 Given the data

0.90	1.42	1.30	1.55	1.63
1.32	1.35	1.47	1.95	1.66
1.96	1.47	1.92	1.35	1.05
1.85	1.74	1.65	1.78	1.71
2.29	1.82	2.06	2.14	1.27

Determine **(a)** the mean, **(b)** median, **(c)** mode, **(d)** range, **(e)** standard deviation, **(f)** variance, and **(g)** coefficient of variation.

14.2 Construct a histogram from the data from Prob. 14.1. Use a range from 0.8 to 2.4 with intervals of 0.2.

14.3 Given the data

29.65	28.55	28.65	30.15	29.35	29.75	29.25
30.65	28.15	29.85	29.05	30.25	30.85	28.75
29.65	30.45	29.15	30.45	33.65	29.35	29.75
31.25	29.45	30.15	29.65	30.55	29.65	29.25

Determine **(a)** the mean, **(b)** median, **(c)** mode, **(d)** range, **(e)** standard deviation, **(f)** variance, and **(g)** coefficient of variation.

(h) Construct a histogram. Use a range from 28 to 34 with increments of 0.4.

(i) Assuming that the distribution is normal, and that your estimate of the standard deviation is valid, compute the range (i.e., the lower and the upper values) that encompasses 68% of the readings. Determine whether this is a valid estimate for the data in this problem.

14.4 Using the same approach as was employed to derive Eqs. (14.15) and (14.16), derive the least-squares fit of the following model:

$$y = a_1 x + e$$

That is, determine the slope that results in the least-squares fit for a straight line with a zero intercept. Fit the following data with this model and display the result graphically.

x	2	4	6	7	10	11	14	17	20
y	4	5	6	5	8	8	6	9	12

14.5 Use least-squares regression to fit a straight line to

x	0	2	4	6	9	11	12	15	17	19
y	5	6	7	6	9	8	8	10	12	12

Along with the slope and intercept, compute the standard error of the estimate and the correlation coefficient. Plot the data and the regression line. Then repeat the problem, but regress x versus y—that is, switch the variables. Interpret your results.

14.6 Fit a power model to the data from Table 14.1, but use natural logarithms to perform the transformations.

14.7 The following data were gathered to determine the relationship between pressure and temperature of a fixed volume of 1 kg of nitrogen. The volume is 10 m^3.

T, °C	−40	0	40	80	120	160
p, N/m^2	6900	8100	9350	10,500	11,700	12,800

Employ the ideal gas law $pV = nRT$ to determine R on the basis of these data. Note that for the law, T must be expressed in kelvins.

15.6 CASE STUDY continued

The result is shown in Fig. 15.5.

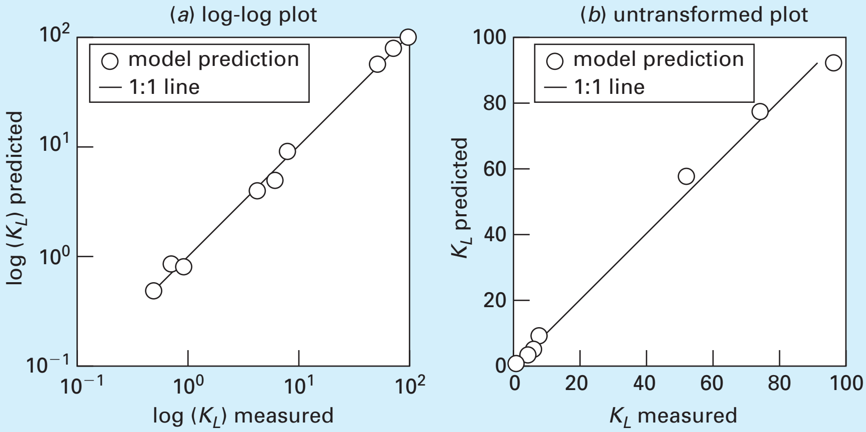


FIGURE 15.5
Plots of predicted versus measured values of the oxygen mass-transfer coefficient as computed with multiple regression. Results are shown for (*a*) log transformed and (*b*) untransformed cases. The 1:1 line, which indicates a perfect correlation, is superimposed on both plots.

PROBLEMS

15.1 Fit a parabola to the data from Table 14.1. Determine the r^2 for the fit and comment on the efficacy of the result.

15.2 Using the same approach as was employed to derive Eqs. (14.15) and (14.16), derive the least-squares fit of the following model:

$$y = a_1 x + a_2 x^2 + e$$

That is, determine the coefficients that result in the least-squares fit for a second-order polynomial with a zero intercept. Test the approach by using it to fit the data from Table 14.1.

15.3 Fit a cubic polynomial to the following data:

x	3	4	5	7	8	9	11	12
y	1.6	3.6	4.4	3.4	2.2	2.8	3.8	4.6

Along with the coefficients, determine r^2 and $s_{y/x}$.

