RUTGERS
School of Engineering

Department of Chemical & Biochemical Engineering
Rutgers, The State University of New Jersey
98 Brett Road
Piscataway, NJ 08854

155:307 CHEMICAL ENGINEERING ANALYSIS II **FALL, 2008**

Lectures: Monday & Wednesday: 10:20 to 11:40 a.m., DSV Lab (SOE room B125)
Exams only: SEC room 203

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Course Description:
Introduction to modeling and simulation techniques in the analysis of chemical, and biochemical engineering systems. Application of numerical methods for the solution of complex process problems. Development and use of MATLAB software for the solution of engineering problems using personal computers.

Course Objectives and Outcomes: In this course, students learn how to apply knowledge of mathematics, science, and engineering to analyze and solve numerically problems encountered in chemical and biochemical engineering. The course gives the student the opportunity to analyze and interpret data, to identify, formulate, and solve engineering problems, an ability to communicate their results effectively, and to use the techniques, skills, and modern engineering tools necessary for engineering practice.

Students will be introduced to the concepts and methods of numerical analysis as applied to the solution of chemical and biochemical engineering problems. Students will be provided with the awareness and the judgment to recognize the accuracy (or inaccuracy) and validity of numerical solutions. They will be familiarized with the strengths and weaknesses of various numerical methods, and give them some criteria for selecting methods to be used for solving of a particular problem. Students will be introduced to the available computational tools in solving engineering problems. Students will achieve the following educational objectives that include:

Outcomes
(a) an ability to apply knowledge of mathematics, science, and engineering
(e) an ability to identify, formulate and solve engineering problems
(g) an ability to communicate effectively
(k) an ability to use the techniques, skills, and modern engineering tools necessary for engineering practice

These outcomes will be assessed according to the procedures described on p. 3.

Textbook (required for all students)
A. Constantinides and N. Mostoufi, *Numerical Methods for Chemical Engineers with MATLAB Applications*, Prentice Hall PTR, Upper Saddle River, NJ, 1999.

Either (A) or (B) is required, depending on which category you will be in:

(A) Software (required, if you will be using your own computer to do the homeworks):
MATLAB & Simulink Student Version (latest release), The Math Works. Can be purchased on line from http://www.mathworks.com/downloads/web_downloads/index_student
or from the University bookstore.

(B) Reference manual (required, if you do not own a computer and will be using Rutgers computers to do the homeworks):
D. Hanselman and B. Littlefield, *Mastering MATLAB 7*, Prentice Hall PTR, Upper Saddle River, NJ, 2005.
or
W. J. Palm, III, *Introduction to MATLAB 7 for Engineers*, 2nd Ed., McGraw-Hill Book Co., New York, NY (2005).

Numerical Methods software
The textbook for this course contains a CD-ROM with Numerical Methods applications software written in the MATLAB language (for all three operating systems: Windows, Unix, and Macintosh). Printing 1 of the textbook (published on 3/10/99) contained Version 1.00 of the software. Printing 2 and 3 contain version 2.00. Some modifications have been made to the software since printings 1 and 2. These changes are included in Version 3.00 of the software, which may be downloaded from the web page of the book:

http://sol.rutgers.edu/~constant

All students in this class who plan to use the Numerical Methods software on their own computers must download and install Version 3.00. This software will be used in this course.

The students will be expected to become familiar with use of the MATLAB computing environment, the MATLAB language, and the Numerical Methods software. Most of the assigned homework in this course will require the writing of computer programs in the MATLAB language and/or the use of the Numerical Methods software for the solution of the problems.

MATLAB and the Numerical Methods software are installed on the computers in the Microlab of the Department (room C233) and in the School of Engineering DSV Lab (rooms B125/B127) and EIT Lab (room D110). If you have your own computer, you should purchase and install the MATLAB Student Version.

Course outline
The course will follow closely the contents of the text. The sections that have been marked with an asterisk (*) in the Contents of the book (pp. vii-xii) will not be covered this semester. A short introduction to MATLAB will be given at the beginning of the semester (Appendix A: Introduction to MATLAB and Mastering MATLAB 7). A week-by-week outline of the course is given on p.4 of this document.

