ChEE 402 & Chemical Engineering Modeling

C E Chavez Bldg, Rm 110 • MWF 8:00-8:50 am

Description of Course

Building models is an important part of chemical engineering. Models predict how a process works and the materials and energy that will be needed as well as whether it will be safe and economical. Designing a process starts with building a model. Models contain a schematic, lists of variables, and equations that describe the most relevant physics and chemistry as you saw in ChEE 201, 202, and 203. We will add a control volume, boundary conditions, and lists of parameters. Some of the equations are exact, whereas others are approximations that depend on experimental data. Exact equations include the conservation of mass, energy, and momentum. Constitutive equations relate two physical quantities and approximate the response of a specific material or process to external forces. Constitutive equations include Henry's law $y = Hx$, Fick's Law $J = -D\frac{dc}{dx}$, and the rate equation $r = -kc$. Armed with an understanding of how to apply these equations, it is surprising the number of interesting problems that can be solved that model real world processes.

Models that describe real chemical processes are often so complex that it is not practical to solve them by hand or analytically. Instead numerical solutions are developed using computers. In this course you will learn how to formulate models of chemical processes and solve them using Matlab. The equations can be linear or nonlinear algebraic equations, differential equations that depend on one or more variables, and integral equations. Models that combine equations of different types are common. For example, a reactor process model will often include a differential equation describing the conservation of mass in the system as well as an algebraic equation describing how the reaction rate changes with temperature and concentration.

Course Prerequisites or Co-requisites

Adv. Stdg: Engineering. CHEE 202, MATH 254, and AME 205.

Instructors, Office Hours, and Contact Information

Anthony Muscat, Tuesday 12-1 PM, Harshbarger Room 108, 520-621-6162, muscat@email.arizona.edu

Teaching assistants

James Makel (TA), Monday 4-5 pm, Harshbarger 118B, 520-626-9186, jamesmakel@gmail.com

Brandon Velasquez (preceptor), Tuesday 5-6 PM and Friday 3-4 PM, Harshbarger 112, bvelasquez@email.arizona.edu

Course Format and Teaching Methods

Lecture with some individual and small-group class activities.

Required and Recommended Texts

Required: Class notes and video lectures posted on D2L.

Recommended:

Professor Saez's class notes from fall 2016 are posted on D2L in the Resources module. Clear description of main concepts and methods used to model chemical processes.

Applied Mathematics and Modeling for Chemical Engineers, Richard G. Rice and Duong D. Do, (John Wiley and Sons, 1995). Excellent reference textbook on a variety of mathematical techniques used in chemical engineering.

A Practical Introduction to Programming and Problem Solving, Stormy Attaway (Butterworth-Heinemann). This book is a good introduction to using the built-in programs in Matlab. Any edition including the first from 2009 will serve you well.

Course Objectives and Expected Learning Outcomes

The purpose of this course is to build skills with mathematical and computational techniques to solve problems in chemical engineering. We will start with finite difference equations and numerical integration using finite differences and move to systems of linear and nonlinear algebraic equations, ordinary differential equations (ODEs), and end with partial differential equations (PDEs). Successful completion of this course will allow you to:

1. Assess chemical engineering processes and systems qualitatively and quantitatively bringing together relevant physical and chemical information.
2. Represent processes and systems with mathematical models.
3. Formulate initial or boundary conditions.
4. Solve model equations using analytical and numerical methods.
5. Code with Matlab to simulate chemical engineering processes.
6. Explain the limitations and practical utility of solutions.

Topics

1. Staged processes in series.
   Finite difference equations. Countercurrent extraction of a gas by a liquid. VLE linear (Henry's law) or nonlinear (relative volatility). Riccati's equation.

2. Perfectly mixed chemical reactors with first-order irreversible reactions.
   Mass and energy balances. Model formulation. Batch reactor. CSTR. First-order ordinary differential equations (ODEs). Finite difference approximations. A first look at Laplace transforms. Reactive membranes. Plug flow reactors without axial diffusion. Batch distillation.

