Department of Chemical Engineering
College of Engineering
University of the Philippines
Diliman, Quezon City

ChE 125

Chemical Reaction Engineering I

Course Description: Kinetics of homogeneous reactions; Analysis of various chemical reactors.

Course Prerequisites: ChE 106, ChE 122, Chem 31

Course Credit: 3.0 units (3 h lecture)

Program Educational Objectives (BS Chemical Engineering)
The program aims to educate students such that three to five years from graduation, they:
1. take leadership roles in their respective fields and/or effectively work in or manage a team;
2. are equipped with the extensive knowledge and relevant skills necessary to succeed in their chosen careers and to become responsive citizens;
3. are able to demonstrate strong research & innovative capability as they recognize and address opportunities and challenges in their respective spheres of influence;
4. have shown strong commitment to the ethical practice of their profession; to health, safety and environment; and service to society.

Course Outcomes
At the end of the course, the student should be able to:
1. Perform mass and energy balances on reacting systems;
2. Analyze experiments and interpret kinetic data to determine rate law parameters;
3. Select from among different types of (ideal) chemical reactors and contacting schemes to meet specific process objectives, and;
4. Apply ideal reactor models and elucidate their limitations in designing and modeling reactors for homogeneous systems.

Student Outcomes Satisfied by Course Outcomes
[a] Ability to apply knowledge of mathematics and science to solve engineering problems
[c] Ability to design a system, component, or process to meet desired needs within realistic constraints such as economic, environmental, social, political, ethical, health and safety, manufacturability, and sustainability, in accordance with standards
[e] Ability to identify, formulate, and solve engineering problems

Course Content

Week	Course Outcomes	Topics
Week 1	▪ Course outline and class policies ▪ Overview of Chemical Reaction Engineering ▪ Define fundamental concepts in stoichiometry	Contexts of chemical reaction.
	▪ Apply the extent of reaction (ξ) concept to single and multiple reaction systems ▪ Relate the composition of a reactor and the extents of independent reactions	Extent of reaction. Reactor composition calculations.
Week 2	▪ Determine the number of independent reactions in a set of multiple chemical reactions ▪ Express the dependent reactions in terms of	Independent and dependent chemical reactions.

Week	Course Outcomes	Topics
	independent reactions in a given multiple reaction system	
Week 3	▪ Characterize reactor feed ▪ Characterize reactor performance	Limiting and excess reactant. Reactant conversion. Product yield and selectivity.
	▪ Determine sets of species compositions that provide independent information on reactor composition	Independent species composition specifications.
Week 4	▪ Define fundamental concepts in chemical kinetics ▪ Dissect the rate law ▪ Write down the rate law for 1. an elementary reaction 2. a single irreversible reaction 3. a reversible reaction 4. multiple reactions	Rate of reaction and its relation to stoichiometry. The rate law and its parts. Simple and complex rate laws. Molecularity and order of a reaction. Empirical versus fundamental rate equations. Temperature effects on reaction rates. Rate constant vs. Equilibrium constant
Week 5	▪ Analyze non-elementary reactions ▪ Obtain the rate law from a reaction mechanism ▪ Apply approximate methods to obtain the rate law from a reaction mechanism ▪ Discuss guidelines in formulating reaction mechanisms	Reaction mechanisms. The quasi-equilibrium hypothesis. The steady-state hypothesis. Guidelines to formulating reaction mechanisms.
Week 6	▪ Explore ways of obtaining kinetic data ▪ Apply methods of analyzing kinetic data to obtain the rate law for constant-density systems	Kinetic measurements. Integral Method of kinetic data analysis.
Week 7	▪ Apply other methods of analyzing kinetic data for constant-density systems ▪ Interpret the results of kinetic data analysis	Other methods of analyzing kinetic data: 1. Fractional Life Method a. Half Life Method 2. Differential Method a. Initial-Rate Method b. Single-Run Differential Method 3. Isolation Method
	▪ Obtain rate law expressions for gas-phase reactions using total pressure data ▪ Perform kinetic data analysis for variable-density systems	Fractional volume change of system (ε) Methods of analyzing kinetic data: 1. Integral Method 2. Differential Method
	LONG EXAM 1	
Week 8	▪ Describe several ideal types of reactors based on the mode of operation (batch or continuous) and ideal flow patterns (backmix or plug flow) for the continuous mode ▪ Set up the material balance for each ideal reactor model	Batch versus continuous operation. The ideal batch reactor. The continuous stirred-tank reactor (CSTR). The plug-flow reactor (PFR). Performance equations of ideal reactors.
Week 9	▪ Perform material balance calculations dealing with ideal isothermal reactors accomplishing a single reaction ▪ Determine the rate law from kinetic data obtained from an ideal isothermal reactor	Kinetic data analysis for 1. an ideal batch reactor 2. a CSTR 3. a PFR a. used as a differential reactor b. used as an integral reactor
Week 10	▪ Design isothermal reactor systems accomplishing a single reaction ▪ Solve problems involving reactor combinations	Size comparison of single reactors. Combinations of reactors: 1. Series and parallel connections 2. Tanks in series