References and additional reading
At the end of each chapter, there is a list of references pertaining to the particular topic of that chapter.

Homework and grading policy
Homework problems will be assigned, collected, and graded. There will be one closed-book midterm examination and one closed-book final examination.
Grading: Homework: 25%
Midterm exam: 30%
Final exam: 40%
Class participation and attendance: 5%.
Completion of assigned homeworks on time, and class participation and attendance are important. The instructor will check student attendance periodically.

ABET Outcomes and Assessment:

Program outcomes achieved in this course

Outcomes
(a) an ability to apply knowledge of mathematics, science, and engineering
(e) an ability to identify, formulate and solve engineering problems
(g) an ability to communicate effectively
(k) an ability to use the techniques, skills, and modern engineering tools necessary for engineering practice

The achievement of outcomes (a), (e), (g), and (k) will be assessed in this course as follows:

Outcome (a): an ability to apply knowledge of mathematics, science, and engineering.
Equations and models used are derived from the transport, thermodynamics, kinetics and other core chemical engineering course material. Correct solution methods for algebraic and differential equations, including analytical solutions, are shown. Concepts from chemistry and physics are correctly incorporated. This outcome is assessed in the evaluation of homeworks and through questions during exams.

Outcome (e): an ability to identify, formulate and solve engineering problems.
Problems are correctly stated and interpreted and the model correctly describes the engineering concepts.

Outcome (g): an ability to communicate effectively.
The homeworks are easy to read, grammatically correct and contain only a few spelling mistakes. The required format for the homework is closely adhered to.

Outcome (k): an ability to use the techniques, skills, and modern engineering tools necessary for engineering practice.
Computational tools (MATLAB, Simulink, FEMLAB), word processing (such as Word), and data analysis packages (such as Excel) are used as needed. Graphical packages are used to generate publication-quality graphics.

The form to be used for the assessment is on p. 4.

155:307 - Chemical and Biochemical Engineering Analysis II
Fall 2008

Assessment Form for Homeworks

Work product: _____

Group/Student: _____

ABET outcomes applicable to this course	**1**	**2**	**3**	**4**	**5**
(a) an ability to apply knowledge of mathematics, science and engineering					
(e) an ability to identify, formulate, and solve engineering problems					
(g) an ability to communicate effectively					
(k) an ability to use the techniques, skills, and modern engineering tools necessary for engineering practice					

Scores are reported as outcomes having been: (1) not demonstrated or evident; (2) minimally demonstrated; (3) satisfactorily demonstrated; and (4) demonstrated in an exceptional manner with (5) clear understanding and critical comparisons to the literature.
Outcomes not relevant to the work being assessed are not scored.

Assessment metrics needed to achieve a satisfactory score (3):

(a) Equations and models used are derived from the transport, thermodynamics, kinetics, and other core chemical engineering course material. Correct solution methods for algebraic and differential equations, including analytical solutions, are shown. Concepts from chemistry and physics are correctly incorporated.

(e) Systematic analysis has been applied for the solution of complex design situations.

(g) The homework is easy to read, grammatically correct and contains only a few spelling mistakes. The required format for the homework is closely adhered to.

(k) Computational tools (MATLAB, Simulink, FEMLAB), word processing (such as Word), and data analysis packages (such as Excel) are used as needed. Graphical packages are used to generate publication-quality graphics.

COURSE OUTLINE

Week	Topic	Chapter[1]
1, 2, & 3	Introduction to MATLAB, Algorithms, and Software	Appendix A, MATLAB text
3 & 4	Solution of Nonlinear Equations	Chapter 1
5 & 6	Solution of Linear Algebraic Equations	Chapter 2
7 & 8	Finite Difference Methods and Interpolation	Chapter 3
9	Midterm Examination (80 minutes)	Location: SEC 203
10 & 11	Numerical Differentiation and Integration	Chapter 4
12 & 13	Solution of Ordinary Differential Equations	Chapter 5
14	Solution of Partial Differential Equations	Chapter 6
15	Final Examination (3 hours)	Location: SEC 203

HOMEWORK ASSIGNMENTS (due on dates shown)