3. Reaction-diffusion (RD) problems in one-dimension.
   Combine reaction at a surface with transport in thin film growth, catalysis, and corrosion. Second-order ordinary differential equations. Plug flow reactor with axial diffusion.

4. Coupled heat or mass transport with reaction, sources, or sinks.
   Systems of ODEs. Numerical solution of initial value problems. Bessel equation. Nonlinear problems. Newton's method.

5. Processes that depend on time.
   Reactor start up and shut down. Stirred tanks with heating elements. Complex variables. The Laplace transform.

6. Processes that depend on time and position.
   Partial differential equations (PDEs). Double-pipe heat exchanger. Coated wall reactor. Sturm-Liouville theory. Heat conduction. Initial and boundary value problems.
   and

Absence and Class Participation Policy

The UA's policy concerning Class Attendance, Participation, and Administrative Drops is available at: http://catalog.arizona.edu/policy/class-attendance-participation-and-administrative-drop

The UA policy regarding absences for any sincerely held religious belief, observance or practice will be accommodated where reasonable, http://policy.arizona.edu/human-resources/religious-accommodation-policy.
Absences pre-approved by the UA Dean of Students (or Dean Designee) will be honored. See: https://deanofstudents.arizona.edu/absences

Participating in the course and attending lectures and other course events are vital to the learning process. As such, attendance is required at all lectures and discussion section meetings. Students who miss class due to illness or emergency are required to bring documentation from their health-care provider or other relevant, professional third parties. Failure to submit third-party documentation will result in unexcused absences.

Course Communications

The instructors will communicate with you using your official UA e-mail address and D2L.

Required or Special Materials

Access to a computer running Matlab and Simulink is required. Matlab is loaded on most University computers. You can load Matlab on your computer for free. The program is available from the UA software licensing website (read the information on the following web page and scroll down to Order/Download).

http://softwarelicense.arizona.edu/mathworks-matlab

Either versions a or b from 2013, 2014, 2015, 2016, or 2017 will be fine for the course. You don't need the latest version, although the interface has been improved. Make sure that you install both Matlab and Simulink. You will be given the option in the installation procedure.

Assignments and Examinations: Schedule/Due Dates

Problem sets will be assigned weekly, typically on Wednesday and is due the following Wednesday. Do all analysis and make plots with Matlab. Please do not use Excel, nor Wolfram Alpha. Clearly document all parameters and variables within a Matlab script or function using comment statements. Use the publish command to output your script and the numerical solution in several different formats such as pdf. In technical writing, clarity and brevity are valued. Provide sufficient detail that an educated reader can follow your method and strive to write concisely.

Submit hard copies of the problem sets including codes and plots. Problem set assignments are due at the beginning of class on the date specified on the problem set. No late problem sets will be accepted unless prior permission is obtained from the instructor. Medical conditions and other circumstances beyond your control will be considered on an individual basis.

There is one quiz on the syllabus to be completed by August 23 and three in-class exams on Friday, September 22, 2017; Friday, October 20, 2017; and Friday, November 17, 2017.

Final Examination

The date and time of the final exam is Wednesday, 12/13/2017, 8:00 am - 10:00 am. Final Exam Regulations, https://www.registrar.arizona.edu/courses/final-examination-regulations-and-information, and Final Exam Schedule, http://www.registrar.arizona.edu/schedules/finals.htm

Grading Scale and Policies

Two problems will be graded on each problem set, the scores averaged, and the result multiplied by the number of problems completed. The total problem set score is 20% of the final grade.

The two highest scores of the three midterm exams are each worth 25% of the final grade.

The final exam is 30% of the final grade.

The problem sets and exams will be graded based on partial credit.

You are encouraged to discuss problem sets with classmates, but everyone must submit their own work. Do not copy someone else's work or submit joint work. This behavior defeats the purpose of the class and will result in a score of 0 for everyone involved.

Final grade based on the following percentages: A > 90%, B > 80%, C > 70%, D > 60%. The cutoffs are based on the difficulty of the problems on the exams and the length of the exams. These values are maximums and typically the cutoffs are 1-3% lower.

