New Jersey Institute of Technology

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Spring 2024

CHE 349-002: Kinetics and Reactor Design

Xianqin Wang

Recommended Citation

Important University Dates (Add/Drop/Refund/Last Day to withdraw/Recess/Finals):

Spring 2024 Academic Calendar			
January	15	Monday	Martin Luther King, Jr. Day
January	16	Tuesday	First Day of Classes
January	20	Saturday	Saturday Classes Begin
January	22	Monday	Last Day to Add/Drop a Class
January	22	Monday	Last Day for 100% Refund, Full or Partial Withdrawal
January	23	Tuesday	W Grades Posted for Course Withdrawals
January	29	Monday	Last Day for 90% Refund, Full or Partial Withdrawal, No Refund for Partial Withdrawal after this
February	12	Monday	Last Day for 50% Refund, Full Withdrawal
March	4	Monday	Last Day for 25% Refund, Full Withdrawal
March	10	Sunday	Spring Recess Begins - No Classes Scheduled - University Open
March	16	Saturday	Spring Recess Ends
March	29	Friday	Good Friday - No Classes Scheduled - University Closed
March	31	Sunday	Easter Sunday - No Classes Scheduled - University Closed
April	1	Monday	Last Day to Withdraw
April	30	Tuesday	Friday Classes Meet
April	30	Tuesday	Last Day of Classes
May	1	Wednesday	Reading Day 1
May	2	Thursday	Reading Day 2
May	3	Friday	Final Exams Begin
May	9	Thursday	Final Exams End
May	11	Saturday	Final Grades Due
May	-	TBA	Commencement

http://www.njit.edu/registrar/calendars/
http://www.njit.edu/registrar/exams/finalexams.php

Type	Time	Days	Where	Date Range	Schedule Type	Instructors
Class	10:00AM-11:20AM	TR	FMH 308	1/16-5/1	Lecture	Xianqin Wang

Remember that you're responsible for in-class topics.

2. **Credits and contact hours**
   (3-0-3) (Lecture hr/wk-lab hr/wk-course credits)

3. **Course coordinator/instructor**

   Dr. **Xianqin Wang**
   xianqin@njit.edu (e-mail)

   Office Hours (Tiernan 360)
   Tuesday and Thursday: 12:00PM-1:00PM

 (note: you can always make appointment with me by email if the office hour time conflicts with your classes)

   Teaching Assistant: Prova Mehedi Joy
            email: **pj56@njit.edu**
   TA Office Hours:
   TA is in charge of grading and posting grades to the class canvas website. TA will also have office hours to help students with their HW assignments.

4. **Specific course information**

General: Derive and solve species and energy balances for single chemical reactors processing liquid and gaseous systems; chemical reactor process safety; multiple reaction applications; catalysis, including mechanisms, rates, reactor design.

Prerequisites: Chem 236 (Physical Chemistry), ChE 342 (Thermodynamics), ChE 370 (Heat & Mass Transfer), Math 222 (Differential Equations)

Textbook   Essentials of Chemical Reaction Engineering, H. S. Fogler, 2nd ed. -- Prentice Hall (2018). The book also contains many links to useful resources. NOTE: Such texts are heavy and often expensive. Feel free to share a copy between a few of you.

Web-Based Textbook Resource: http://www.umich.edu/~essen/

Assigned Readings: The semester schedule (separate posting) lists recommended readings in the Fogler text. Ultimately, for quizzes and exams, you are responsible for the material *covered in class.*

Recommended Link: You should check out this link: www.essentialchemicalindustry.org
            This is a treasure of information about our profession.

Math Solver: You must have access to and know how to use one math solver software package. Examples include *Polymath, Maple, Matlab, Mathcad,* and *Mathematica.* It will be needed for the term project and some homework.

Polymath is available and will be provided by the department. Please contact Shawn Yetman (shawn.yetman@njit.edu) if you do not have the software yet.