15.4 Develop an M-file to implement polynomial regression. Pass the M-file two vectors holding the x and y values along with the desired order m. Test it by solving Prob. 15.3.

15.5 For the data from Table P15.5, use polynomial regression to derive a predictive equation for dissolved oxygen concentration as a function of temperature for the case where the chloride concentration is equal to zero. Employ a polynomial that is of sufficiently high order that the predictions match the number of significant digits displayed in the table.

15.6 Use multiple linear regression to derive a predictive equation for dissolved oxygen concentration as a function of temperature and chloride based on the data from Table P15.5. Use the equation to estimate the concentration of dissolved oxygen for a chloride concentration of 15 g/L at $T = 12$ °C. Note that the true value is 9.09 mg/L. Compute the percent

14.8 Beyond the examples in Fig. 14.13, there are other models that can be linearized using transformations. For example,

$$y = \alpha_4 x e^{\beta_4 x}$$

Linearize this model and use it to estimate α_4 and β_4 based on the following data. Develop a plot of your fit along with the data.

x	0.1	0.2	0.4	0.6	0.9	1.3	1.5	1.7	1.8
y	0.75	1.25	1.45	1.25	0.85	0.55	0.35	0.28	0.18

14.9 The concentration of *E. coli* bacteria in a swimming area is monitored after a storm:

t (hr)	4	8	12	16	20	24
c (CFU/100 mL)	1600	1320	1000	890	650	560

The time is measured in hours following the end of the storm and the unit CFU is a "colony forming unit." Use this data to estimate (**a**) the concentration at the end of the storm ($t = 0$) and (**b**) the time at which the concentration will reach 200 CFU/100 mL. Note that your choice of model should be consistent with the fact that negative concentrations are impossible and that the bacteria concentration always decreases with time.

14.10 Rather than using the base-e exponential model (Eq. 14.22), a common alternative is to employ a base-10 model:

$$y = \alpha_5 10^{\beta_5 x}$$

When used for curve fitting, this equation yields identical results to the base-e version, but the value of the exponent parameter (β_5) will differ from that estimated with Eq.14.22 (β_1). Use the base-10 version to solve Prob. 14.9. In addition, develop a formulation to relate β_1 to β_5.

14.11 Determine an equation to predict metabolism rate as a function of mass based on the following data. Use it to predict the metabolism rate of a 200-kg tiger.

Animal	Mass (kg)	Metabolism (watts)
Cow	400	270
Human	70	82
Sheep	45	50
Hen	2	4.8
Rat	0.3	1.45
Dove	0.16	0.97

14.12 On average, the surface area A of human beings is related to weight W and height H. Measurements on a number of individuals of height 180 cm and different weights (kg) give values of A (m^2) in the following table:

W (kg)	70	75	77	80	82	84	87	90
A (m^2)	2.10	2.12	2.15	2.20	2.22	2.23	2.26	2.30

Show that a power law $A = aW^b$ fits these data reasonably well. Evaluate the constants a and b, and predict what the surface area is for a 95-kg person.

14.13 Fit an exponential model to

x	0.4	0.8	1.2	1.6	2	2.3
y	800	985	1490	1950	2850	3600

Plot the data and the equation on both standard and semi-logarithmic graphs with the MATLAB `subplot` function.

14.14 An investigator has reported the data tabulated below for an experiment to determine the growth rate of bacteria k (per d) as a function of oxygen concentration c (mg/L). It is known that such data can be modeled by the following equation:

$$k = \frac{k_{max} c^2}{c_s + c^2}$$

where c_s and k_{max} are parameters. Use a transformation to linearize this equation. Then use linear regression to estimate c_s and k_{max} and predict the growth rate at $c = 2$ mg/L.

c	0.5	0.8	1.5	2.5	4
k	1.1	2.5	5.3	7.6	8.9

14.15 Develop an M-file function to compute descriptive statistics for a vector of values. Have the function determine and display number of values, mean, median, mode, range, standard deviation, variance, and coefficient of variation. In addition, have it generate a histogram. Test it with the data from Prob. 14.3.

14.16 Modify the `linregr` function in Fig. 14.15 so that it **(a)** computes and returns the standard error of the estimate, and **(b)** uses the `subplot` function to also display a plot of the residuals (the predicted minus the measured y) versus x.

14.17 Develop an M-file function to fit a power model. Have the function return the best-fit coefficient α_2 and power β_2 along with the r^2 for the untransformed model. In addition, use the `subplot` function to display graphs of both the transformed and untransformed equations along with the data. Test it with the data from Prob. 14.11.

14.18 The following data show the relationship between the viscosity of SAE 70 oil and temperature. After taking the log of the data, use linear regression to find the equation of the line that best fits the data and the r^2 value.

Temperature, °C	26.67	93.33	148.89	315.56
Viscosity, μ, N·s/m²	1.35	0.085	0.012	0.00075

14.19 You perform experiments and determine the following values of heat capacity c at various temperatures T for a gas:

T	−50	−30	0	60	90	110
c	1250	1280	1350	1480	1580	1700

Use regression to determine a model to predict c as a function of T.