Week	Course Outcomes	Topics
	(series and parallel)	
Week 11	▪ Describe the recycle reactor and its performance equation ▪ Optimize recycle operations	The recycle reactor. Optimum recycle ratio.
	LONG EXAM 2	
Week 12	▪ Determine qualitatively the most favorable contacting scheme to optimize the reaction process of isothermal systems	Contacting patterns.
	▪ Describe reactor operations in terms of intensive dimensionless quantities ▪ Determine the characteristic reaction time ▪ Derive the reaction-based design equations for the three ideal reactor models with multiple reactions	Dimensionless extents. Characteristic reaction time. Dimensionless design equations.
Week 13	▪ Apply the design formulation of isothermal reactors with multiple reactions for various types of chemical reactions	Isothermal operations with multiple reactions of ideal reactors.
	LONG EXAM 3	
Week 14	▪ Determine qualitatively the most favorable contacting scheme to optimize the reaction process of non-isothermal systems ▪ Set up the energy balance equations for each ideal reactor model ▪ Examine adiabatic and nonisothermal operation	Nonisothermal operations of ideal reactors.
Week 15	▪ Describe how multiple steady states arise and their consequences ▪ Discuss how mathematical analysis can reveal these behaviors	Heat generation and removal functions. Ignition-extinction curve. Runaway reactions in a CSTR. Stability diagram.
	LONG EXAM 4	

Course Assessment

Long Examinations	70%
Class Work	15%
Finals	15%

Course Policies

1. **Attendance**
   a) Attendance shall be checked by the instructor every meeting. A student arriving twenty five (25) minutes beyond the start of the class will be considered absent.
   b) A student may only incur a maximum of 6 total absences. Should the student go beyond the maximum number of absences, s/he will be given a grade of 5.0 unless s/he drops from the class.
2. **Long Examinations**
   a) There will be four (4) Long Examinations (all shall be closed notes and closed book exam, unless stated by the instructor) for the entire course.
   b) At least 10 sheets of neat legal sized paper, with ONLY the class number and student number written on every upper right portion of the pages, must be submitted at the end of the last class before the scheduled exam. Late submission of answer sheets will be penalized with a **10% deduction** from the long exam grade.
   c) Answers should be written legibly in black/blue ink only; otherwise, the student forfeits his/her right to seek any corrections after. Solutions written in pencil will not be considered.

d) A student who misses an exam with a valid excuse must approach his/her instructor to discuss the options that can be taken. This should be done on or before the schedule of the next long exam; otherwise, a score of zero will be given for the missed exam. Only one (1) excused missed long exam is allowed.
e) The students shall be given **five (5) days** (excluding Saturdays, Sundays, and holidays) after the release of exam results to seek corrections. **All grievances (for whatever reason) will not affect the grades if it is raised after the 5-day grace period.**
f) Cheating during the examinations will be penalized with a grade of **5.00** in the course and possibly, expulsion.

3. **Classwork**
The grades for classwork in this course shall come from problem sets, homework, seatwork and quizzes. There shall be no make-up activity for any missed classwork. **LATE CLASSWORK WILL NOT BE ACCEPTED.**

4. **Design Project**
A design project shall be given for each group of three to four students that will gauge their understanding on the concepts covered on reactor design. The design problem will be given after the 2nd Long Exam, and will be submitted during the finals week. Consultation periods will be set in order to ensure the groups have significant progress.

5. **General Guidelines**
a) Any form of cheating is punishable by expulsion from the university.
b) Courtesy towards each person in this class is expected. Thus, any behavior that will impede learning should be avoided. **Refrain from sending messages and making calls through your cellular phones during class hours. Keep your cellular phones in mute or silent mode or turn it OFF while in class.**
c) **Refrain from frequently exiting and re-entering the room during class hours.**
d) Read the recommended or related materials pertaining to the subject matter prior to coming to class. Always be prepared physically, mentally and emotionally. **Study regularly.**
e) Requirements not submitted on time **will not be graded** (i.e. will be given a grade of zero).

6. **The instructor reserves the right to amend class policies when deemed necessary.**

Grading System

1.00	1.25	1.50	1.75	2.00	2.25	2.5	2.75	3.00	5.00
[92,100]	[88,92)	[84,88)	[80,84)	[76,80)	[72,76)	[68,72)	[64,68)	[60,64)	[0,60)

List of Instructors
Dr. Terence Tumolva
Prof. Kristian July Yap
Prof. Charlimagne Montealegre
Engr. Bemboy Niño Subosa
Engr. Michael Sean Deang

References

1. Coker, A. Kayode. Modeling of Chemical Kinetics and Reactor Design. 1st Ed. Boston, MA: Gulf Professional Pub., 2001.
2. Davis, Mark E., et al. Fundamentals of Chemical Reaction Engineering. 1st Ed. New York: McGraw-Hill, 2003.
3. Fogler, H. Scott. Elements of Chemical Reaction Engineering. 4th Ed. New Jersey: Pearson Education, Inc., 2006.
4. Hill, Charles. An Introduction to Chemical Engineering Kinetics and Reactor Design. 1st Ed. John Wiley and Sons, 1977.
5. Levenspiel, Octave. Chemical Reaction Engineering. 3rd Ed. New York: John Wiley and Sons, 1999.
6. Mann, Uzi. Principles of Chemical Reactor Analysis and Design. 2nd Ed. New Jersey: John Wiley and Sons, 2009.
7. Missen, Ronald W., et al. Introduction to Chemical Reaction Engineering and Kinetics. 1st Ed. New York: John Wiley and Sons, 1999.