

Chemical Engineering Kinetics

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: New Engineering Building (NEB) 201

Academic Term: Spring 2020

Instructor:

David Hibbitts

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352-392-0751

CHE 221

Faculty Office Hours: Mondays and Thursdays: 10:30 AM – 12:00 PM

Recitation: Narrated homework solutions to be uploaded by S.T. (who is a remote student).

Supervised Teacher:

Nicholas Schwartz, nrschwartz@ufl.edu

TA Office Hours:

See recitation. Nicholas will also be free to answer questions via email / skype / Canvas.

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 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

Irregular Faculty Office Hours

Office hours will not be held on:

Thursday, 1/9
Thursday, 4/9

and otherwise by announcement on Canvas.

Class Policies

Please refrain from the use of cell phones and laptops during 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 midterm is tentatively scheduled for the last week of February (before spring break). It will be in the evening on Thursday or Friday, the 27th or 28th.

The final exam slot is 3:00 PM – 5:00 PM, Thursday, April 30th 2020, but we will try to have the final exam, instead, be during class time on the last day of class: April 21st 2020.

Course Schedule

Week	Date	Class/Video	HW	Unit	Topic
1	01/07 01/09	01–02 03		I	Introduction, Reaction Rates, Mole Balances Design Equations, Energy Diagrams
2	01/14 01/16	04–05 06	1	II	Kinetics of Complex Reactions, Pseudo-steady-state hypothesis, Regular Perturbation Theory Mechanism of homogeneous reactions, Unimolecular decomposition and thermal cracking reactions.
3	01/21 01/23	07–08 09	2		Complex kinetics, continuous and discrete lumping models. Sensitivity analysis and mechanism of complex reaction pathways.
4	01/28 01/30	10–11 12	3		Collision theory and transition state theory Estimations of activation and reaction energies, quantum chemistry and density functional theory
5	02/04 02/06	13–14 15	4		Adsorption-Desorption processes, Adsorption on non-uniform surfaces, Catalytic reactions on uniform surfaces Quasi-equilibrated and Kinetically relevant steps in catalytic reaction sequences, Non-equilibrium kinetics
6	02/11 02/13	16–17 18	5		Kinetics of surface-catalyzed reactions: CO oxidation, NH ₃ synthesis, CH ₄ activation. Experimental methods for confirming mechanistic hypotheses. Adsorption and chemical reactions on non-uniform surfaces
7	02/18 02/20	19–20 21	6	III	External mass and heat transfer restrictions in catalytic systems Structural models of porous solids and effective transport coefficients within pore networks, intraparticle transfer.
8	02/25 02/27 02/27– 02/28	22–23 24	7		Intraparticle mass and heat transport effects in porous catalysts Generalized Thiele modulus and effectiveness factors Midterm Exam: Thursday or Friday Evening, Exact time TBD
9	03/03 03/05	No Class No Class			Spring Break Spring Break
10	03/10 03/12	24–25 26		IV	Design of Chemical Reactors: material, momentum, and energy balances. Stirred tank reactors, bifurcation theory, multiple steady states, local stability analysis.
11	03/17 03/19	27–28 29	8		Plug-flow reactors, recycle reactors, tubular reactors with permeable walls (membrane reactors) Packed-bed reactors, hot spots and thermal runaway
12	03/24 03/26	30–31 32	9		One-dimensional pseudo-homogeneous reactor models with axial dispersion Two-dimensional pseudo-homogeneous reactor models, asymptotic reduction of 2-D to 1-D models
13	03/31 04/02	33–34 35	10		Perturbation analysis of reactors with axial and radial gradients Heterogeneous reactor models and averaging of local gradients, Multiphase reactors: fluid bed reactor models and applications
14	04/07 04/09	36–37 38	11	V	Multiphase reactors: slurry bubble column and trickle-bed reactor models and applications Hydrodynamically non-ideal chemical reactors, tracer methods and residence time distributions (video lecture only)
15	04/14 04/16	39–40 41	12		Zero-parameter (segregated flow, maximum mixedness) and one-parameter (axial dispersion, tanks-in-series) models of non-ideal reactors Course summary (and padding)
16	04/21 04/30	42–43 Final Slot			Final Exam (During Class Time) (3:00 PM - 5:00 PM) Unused if we don't fall behind.

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 feedback on the quality of instruction in this course by completing online evaluations at <https://evaluations.ufl.edu/evals>. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at <https://evaluations.ufl.edu/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://www.dso.ufl.edu/sccr/process/student-conduct-honor-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.

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:

<http://registrar.ufl.edu/catalog0910/policies/regulationferpa.html>

Campus Resources:

Health and Wellness

U Matter, We Care:

If you or a friend is in distress, please contact umatter@ufl.edu or 352 392-1575 so that a team member can reach out to the student.

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 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 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://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://www.dso.ufl.edu/documents/UF_Complaints_policy.pdf.

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