Fall 2021

# CHE 349-001: Kinetics and Reactor Design

Xianqin Wang

| 2021F Calendar | | | |
|---|---|---|---|
| September | 1 | Wednesday | First Day of Classes |
| September | 4 | Saturday | Saturday Classes Begin |
| September | 6 | Monday | Labor Day |
| September | 8 | Wednesday | Monday Classes Meet |
| September | 8 | Wednesday | Last Day to Add/Drop a Class |
| September | 8 | Wednesday | Last Day for 100% Refund, Full or Partial Withdrawal |
| September | 9 | Thursday | W Grades Posted for Course Withdrawals |
| September | 15 | Wednesday | No Refund for Partial Withdrawal after this date |
| September | 29 | Wednesday | Last Day for 50% Refund, Full Withdrawal |
| October | 20 | Wednesday | Last Day for 25% Refund, Full Withdrawal |
| November | 10 | Wednesday | Last Day to Withdraw from Classes |
| November | 25 | Thursday | Thanksgiving Recess Begins |
| November | 28 | Sunday | Thanksgiving Recess Ends |
| December | 10 | Friday | Last Day of Classes |
| December | 11 | Saturday | Saturday Classes Meet |
| December | 12 | Sunday | Sunday Classes Meet |
| December | 13 | Monday | Reading Day 1 |
| December | 14 | Tuesday | Reading Day 2 |
| December | 15 | Wednesday | Final Exams Begin |
| December | 21 | Tuesday | Final Exams End |
| December | 23 | Thursday | Final Grades Due |

1. **ChE 349 Kinetics and Reactor Design, Fall 2021**

| Type | Time | Days | Where | Date Range | Schedule Type | Instructors |
|---|---|---|---|---|---|---|
| Class | 1:00pm-2:20pm | TR | Kupfrian Hall 203 | Sep 01, 2021 - Dec 21, 2021 | 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: 10:00AM-12:00PM

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

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 homeworks.

*Polymath* is available and will be provided by the department.

## 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. Express concentrations in terms of conversion for both liquid and gas catalytic systems using stoichiometry and feed/charge conditions
14. Calculate the required unknowns (e.g. volume, time) using the appropriate species balance for assigned catalytic reactor

15. Derive species net reaction rates from multiple reaction networks
16. Design the required reactor using the energy and species balances in a multiple reaction problem
17. Complete a team-based term project by preparing the basic reactor design using energy and species balances
18. Produce a professional, team-based memo with sound presentation of results and quality graphs
19. Solve algebraic (linear, quadratic) equations and ODEs (separation of variables) analytically (by hand)
20. Solve term project multiple-equation (algebraic, ODEs) problems using computer-based numerical software

**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 (team work) | 100 pts | (10%) |
| Team project (team work) | 100 pts | (10%) |
| 1st term exam (individual) | 250 pts | (25%) |
| 2nd term exam (individual) | 250 pts | (25%) |
| Final exam (individual) | 300 " | (30%) |

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 " |

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

**Homework:** Homework assignments will be collected and graded. 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".** All solutions will be posted on the course *Canvas* site. All homework assignments, however, must be *submitted before the solutions are reviewed in class*.

**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 13th 2021. Submission of the form after Dec. 13th 2021 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 open **textbook/ instructor lecture** notes. Graded homework problems **cannot** be used during exams. Additional personal notes on the course (or solutions to additional problems), copies of class notes, as well as copies of the instructor's solutions to homework problems are also **not allowed** to be used during exams. Graded exams will be returned in about a week after they are taken.

1) **Cheating on exams will not be tolerated.**
2) **Your textbook, class notes and calculator are the only things allowed**
3) **Cellphone MUST be OFF except that you use your cellphone camera for your exam!**
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. A student who cannot make it to an exam needs to either e-mail or call and leave a voice message for the instructor **before** the exam is held. **A single (comprehensive) make-up exam will be given on the reading day (Dec. 13th 2021) 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 Spring 2022 (grade to count towards 30% of the composite). If the course is not offered in Spring 2022, a special make-up final will be scheduled during the Spring 2022 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 recommended, but not mandatory.