5. Topics

Constant density (liquid) reactors – species balance
Variable density (gas) reactors – species balance
Simultaneous species and energy balances
Chemical reactor process safety
Multiple reaction systems
Catalysis – homogeneous and heterogeneous
Steady-state energy balance and reactor design

6. Specific course objectives

a. Students will be able to:

1. Write reaction rate laws for single elementary reactions and/or stated complex liquid phase reactions
2. Express concentrations in terms of conversion for liquid (constant density) systems using the given reaction stoichiometry and reactor feed
3. Calculate the requested unknown (e.g. volume, space time) using the appropriate species balance for the assigned liquid phase steady-state flow reactor (CSTR, PFR)
4. Write reaction rate laws for single elementary reactions and/or stated complex gas phase reactions
5. Express concentrations in terms of conversion for gas (variable density) systems using the given reaction stoichiometry and reactor feed
6. Simplify concentration expressions for dilute gas systems using problem-specific appropriate assumptions
7. Calculate the requested unknown (e.g. volume, space time) using the appropriate species balance for the assigned gas phase steady-state flow reactor (CSTR, PFR)
8. Derive the appropriate energy balance for the assigned steady-state flow reactor
9. Combine species, energy balances to determine unknown quantity (time, conversion, energy transfer rate, temperature) for steady-state flow reactors
10. Model (species, energy balances) the pre-upset (steady-state) condition for a CSTR with emphasis on process safety (e.g. runaway)
11. Model (species, energy balances) the upset (transient) condition for a CSTR and for a batch reactor with emphasis on process safety (e.g. runaway)
12. Derive a rate expression based on an elementary mechanism using the Pseudo Steady State Hypothesis or Langmuir–Hinshelwood algorithm for homogeneous and heterogeneous catalytic systems
13. Calculate the required unknowns (e.g. volume, time) using the appropriate species balance for assigned catalytic reactor
14. Derive species net reaction rates from multiple reaction networks
15. Design the required reactor using the energy and species balances in a multiple reaction problem

16. Complete a team-based term project by preparing the basic reactor design using energy and species balances
17. Produce a professional, team-based memo with sound presentation of results and quality graphs
18. Solve algebraic (linear, quadratic) equations and ODEs (separation of variables) analytically (by hand)
19. Solve term project multiple-equation (algebraic, ODEs) problems using computer-based numerical software
20. Identify effects of particular chemical process on political, social, legal, environmental, health, safety, loss prevention, cultural, and demographic situations
21. Communicate data, ideas, analysis, results orally considering a wider audience

b. This course explicitly addresses ABET student outcomes 1, 2, 3, 4:

1. An ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics
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
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

7. **Grading**

The final grade on a 1000-point basis as follows:

Homework (individual work)	100 pts	(10%)
Team project (team work)	100 pts	(10%)
Popup quiz (individual work)	50 pts	(5%)
1st term exam (individual)	250 pts	(25%)
2nd term exam (individual)	250 pts	(25%)
Final exam (individual)	250 pts	(25%)

Letter grades will be awarded for the following totals:

A	850 and above
B+	800-849 "
B	750-799 "
C+	700-749 "
C	650-699 "
D	550-649 "
F less than	550 "

There may be a gray area between each two letter grades in the final distribution, so that two students getting similar weighted average, at the border of grade categories, could get different letter grades. If you are in one of these gray areas, whether you get the higher or lower grade depends on whether your performance has been improving or declining over the course period and on your overall class participation (attendance/discussion etc.).

8. **Policies on assignments/exams and classroom policy**

   Class Attendance: Students must be present in class to receive any credit on the quizzes, labs, assignments or tests that occurred during it. Also, experience shows that students who do not regularly attend class typically perform poorly in the course. In addition, examples are worked out during the lectures. These examples are may not be posted online. Students are responsible for all material covered in class.

   Cell phones and other electronic devices: must be turned off during both lectures and exams, unless specifically permitted by the instructor. For example, the use of cellphone or tablet devices for scanning exams or HWs to submit to Canvas system.

