Chemical Engineering Analysis 1

ChE 735 **Course Introduction** **Fall 2019**

10:30 MWF—DUE 0096

Description: The mathematical formulation of problems in chemical engineering with emphasis upon the solution of both ordinary and partial differential equations by analytic and numerical means. Examples in this course are drawn from transport phenomena, chemical reaction engineering, and process dynamics and control.

Required book: Glasgow, L. A. *Applied Mathematics for Science and Engineering*, John Wiley & Sons (2014), ISBN 978-1-118-74992-0.

Supplementary resources:

M. R. Spiegel, *Fourier Analysis with Applications to Boundary Value Problems,* McGraw-Hill (1974).

E. Kreyszig, *Advanced Engineering Mathematics (any Edition,3 through 8)*, Wiley (1972 through 1999).

Course meets: MWF, 10:30 AM, DUE 0096

Instructor: Larry A. Glasgow, PhD, University of Missouri (1977)

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Grading: There will be 14 or 15 assigned problems, each worth approximately 20 points. We will also have two examinations (or exercises), one at mid-term and a final (each worth about 60 points). Course grades will be determined from the class distribution. The final exam/problem will be distributed in December 2019.

Objectives of course:

Acquaint student with problem formulation in chemical engineering.

Familiarize student with important solution techniques, emphasizing ordinary and partial differential equations.

Prepare student for success in graduate-level chemical engineering coursework and research.

Philosophy:

The long-term value of graduate-level coursework depends almost entirely upon effort expended by the student. The instructor's role is to focus and guide the classroom discussions to facilitate student inquiry and increase the efficiency of the learning process. In that regard, we emphasize that a participatory classroom experience benefits everybody.

Expectations:

It is expected that all academic work for ChE 735 be *performed solely by you*. Do not collaborate on any academic work unless you obtain prior approval from the instructor. Sanctions will be imposed upon any student found in violation of this policy.

- **Statement Regarding Academic Honesty**

Kansas State University has an Honor System based on personal integrity, which is presumed to be sufficient assurance that, in academic matters, one's work is performed honestly and without unauthorized assistance. Undergraduate and graduate students, by registration, acknowledge the jurisdiction of the Honor System. The policies and procedures of the Honor System apply to all full and part-time students enrolled in undergraduate and graduate courses on-campus, off-campus, and via distance learning. The honor system website can be reached via the following URL: www.ksu.edu/honor . A component vital to the Honor System is the inclusion of the Honor Pledge which applies to all assignments, examinations, or other course work undertaken by students. The Honor Pledge is implied, whether or not it is stated: "On my honor, as a student, I have neither given nor received unauthorized aid on this academic work." A grade of XF can result from a breach of academic honesty. The F indicates failure in the course; the X indicates the reason is an Honor Pledge violation.

- **Statements for Academic Accommodations for Students with Disabilities***

"Any student with a disability who needs a classroom accommodation, access to technology or other academic assistance in this course should contact Disability Support Services (dss@k-state.edu) and/or the instructor. DSS serves students with a wide range of disabilities including, but not limited to, physical disabilities, sensory impairments, learning disabilities, attention deficit disorder, depression, and anxiety."

Kansas State University is vitally interested in the well-being and the academic progress of every student. Should you have need for an accommodation, please see the instructor as soon as possible.

Course outline:

1. Review of algebraic equations with a survey of solution techniques for simultaneous nonlinear algebraic equations.
2. Numerical quadrature.
3. Classification of differential equations by type, order, and linearity.
4. Boundary conditions: Dirichlet, Neumann, and Robin's type.
5. Formulation of first-order ordinary differential equations by mass and energy balances.
6. Formulation of second-order differential equations by force balance.
7. Solution of ordinary differential equations: analytic techniques and numerical methods.
8. Use of the Laplace transform for temporal problems with constant coefficients; applications to process control.
9. Formulation of partial differential equations in transport phenomena.

