Chemical Kinetics and Reactor Design

ECH 4504

Class Periods: T,R | Period 8 - 9 (3:00 PM - 4:55 PM)

Location: LAR 0330

Academic Term: Spring 2021

Instructor:
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Office Hours: M, W: 5-6 PM

TA: Alexander Jess
Email:
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Course Description

Homogeneous and heterogeneous reaction kinetic modeling and data analysis. Analysis and design of ideal batch, mixed, plug and recycle reactors. Heterogeneous catalysis and reactor design.

Course Pre-Requisites / Co-Requisites

ECH 3264 and ECH 4123

Course Objectives

Chemical Kinetics and Reactor Design is a unique course in the chemical engineering curriculum that distinguishes this field from other engineering disciplines. In this regard, this course can be viewed as a culmination of your undergraduate education in chemistry, material and energy balances, transport phenomena, numerical methods, and thermodynamics. Upon completion of this course, a student should be able to:

1. Express reaction rate dependence on temperature and species concentration
2. Formulate rate equations based on a sequence of elementary reactions
3. Evaluate rate equations based on experimental data
4. Apply material balances to size and analyze reactors
5. Apply energy balances to size and analyze reactors
6. Evaluate catalyst performance and recognize transport effects in heterogeneous catalysis

Professional Component (ABET):

State the contribution of the course to meeting the professional components of the ABET-accredited degree.

Relation to Program Outcomes (ABET):

The table below is an example. Please consult with your department's ABET coordinator when filling this out.

Outcome	**Coverage***
1. An ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics	High
2. An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors	Medium
3. An ability to communicate effectively with a range of audiences	
4. An ability to recognize ethical and professional responsibilities in engineering situations and make	

informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts	
5. An ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives	Low
6. An ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions	Low
7. An ability to acquire and apply new knowledge as needed, using appropriate learning strategies	Medium

*Coverage is given as high, medium, or low. An empty box indicates that this outcome is not covered or assessed in the course.

Required Textbook

- Chemical Reactions and Chemical Reactors (At least one book on reserve in UF MARSTON LIBRARY)
- George W. Roberts
- 2009
- ISBN-13 978-0471742203

Required software

- Python, Solver add-in in Excel

Course notes are developed by the instructor and not from published sources

Additional recommended materials

- Essentials of Chemical Reaction Engineering (2016). Scott Fogler
- Learn ChemE , Educational Resources from ChemE from University of Colorado Boulder (http://www.learncheme.com/screencasts/kinetics-reactor-design).
- http://www.umich.edu/~elements/5e/

A few illustrative examples and quiz questions may be taken from this resource.

Tentative Course Schedule

Date	Topic	Reading	HW due	Quiz
12-Jan	Introduction, reactions and stoichiometric relations	Ch. 1.1-1.3		
14-Jan	Components of the rate law – generalizations	Ch. 1.4, 2		
19-Jan	Ideal reactors	Ch. 3		#1
21-Jan	Ideal reactors	Ch. 3	#1	
26-Jan	Design equations and reactor sizing – Homogeneous reactions in batch reactors	Ch. 3-4/Notes		
28-Jan	Design equations and reactor sizing – Flow systems (CSTR, PFR, PBR)			#2
2-Feb			#2	
4-Feb	Reactor sizing – Pressure drop in PBR, recycle reactors			
9-Feb	Reactor sizing –Recycle reactors, multiple reactors	Ch. 4		#3