   Office Hours Attendance: This time is for you to come and seek help in case: you don't understand the material, have an English problem, or are concerned about your grade. Coming to office hours shows that you care about learning and positively affects both your performance and evaluation. Do not wait until the very end of semester to do this!

   Homework: HW problems are the examples problems covered in the lectures. Homework assignments are the responsibility of the students. You are strongly advised to work on the homework problems because you will <u>NOT</u> learn this material unless you get into the materials **"Hands-on".**

   HW submission: Homework assignments will be collected. You MUST submit each HW in a PDF file through your NJIT Canvas before the due date.

   Popup quiz:
   There will be no makeup quizzes. I will give one or two extra quizzes (in case you have to miss one due to emergency), but only 5 quizzes with top scores will be counted.

   Group activities policy:
   Everyone within a Term Project group must contribute effort equally. A Peer & Self Evaluation will be done after the group projects are submitted. Each student will be asked at the end of the semester to confidentially rate his/her performance/effort as well as that of all his/her group-mates. The completed evaluation form has to be attached to an e-mail to the instructor. Evaluation forms are due on May 2nd 2024. Submission of the form after May 2nd 2024 and before the final exam will result to the late submitter getting 75% of the credit that he/she would had received if the form was submitted timely. Submission of the form at the final exam will lead to a further 25% reduction of the credit. No student will be allowed to take the final exam without prior submission of the self & peer evaluation form.

   Exam policy: All exams are **close textbook/ instructor lecture notes**. You are allowed to have two pages of cheat sheets (A-4 paper) and you can write on both sides if you wish. Graded exams will be returned in about a week after they are taken.

1) **Cheating on exams will not be tolerated.**
2) **Your two-page cheat sheets and calculator are the only things allowed**
3) **Cellphone MUST be OFF!**
4) **It is your own responsibility to make sure you submit all the pages of your exam!!!!**

   Policy on exams (other than final): A student must have a compelling reason to miss an exam. Documentation of the reason (e.g., doctor's note) is needed for the instructor to

consider giving a make-up exam. The documents should be submitted to DOS@njit.edu for their approval. The office will notify the instructor directly. Only one term exam can be missed with the approval from the office of the Dean of Students. **A single (comprehensive) make-up exam will be given on the reading day (May 1st 2024) for those who have missed an exam for documented/ legitimate reasons.**

Policy on final exam: The final exam will be based on the entire course material. Students missing the final exam without a documented serious excuse fail the course. Students missing the final exam with a documented serious reason get an Incomplete. The Incomplete will be removed after students take the final exam in the Fall 2024 (grade to count towards 30% of the composite). If the course is not offered in the Fall 2024, a special make-up final will be scheduled during the Fall 2024 finals week.

Disputing a grade on tests/assignments: If a student has questions about the grade he/she has received on an exam, homework, or group activity he/she must talk to the instructor (or the teaching assistant where appropriate) **no later than a week after the graded activity has been returned to students. No grade change will be made after the one-week period.**

Term Project: Work in groups (you form). A Peer & Self Evaluation will be done at the conclusion of the project that will impact your grade; more details later. A group project presentation is required at the end of the semester. Everyone should present part of their project. A group project report is due on April 25th 2024.

Canvas **Site:** http://canvas.njit.edu --- Please check this site and your email often (at least once a day). Practice problems will be posted, as well as HW and test solutions, group projects, some in-class work, and useful memos.

Policy on Integrity: Professional behavior is expected at all times in this course.

- On-time arrival for the start of class is expected.
- Cheating on exams will not be tolerated. If calculations are required, only calculators are permitted. All cell phones must be turned off during exams.
- All homework assignments must be *submitted before the solutions are reviewed in class*.
- Everyone within a Term Project group must contribute effort equally. A Peer & Self Evaluation will be done after the group projects are submitted.
- If you use *Polymath*, you must obey the license terms – no commercial use; for education use only.