14.20 It is known that the tensile strength of a plastic increases as a function of the time it is heat treated. The following data are collected:

Time	10	15	20	25	40	50	55	60	75
Tensile Strength	5	20	18	40	33	54	70	60	78

(a) Fit a straight line to these data and use the equation to determine the tensile strength at a time of 32 min.

(b) Repeat the analysis but for a straight line with a zero intercept.

14.21 The following data were taken from a stirred tank reactor for the reaction $A \rightarrow B$. Use the data to determine the best possible estimates for k_{01} and E_1 for the following kinetic model:

$$-\frac{dA}{dt} = k_{01}e^{-E_1/RT}A$$

where R is the gas constant and equals 0.00198 kcal/mol/K.

$-dA/dt$ (moles/L/s)	460	960	2485	1600	1245
A (moles/L)	200	150	50	20	10
T (K)	280	320	450	500	550

14.22 Concentration data were collected at 15 time points for the polymerization reaction:

$$xA + yB \rightarrow A_xB_y$$

We assume the reaction occurs via a complex mechanism consisting of many steps. Several models have been hypothesized, and the sum of the squares of the residuals had been calculated for the fits of the models of the data. The results are shown below. Which model best describes the data (statistically)? Explain your choice.

	Model A	Model B	Model C
S_r	135	105	100
Number of Model Parameters Fit	2	3	5

14.23 Below are data taken from a batch reactor of bacterial growth (after lag phase was over). The bacteria are allowed to grow as fast as possible for the first 2.5 hours, and then they are induced to produce a recombinant protein, the production of which slows the bacterial growth significantly. The theoretical growth of bacteria can be described by

$$\frac{dX}{dt} = \mu X$$

where X is the number of bacteria, and μ is the specific growth rate of the bacteria during exponential growth. Based on the data, estimate the specific growth rate of the bacteria during the first 2 hours of growth and during the next 4 hours of growth.

Time, h	0	1	2	3	4	5	6
[Cells], g/L	0.100	0.335	1.102	1.655	2.453	3.702	5.460

14.24 A transportation engineering study was conducted to determine the proper design of bike lanes. Data were gathered on bike-lane widths and average distance between bikes and passing cars. The data from 9 streets are

Distance, m	2.4	1.5	2.4	1.8	1.8	2.9	1.2	3	1.2
Lane Width, m	2.9	2.1	2.3	2.1	1.8	2.7	1.5	2.9	1.5

(a) Plot the data.

(b) Fit a straight line to the data with linear regression. Add this line to the plot.

(c) If the minimum safe average distance between bikes and passing cars is considered to be 1.8 m, determine the corresponding minimum lane width.

14.25 In water-resources engineering, the sizing of reservoirs depends on accurate estimates of water flow in the river that is being impounded. For some rivers, long-term historical records of such flow data are difficult to obtain. In contrast, meteorological data on precipitation are often available for many years past. Therefore, it is often useful to determine a relationship between flow and precipitation. This relationship can then be used to estimate flows for years when only precipitation measurements were made. The following data are available for a river that is to be dammed:

Precip., cm/yr	88.9	108.5	104.1	139.7	127	94	116.8	99.1
Flow, m³/s	14.6	16.7	15.3	23.2	19.5	16.1	18.1	16.6

(a) Plot the data.
(b) Fit a straight line to the data with linear regression. Superimpose this line on your plot.
(c) Use the best-fit line to predict the annual water flow if the precipitation is 120 cm.
(d) If the drainage area is 1100 km^2, estimate what fraction of the precipitation is lost via processes such as evaporation, deep groundwater infiltration, and consumptive use.

14.26 The mast of a sailboat has a cross-sectional area of 10.65 cm^2 and is constructed of an experimental aluminum alloy. Tests were performed to define the relationship between stress and strain. The test results are

Strain, cm/cm	0.0032	0.0045	0.0055	0.0016	0.0085	0.0005
Stress, N/cm²	4970	5170	5500	3590	6900	1240

The stress caused by wind can be computed as F/A_c where $F =$ force in the mast and $A_c =$ mast's cross-sectional area. This value can then be substituted into Hooke's law to determine the mast's deflection, $\Delta L =$ strain $\times$ L, where $L =$ the mast's length. If the wind force is 25,000 N, use the data to estimate the deflection of a 9-m mast.

14.27 The following data were taken from an experiment that measured the current in a wire for various imposed voltages:

***V*, V**	2	3	4	5	7	10
***i*, A**	5.2	7.8	10.7	13	19.3	27.5

(a) On the basis of a linear regression of this data, determine current for a voltage of 3.5 V. Plot the line and the data and evaluate the fit.
(b) Redo the regression and force the intercept to be zero.

14.28 An experiment is performed to determine the % elongation of electrical conducting material as a function of temperature. The resulting data are listed below. Predict the % elongation for a temperature of 400 °C.

