

Chemical Engineering Kinetics, Reactor Design, and Optimization

ECH 6526

Class Periods: Tuesdays: 8:30 AM – 10:25 AM (T: Periods 2–3)

Thursdays: 9:35 AM – 10:25 AM (R: Period 3)

Location: Comp. Sci./Eng. (CSE) E118

Academic Term: Spring 2022

Instructor:

David Hibbitts

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352-392-0751

CHE 221

Faculty Office Hours: TBD

Supervised Teacher:

None Assigned.

Course Description (3 credits)

Fundamentals of heterogeneous reactor design including the characterization of catalytic reactions and support, the development of global rate of the intrinsic reaction affected by chemical and physical deactivation of catalyst, intraphase and interphase mass and heat transfer, and the design and optimization of various types of heterogeneous reactors.

Recommended Materials

- (No required textbook)
- *Elements of Chemical Reaction Engineering*, H.S. Fogler, 5th Ed., ISBN: 0-13-388751-0
- *Fundamentals of Chemical Reaction Engineering*, M. E. Davis and R. J. Davis, 1st Ed., McGraw-Hill, 2003. (Note: Available online for free at <http://resolver.caltech.edu/CaltechBOOK:2003.001>)
- *Chemical Reactor Analysis and Design*, G. F. Froment, K. B. Bischoff and J. D. Wylde, 3rd Ed., Wiley, 2010.
- *Kinetics of Chemical Processes*, M. Boudart, Prentice Hall, 1968.
- *Chemical Kinetics*, K.J. Laidler, Harper Collins (1987).
- *Statistical Mechanics*, D.A. McQuarrie, University Science Books. ISBN: 1891389157
- *An Introduction to Statistical Thermodynamics*, T.L. Hill, Dover (1986). ISBN: 0-486-65242-4.

Course Modality

Students do not have to attend class in-person. In addition to the in-person lectures, courses will be broadcast over zoom (and students will be able to ask questions), and lectures will be recorded and posted online. Students are expected to watch all lectures (in-person, zoom broadcast, recording).

Review Materials

Students are expected to have taken an undergraduate level kinetics and reactor design course (ECH 4504 or equivalent). To assist students that may need to review these concepts, course notes and lecture videos for ECH 4504 will be provided via Canvas.

Course Topics

The course will mainly be divided into 5 units, the table below shows which lectures and which chapters of the recommended textbooks each unit will cover. Some of these units (in part or in whole) review material covered in undergraduate chemical engineering kinetics and reactor design courses (ECH 4504 or equiv.).

Unit	Lectures	Fogler	Davis & Davis
I. Basic chemical reactor design (mole balances)	1–2	Ch. 1, 2, 3	Ch. 1, 3
II. Chemical kinetics and mechanisms (homogeneous and heterogeneous)	3–12	Ch. 6, 7, 10	Ch. 2, 4, 5, 7
III. Coupled reaction and transport phenomena in catalyst particles	13–17	Ch. 5, 11, 12	Ch. 6
IV. Advanced chemical reactor design (energy balances, multiple phases)	18–26	Ch. 4, 8, 9	Ch. 9, 10
V. Non-ideal flow models and residence time distributions	27–28	Ch. 13, 14	Ch. 8

Class Policies

Please refrain from the use of cell phones and laptops during in-person class.

Grading Policy

Homework problems will not be collected or graded.

Evaluation of Grades

Assignment	Percentage of Final Grade
Exam w/ Best Grade	55%
Other Exam	45%

The first exam is tentatively scheduled for the first week of March (before spring break). It will be an evening exam (period E2-E3, 8:20 PM – 10:10 PM) on March 2nd, 3rd, or 4th.

The final exam will be 4/25/2022 3:00 PM – 5:00 PM.

