

Fall 2018

CHE 365 - Chemical Engineering Computing

Roman Voronov

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Sample Course Syllabi:

ChE365 – Chemical Engineering Computing

Fall 2018

Otto H. York Department of Chemical, Biological & Pharmaceutical Engineering
New Jersey Institute of Technology

Course Schedule: W:600PM - 905PM, TIER411

Office Hours: Friday 3:00-5:00 PM and other times strictly by appointment (e-mail)

Instructor: Dr. Roman S. Voronov, Assistant Professor

Instructor Contact: Tiernan Hall 378, 1.973.642.4762 (voicemail=slow), rvoronov@njit.edu
(fast)

Instructor Webpage: <http://chemicaleng.njit.edu/people/rvoronov.php>

Please add ChE365 in the subject of your emails

Catalog Description:

Introduction to basic concepts of computational methods for solving chemical engineering problems and performing process simulations. Topics include common numerical techniques encountered in chemical engineering, for the solution of linear and non-linear algebraic equations and ordinary differential equations, differentiation/integration, optimization and interpolation/regression of data. Students will be exposed to modern computational software and commercial chemical processes simulators.

Pre-requisites: CHE 370. Corequisite: CHE 360

Course Objectives:

1. Select and apply appropriate numerical methods for root searching, optimization, solving systems of linear algebraic equations, curve fitting, interpolation, differentiation, integration and ordinary differential equations when applied to a range of chemical engineering problems.
2. Analyze various sources of errors in computation and model building, define error types and convergence
3. Develop an understanding for how numerical methods afford a means to generate solutions to chemical engineering problems, in a manner that can be implemented on digital computers.
4. Apply the built-in functions in MATLAB®/Mathematica® and EXCEL® to solve numerical engineering problems, as well as develop an understanding for how they work “behind the scenes”.
5. Work on group exercises and apply a range of numerical methods to evaluate solutions to engineering problems
6. Become acquainted with advanced modeling packages like COMSOL® and Aspen®

Textbooks: Required –

1) Connect Access Card for Applied Numerical Methods with MATLAB for Engineers and Scientists by Chapra, 4th edition, ISBN: 9781259547669

Note: Students may additionally purchase the hard copy of Applied Numerical Methods with MATLAB for Engineers and Scientists / Edition 4 by Steven Chapra. ISBN-13: 978-0073397962; ISBN-10: 0073397962. Alternatively, you may be able to get away with using the cheaper international or 3rd editions, at your own risk. The purchase of the hard copy is optional.

2) You already have the electronic copy of this book through NJIT libraries, so do NOT need to buy the hard copy (unless you really want to). Introduction to Chemical Engineering Computing 2nd Edition by Bruce A. Finlayson. ISBN-13: 978-1118888315; ISBN-10: 1118888316.

Recommended/Alternative Resources – 1) Numerical Methods for Chemical Engineers Using Excel, VBA, and MATLAB by Victor J. Law. ISBN-13: 9781466575349; 2) Numerical Methods for Engineers - 7th edition ISBN13: 9780073397924; ISBN10: 007339792X

Required Software: Latest versions of Matlab, MS Office, Adobe Reader (available through the CME department, while the rest of the software can be downloaded from the NJIT IST website). Student Mall and CME department PC lab have most of the software. Please see Highlander Pipeline for Matlab tutorial and example programs.

Clickers: Required – we will use them to take some of the quizzes.

Grading (curved at the end of the course):

HOMEWORK (HW) — 10%

LABORATORY* – 25%

QUIZES – 10%

MIDTERM – 20%

INDIVIDUAL PROJECT — 15%

FINAL — 20%

*This course will implement an “active learning” environment. Therefore, a significant portion of the grade will depend on interactive assignments during class.

Grade Cut-offs

A = Above 90%

B+ = 80-89%

B = 70-79%

C+ = 65-69%

C = 60-64%

D = 50-59%

F = below 50%

Homework will be assigned through either Moodle: <http://moodle.njit.edu> – Or McGraw Hill Connect. Please check these sites and your email often. Most of the homework, quizzes and solutions will be on these sites, as well important course announcements.

There may be a gray area between each two letter grades in the final distribution, so that two students getting similar weighted average, at the border of grade categories, could get different letter grades. If you are in one of these gray areas, whether you get the higher or lower grade depends on whether your performance has been improving or declining over the course period and on your overall class participation (attendance/discussion etc.).