Temperature, °C	200	250	300	375	425	475	600
% Elongation	7.5	8.6	8.7	10	11.3	12.7	15.3

14.29 The population p of a small community on the outskirts of a city grows rapidly over a 20-year period:

t	0	5	10	15	20
p	100	200	450	950	2000

As an engineer working for a utility company, you must forecast the population 5 years into the future in order to anticipate the demand for power. Employ an exponential model and linear regression to make this prediction.

14.30 The velocity u of air flowing past a flat surface is measured at several distances y away from the surface. Fit a curve to this data assuming that the velocity is zero at the surface ($y = 0$). Use your result to determine the shear stress (du/dy) at the surface.

***y*, m**	0.002	0.006	0.012	0.018	0.024
***u*, m/s**	0.287	0.899	1.915	3.048	4.299

14.31 *Andrade's equation* has been proposed as a model of the effect of temperature on viscosity:

$$\mu = De^{B/T_a}$$

where $\mu =$ dynamic viscosity of water (10^{-3} N·s/m^2), $T_a =$ absolute temperature (K), and D and B are parameters. Fit this model to the following data for water:

T	0	5	10	20	30	40
μ	1.787	1.519	1.307	1.002	0.7975	0.6529

14.32 Perform the same computation as in Example 14.2, but in addition to the drag coefficient, also vary the mass uniformly by ±10%.

14.33 Perform the same computation as in Example 14.3, but in addition to the drag coefficient, also vary the mass normally around its mean value with a coefficient of variation of 5.7887%.

14.34 Manning's formula for a rectangular channel can be written as

$$Q = \frac{1}{n_m} \frac{(BH)^{5/3}}{(B + 2H)^{2/3}} \sqrt{S}$$

where Q = flow (m^3/s), n_m = a roughness coefficient, B = width (m), H = depth (m), and S = slope. You are applying this formula to a stream where you know that the width = 20 m and the depth = 0.3 m. Unfortunately, you know the roughness and the slope to only a ±10% precision. That is, you know that the roughness is about 0.03 with a range from 0.027 to 0.033 and the slope is 0.0003 with a range from 0.00027 to 0.00033. Assuming uniform distributions, use a Monte Carlo analysis with n = 10,000 to estimate the distribution of flow.

14.35 A Monte Carlo analysis can be used for optimization. For example, the trajectory of a ball can be computed with

$$y = (\tan\theta_0)x - \frac{g}{2v_0^2 \cos^2\theta_0} x^2 + y_0 \qquad \text{(P14.35)}$$

where y = the height (m), θ_0 = the initial angle (radians), v_0 = the initial velocity (m/s), g = the gravitational constant = 9.81 m/s^2, and y_0 = the initial height (m). Given y_0 = 1 m, v_0 = 25 m/s, and θ_0 = 50°, determine the maximum height and the corresponding x distance (**a**) analytically with calculus and (**b**) numerically with Monte Carlo simulation. For the latter, develop a script that generates a vector of 10,000 uniformly-distributed values of x between 0 and 60 m. Use this vector and Eq. P14.35 to generate a vector of heights. Then, employ the `max` function to determine the maximum height and the associated x distance.

TABLE P15.5 Dissolved oxygen concentration in water as a function of temperature (°C) and chloride concentration (g/L).

	Dissolved Oxygen (mg/L) for Temperature (°C) and Concentration of Chloride (g/L)		
T, °C	**c = 0 g/L**	**c = 10 g/L**	**c = 20 g/L**
0	14.6	12.9	11.4
5	12.8	11.3	10.3
10	11.3	10.1	8.96
15	10.1	9.03	8.08
20	9.09	8.17	7.35
25	8.26	7.46	6.73
30	7.56	6.85	6.20

relative error for your prediction. Explain possible causes for the discrepancy.

15.7 As compared with the models from Probs. 15.5 and 15.6, a somewhat more sophisticated model that accounts for the effect of both temperature and chloride on dissolved oxygen saturation can be hypothesized as being of the form

$$o = f_3(T) + f_1(c)$$

That is, a third-order polynomial in temperature and a linear relationship in chloride is assumed to yield superior results. Use the general linear least-squares approach to fit this model to the data in Table P15.5. Use the resulting equation to estimate the dissolved oxygen concentration for a chloride concentration of 15 g/L at $T = 12$ °C. Note that the true value is 9.09 mg/L. Compute the percent relative error for your prediction.

15.8 Use multiple linear regression to fit

x_1	0	1	1	2	2	3	3	4	4
x_2	0	1	2	1	2	1	2	1	2
y	15.1	17.9	12.7	25.6	20.5	35.1	29.7	45.4	40.2

Compute the coefficients, the standard error of the estimate, and the correlation coefficient.