Date due	Topic	Homework [2]
Sept. 17	Use of MATLAB	Homework #1: MATLAB Exercises
Oct. 1	Solution of Nonlinear Equations	Homework #2: Newton-Raphson method Homework #3: Fanning Friction Factor
Oct. 8	Solution of Nonlinear Equations	1.1, 1.2 1.4
Oct. 15	Solution of Linear Algebraic Equations	2.1, 2.3 (a, b, c), 2.4
Oct. 22	Finite Difference Methods	3.2, 3.3
Nov. 5	Numerical Differentiation and Integration	4.1, 4.2, 4.3, 4.5, 4.8
Nov. 19	Solution of Ordinary Differential Equations	5.3, 5.7, 5.8
Dec. 8	Solution of Partial Differential Equations	Handout

Errata for the text

Corrections have been made to the text since the first printing of the book. For your convenience, the list of errata for the 2nd and 3rd printings is attached to this outline (pages 6-8 of this document). If you own the 1st printing of the book, please obtain the errata list from our web site:

(http://sol.rutgers.edu/~constant)

Please make these corrections to your copy of the textbook.

[1] The course will follow closely the contents of the text. The sections that have been marked with an asterisk (*) in the Contents of the book (pp. vii-xii) will not be covered this semester.

[2] Additional homeworks may be assigned, as needed.

Numerical Methods for Chemical Engineers
with MATLAB Applications
by Alkis Constantinides & Navid Mostoufi
Prentice Hall PTR, 1999

These are the errata for the 2nd and 3rd printing of this book. Please make these corrections to your copy of the book.

Page	Location	Correction
29	Line 7	Change "temperatures" to "pressures
50	Line 13	Change "TOL or TRACE" to "RHO or TOL"
61	Line 3	Change "... water at 50^{o}C ..." to "... water at 20^{o}C..."
62	Line 4	Change “Davidson, B. D.” to “Davidson, B. Z.”
64	Eq. (2.6)	Change " V_i " to " V_j "
91	Eq. (2.108)	Replace "c_{ij}" with "c_i"
91	Eq. (2.109)	Delete $\sum$ at the beginning of the equation
122	Line below Eq. (2.148)	Change "$(\mathbf{A} - \lambda\mathbf{x})$" to "$(\mathbf{A} - \lambda\mathbf{I})$"
122	Eq. (2.152)	Change " - a_n" to " - $a_n\mathbf{I}$ "
147	Eq. (3.14)	Change " $(h^3/3!)Dy(x)$ " to " $(h^3/3!)D^3y(x)$ "
156	Eq. (3.68)	Change " δ_{i+1}" to "δy_{i+1}"
157	Eq. (3.70)	Change " - $y_{i - 1/2}$ " to " - $10y_{i - 1/2}$ "
179	Eq. (3.133)	Change " $p_k(x)$ " to " $p_k(x_i)$ "
182	Eq. (3.145)	Change " y'_{i-1} " to " y'_{i+1} "
215	After line 20	Add: "options = optimset;"
215	Line 21	Replace "phi = fzero(phifile,1,[ ], [ ], x0)" with "phi = fzero(phifile, 1, options, x0);"
217	Line 9	Remove the command "break"
222	Line 16	Change " (-dp-0*rhog*g) " to " (-dp-rhog*g) "
222	Lines 4-5 in deriv.m	Replace with: % DERIV(Y) calculates the first-order derivative % of each column of matrix Y by central finite % differences,using unity as the independent % variable interval. If Y is a row vector, then Y % is converted to a column vector.
223	Line 26	Change "(err ~= 2 | err ~= 4)" to "(err = = 2 | err = = 4)"
227	Line 12	Change "... = 3.26% " to "... = 3.21% "
231	Figure 4.2	Change the labels on the horizontal axis from " x_1 x_0 " to " x_0 x_1 "
235	Eq. (4.83)	Change upper limit on the two integrals from " x_2 " to " x_3 "
243	Eq. (4.93)	Move this equation one line down (below the line "For converting to ....")
243	Eq. (4.92)	This equation is missing: (x - a)/(b - a) = (z - c)/(d - c) Add it in the place previously occupied by Eq. (4.93):