11-Feb	Exam review and catchup		#3	
16-Feb	**Exam I**			
18-Feb	Reaction rate fundamentals – Elementary reactions and the Steady-State Approximation (SSA)	Ch. 5.1-5.3		
23-Feb	Reaction rate fundamentals – Closed Sequences and the Rate-Limiting Step (RLS)	Ch. 5-4, 5-6		#4
25-Feb	**Recharge Day (No Class)**			
2-Mar	Enzyme kinetics – Michaelis-Menten (types of inhibition) Bioreactors	Notes	#4	
4-Mar	Bioreactors – Analysis and correlation of kinetic data	Ch. 6/Notes		
9-Mar	Analysis and correlation of kinetic data	Ch. 6		
11-Mar	Reactor design and analysis for multiple reactions - Conversion, selectivity and yield	Ch. 7		#5
16-Mar	Conversion, selectivity and yield	Ch. 7/Notes	#5	
18-Mar	**Exam II**			
23-Mar	Macroscopic energy balances (heat effects) Isothermal and adiabatic reactors	Ch. 8		
25-Mar	Macroscopic energy balances (heat effects) Isothermal and adiabatic reactors	Ch 8		
30-Mar	Multiple steady states, blowout and hysteresis (CSTR)	Ch. 8		#6
1-Apr	Flow reactors with heat exchange	Notes	#6	
6-Apr	Reversible reactions with heat effects – Review for Exam III	Notes		
8-Apr	**Exam III**			
13-Apr	Heterogeneous catalysis – Internal transport	Ch. 9		
15-Apr	Heterogeneous catalysis – Internal and external transport	Ch. 9		#7
21-Apr	**No class/unless needed for catching up and review for final**		#7	
28-Apr	**Final Exam (not cumulative)**			

Attendance Policy, Class Expectations, and Make-Up Policy

This course is fully online. Attendance is not required and is not monitored. Lectures will be recorded and will be made available shortly after class.

This statement is required: Excused absences must be consistent with university policies in the Graduate Catalog (http://gradcatalog.ufl.edu/content.php?catoid=10&navoid=2020#attendance) and require appropriate documentation. Additional information can be found here:
https://catalog.ufl.edu/ugrad/current/regulations/info/attendance.aspx

Quizzes

The quizzes will cover lecture material from the previous few class periods and will require 10-15 minutes to complete. Quiizzes will be administered via honorlock through Canvas. Students are expected to abide by honorlock code of conduct. Quiz solutions will be posted on Canvas. Quizzes are closed book, closed notes. Use of

cell phones is not allowed. If a student has a conflict and cannot take the quiz during class, a previous arrangement can be made to take quizzes at an agreed upon time.

Homework grading policy
Homework will be used to give you a maximum of 5 extra points. Homework problems will be graded on a 0-2 scale (0 = no effort, 1 = little effort, 2 = significant effort). No credit will be given without work being shown. The lowest homework score/missing HWs will be dropped. HW due dates are on the schedule and should be turned in on Canvas before 11:59 PM. Late HW is docked 50% if it is a day late. HW *will not* be accepted beyond 24 hours after the due date (so 11:59 PM the following day). Students are encouraged to help each other on HW, but copying someone else's solution or allowing someone else to copy yours is cheating and a violation of academic honesty policy. Rule of thumb: Discuss the HW, but don't look at anyone else's work or show them your work. Homework solutions will be posted on canvas two days after the due date.

Exams
Exams (except for the final) will be fully in-class exams or will be a combination of take-home and in-class (honorlock).

Evaluation of Grades
Table 1. Grade evaluation if homework is counted towards final grade

Assignment	Percentage of Final Grade
Homework	0-5%
Quizzes	20%
Exam with the lowest grade	10%
Three remaining exams (including the final)	70%/3

Grading Policy
The final grade will be determined by scaling every score to the highest score, and then choosing cutoffs for grades A, A- and so on.

More information on UF grading policy may be found at:
https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

Students Requiring Accommodations
Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, https://www.dso.ufl.edu/drc) by providing appropriate documentation. Once registered, students will receive an accommodation letter which must be presented to the instructor when requesting accommodation. Students with disabilities should follow this procedure as early as possible in the semester.

Course Evaluation
Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at https://gatorevals.aa.ufl.edu/students/. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via https://ufl.bluera.com/ufl/. Summaries of course evaluation results are available to students at https://gatorevals.aa.ufl.edu/public-results/.