15.9 The following data were collected for the steady flow of water in a concrete circular pipe:

Experiment	Diameter, m	Slope, m/m	Flow, m³/s
1	0.3	0.001	0.04
2	0.6	0.001	0.24
3	0.9	0.001	0.69
4	0.3	0.01	0.13
5	0.6	0.01	0.82
6	0.9	0.01	2.38
7	0.3	0.05	0.31
8	0.6	0.05	1.95
9	0.9	0.05	5.66

Use multiple linear regression to fit the following model to this data:

$$Q = \alpha_0 D^{\alpha_1} S^{\alpha_2}$$

where Q = flow, D = diameter, and S = slope.

15.10 Three disease-carrying organisms decay exponentially in seawater according to the following model:

$$p(t) = Ae^{-1.5t} + Be^{-0.3t} + Ce^{-0.05t}$$

Estimate the initial concentration of each organism (A, B, and C) given the following measurements:

t	0.5	1	2	3	4	5	6	7	9
$p(t)$	6	4.4	3.2	2.7	2	1.9	1.7	1.4	1.1

15.11 The following model is used to represent the effect of solar radiation on the photosynthesis rate of aquatic plants:

$$P = P_m \frac{I}{I_{sat}} e^{-\frac{I}{I_{sat}}+1}$$

where P = the photosynthesis rate (mg m^{-3}d^{-1}), P_m = the maximum photosynthesis rate (mg m^{-3}d^{-1}), I = solar radiation (μE m^{-2}s^{-1}), and I_{sat} = optimal solar radiation (μE m^{-2}s^{-1}). Use nonlinear regression to evaluate P_m and I_{sat} based on the following data:

I	50	80	130	200	250	350	450	550	700
P	99	177	202	248	229	219	173	142	72

15.12 The following data are provided

x	1	2	3	4	5
y	2.2	2.8	3.6	4.5	5.5

Fit the following model to this data using MATLAB and the general linear least-squares model

$$y = a + bx + \frac{c}{x}$$

15.13 In Prob. 14.8 we used transformations to linearize and fit the following model:

$$y = \alpha_4 x e^{\beta_4 x}$$

Use nonlinear regression to estimate α_4 and β_4 based on the following data. Develop a plot of your fit along with the data.

x	0.1	0.2	0.4	0.6	0.9	1.3	1.5	1.7	1.8
y	0.75	1.25	1.45	1.25	0.85	0.55	0.35	0.28	0.18

15.14 Enzymatic reactions are used extensively to characterize biologically mediated reactions. The following is an example of a model that is used to fit such reactions:

$$v_0 = \frac{k_m [S]^3}{K + [S]^3}$$

where v_0 = the initial rate of the reaction (M/s), $[S]$ = the substrate concentration (M), and k_m and K are parameters. The following data can be fit with this model:

$[S]$, M	v_0, M/s
0.01	6.078×10^{-11}
0.05	7.595×10^{-9}
0.1	6.063×10^{-8}
0.5	5.788×10^{-6}
1	1.737×10^{-5}
5	2.423×10^{-5}
10	2.430×10^{-5}
50	2.431×10^{-5}
100	2.431×10^{-5}

(a) Use a transformation to linearize the model and evaluate the parameters. Display the data and the model fit on a graph.

(b) Perform the same evaluation as in **(a)** but use nonlinear regression.

15.15 Given the data

x	5	10	15	20	25	30	35	40	45	50
y	17	24	31	33	37	37	40	40	42	41

use least-squares regression to fit **(a)** a straight line, **(b)** a power equation, **(c)** a saturation-growth-rate equation, and **(d)** a parabola. For **(b)** and **(c)**, employ transformations to linearize the data. Plot the data along with all the curves. Is any one of the curves superior? If so, justify.

15.16 The following data represent the bacterial growth in a liquid culture over of number of days:

Day	0	4	8	12	16	20
Amount × 10^6	67.38	74.67	82.74	91.69	101.60	112.58

Find a best-fit equation to the data trend. Try several possibilities—linear, quadratic, and exponential. Determine the best equation to predict the amount of bacteria after 30 days.

15.17 Dynamic viscosity of water $\mu(10^{-3}\ \mathrm{N \cdot s/m^2})$ is related to temperature $T(°\mathrm{C})$ in the following manner:

T	0	5	10	20	30	40
μ	1.787	1.519	1.307	1.002	0.7975	0.6529

(a) Plot this data.

(b) Use linear interpolation to predict μ at $T = 7.5$ °C.

(c) Use polynomial regression to fit a parabola to the data in order to make the same prediction.

15.18 Use the following set of pressure-volume data to find the best possible virial constants (A_1 and A_2) for the following equation of state. R = 82.05 mL atm/gmol K, and T = 303 K.

$$\frac{PV}{RT} = 1 + \frac{A_1}{V} + \frac{A_2}{V^2}$$

***P* (atm)**	0.985	1.108	1.363	1.631
***V* (mL)**	25,000	22,200	18,000	15,000

15.19 Environmental scientists and engineers dealing with the impacts of acid rain must determine the value of the ion product of water K_w as a function of temperature. Scientists have suggested the following equation to model this relationship:

$$-\log_{10} K_w = \frac{a}{T_a} + b \log_{10} T_a + cT_a + d$$

where T_a = absolute temperature (K), and a, b, c, and d are parameters. Employ the following data and regression to estimate the parameters with MATLAB. Also, generate a plot of predicted K_w versus the data.

