

Fall 2024

## CHE 612-101: Kinetics of Reactions and Reactor Design

Xianqin Wang

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

<b>Sept</b>	<b>2</b>	<b>Labor Day. University Closed</b>
<b>Sept</b>	<b>3</b>	<b>First Day of Classes</b>
<b>Sept</b>	<b>9</b>	<b>Last Day to Add/Drop a Class</b>
<b>Sept</b>	<b>9</b>	<b>Last Day for 100% Refund, Full or Partial Withdrawal</b>
<b>Sept</b>	<b>10</b>	<b>W Grades Posted for Course Withdrawals</b>
<b>Sept</b>	<b>16</b>	<b>Last Day for 90% Refund, Full or Partial Withdrawal - No Refund for Partial Withdrawal after this date</b>
<b>Sept</b>	<b>30</b>	<b>Last Day for 50% Refund, Full Withdrawal</b>
<b>Oct</b>	<b>21</b>	<b>Last Day for 25% Refund, Full Withdrawal</b>
<b>Nov</b>	<b>11</b>	<b>Last Day to Withdraw from Classes</b>
<b>Nov</b>	<b>26</b>	<b>Thursday Classes Meet</b>
<b>Nov</b>	<b>27</b>	<b>Friday Classes Meet</b>
<b>Nov</b>	<b>28</b>	<b>Thanksgiving Recess Begins. No Classes</b>
<b>Dec</b>	<b>1</b>	<b>Thanksgiving Recess Ends</b>
<b>Dec</b>	<b>11</b>	<b>Last Day of Classes</b>
<b>Dec</b>	<b>12</b>	<b>Reading Day 1</b>
<b>Dec</b>	<b>13</b>	<b>Reading Day 2</b>
<b>Dec</b>	<b>14</b>	<b>Saturday Classes Meet</b>
<b>Dec</b>	<b>15</b>	<b>Final Exams Begin</b>
<b>Dec</b>	<b>21</b>	<b>Final Exams End</b>
<b>Dec</b>	<b>23</b>	<b>Final Grades Due</b>

<http://www.njit.edu/registrar/calendars/>

<http://www.njit.edu/registrar/exams/finalexams.php>

## 1. ChE 612 Kinetics of Reactions and Reactor Design, Fall 2024

Type	Time	Days	Where	Date Range	Schedule Type	Instructors
Class	6:00-8:50pm	W	Tier106	9/4-12/15	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](mailto:xianqin@njit.edu) (e-mail)

**Office Hours** (Tiernan 360)

**Wed: 4:00PM-5:00PM**

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

TA: TBD

TA Office hour: TBD

### 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, steady state isothermal and nonisothermal reaction design, unsteady state isothermal and nonisothermal reactor design, study of various models for catalytic reaction with/without mass transfer limitations.

Prerequisites: Prerequisites: Undergraduate course in chemical engineering kinetics or equivalent. Elements of optimum design for various reactor types, multiple reactions, and temperature effects. Yield and selectivity optimization with emphasis on small-scale pharmaceutical production. Introduction to non-ideal reactor design. Study of various models for catalytic and non-catalytic solid-fluid reactions.

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](http://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](mailto:shawn.yetman@njit.edu)) if you do not have the software yet.

#### 4. 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  
Nonsteady-state energy balance and reactor design

#### 5. 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. Design the required reactor using the energy and species balances for catalytic reaction with and without mass transfer limitation
17. Design the required reactor for non-steady state reaction system
18. Complete a team-based term project by preparing the basic reactor design using energy and species balances
19. Produce a professional, team-based memo with sound presentation of results and quality graphs
20. Solve algebraic (linear, quadratic) equations and ODEs (separation of variables) analytically (by hand)
21. Solve term project multiple-equation (algebraic, ODEs) problems using computer-based numerical software
22. Identify effects of particular chemical process on political, social, legal, environmental, health, safety, loss prevention, cultural, and demographic situations
23. 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

## 6. Grading

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

Team project (team work)	200 pts	(20%)
Popup quiz (individual work)	50 pts	(5%)
1 <sup>st</sup> term exam (individual)	250 pts	(25%)
2 <sup>nd</sup> term exam (individual)	250 pts	(25%)
Final exam (individual)	250 pts	(25%)
HW assignments (individual)	0	(0)

or

Team project (team work)	300 pts	(30%)
Popup quiz (individual work)	100 pts	(10%)
1 <sup>st</sup> term exam (individual)	300 pts	(30%)
2 <sup>nd</sup> term exam (individual)	300 pts	(30%)
HW assignments (individual)	0	(0)

Doing HW problems are good practice for preparing for exams!