251	Middle of page	Delete " Initial value of "
271	Bottom line	Change " = dy_3 /dt " to " = dy_3 /dx "
279	Lines 5,6	Enter " method =1; " between lines 5 and 6
279	Line 12	Delete " method =1; " at line 12
283	Line 3 (bottom of page)	Change "The vector of dependent variable" to "The vector of independent variable"
294	Eq. (5.96)	Last term is " 9$f(x_{i-3}, y_{i-3})$] "
294	Eq. (5.97)	Last term is " $f(x_{i-2}, y_{i-2})$] "
295	Line 3	Change "value" to "values"
301	Line 6	Change "F(X,P1,P2,...)" to "F(X,Y,P1,P2,...)"
301	Line 2 (bottom of page)	Change "F(X,P1,P2,...)" to "F(X,Y,P1,P2,...)"
302	Line 4 (bottom of page)	Change "F(X,P1,P2,...)" to "F(X,Y,P1,P2,...)"
304	Line 12 in Adams.m	Change "F(X,P1,P2,...)" to "F(X,Y,P1,P2,...)"
305	Line 13 in AdamsMoulton.m	Change "F(X,P1,P2,...)" to "F(X,Y,P1,P2,...)"
314	Line 1 (bottom of page)	Change "t_1=4.36" to "t_1=4.36e-2"
315	Eq. (2)	The term $\left(\frac{d\Phi}{d\eta}\right)$ in the denominator should be raised to the power of 2.
315	Eq. (3)	The term y_1 in the denominator should be raised to the power of 2.
317	Line 17 (bottom of page)	Change "Inside diameter" to "Inside radius"
317	Line 4 (bottom of page)	Change "/vmax" to "/vstar"
318	Line 13	Change "lambda^2*y(1)" to "lambda^2*y(1)^2"
320	Middle of page	Change "Inside diameter" to "Inside radius"
320	Bottom of page	Change "Volumetric flow rate = 2.91" to "Volumetric flow rate = 8.00"
320	Line 2 (Discussion of Results)	Change "2.91 L/s" to "8.00 L/s"
321	Figure E5.4b	Has changed because of the above changes to the program.
328	Eq. (5.151a & b)	Change "j=0" to "i=0" under the summation signs
334	Line 4 (bottom of page)	Add: "options = optimset;"
334	Line 3 (bottom of page)	Replace "theta(k) = fzero(fth,30,1e-6,0, y(:,k),w)" with "theta(k) = fzero(fth,30,options, y(:,k),w)";"
335	Line 22	Add: "options = optimset;"
334-335		Example5_5.m and Ex5_5_func.m have changed. Please download the updated software and re-install.

335	Line 23	Replace "theta = fzero(fth,30,1e-6,0, y,w)" with "theta = fzero(fth,30,options, y,w)";"
345	Middle of page (above Eq. (5.189))	Change "implicit Euler" to "explicit Euler"
350	Eq. (5.223)	Change "y_{n+2}" to "y_{n+1}" on the left-hand-side
356	Line 1 (bottom of page)	Delete ".1"
357	Problem 5.7 Line 2	Change "Lokta" to "Lotka"
372	Line 1	Change "independent" to "dependent"
383	Part (b)	Change the partial derivative in the 4th boundary condition to be with respect to y (not x)
385-393		Example6_1.m and elliptic.m have been changed. Please go to http://sol.rutgers.edu/~constant to obtain software updates.
407	Line 10	Change " DY = " to " DT = "
413-416		Example6_3.m has been changed. Please go to http://sol.rutgers.edu/~constant to obtain software updates.
416	Line 15 from bottom	Change " by Crank-Nicolson implicit " to " by explicit (6.66) "
469	Line 1	Change "in independent" to "is independent"
477	Eq. (7.114)	Move equation down one line (below the first line of item 2.)
508	Line 10	Change " independent " to " dependent " (Note: The MATLAB script**,** Example7_1.m, should also be modified. You may make the change yourself or download the updated software from http://sol.rutgers.edu/~constant and re-install.