T (°C)	K_w
0	1.164×10^{-15}
10	2.950×10^{-15}
20	6.846×10^{-15}
30	1.467×10^{-14}
40	2.929×10^{-14}

15.20 The distance required to stop an automobile consists of both thinking and braking components, each of which is a function of its speed. The following experimental data were collected to quantify this relationship. Develop best-fit equations for both the thinking and braking components. Use these equations to estimate the total stopping distance for a car traveling at 110 km/h.

Speed, km/h	30	45	60	75	90	120
Thinking, m	5.6	8.5	11.1	14.5	16.7	22.4
Braking, m	5.0	12.3	21.0	32.9	47.6	84.7

15.21 An investigator has reported the data tabulated below. It is known that such data can be modeled by the following equation

$$x = e^{(y-b)/a}$$

where a and b are parameters. Use nonlinear regression to determine a and b. Based on your analysis predict y at $x = 2.6$.

x	1	2	3	4	5
y	0.5	2	2.9	3.5	4

15.22 It is known that the data tabulated below can be modeled by the following equation

$$y = \left(\frac{a + \sqrt{x}}{b\sqrt{x}}\right)^2$$

Use nonlinear regression to determine the parameters a and b. Based on your analysis predict y at $x = 1.6$.

x	0.5	1	2	3	4
y	10.4	5.8	3.3	2.4	2

15.23 An investigator has reported the data tabulated below for an experiment to determine the growth rate of bacteria k (per d), as a function of oxygen concentration c (mg/L). It is known that such data can be modeled by the following equation:

$$k = \frac{k_{\max} c^2}{c_s + c^2}$$

Use nonlinear regression to estimate c_s and $k_{\max}$ and predict the growth rate at $c = 2$ mg/L.

c	0.5	0.8	1.5	2.5	4
k	1.1	2.4	5.3	7.6	8.9

15.24 A material is tested for cyclic fatigue failure whereby a stress, in MPa, is applied to the material and the number of cycles needed to cause failure is measured. The results are in the table below. Use nonlinear regression to fit a power model to this data.

N, cycles	1	10	100	1000	10,000	100,000	1,000,000
Stress, MPa	1100	1000	925	800	625	550	420

15.25 The following data shows the relationship between the viscosity of SAE 70 oil and temperature. Use nonlinear regression to fit a power equation to this data.

Temperature, T, °C	26.67	93.33	148.89	315.56
Viscosity, μ, N·s/m^2	1.35	0.085	0.012	0.00075

15.26 The concentration of *E. coli* bacteria in a swimming area is monitored after a storm:

t (hr)	4	8	12	16	20	24
c(CFU/100 mL)	1590	1320	1000	900	650	560

The time is measured in hours following the end of the storm and the unit CFU is a "colony forming unit." Employ nonlinear regression to fit an exponential model (Eq. 14.22) to this data. Use the model to estimate **(a)** the concentration at the end of the storm ($t = 0$) and **(b)** the time at which the concentration will reach 200 CFU/100 mL.

15.27 Use the following set of pressure-volume data to find the best possible virial constants (A_1 and A_2) for the equation of state shown below. $R = 82.05$ mL atm/gmol K and $T = 303$ K.

$$\frac{PV}{RT} = 1 + \frac{A_1}{V} + \frac{A_2}{V^2}$$

***P* (atm)**	0.985	1.108	1.363	1.631
***V* (mL)**	25,000	22,200	18,000	15,000

15.28 Three disease-carrying organisms decay exponentially in lake water according to the following model:

$$p(t) = Ae^{-1.5t} + Ae^{-0.3t} + Ae^{-0.05t}$$

Estimate the initial population of each organism (A, B, and C) given the following measurements:

***t*, hr**	0.5	1	2	3	4	5	6	7	9
***p*(*t*)**	6.0	4.4	3.2	2.7	2.2	1.9	1.7	1.4	1.1

14.1 The data can be ordered and tabulated as

i	y	$(y_i - \bar{y})^2$
1	0.9	0.524755
2	1.05	0.329935
3	1.27	0.125599
4	1.3	0.105235
5	1.32	0.092659
6	1.35	0.075295
7	1.35	0.075295
8	1.42	0.041779
9	1.47	0.023839
10	1.47	0.023839
11	1.55	0.005535
12	1.63	3.14E-05
13	**1.65**	**0.000655**
14	1.66	0.001267
15	1.71	0.007327
16	1.74	0.013363
17	1.78	0.024211
18	1.82	0.038259
19	1.85	0.050895
20	1.92	0.087379
21	1.95	0.106015
22	1.96	0.112627
23	2.06	0.189747
24	2.14	0.265843
25	2.29	0.443023
Σ	**40.61**	**2.764416**

(a) $\bar{y} = \dfrac{40.61}{25} = 1.6244$

(b) 1.65

(c) There are two values that occur most frequently: 1.35 and 1.47.

