ChEE 402 Chemical Engineering Modeling

Building: _____, Rm _____ • Day(s) Time

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 reaction 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, Wednesday 5-6 PM and by appointment, Harshbarger Room 108/120, 520-621-6162, muscat@email.arizona.edu

Teaching assistant, _____ (TA), Weekday, Time, Office Location, 520-62x-xxxx, ----------@email.arizona.edu

Course Format and Teaching Methods

On D2L you will find videos and notes containing the course material and the problem packet for that section of the course. Before coming to class, please view the videos and lecture notes on the module that we are working on. Although you have my notes, I suggest that you take your own notes or annotate my notes. Also please come to class with access to the problem packet. You can print the problems or access them electronically from the D2L site. It is important that everyone have access to the problem packet because you may be at different points in working the problems. We will spend class time working individually and in small groups. We will formulate problems by asking high quality questions, solve problems, and make concept maps.

How to Learn

Research shows that our performance in activities as different as playing tennis or the violin to memorizing long strings of 86 digits or playing a game like chess is not determined by the genes that we are born with, rather by the way that we practice and learn the activity and our mental attitude.* The book "Make It Stick" by Peter Brown, Henry Roediger, and Mark McDaniel suggests the following for optimal learning:

(i) learning is more durable and lasting when we put effort in to it (after all, the brain needs to physically change for us to learn new things),

(ii) re-reading text or a problem solution and cramming are ineffective (these are typically low activity or passive practices),

(iii) recalling information (or simple self-testing) is more effective than re-reading (self-testing is very active learning). For example, try to summarize or outline what you have heard or read. Work an example problem from the course videos and notes or the problem packet or that you found on the internet without assistance. Also try working or re-working a problem in the problem packet without using your notes.

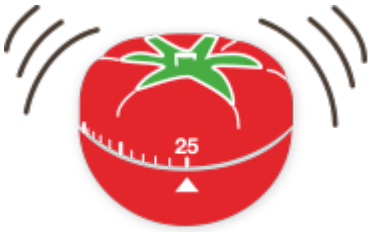
(iv) several "short" intense study sessions spread out over an extended period (many days or weeks) is more effective than one "long" study session (I recommend turning off electronic devices and other distractions), and

(v) trying (really hard) to solve a problem prior to being taught the solution leads to much better learning (again, this is very active learning and what you will be expected to do once you are on the job in industry).

Portions of "Make it Stick" are available for free on http://books.google.com/.

You may also wish to check out the free Coursera online course entitled "Learning How to Learn": https://www.coursera.org/learn/learning-how-to-learn. In this course the so-called "Pomodoro Technique" is described and this may be helpful to you.

Here is how the pomodoro technique works:



1. Choose the task you will work on from your priority list.
2. Set your timer (the pomodoro – tomato in Italian) for 25 minutes. Turn off your cell phone (and eliminate other distractions).
3. Immerse yourself in the task for 25 minutes. If you think of something you need/want to do in the future make a quick note of it so that you can remember to address this at the end of 25 minutes.
4. When the pomodoro buzzes feel free to take a break (or continue with work if that feels right).
5. Start over after your break.

Required and Recommended Course Materials

Required: Class notes and video lectures and problem packets posted on D2L.
Recommended:

* Original research is cited in the books "Peak" by Anders Ericsson, "Mindset" by Carol Dweck, and "Make It Stick" by Peter Brown, Henry Roediger, and Mark McDaniel, whereas "Mastery" by Robert Greene and "The Talent Code" by Dan Coyle are popularizations of the research. Both approaches have their place and all of these books are well worth the time spent reading them and thinking about what they say.

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 a review of the most common analytical methods to solve ordinary differential equations (ODEs). You will learn to integrate an ODE numerically by writing scripts and functions in Matlab. We will discuss how to model a chemical process and solve the resulting ODE in one-dimension or time using common engineering analytical methods (separation of variables, Laplace transforms, and series solutions i.e. Bessel functions) and numerical methods using the solvers in Matlab. We will model processes in more than one variable and solve the partial differential equation (PDE) both analytically and numerically.

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. Review of ordinary differential equations.
   Integrating factor; characteristic equation; undetermined coefficients; variation of parameters.

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.

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. It is important to your learning that you attend all lectures. I will do my best to make the lectures worth attending. 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, 2017, or 2018 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

There are no homework assignments in this course! Well sort of. We will spend class time formulating and doing problems and you are expected to continue this process outside of class. The problems in the problem packets were chosen to guide your thinking and develop your skills. I suggest that you do the problems more or less in numerical order. Generally the problems at the end of the packet are from old exams.

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.

Quizzes. In order to assess how your skills are developing and to encourage you to consistently devote time to the material, there will be a quiz almost every class meeting. The quizzes are closed book and notes and most are conceptual so will not require a calculator or computer. Some of the quizzes will require a calculator so please bring one to every class. In order to be fair to your peers, please stop working when we ask you to stop. I will enforce this policy so that everyone is treated fairly. You will receive (full) credit on the quiz if your answer is close to perfect. If there is a major error then you will receive a zero on that quiz. This all or nothing grading on quizzes is to encourage you to be careful and thoughtful. There will be around 25

quizzes during the semester. No makeup quizzes will be given.

Midterm Exams. The midterms exams will be held on Weekday, Month XX, 20XX; Weekday, Month XX, 2018; and Weekday, Month XX, 20XX. Exams cannot be made up. If a midterm exam is missed due to illness or family emergency or a trip, then the final exam score will be substituted for the missed exam. This can only be done once. A score of zero will be given on the second and third missed exams.

Final Examination

The date and time of the final exam is Weekday, Month XX, 201X, Time. 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

Quizzes	15%
Midterm exam 1	18.33% (55%/3)
Midterm exam 2	18.33%
Midterm exam 3	18.33%
Final exam	30%
Total	100%

Final grades are based on the following percentages: A > 90%, B > 80%, C > 70%, D > 60%.

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

Dispute of Grade Policy: If you have questions how a problem was graded on your exam, please write a note describing the issue, attach the note to your exam, and give the exam and note to me. Resubmissions must be done by the next class period after an exam is returned, otherwise I will not regrade your exam.

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 me 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.

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.