Fall 2020

CHE 349-001: Kinetics & Reactor Design

Xianqin Wong

September	1	Tuesday	First Day of Classes
September	5	Saturday	Saturday Classes Begin
September	7	Monday	Labor Day
September	8	Tuesday	Monday Classes Meet
September	8	Tuesday	Last Day to Add/Drop a Class
September	8	Tuesday	Last Day for 100% Refund, Full or Partial Withdrawal
September	9	Wednesday	W Grades Posted for Course Withdrawals
September	14	Monday	Last Day for 90% Refund, Full or Partial Withdrawal - No Refund for Partial Withdrawal after this date
September	28	Monday	Last Day for 50% Refund, Full Withdrawal
October	19	Monday	Last Day for 25% Refund, Full Withdrawal
November	9	Monday	Last Day to Withdraw
November	25	Wednesday	Friday Classes Meet
November	26	Thursday	Thanksgiving Recess Begins
November	29	Sunday	Thanksgiving Recess Ends
December	10	Thursday	Last Day of Classes
December	11	Friday	Reading Day 1
December	14	Monday	Reading Day 2
December	15	Tuesday	Final Exams Begin
December	21	Monday	Final Exams End
December	23	Wednesday	Final Grades Due

1. **ChE 349 Kinetics and Reactor Design, Fall 2020**

Type	Time	Days	Where	Date Range	Schedule Type	Instructors
Class	9:00 am - 10:20 am	T	Webex	Sep 01, 2020 - Dec 21, 2020	Lecture	Xianqin Wang
Class	11:00 am - 12:20 pm	R	Webex	Sep 01, 2020 - Dec 21, 2020	Lecture	Xianqin Wang

Webex link: https://njit.webex.com/meet/xianqin

Try to make the Webex classes. 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/TA**

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

   Office Hours (via Webex)
   Tuesday: 10:30AM-11:30AM
   Thursday: 10:00AM - 11:00 AM

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

ChE349 TA : Siming Huo, sh533@njit.edu
You can consult with TA on questions about the grading of homework assignments, quizzes and/or exams.

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	(15%)
Team project (team work)	100 pts	(15%)
1st term exam (individual)	250 pts	(25%)
2nd term exam (individual)	250 pts	(25%)
Final exam (individual)	200 "	(20%)

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 "

Before the final exam, those students, who can get above 95% from all homework, all term exams and team project, can be exempted from final exam.

8. Policies on assignments/exams and classroom policy

Homework: Problem sets will be assigned, collected, T/A graded, and then returned. Solutions will be reviewed in class as time allows. All solutions will be posted on the course *Canvas* site. If you have questions about HW grading, contact the T/A directly.

Homework Grader: Siming Huo, sh533@njit.edu
– If you have questions about HW grading, contact the grader.
For questions about course material, see the instructor. The tests and the Term Project are all graded by the instructor.

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.

***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.
- Collaboration on homework assignments is not discouraged. In fact, homework and study groups might be helpful. All homework assignments, however, must be individually *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. Tentative Schedule

			Tentative Topics	HW assignments	HW due date
week1	9/1/2020	Tuesday	Chapter 1, Introduction, POLYMATH, Mole balances	HW1: P1-1A, P1-6B	
	9/3/2020	Thursday	Chapter 1, Introduction, POLYMATH, Mole balances		
week2	9/8/2020	Tuesday	No class, Monday schedule		
	9/10/2020	Thursday	Chapter 2, Conversion Reactor sizing	HW2: P2-1A, P2-7B	HW1 due
week3	9/15/2020	Tuesday	Chapter 2, Conversion Reactor sizing		
	9/17/2020	Thursday	Chapter 3, Rate Laws	HW3: P3-5A, P3-8B, P3-11B, P3-13A	HW2 due
week4	9/22/2020	Tuesday	Chapter 3, Rate Laws		
	9/24/2020	Thursday	Chapter 4, Stoichiometry Batch Systems	HW4: P4-3A, P4-4B, P4-5B	HW3 due
week5	9/29/2020	Tuesday	Chapter 4, Stoichiometry Flow Systems		
	10/1/2020	Thursday	Chapter 5, Isothermal reactor design: Conversion	HW5: P5-3_A, P5-4_B, P5-8_B, P5-11A	HW4 due
week6	10/6/2020	Tuesday	Chapter 5, Isothermal reactor design: Conversion		
	10/8/2020	Thursday	Chapter 6, Isothermal reactor design: Moles and molar flowrate	HW6: P6-4_B delete part (c), P6-5_B	HW5 due
week7	10/13/2020	Tuesday	Chapter 7, Collection and analysis of rate data	HW7: P7-7_A, P7-8_A.	HW6 due
	10/15/2020	Thursday	Chapter 7, Collection and analysis of rate data		
week8	10/20/2020	Tuesday	1st term exam		HW7 due
	10/22/2020	Thursday	Chapter 8, Multiple Reactions	HW8: P8-2_B, P8-6_B, P8-7_C (a), (b), (c)	
week9	10/27/2020	Tuesday	Chapter 8, Multiple Reactions		
	10/29/2020	Thursday	Chapter 9: Reaction mechanisms, pathways	HW9: P9-3C, P9-8B	HW8 due
week10	11/3/2020	Tuesday	Chapter 9: Reaction mechanisms, pathways		
	11/5/2020	Thursday	Chapter 9: Bioreaction and bioreactors		
week11	11/10/2020	Tuesday	Chapter 10: Catalysis and catalytic reactors	HW10: P10-12B, P10-18B	HW9 due
	11/12/2020	Thursday	Chapter 10: Catalysis and catalytic reactors		
week12	11/17/2020	Tuesday	Chapter 10: Catalysis and catalytic reactors		
	11/19/2020	Thursday	Chapter 11: Non-isothermal reactor design-energy balance	HW11: P11-7B	HW10 due
week13	11/24/2020	Tuesday	Chapter 11: Non-isothermal reactor design-Adiabatic PFR		
	11/26/2020	Thursday	No class, Thanksgiving		
week14	12/1/2020	Tuesday	Chapter 12: Steady-state nonisothermal reactor design	HW12: P12-9A	HW11 due
	12/3/2020	Thursday	Chapter 12: Steady-state nonisothermal reactor design		
week15	12/8/2020	Tuesday	2nd term exam		HW12 due
	12/10/2020	Thursday	Review lecture		
week16	12/11/2020	Friday	reading day 1		
	12/14/2020	Monday	reading day 2 Makeup exam		
	TBA		Final exam		