(d) range = maximum – minimum = 2.29 – 0.9 = 1.39

(e) $s_y = \sqrt{\dfrac{2.764416}{25-1}} = 0.339388$

(f) $s_y^2 = 0.339388^2 = 0.115184$

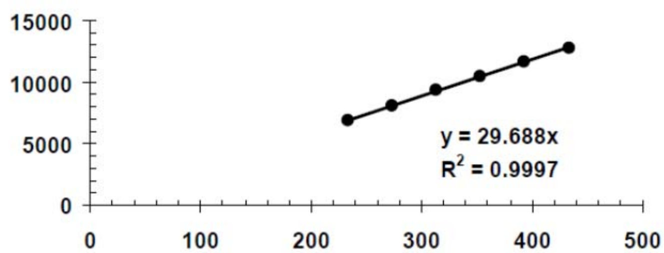
(g) $\text{c.v.} = \dfrac{0.339388}{1.6244} \times 100\% = 20.89\%$

Here is how the problem would be answered using MATLAB's built-in functions:

```
clear, clc
y=[0.9 1.32 1.96 1.85 2.29 1.42 1.35 1.47 1.74 1.82 ...
  1.3 1.47 1.92 1.65 2.06 1.55 1.95 1.35 1.78 2.14 ...
  1.63 1.66 1.05 1.71 1.27];
>> m=mean(y)
m =
    1.6244
>> median(y)
ans =
    1.6500
```

```
>> mode(y)
ans =
    1.3500
>> range=max(y)-min(y)
range =
    1.3900
>> s=std(y)
s =
    0.3394
>> var(y)
ans =
    0.1152
>> cv=s/m
cv =
    0.1152
```

14.7 Linear regression with a zero intercept gives [note that $T(\text{K}) = T(^\circ\text{C}) + 273.15$].



Thus, the fit is

$$p = 29.688T$$

Using the ideal gas law

$$R = \left(\frac{p}{T}\right)\frac{V}{n}$$

For our fit, $p/T = 29.688$. For nitrogen,

$$n = \frac{1\text{ kg}}{28\text{ g/mole}}$$

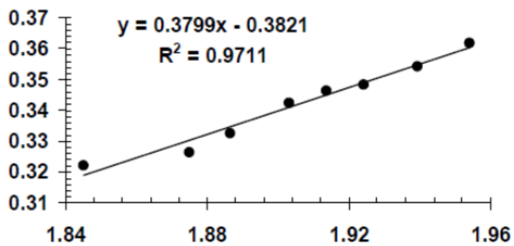
Therefore,

$$R = 29.728\left(\frac{10}{10^3/28}\right) = 8.31264$$

This is close to the standard value of 8.314 J/gmole.

14.12 The power fit can be determined as

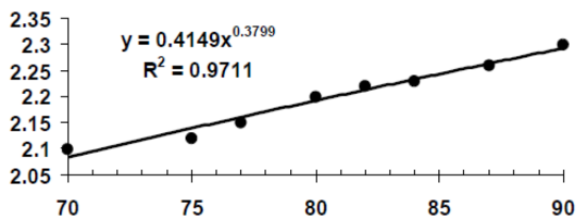
W (kg)	A (m^2)	log W	log A
70	2.10	1.845098	0.322219
75	2.12	1.875061	0.326336
77	2.15	1.886491	0.332438
80	2.20	1.90309	0.342423
82	2.22	1.913814	0.346353
84	2.23	1.924279	0.348305
87	2.26	1.939519	0.354108
90	2.30	1.954243	0.361728



Therefore, the power is $b = 0.3799$ and the lead coefficient is $a = 10^{-0.3821} = 0.4149$, and the fit is

$$A = 0.4149W^{0.3799}$$

Here is a plot of the fit along with the original data:



The value of the surface area for a 95-kg person can be estimated as

$$A = 0.4149(95)^{0.3799} = 2.34 \text{ m}^2$$

15.3 The data can be tabulated and the sums computed as

i	x	y	x^2	x^3	x^4	x^5	x^6	xy	x^2y	x^3y
1	3	1.6	9	27	81	243	729	4.8	14.4	43.2
2	4	3.6	16	64	256	1024	4096	14.4	57.6	230.4
3	5	4.4	25	125	625	3125	15625	22	110	550
4	7	3.4	49	343	2401	16807	117649	23.8	166.6	1166.2
5	8	2.2	64	512	4096	32768	262144	17.6	140.8	1126.4
6	9	2.8	81	729	6561	59049	531441	25.2	226.8	2041.2
7	11	3.8	121	1331	14641	161051	1771561	41.8	459.8	5057.8
8	12	4.6	144	1728	20736	248832	2985984	55.2	662.4	7948.8
Σ	59	26.4	509	4859	49397	522899	5689229	204.8	1838.4	18164

