COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK
DEPARTMENT OF CHEMICAL ENGINEERING

CHEN E4010 Mathematical Methods in Chemical Engineering

Syllabus and Lectures Schedule – Spring 2020

Welcome!

CHEN E4010 *Mathematical Methods in Chemical Engineering* is a rigorous course that is an important component of the foundations of your graduate education in chemical engineering. I love math for its *inherent beauty* and *awesome power* in solving practical problems in almost any field. In this course, you will have an opportunity to appreciate this in the context of chemical engineering problems.

1. **CHEN E4010 Math Methods in Chemical Engineering -** 3.0 pts
Prerequisites: CHEN E3120 and E4230, or equivalent, or instructor's permission. Mathematical description of chemical engineering problems and the application of selected methods for their solution. General modeling principles, including model hierarchies. Linear and nonlinear ordinary differential equations and their systems, including those with variable coefficients. Partial differential equations in Cartesian and curvilinear coordinates for the solution of chemical engineering problems. (http://www.columbia.edu/cu/bulletin/uwb/)

2. **Instructor:**
Professor Venkat Venkatasubramanian
Mudd 819
212-854-4453, venkat@columbia.edu

Teaching Assistant
Mr. Jagan Mohan Sanghishetty email: js5521@columbia.edu

3. **Class Hours/Office Hours:**
   a. Class Hours: Tue and Thu - 10:10 AM – 11:25 AM
   b. Office Hours: Thursday 4 – 5 PM in Mudd 233. Otherwise by appointment.
   Email contact is the preferred method of contact for ease of recording information.
   c. TA Office Hours: TBA

4. **Classroom: Mudd 233**

5. **Textbook and Materials (required and supplemental):**

   a.**Textbook (Required):**
   Rice, Richard G. and Duong D. Do Applied Mathematics and Modeling for Chemical Engineers 2nd Edition, New York, Wiley 2012. ISBN-13: 978-1118024720
   ISBN-10: 1118024729

(Suggested):

Francis B. Hildebrand, *Advanced Calculus for Applications,* 2nd Edition, Prentice-Hall (1976). ISBN-13: 978-0130111890, ISBN-10: 0130111899

b. **Materials(required):**

1. CHEN E4010 CourseWork's web site https://courseworks2.columbia.edu/welcome/

c. **Materials (supplemental)**

1. Reference books and internet sites

Abramowitz, Milton and Irene A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, New York: Dover, 1965 9th printing.

Billo, E. Joseph*, Excel for Scientists and Engineers, Numerical Methods*, Hoboken, NJ: Wiley, 2007

Fogler, H. Scott, *Elements of Chemical Reaction Engineering 4th Edition (3rd Printing)*, New York: Prentice Hall, 2006

Fong, C.F. Chan Man, D. De Kee and P.N. Kaloni, *Advanced Mathematics for Applied and Pure Sciences*, Canada: Gordon Breach Science Publishers, 1997.

(http://cuit.columbia.edu/mathematica-students accessed Jan 5, 2017)

(http://www.mathworksheetsgo.com/trigonometry-calculators/inverse-cosine-calculator.php accessed Jan 5, 2017)

(http:// http://integrals.wolfram.com/index.jsp accessed Jan 5, 2017)

Aris, Rutherford, *Vectors, Tensors, and the Basic Equations of Fluid Mechanics*. New York: Dover Publications Inc. 1962.

Stewart, James, *Calculus Concepts and Contexts*, New York: Brooks/Cole Publishing. 1998, P402 -408, Section 5.6 Integration by parts

Strang, Gilbert, *Introduction to Linear Algebra*, Wellesley-Cambridge Press and SIAM, Fifth Edition (2016). Excellent introduction to the subject.

Zill, Dennis G. and Warren S. Wright, *Advanced Engineering Mathematics*, Burlington, MA: Jones and Bartlett Learning LLC, 2014. Engineering mathematics textbook.

2. Other supplemental material, notes, and problems will be posted on the CourseWorks web page, which will be updated throughout the course.