Academic Integrity is the cornerstone of higher education and is central to the ideals of this course and the university. Cheating is strictly prohibited and devalues the degree that you are working on. As a member of the NJIT community, it is your responsibility to protect your educational investment by knowing and following the academic code of integrity policy that is found at: http://www5.njit.edu/policies/sites/policies/files/academic-integrity-code.pdf Please note that it is my professional obligation and responsibility to report any academic misconduct to the Dean of Students Office. Any student found in violation of the code by cheating, plagiarizing or using any online software inappropriately will result in disciplinary action. This may include a failing grade of F, and/or suspension or dismissal from the university. If you have any questions about the code of Academic Integrity, please contact the Dean of Students Office at dos@njit.edu.

Seating Chart: The instructor reserves the right to assign seating during the class lecture.

NJIT Honor Code: The NJIT honor code is being upheld on all issues related to the course. Students are expected to be familiar with the code and conduct themselves accordingly. Any violations will be brought to the immediate attention of the Dean of Students.

9: **Exam preparation**
1. Understand lecture materials and basic concepts
2. Do example problems covered in lectures
3. Do HW problems

University statement on academic integrity:

o **"Academic Integrity is the cornerstone of higher education and is central to the ideals of this course and the university. Cheating is strictly prohibited and devalues the degree that you are working on. As a member of the NJIT community, it is your responsibility to protect your educational investment by knowing and following the academic code of integrity policy that is found at: *http://www5.njit.edu/policies/sites/policies/files/academic-integrity-code.pdf*.**

Please note that it is my professional obligation and responsibility to report any academic misconduct to the Dean of Students Office. *Any student found in violation of the code by cheating, plagiarizing or using any online software inappropriately will result in disciplinary action. This may include a failing grade of F, and/or suspension or dismissal from the university.* If you have any questions about the code of Academic Integrity, please contact the Dean of Students Office at *dos@njit.edu*"

Policies and Expectations about Exams/Grades

• The course letter grade will be assigned and rounded automatically by Excel (no emotions attached). The assigned letter grade is FINAL without subject to negotiation!
• Any excuses used to drop missed assignments or exams must first be documented with the Dean of Students.
• Students have to plan, study and do well in exams/assignments if they want to get a good grade in this class. Instructor will NOT change letter grades to accommodate any special circumstances (unless excused by the Dean of Students). The student will get the letter grade he/she deserves.
• Students can dispute the assignment and exam scores within a week following the announcement of the score. Students cannot dispute their prior exams or assignments after one week or at the end of the semester! Furthermore, upon requesting grade review the student accepts the possibility of instructor both removing points, as well as giving points, in case grading mistakes are found.
• Student handwriting must be legible in order to receive points.
• The graded exams must be returned within a week to be saved for the department course assessment initiative.
• Students will get 0 for not showing up to exams, or any other course activity.
If a student misses an exam due to extreme circumstances (such as a medical problem or a death in the family), he/she needs to notify the instructor via email before the beginning of the exam, and provide proof of the circumstance to the Dean of Student's office. Only in this case of official approval from the Dean of Student's office, may a make-up be given. When a student invokes extenuating circumstances for any reason (late withdrawal from a course, request for a make-up exam, request for an Incomplete grade) the student will be sent to the Dean of Students Office. The Dean of Students will be making the determination of whether extenuating circumstances exist or not and will be notifying the instructor accordingly. Instructors will never request or