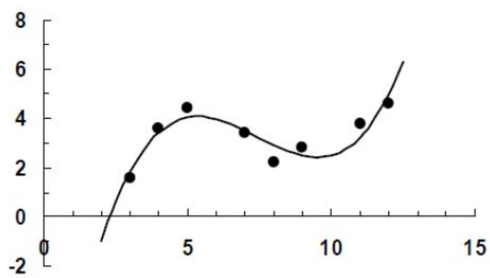
Normal equations:

$$\begin{bmatrix} 8 & 59 & 509 & 4859 \\ 59 & 509 & 4859 & 49397 \\ 509 & 4859 & 49397 & 522899 \\ 4859 & 49397 & 522899 & 5689229 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{Bmatrix} = \begin{Bmatrix} 26.4 \\ 204.8 \\ 1838.4 \\ 18164 \end{Bmatrix}$$

which can be solved for the coefficients yielding the following best-fit polynomial

$$y = -11.4887 + 7.143817x - 1.04121x^2 + 0.046676x^3$$

Here is the resulting fit:



The predicted values can be used to determined the sum of the squares. Note that the mean of the y values is 3.3.

i	x	y	y_{pred}	$(y_i - \bar{y})^2$	$(y - y_{pred})^2$
1	3	1.6	1.83213	2.8900	0.0539
2	4	3.6	3.41452	0.0900	0.0344
3	5	4.4	4.03471	1.2100	0.1334
4	7	3.4	3.50875	0.0100	0.0118
5	8	2.2	2.92271	1.2100	0.5223
6	9	2.8	2.4947	0.2500	0.0932
7	11	3.8	3.23302	0.2500	0.3215
8	12	4.6	4.95946	1.6900	0.1292
Σ				7.6000	1.2997

The coefficient of determination can be computed as

$$r^2 = \frac{7.6 - 1.2997}{7.6} = 0.829$$

Note that the above solution can also be easily obtained with the following MATLAB script:

```
clear,clc,format short g
x=[3 4 5 7 8 9 11 12]'; y=[1.6 3.6 4.4 3.4 2.2 2.8 3.8 4.6]';
Z = [ones(size(x)) x x.^2 x.^3];
a = (Z'*Z)\(Z'*y)
Sr = sum((y-Z*a).^2)
r2 = 1-Sr/sum((y-mean(y)).^2)
```

Running this script yields:

```
a =
       -11.489
        7.1438
       -1.0412
      0.046676
Sr =
        1.2997
r2 =
       0.82898
```

15.10 The linear regression model to evaluate is

$$p(t) = Ae^{-1.5t} + Be^{-0.3t} + Ce^{-0.05t}$$

The unknowns can be entered and the [Z] matrix can be set up as in

```
>> p = [6 4.4 3.2 2.7 2 1.9 1.7 1.4 1.1]';>> t = [0.5 1 2 3 4 5 6 7 9]';
>> Z = [exp(-1.5*t) exp(-0.3*t) exp(-0.05*t)];
```

Then, the coefficients can be generated by solving Eq.(15.10)

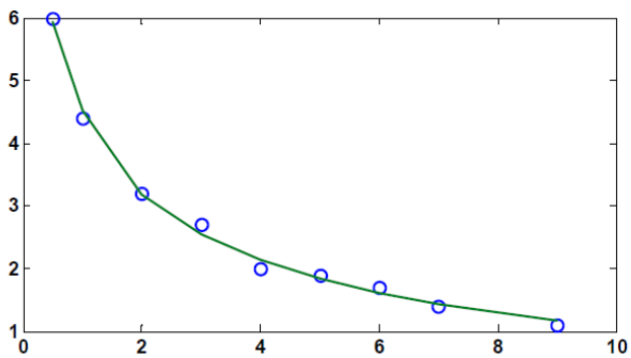
```
>> a = (Z'*Z)\[Z'*p]
a =
    4.1375
    2.8959
    1.5349
```

Thus, the least-squares fit is

$$p(t) = 4.1375e^{-1.5t} + 2.8959e^{-0.3t} + 1.5349e^{-0.05t}$$

The fit and the data can be plotted as

```
>> pp = Z*a;
>> plot(t,p,'o',t,pp)
```



15.18 The equation can be expressed in the form of the general linear least-squares model,.

$$\frac{PV}{RT} - 1 = A_1 \frac{1}{V} + A_2 \frac{1}{V^2}$$

```
>> R=82.05;T=303; P=[0.985 1.108 1.363 1.631]'; V=[25000 22200 18000 15000]';
>> y=P.*V/R/T-1;
>> Z=[1./V 1./V.^2];
>> a=(Z'*Z)\(Z'*y)

a =
      -231.67
 -1.0499e+005
```