6. **Course Objectives:**

a. Be able to mathematically describe chemical engineering problems and the application of selected methods for their solution.

b. Apply general modeling principles, including model hierarchies.

c. Solve linear and nonlinear ordinary differential equations and their systems, including those with variable coefficients.

d. Solve partial differential equations in Cartesian and curvilinear coordinates for the solution of chemical engineering problems.

e. Hopefully, learn to love and admire mathematics for its *inherent beauty* and its almost *magical power* in solving practical problems.

7. Classroom Procedures:

a. *What you should to bring to class:* A calculator, writing implement, a notebook, textbook, computer laptop as desired.

b. *What **not** to bring to class:* Anything that could disturb others around you. Anything that would distract you or others from the guest speaker such as but not limited to a plate of food, computer games, any device that make sounds, course work from another class, social media connecting devices, etc.

c. *Be on time for class and actively participate*. Being on time for class means that you are seated, ready to take notes, solve problems, listen to lecture, and take other class room instructions prior to the start time. You are also expected not to chat and distract. This standard is adopted in order to provide the best class experience possible. Class participation is part of your grade. You are required to be in class and seated ready to go at the start time. If you are found to be a distraction, you may be asked to leave.

d. *Web Site*. The web site for this class contains important administrative and scheduling information, and is located at the Columbia Course Works web site: https://courseworks.columbia.edu/welcome/ I will update the site with lecture slides and links to articles and resources as appropriate.

8. **Course Grade:** The final grade in this course will be based on points awarded according to the following system:

a. **Final grade**: 50 % midterms (two midterms, 25% each) + 50 % final

b. **References for In-Class Exams:** The exams are **closed book** and **closed notes**. You are **not allowed** to use any books or notes of any sort during the exams, except for a "crib sheet" (**one page** for all exams) as a concise set of notes used for quick reference. Exam "Blue books" will be provided for you. You are not allowed to use any cell phones, calculators, computers, or any device that allows for storage of data during the exams. Any exceptions to this policy will be announced by the instructor prior to the specific event.

9. **Homework:** Homework problems will be assigned and completion dates suggested. *However, homework will not be collected or graded.* You are ultimately responsible for knowing all aspects of the problems. To help you learn, homework solutions will be made available through the TA. A student in the course can do the work and contact TA for assistance in order to learn the material. Copying solutions will not achieve this and is against Columbia University Policy. (http://bulletin.engineering.columbia.edu/policy-conduct-and-discipline). The re-distribution of the homework solutions in CHEN E4010 is not authorized. The TA has office hours so that you can meet and cover homework problems that you have attempted or perhaps need assistance or clarification with the solution. While the homework in the math methods course is not graded, the homework is still an assignment for a student in the course and are assigned to help your learning.

10. **Academic integrity:** If a student is suspected of a breach of academic integrity, the student will be referred to the university office on matters of honor and academic integrity. As your grade is determined based on in-class examinations, it is imperative that you do your own work. Do not cheat on any exams. Students who are suspected of cheating on an exam will be reported to the School of Engineering and Applied Science for further processing, which can result in dismissal from Columbia. All students are reminded of the following information from the Columbia University Web site:
"Academic integrity defines a university and is essential to the mission of education. At Columbia students are expected to participate in an academic community that honors intellectual work and respects its origins….As such, a violation of academic integrity is one of the most serious offenses a student can commit at Columbia and can result in dismissal."
(http://bulletin.engineering.columbia.edu/policy-conduct-and-discipline, accessed 23 Jan 2016)

"Academic Integrity Policies and Expectations: Violations of policy may be intentional or unintentional and may include dishonesty in academic assignments or in dealing with University officials, including faculty and staff members. Moreover, dishonesty during the Dean's Discipline hearing process may result in more serious consequences"
(http://bulletin.engineering.columbia.edu/policy-conduct-and-discipline, accessed 23 Jan 2016)
"Common types of academic integrity violations:

-Plagiarism: the use of words, phrases, or ideas belonging to another, without properly citing or acknowledging the source
-Self-plagiarism: the submission of one piece of work in more than one course without the explicit permission of the instructors involved
-Falsification or misrepresentation of information in course work or lab work; on any application, petition, or forms submitted to the School
-Fabrication of credentials in materials submitted to the University for administrative or academic review
-Violating the limits of acceptable collaboration in course work set by a faculty member or department
-Facilitating academic dishonesty by enabling another to engage in such behavior