10. Application of similarity transformations to problems in boundary-layer theory.
11. Applications of the product method (separation of variables) to parabolic, hyperbolic, and elliptic PDE’s; Fourier series and orthogonal functions.
12. Finite difference representations for PDE’s; discretization.
13. Iterative solution of elliptic partial differential equations: Gauss-Seidel and successive over-relaxation (SOR), with applications to fluid-flow, and heat and mass transfer.
14. Explicit solution of parabolic PDE’s—numerical stability.
15. Convective transport terms and the use of upwind differencing.
16. Fully-implicit solution techniques for PDE’s.
17. Elementary topics in CFD (computational fluid dynamics).

The First Assigned Problem (due August 30, 2019)**:**

Part 1. Consider the following set of simultaneous, linear algebraic equations:

$$3X_1 - 2X_2 + 6.2X_3 = 6.01$$

$$-X_1 + 2.7X_2 + X_3 = 0.9025$$

$$4X_1 - 6X_2 - 5X_3 = -0.87$$

The augmented coefficient matrix is simply:

3	-2	6.2	6.01
-1	2.7	1	0.9025
4	-6	-5	-0.87

Use the technique of your choice to show that the three unknowns are: 1.42, 0.675, and 0.5, respectively. Provide enough detail so that I can follow your procedure. Note that you have *many* options for problems of this type; for example, if you have a TI-85 or a TI-89 you can use SIMULT. With Mathcad you can use lsolve(M,v). You could also use PolyMath, MATLAB, or Excel, and you could--in desperation--use pencil and paper (direct elimination).

Part 2. Then, examine the following set of nonlinear equations:

$$3X_1^{\,2} X_2 + X_3 = 25.032$$

$$X_1 X_3 / X_2^{\,1.5} = 2.1896$$

$$\sqrt{X_3}\,(X_1^{\,3} + X_2) = 15.7171$$

See if you can find values for the variables in this case (all three are positive). *Be forewarned: There is no guarantee that any method will produce the desired solution!* Among your options in this case are successive substitution, Newton's method, Excel's Solver add-in, and differential homotopy (continuation). *Please note that X_1, X_2, and X_3 are all positive numbers between 0 and 10.*

Some additional notes for simultaneous linear algebraic equations:

Consider the following set of equations:

$$X_1 + 2X_2 + 3X_3 + X_4 = 8.98958$$

$$X_1 + X_2 - 9X_3 + X_4 = 0.65625$$

$$X_1 + 6X_3 - X_4 = 4.01042$$

$$5X_1 - 2X_2 - X_3 + 7X_4 = 2.14931,$$

with the solution: 1.5, 3.0, 0.444444, and 0.15625 for X_1 through X_4, respectively. We can write this set of equations alternatively as: **AX=C.** If the coefficient matrix, **A**, is nonsingular, then an inverse matrix exists such that: $\mathbf{A}^{-1}\mathbf{A}=\mathbf{I}$. The right-hand side is the identity matrix which consists of 1's on the diagonal and zeroes elsewhere. This suggests the following multiplication: $\mathbf{A}^{-1}\mathbf{A}\,\mathbf{X}=\mathbf{A}^{-1}\,\mathbf{C}$. Consequently, $\mathbf{X}=\mathbf{A}^{-1}\,\mathbf{C}$, and the solution is at hand. So, how does one determine the inverse of **A**?