***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 away 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.

## 9: Exam preparation

1. Understand lecture materials and basic concepts
2. Do all homework problems
3. Do example problems covered in lectures

**Group Project: Details for the group project and requirements will be sent in a separate file!**

## 10: Tentative Schedule

| | | | Tentative Topics | HW assignments (Due date is announced in lectures based on progress) |
|---|---|---|---|---|
| week1 | 9/2/2021 | Thursday | Chapter 1, Introduction, POLYMATH, Mole balances | HW1: P1-5A, P1-8A |
| week2 | 9/7/2021 | Tuesday | Chapter 1, Introduction, POLYMATH, Mole balances | |
| | 9/9/2021 | Thursday | Chapter 2, Conversion Reactor sizing | HW2: P2-1A, P2-7B |
| week3 | 9/14/2021 | Tuesday | Chapter 2, Conversion Reactor sizing | |
| | 9/16/2021 | Thursday | Chapter 3, Rate Laws | HW3: P3-5A, P3-8B, P3-11B |
| week4 | 9/21/2021 | Tuesday | Chapter 3, Rate Laws | P3-13A (excluding part b) |
| | 9/23/2021 | Thursday | Chapter 4, Stoichiometry Batch Systems | HW4: P4-3A, P4-4B, P4-5A |
| week5 | 9/28/2021 | Tuesday | Chapter 4, Stoichiometry Flow Systems | |
| | 9/30/2021 | Thursday | Chapter 4, Stoichiometry Flow Systems | |
| week6 | 10/5/2021 | Tuesday | Chapter 5, Isothermal reactor design: Conversion | HW5: P5-$3_A$, P5-$4_B$, P5-$8_B$, P5-11B |
| | 10/7/2021 | Thursday | Chapter 5, Isothermal reactor design: Conversion | |
| week7 | 10/12/2021 | Tuesday | Chapter 5, Isothermal reactor design: Conversion | |
| | 10/14/2021 | Thursday | Chapter 5, Isothermal reactor design: Conversion | |
| week8 | 10/19/2021 | Tuesday | Chapter 6, Isothermal reactor design: Moles and molar flowrate | HW6: P6-$4_B$ delete part (c), P6-$5_B$ |
| | 10/21/2021 | Thursday | Chapter 6, Isothermal reactor design: Moles and molar flowrate | |
| week9 | 10/26/2021 | Tuesday | Chapter 6, Isothermal reactor design: Moles and molar flowrate | |
| | 10/28/2021 | Thursday | 1st term exam | |
| week10 | 11/2/2021 | Tuesday | Chapter 7, Collection and analysis of rate data | HW7: P7-$7_A$, P7-$8_A$. |
| | 11/4/2021 | Thursday | Chapter 8, Multiple Reactions | HW8: P8-$3_B$, P8-$6_B$, P8-$7_C$ (a), (b), (c) |
| week11 | 11/9/2021 | Tuesday | Chapter 8, Multiple Reactions | |
| | 11/10/2021 | Wednesday | Last day to withdraw | |
| | 11/11/2021 | Thursday | Chapter 10: Catalysis and catalytic reactors | HW10: P10-12B, P10-18B |
| week12 | 11/16/2021 | Tuesday | Chapter 10: Catalysis and catalytic reactors | |
| | 11/18/2021 | Thursday | Chapter 10: Catalysis and catalytic reactors | |
| week13 | 11/23/2021 | Tuesday | Chapter 10: Catalysis and catalytic reactors | |
| | 11/25/2021 | Thursday | No class, Thanksgiving | |
| week14 | 11/30/2021 | Tuesday | Chapter 11: Non-isothermal reactor design-energy balance | HW11: P11-7B |
| | 12/2/2021 | Thursday | Chapter 12: Steady-state nonisothermal reactor design | HW12: P12-9A |
| week15 | 12/7/2021 | Tuesday | 2nd term exam | |
| | 12/9/2021 | Thursday | Review lecture | |
| week16 | 12/13/2021 | Monday | Reading day 1 | |
| | 12/14/2021 | Tuesday | reading day 2 Makeup exam day | |
| | TBA | | Final exam | |