University policy regarding grades and grading systems is available at http://catalog.arizona.edu/policy/grades-and-grading-system

Dispute of Grade Policy: On problem sets or exams that you do not agree with the grading, please write a short description describing why and submit to Professor Muscat within one week after the work is returned in class.

Requests for incomplete (I) or withdrawal (W) must be made in accordance with University policies, which are available at http://catalog.arizona.edu/policy/grades-and-grading-system#incomplete and http://catalog.arizona.edu/policy/grades-and-grading-system#Withdrawal respectively.

Honors Credit

Students wishing to contract this course for Honors Credit should email Professor Muscat to set up an appointment to discuss the terms of the contract. Information on Honors Contracts can be found at https://www.honors.arizona.edu/honors-contracts.

Scheduled Topics/Activities

Please consult the course homepage on D2L for the weekly schedule.

Classroom Behavior Policy

To foster a positive learning environment, students and instructors have a shared responsibility. We want a safe, welcoming, and inclusive environment where all of us feel comfortable with each other and where we can challenge ourselves to succeed. To that end, our focus is on the tasks at hand and not on extraneous activities (e.g., texting, chatting, reading a newspaper, making phone calls, web surfing, etc.).

Students are asked to refrain from disruptive conversations with people sitting around them during lecture. Students observed engaging in disruptive activity will be asked to cease this behavior. Those who continue to disrupt the class will be asked to leave lecture or discussion and may be reported to the Dean of Students.

Threatening Behavior Policy

The UA Threatening Behavior by Students Policy prohibits threats of physical harm to any member of the University community, including to oneself. See http://policy.arizona.edu/education-and-student-affairs/threatening-behavior-students.

Accessibility and Accommodations

Our goal in this classroom is that learning experiences be as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, please let Professor Muscat know immediately so that we can discuss options. You are also welcome to contact the Disability Resource Center (520-621-3268) to establish reasonable accommodations. For additional information on the Disability Resource Center and reasonable accommodations, please visit http://drc.arizona.edu.

If you have reasonable accommodations, please plan to meet with Professor Muscat by appointment or during office hours to discuss accommodations and how the course requirements and activities may impact your ability to fully participate.

Please be aware that the accessible table and chairs in this room should remain available for students who find that standard classroom seating is not usable.

Code of Academic Integrity

Students are encouraged to share intellectual views and discuss freely the principles and applications of course materials. However, graded work/exercises must be the product of independent effort unless otherwise instructed. Students are expected to adhere to the UA Code of Academic Integrity as described in the UA General Catalog. See: http://deanofstudents.arizona.edu/academic-integrity/students/academic-integrity.

The University Libraries have some excellent tips for avoiding plagiarism, available at http://new.library.arizona.edu/research/citing/plagiarism.

Selling class notes and/or other course materials to other students or to a third party for resale is not permitted without the instructor's express written consent. Violations to this and other course rules are subject to the Code of Academic Integrity and may result in course sanctions. Additionally, students who use D2L or UA e-mail to sell or buy these copyrighted materials are subject to Code of Conduct Violations for misuse of student e-mail addresses. This conduct may also constitute copyright infringement.

UA Nondiscrimination and Anti-harassment Policy

The University is committed to creating and maintaining an environment free of discrimination; see http://policy.arizona.edu/human-resources/nondiscrimination-and-anti-harassment-policy

Our classroom is a place where everyone is encouraged to express well-formed opinions and their reasons for those opinions. We also want to create a tolerant and open environment where such opinions can be expressed without resorting to bullying or discrimination of others.

Additional Resources for Students

UA Academic policies and procedures are available at http://catalog.arizona.edu/policies

Student Assistance and Advocacy information is available at http://deanofstudents.arizona.edu/student-assistance/students/student-assistance

Confidentiality of Student Records

http://www.registrar.arizona.edu/personal-information/family-educational-rights-and-privacy-act-1974-ferpa?topic=ferpa

Subject to Change Statement

Information contained in the course syllabus, other than the grade and absence policy, may be subject to change with advance notice, as deemed appropriate by the instructor.