University Honesty Policy
UF students are bound by The Honor Pledge which states, "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code. On all work submitted for credit by students at the University of Florida, the following pledge is either required or

implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment." The Honor Code (https://sccr.dso.ufl.edu/policies/student-honor-code-student-conduct-code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class.

Commitment to a Safe and Inclusive Learning Environment

The Herbert Wertheim College of Engineering values broad diversity within our community and is committed to individual and group empowerment, inclusion, and the elimination of discrimination. It is expected that every person in this class will treat one another with dignity and respect regardless of gender, sexuality, disability, age, socioeconomic status, ethnicity, race, and culture.

If you feel like your performance in class is being impacted by discrimination or harassment of any kind, please contact your instructor or any of the following:

- Your academic advisor or Graduate Program Coordinator
- Robin Bielling, Director of Human Resources, 352-392-0903, rbielling@eng.ufl.edu
- Curtis Taylor, Associate Dean of Student Affairs, 352-392-2177, taylor@eng.ufl.edu
- Toshikazu Nishida, Associate Dean of Academic Affairs, 352-392-0943, nishida@eng.ufl.edu

Software Use

All faculty, staff, and students of the University are required and expected to obey the laws and legal agreements governing software use. Failure to do so can lead to monetary damages and/or criminal penalties for the individual violator. Because such violations are also against University policies and rules, disciplinary action will be taken as appropriate. We, the members of the University of Florida community, pledge to uphold ourselves and our peers to the highest standards of honesty and integrity.

Student Privacy

There are federal laws protecting your privacy with regards to grades earned in courses and on individual assignments. For more information, please see: https://registrar.ufl.edu/ferpa.html

Campus Resources:

Health and Wellness

U Matter, We Care:

Your well-being is important to the University of Florida. The U Matter, We Care initiative is committed to creating a culture of care on our campus by encouraging members of our community to look out for one another and to reach out for help if a member of our community is in need. If you or a friend is in distress, please contact umatter@ufl.edu so that the U Matter, We Care Team can reach out to the student in distress. A nighttime and weekend crisis counselor is available by phone at 352-392-1575. The U Matter, We Care Team can help connect students to the many other helping resources available including, but not limited to, Victim Advocates, Housing staff, and the Counseling and Wellness Center. Please remember that asking for help is a sign of strength. In case of emergency, call 9-1-1.

Counseling and Wellness Center: http://www.counseling.ufl.edu/cwc, and 392-1575; and the University Police Department: 392-1111 or 9-1-1 for emergencies.

Sexual Discrimination, Harassment, Assault, or Violence

If you or a friend has been subjected to sexual discrimination, sexual harassment, sexual assault, or violence contact the **Office of Title IX Compliance**, located at Yon Hall Room 427, 1908 Stadium Road, (352) 273-1094, title-ix@ufl.edu

Sexual Assault Recovery Services (SARS)

Student Health Care Center, 392-1161.

University Police Department at 392-1111 (or 9-1-1 for emergencies), or http://www.police.ufl.edu/.

Academic Resources

E-learning technical suppor*t*, 352-392-4357 (select option 2) or e-mail to Learning-support@ufl.edu. https://lss.at.ufl.edu/help.shtml.

Career Resource Center, Reitz Union, 392-1601. Career assistance and counseling. https://www.crc.ufl.edu/.

Library Support, http://cms.uflib.ufl.edu/ask. Various ways to receive assistance with respect to using the libraries or finding resources.

Teaching Center, Broward Hall, 392-2010 or 392-6420. General study skills and tutoring. https://teachingcenter.ufl.edu/.

Writing Studio, 302 Tigert Hall*,* 846-1138. Help brainstorming, formatting, and writing papers. https://writing.ufl.edu/writing-studio/.

Student Complaints Campus*:* https://care.dso.ufl.edu.

On-Line Students Complaints*:* http://www.distance.ufl.edu/student-complaint-process.