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.).

## 7. 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 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 NOT learn this material unless you get into the materials “**Hands-on**”.

**HW submission:** Homework assignments will NOT be collected.

**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 **Dec 12<sup>th</sup> 2024**. Submission of the form after **Dec. 12<sup>th</sup> 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](mailto: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 (Dec 12<sup>th</sup> 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 2025 (grade to count towards 30% of the composite). If the course is not offered in the Fall 2025, a special make-up final will be scheduled during the Fall 2025 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 Dec 12<sup>th</sup> 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.

**Calculator:** A high-end calculator (TI-83, TI-84 or TI-84SE) is required for solving exam problems.

**Software:** Use of Matlab, Python or other computational software is strongly recommended for working on homework assignments.

**Needs-Requirements for Remote Learning:** During school closure, access to a computer or laptop with high-speed internet connection, webcam, microphone, and audio is required. Note that if you have any issues with accessibility to Webex/Canvas and webcams, you must resolve them as soon as possible by contacting the Dean of Students and/or the chair of the Chemical and Materials Engineering department. Inaction on your part is not an acceptable excuse for any issues you may face during the online lectures, quizzes, and exams



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

- Attendance is strongly recommended. The examples discussed in the class are not necessarily from the main textbook and therefore missing a class will have consequences for preparation for quizzes and exams.
- Cheating on exams will not be tolerated. If calculations are required, only calculators are permitted. All cell phones must be turned off during exams.
- 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.
- The classes start at 6:00 PM, and the students must be in class by that time. Being late to class may have consequences for the grade, since many of the classes will start from quizzes.

**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.

#### **CRITICAL NOTES TO STUDENTS FOR EXAMS**

1. **SHOW ALL WORK, do not skip anything!!!** Write down all fundamental equations, numerical values/units of all variables and parameters. Show all intermediate calculations by plugging numbers into the equations. Show results of intermediate calculations. You will lose a lot of points if your equations are missing. **You will get minimal score, mostly 0, for each step regardless whether your answer is correct or not if the calculations and numbers leading to the answer are missing.**
2. **If the values of parameters, variables, and intermediate calculations are missing or incorrect, yet your intermediate calculations and/or final answer are correct, first you will get minimal partial scores, close to 0 points per step, and additionally your paper will be flagged for misconduct investigation.**

## 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](mailto: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 for 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

### Review lectures for exams?

Week	Date	Tentative topics
1	9/4/2024	Mole Balance Ch1, Ch2
2	9/11/2024	Rate Laws, Ch3, Ch9, Ch10
3	9/18/2024	Rate Model Selection, Ch7 and Ch10
4	9/25/2024	Stoichiometry Ch4
5	10/2/2024	Isothermal reactor design (X) Ch5, Ch6
6	10/9/2024	Multiple reaction system, catalytic reaction system Ch8 Ch10
7	10/16/2024	1st term exam
8	10/23/2024	Nonisothermal Reactor Design Ch11
9	10/30/2024	Steady-State Nonisothermal Reactor Design Ch12
10	11/6/2024	Unsteady-State Nonisothermal Reactor Design Ch13
11	11/13/2024	Mass Transfer and Diffusion Ch14 Ch15
12	11/20/2024	Distribution of residence times, nonideal reactors Ch16-18
13	11/27/2024	Friday Schedule, No Class
14	12/4/2024	2nd term exam
15	12/11/2024	Team Project Presentation
16	TBD	Final exam