Course Schedule

Week	Date	Class/Video	HW	Unit	Topic
1	01/06	01		I	Introduction
2	01/11	02–03			Reaction rates, mole balances
	01/13	04			design equations, energy diagrams
3	01/18	05–06	1	II	Kinetics of complex reactions, pseudo-steady-state hypothesis, regular perturbation theory.
	01/20	07			Mechanism of homogeneous reactions, unimolecular decomposition and thermal cracking reactions.
4	01/25	08–09	2		Complex kinetics, continuous and discrete lumping models.
	01/27	10			Sensitivity analysis and mechanism of complex reaction pathways.
5	02/01	11–12	3		Collision theory and transition state theory.
	02/03	13			Estimations of activation and reaction energies, quantum chemistry and density functional theory.
6	02/08	13–14	4		Adsorption-desorption processes, adsorption on non-uniform surfaces, catalytic reactions on uniform surfaces.
	02/10	15			quasi-equilibrated and kinetically relevant steps in catalytic reaction sequences, non-equilibrium kinetics.
7	02/15	16–17	5		Kinetics of surface-catalyzed reactions: CO oxidation, NH ₃ synthesis, CH ₄ activation. Experimental methods for confirming mechanistic hypotheses.
	02/17	18			Adsorption and chemical reactions on non-uniform surfaces.
8	02/22	19–20	6	III	External mass and heat transfer restrictions in catalytic systems.
	02/24	21			Structural models of porous solids and effective transport coefficients within pore networks, intraparticle transfer.
9	03/01	22–23			Intraparticle mass and heat transport effects in porous catalysts.
	03/03	24	7		Generalized Thiele modulus and effectiveness factors.
	03/02– 03/04				Midterm Exam: Evening of Wed., Thurs., or Friday of this week.
10	03/08	No Class			Spring Break
	03/10	No Class			Spring Break
11	03/15	24–25		IV	Design of Chemical Reactors: material, momentum, and energy balances.
	03/17	26			Stirred tank reactors, bifurcation theory, multiple steady states, local stability analysis.
12	03/22	27–28	8		Plug-flow reactors, recycle reactors, tubular reactors with permeable walls (membrane reactors).
	03/24	29			Packed-bed reactors, hot spots and thermal runaway.
13	03/29	30–31	9		One-dimensional pseudo-homogeneous reactor models with axial dispersion.
	03/31	32			Two-dimensional pseudo-homogeneous reactor models, asymptotic reduction of 2-D to 1-D models.
14	04/05	33–34	10		Perturbation analysis of reactors with axial and radial gradients.
	04/07	35			Heterogeneous reactor models and averaging of local gradients, Multiphase reactors: fluid bed reactor models and applications.
15	04/12	36–37	11		Multiphase reactors: slurry bubble column and trickle-bed reactor models and applications.
	04/14	38		V	Hydrodynamically non-ideal chemical reactors, tracer methods and residence time distributions.
16	04/19	39–40	12		Zero-parameter (segregated flow, maximum mixedness) and one-parameter (axial dispersion, tanks-in-series) models of non-ideal reactors.
	04/25	Final Slot			(10:00 AM – 12:00 PM) May move this to 4/19 based on course progress.

Students Requiring Accommodations

Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center by visiting <https://disability.ufl.edu/students/get-started/>. It is important for students to share their accommodation letter with their instructor and discuss their access needs, 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/>.

In-Class Recording

Students are allowed to record video or audio of class lectures. However, the purposes for which these recordings may be used are strictly controlled. The only allowable purposes are (1) for personal educational use, (2) in connection with a complaint to the university, or (3) as evidence in, or in preparation for, a criminal or civil proceeding. All other purposes are prohibited. Specifically, students may not publish recorded lectures without the written consent of the instructor.

A “class lecture” is an educational presentation intended to inform or teach enrolled students about a particular subject, including any instructor-led discussions that form part of the presentation, and delivered by any instructor hired or appointed by the University, or by a guest instructor, as part of a University of Florida course. A class lecture does not include lab sessions, student presentations, clinical presentations such as patient history, academic exercises involving solely student participation, assessments (quizzes, tests, exams), field trips, private conversations between students in the class or between a student and the faculty or lecturer during a class session.

Publication without permission of the instructor is prohibited. To “publish” means to share, transmit, circulate, distribute, or provide access to a recording, regardless of format or medium, to another person (or persons), including but not limited to another student within the same class section. Additionally, a recording, or transcript of a recording, is considered published if it is posted on or uploaded to, in whole or in part, any media platform, including but not limited to social media, book, magazine, newspaper, leaflet, or third party note/tutoring services. A student who publishes a recording without written consent may be subject to a civil cause of action instituted by a person injured by the publication and/or discipline under UF Regulation 4.040 Student Honor Code and Student Conduct Code.

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 Conduct Code (<https://sccr.dso.ufl.edu/process/student-conduct-code/>) specifies a number of behaviors that are in violation of this code and the possible sanctions. 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
- Jennifer Nappo, Director of Human Resources, 352-392-0904, jpennacc@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: <https://counseling.ufl.edu>, 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/>.

COVID-19

- You are expected to wear approved face coverings at all times during class and within buildings even if you are vaccinated.
- If you are sick, stay home and self-quarantine. Please visit the UF Health Screen, Test & Protect website about next steps, retake the questionnaire and schedule your test for no sooner than 24 hours after your symptoms began. Please call your primary care provider if you are ill and need immediate care or the UF Student Health Care Center at 352-392-1161 (or email covid@shcc.ufl.edu) to be evaluated for testing and to receive further instructions about returning to campus.

- If you are withheld from campus by the Department of Health through Screen, Test & Protect, you are not permitted to use any on campus facilities. Students attempting to attend campus activities when withheld from campus will be referred to the Dean of Students Office.
- UF Health Screen, Test & Protect offers guidance when you are sick, have been exposed to someone who has tested positive or have tested positive yourself. Visit the [UF Health Screen, Test & Protect website](#) for more information.
- Please continue to follow healthy habits, including best practices like frequent hand washing. Following these practices is our responsibility as Gators.

Academic Resources

E-learning technical support, 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://career.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://sccr.dso.ufl.edu/policies/student-honor-code-student-conduct-code/>;
<https://care.dso.ufl.edu>.

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