-Cheating on examinations, tests, or homework assignments

-Unauthorized collaboration on an assignment

-Receiving unauthorized assistance on an assignment

-Copying computer programs

-Unauthorized distribution of assignments and exams

-Lying to a professor or University officer

-Obtaining advance knowledge of exams or other assignments without permission "
(http://bulletin.engineering.columbia.edu/policy-conduct-and-discipline, accessed 23 Jan 2016)

11. Lecture Schedule

(*Note:* **(1) 1/21** *– Lecture # and Date; Pages in parentheses refer to Rice & Do; Schedule and topics might change somewhat depending on the course progress.)*

I. Model formulation (1) 1/21

A. General modeling principles (pp. 3-10)
B. Model hierarchies (pp. 19-25)
C. Typical ChE model formulation examples

II. Review of Linear Algebra

A. Vectors and Matrices (pp. 10-17; Strang, Ch. 1-2) **(2) 1/23**
B. Solving linear equations **(3) 1/28**
C. Vector Subspaces, Orthogonality, Determinants (Strang, Ch. 3-5) **(4) 1/30,(5) 2/4**
D. Eigenvalues and Eigenvectors, Linear transformations (Strang, Ch. 6, 8) **(6) 2/6**

III. Linear ODEs (7) 2/11

A. First order (pp. 32-33)
B. Systems of linear first order ODEs (pp. 55-60) **(8) 2/13**
C. Higher order with constant coefficients **(9) 2/18**
    1. Homogeneous (pp. 42-47)
    2. Non-homogeneous (pp. 47-50, 54-55)
D. Systems with constant coefficients (pp. 55-60)

Midterm Exam 1 on 2/20

E. Higher order with variable coefficients **(10) 2/25**
    1. Special cases and strategies (p. 40, 41)
    2. Power series solutions (pp. 75-77) **(11) 2/27**
    3. Method of Frobenius (pp. 77-86) **(12) 3/3**
    4. Bessel and Gamma functions (pp. 86-92, 98-99) **(13) 3/5**
    5. Legendre polynomials (Hildebrand pp. 159-165) **(14) 3/10**

F. Eigenvalue problems **(15) 3/12**

Spring Recess (3/16-20)

IV. Linear PDEs (pp. 229-233) **(16) 3/24**

A. Separation of variables (pp. 238-248)
   1. Sturm-Liouville Problems, Cartesian Parabolic PDEs
   2. Cylindrical Parabolic PDEs **(17) 3/26**
   3. Parabolic PDEs with non-homogeneities **(18) 3/31**
   4. Elliptic PDEs **(19) 4/2**

B. Finite Fourier Transforms (pp. 273-289) **(20) 4/7**
   Midterm Exam 2 on 4/9

C. Combination of variables/Similarity transform (pp. 233-8; 97-8) **(21) 4/14**
   1. Rayleigh problem and error function **(22) 4/16**

V. Nonlinear ODEs (23) 4/21

A. First order strategies (pp. 33-37)
B. Second order strategies (pp. 37-42) **(24) 4/23**
C. Systems of nonlinear ODEs
D. Linearization

VI. Laplace transforms (pp. 204-215, 248-253) **(25) 4/28**

A. Solving ODEs, systems of ODEs, and PDEs
B. Inversion: practical guidelines

VII. Numerical Solution Methods (pp. 139-156) **(26) 4/30**

A. Euler's method, Midpoint method, Trapezoidal method
B. Runge-Kutta
C. Stiff differential equations, Implicit Euler's method
D. MATLAB ODE Suite

Exam Schedule

Midterm Exam 1: Modeling principles, Linear Algebra, Linear ODEs with constant coefficients, Systems of linear ODEs with constant coefficients – **2/19**

Midterm Exam 2: Higher order linear ODEs with variable coefficients, Eigenvalue problems, Linear PDEs by separation of variables -- **4/9**

Final Exam: All course topics – **TBA**

12. Acknowledgements:
This document is based on earlier versions prepared by Mr. Michael Hill and Dr. Robert Bozic, who had taught this course in previous years. I have benefited greatly from their input about the course.