Since $\mathbf{A}^{-1}\mathbf{A}=\mathbf{I}$, we can obtain the result we seek by applying the Gauss-Jordan method to the *augmented* matrix:

1	2	3	1	1	0	0	0
1	1	-9	1	0	1	0	0
1	0	6	-1	0	0	1	0
5	-2	-1	7	0	0	0	1

See if you can verify that the inverse we are looking for is:

-0.113	0.323	0.548	0.048
0.381	0.084	-0.077	-0.077
0.052	-0.090	0.00645	0.00645
0.197	-0.219	-0.413	0.087

You might do this using Excel's MINVERSE (=MINVERSE(A1:D4), for example) to obtain:

-0.1129	0.322581	0.548387	0.048387
0.380645	0.083871	-0.07742	-0.07742
0.051613	-0.09032	0.006452	0.006452
0.196774	-0.21935	-0.4129	0.087097

Use of search techniques for more challenging problems:

Suppose we are interested in the following algebraic equation:

$$f(x) = 3x - x^2 + \tfrac{1}{3}x^3 - \tfrac{1}{4}x^4.$$

Let's assume we need to identify the value of *x* for which *f(x)*=0. One of the possibilities is to seek the maximum value of $\frac{1}{[f(x)]^2}$ using an appropriate search procedure. We will employ the dichotomous search on the initial interval $1 \le x \le 9$, and refine Δ successively; this produces the following pairs of search endpoints:

2.1086 and 2.1286
2.11667 and 2.12068
2.11848 and 2.11888.

Note that $f(x = 2.11868) = -0.000025$. The logic required for this process is provided immediately below.

```
#COMPILE EXE
#DIM ALL
    REM *** dichotomous search for solution of an algebraic equation
                GLOBAL delta,MP,x1,x2,xl,xh,x,FL,FH,test,trial,FX,ZZ AS
SINGLE
FUNCTION PBMAIN
            INPUT "Specify delta:";delta
            INPUT "Select x1:";x1
            INPUT "Select x2:";x2
                    OPEN "c:dichoto2.dat" FOR OUTPUT AS #1
    100 REM *** continue
                MP=(x1+x2)/2
                    xl=mp-delta
                    xh=mp+delta
                    x=xl
                        GOSUB 300
                        FL=FX
                    x=xh
                        GOSUB 300
                        FH=FX
                    test=FH-FL
                IF test>0 THEN x1=xl ELSE x2=xh
```

```
                PRINT x1,x2
                WRITE#1,x1,x2
                    trial=trial+1
                        IF trial>25 THEN 200 ELSE 100
200 REM *** continue
                INPUT "Shall we continue?";ZZ
                IF ZZ>0 THEN CLOSE
                END
300 REM *** subroutine for function evaluation
            FX=1/(-0.25*x^4+1/3*x^3-x^2+3*x)^2
            RETURN
```

The same basic idea can be used for nonlinear algebraic problems with multiple variables. Suppose for example that you need to estimate the rate of heat transfer in some piece of process equipment. We *presume* that

$$Nu = \frac{hd}{k} = f(\mathrm{Re}, \mathrm{Pr}, L/d, \mu/\mu_0, \ldots..).$$

We might then use experimental data to seek a correlation of the form:

$$Nu = a\,\mathrm{Re}^b\,\mathrm{Pr}^c\,(L/d)^d\,(\mu/\mu_0)^e \ldots.$$

Our task would be to determine the “best” values for *a, b, c, d, e,…. etc.* So, we take the laboratory data from our experimental measurements of *h*, and try to minimize the sum:

$$\sum\left[Nu_{\exp} - a\,\mathrm{Re}^b\,\mathrm{Pr}^c\,(L/d)^d\,(\mu/\mu_0)^e\right]^2.$$

Such correlations have been developed and used extensively in engineering practice over the past 150 years; to illustrate, Churchill and Brier (1955) studied heat transfer from cylinders for large thermal driving forces and found:

$$Nu_m = 0.60\,\mathrm{Re}^{0.5}\,\mathrm{Pr}^{0.33}(T_\infty/T_w)^{0.12}.$$

Of course, experimental data are usually accompanied by error, and in heat and mass transfer studies ±20% would not be unusual. Thus the analyst would want to employ an optimization routine that could cope with such large variability.