Important University Dates (Add/Drop/Refund/Last Day to Withdraw/Recess/Finals):

<http://www.njit.edu/registrar/calendars/>

<http://www.njit.edu/registrar/exams/finalexams.php>

Make-up sessions — If classes are cancelled due to inclement weather, students will be asked to attend make-up session(s) on a Saturday (TBA).

Class Attendance: Experience shows that students who do not regularly attend class typically perform poorly in the course. In addition, examples are worked out during the lectures. These examples are may not be posted online. Students are responsible for all material covered in class.

Office Hours Attendance: This time is for you to come and seek help in case you don't understand the material, have an English problem, or are concerned about your grade. Coming to office hours shows that you care about learning and positively affects both your performance and evaluation. Do not wait until the very end to do this!

Seating Chart: The instructor reserves the right to assign seating during the class lecture.

NJIT Honor Code: The NJIT honor code is being upheld on all issues related to the course. Students are expected to be familiar with the code and conduct themselves accordingly. Any violations will be brought to the immediate attention of the Dean of Students.

A TENTATIVE SCHEDULE FOR THE SEMESTER:

Lecture #	Date	Numerical method (Typical example or module)*
PART I		
1	09/05/18	INTRO TO COMPUTERS & CHE MODELING
2	09/12/18	CHE COMPUTING FUNDAMENTALS
3	09/19/18	ROUND OFF AND TRUNCATION ERRORS, CONVERGENCE
4	09/26/18	ROOTS BRACKETTING & OPEN METHODS (SOLVING CUBIC EQUATION OF STATE)
5	10/03/18	OPTIMIZATION
6	10/10/18	SOLVING LINEAR SYSTEMS OF EQUATIONS (CHEMICAL REACTORS LINKED BY PIPES)
PART II		
7	10/17/18	CURVE FITTING (DETERMINING REACTION RATE CONSTANTS)
8	10/24/18	INTERPOLATION
9	10/31/18	TBA (AICHE CONFERENCE)

11	11/07/18	NUMERICAL INTEGRATION
12	11/14/18	NUMERICAL DIFFERENTIATION (REACTION RATE CONSTANTS)
PART III ADVANCED COMPUTATIONAL MODELING		
13	11/21/18	FRIDAY CLASSES MEET
14	11/28/18	ORDINARY DIFFERENTIAL EQUATIONS
15	12/05/18	ADVANCED COMPUTATION TOPICS
16	12/12/18	ADVANCED COMPUTATION TOPICS
17	TBA	FINAL

* While topics remain identical, the example and module titles may be subject to change.

Policies and Expectations about Exams/Grades

- The course letter grade will be assigned and rounded automatically by an Excel code (no emotions attached). The assigned letter grade is FINAL without subject to negotiation!
- Students have to plan, study and do well in exams/HW if they want to get a good grade in this class. Instructor will NOT change letter grades to accommodate any special circumstances. The student will get the letter grade he/she deserves.
- Students can dispute the exam scores within a week following the announcement of the score. Students cannot dispute their prior exams or HWs after one week or at the end of the semester! After first review of the dispute, if the score is not modified, but the student is unconvinced and asks for an additional review, then he/she assumes the possibility of instructor removing points as well as giving points.
- Student handwriting must be legible in order to receive points.
- The graded exams must be returned within a week to be saved for the department course assessment initiative.
- Students will get 0 for not showing to quizzes, participation, exams, or any other course activity. If a student misses an exam due to extreme circumstances (such as a medical problem or a death in the family), he/she needs to notify the instructor via email before the beginning of the exam, and bring proof of the circumstance to the Dean of Student's office. Only in this case of official approval from the Dean of Student's office, may a make-up be given.
- Extra credit may be assigned during the semester, at the digression of the instructor. There will be no make-ups, extra credit, or any additional projects/assignments given beyond the semester's completion.
- If you need accommodations due to a disability please contact Chantonette Lyles, Associate Director of Disability Support Services, Fenster Hall Room 260 to discuss your specific needs. A Letter of Accommodation Eligibility from the Disability Support Services office authorizing your accommodations will be required.

Most important: Have lots of fun!