accept medical or other documents from students; such documents need to be submitted by the student to the Dean of Students. Except for cases determined by law, an instructor is not required to accommodate student requests even when extenuating circumstances are certified by the Dean of Students; however, all efforts should be made to ensure a student-friendly environment.
• Extra credit may be assigned during the semester, at the discretion of the instructor. There will be no make-ups, extra credit, or any additional projects/assignments given beyond the semester's completion.
• Students may NOT seek help from someone outside of the class on any of the in class exercises, homework assignments, tests or projects.
• Students may NOT use course materials from the previous semesters, unless such materials have been explicitly shared with them by the instructor.
• Students may NOT post course materials to external resources, such as Chegg.com and others.
• Students may NOT share course materials with other students or persons, even after course completion. Doing so may result in penalties to the grade that has already been earned.
• If multiple students turn in identical (or very similar) projects, this is considered to be a violation and the case will be turned over to the Dean of Students for further examination.
• If you need accommodations due to a disability please contact the Associate Director of Disability Support Services, Fenster Hall Room 260 to discuss your specific needs. A Letter of Accommodation Eligibility from the Disability Support Services office authorizing your accommodations will be required.
• NJIT policy requires that all the exams must be proctored, regardless of delivery mode, in order to increase academic integrity. Note that this does not apply to essay or authentic based assessments.
• Class Recordings: Class sessions may be recorded by the instructor. These recordings shall only be used as an educational resource and are not to be distributed or used outside of this class. Information on how to access recorded lectures will be made available by your instructor. Any recordings that contain identifiable information about students will not be used beyond this semester.
Class Recording Etiquette: Students are expected to respect their fellow students' privacy and freedom to learn without disruption. Students are not allowed to capture or reproduce anyone's name, image, or voice without permission. They must be polite and respectful in the online chat. Informal chat is okay, but typing is restricted to things that one would say out loud in front of the entire class. Students must always conduct themselves on their webcam video as they would in person in a classroom.

10: Tentative Schedule

			Tentative Topics and schedule
week1	1/16/2024	Tuesday	Chapter 1, Introduction, POLYMATH, Mole balances
	1/18/2024	Thursday	Chapter 1, Introduction, POLYMATH, Mole balances
week2	1/23/2024	Tuesday	Chapter 2, Conversion Reactor sizing
	1/25/2024	Thursday	Chapter 2, Conversion Reactor sizing
week3	1/30/2024	Tuesday	Chapter 3, Rate Laws (mostly homogenous reaction)
	2/1/2024	Thursday	Chapter 3, Rate Laws (mostly homogenous reaction)
week4	2/6/2024	Tuesday	Chapter 10: Catalysis and rate (heterogenous reaction)
	2/8/2024	Thursday	Chapter 10: Catalysis and rate (heterogenous reaction)
week5	2/13/2024	Tuesday	Chapter 10: Catalysis and rate (heterogenous reaction)
	2/15/2024	Thursday	Chapter 10: Catalysis and rate (heterogenous reaction)
week6	2/20/2024	Tuesday	Chapter 7: Collection and analysis of rate data
	2/22/2024	Thursday	Chapter 4, Stoichiometry Flow Systems
week7	2/27/2024	Tuesday	Chapter 4, Stoichiometry Flow Systems
	2/29/2024	Thursday	Chapter 4, Stoichiometry Flow Systems
week8	3/5/2024	Tuesday	**1st term exam**
	3/7/2024	Thursday	Chapter 5, Isothermal reactor design: Conversion
week9	3/12/2024	Tuesday	Spring break
	3/14/2024	Thursday	Spring break
week10	3/19/2024	Tuesday	Chapter 5, Isothermal reactor design: Conversion
	3/21/2024	Thursday	Chapter 5, Isothermal reactor design: Conversion
week11	3/26/2024	Tuesday	Chapter 6, Isothermal reactor design: Moles and molar flowrate
	3/28/2024	Thursday	Chapter 6, Isothermal reactor design: Moles and molar flowrate
week12	4/2/2024	Tuesday	Chapter 6, Isothermal reactor design: Moles and molar flowrate
	4/4/2024	Thursday	Chapter 8, Multiple Reactions
week13	4/9/2024	Tuesday	Chapter 8, Multiple Reactions
	4/11/2024	Thursday	Chapter 8, Multiple Reactions
week14	4/16/2024	Tuesday	Chapter 10: Catalysis and catalytic reactors
	4/18/2024	Thursday	Chapter 10: Catalysis and catalytic reactors
week15	4/23/2024	Tuesday	**2nd term exam**
	4/25/2024	Thursday	**Review lecture (can be rescheduled to 1st reading day)**
week16	5/1/2024	Wednesday	Reading day makeup exam day
	TBD		**Final exam**

HW problems and due date will be announced during the lectures and posted in the assignment in Canvas