A preview of something that will be incredibly useful to us later in the semester, the Fourier series:

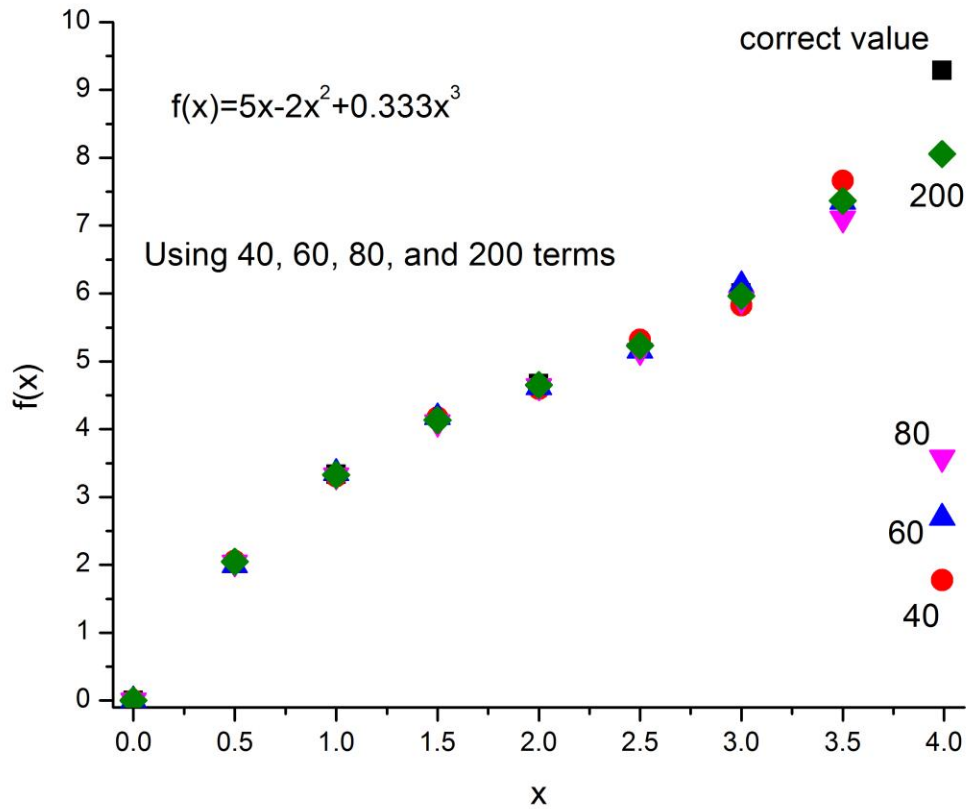
Let’s think about the function, $f(x) = 5x - 2x^2 + \frac{1}{3}x^3$, for $0 \le x \le 4$. We see that $f(1)=3.3333$, $f(2)=4.6667$, $f(3)=6$, etc. If you do not have any experience with Fourier series, then consider the likelihood that we can adequately represent $f(x)$ as:

$$f(x) = \sum_{n=1}^{\infty} A_n \sin\frac{n\pi x}{4}.$$

What do we know about *sine*? It is an *odd* function, and it is *periodic*. Anything else? Fourier proposed that the $A_n's$ could be determined for the infinite series approximating *f*(*x*):

$$A_n = \frac{2}{L}\int_0^L f(x)\sin\frac{n\pi x}{L}dx$$, where *L*=4 of course.

We will find these coefficients by integration (I usually do this numerically and I found A_1 and A_2 to be 5.94176 and -1.93882) and then check our results for *f(x)* against the original function We should expect the approximation to improve as we increase the number of terms in the series:



Notice that the approximation is very good *until* we approach *x*=4; if we want to obtain an accurate value for *f*(*x*=4) we will need *many* terms in the infinite series! This has a number of important implications for our work later in the semester. *If you have a few moments to spare*, try to determine how large *n* must be for us to be within 1% of *f*(*x*=4)?