18 APR 2018 CC/ 28 MAY 2018 UC

DEPARTMENT OF CHEMICAL ENGINEERING
College of Engineering
University of the Philippines Diliman, Quezon City

COURSE SYLLABUS
ChemE 128 Chemical Reaction Engineering

A. Course Catalogue Description

1. **Course Number:** ChemE 128
2. **Course Title:** Chemical Reaction Engineering
3. **Course Description:** Kinetics of homogeneous and heterogeneous reactions; application of thermodynamics and transport processes in the analysis and design of reactors
4. **Prerequisite:** Chem 31 Elementary Organic Chemistry
   ChemE 123 Chemical Engineering Thermodynamics II and
   ChemE 131 Thermal Systems
5. **Corequisite:** ChemE 132 Separation Processes I
6. **Semester Offered:** First Semester
7. **Course Credit:** 4u
8. **Number of Hours:** 4h
9. **Meeting Type:** lecture
10. **Course Goals:** To discuss the analysis of the kinetics of homogeneous and heterogeneous reactions; to perform basic design calculations of different types of reactors, and to evaluate reactor performance and efficiency within safety and economic limits

B. Rationale

This course introduces the key concepts of chemical reaction engineering, which is the core discipline in the study of chemical engineering. It relates the principles of chemical reaction kinetics, reaction equilibrium, and transport phenomena to the proper design of a given chemical reactor system.

C. Course Outline

1. Course Outcomes (CO)

Upon completion of the course, students must be able to:

- **CO 1.** perform mass and energy balances on reacting systems;
- **CO 2.** interpret kinetic data to determine rate law parameters;
- **CO 3.** select from among different types of ideal reactors and contacting schemes to meet specific process objectives;
- **CO 4.** utilize ideal models for the design of reactors for homogeneous systems;
- **CO 5.** apply the concepts of chemical kinetics and transport phenomena in determining the overall kinetic equations of heterogeneous reactions; and
- **CO 6.** formulate a basic design of heterogeneous packed-bed reactors for desired process requirements.

Course Outcomes and Relationship to Program Learning Objectives

Course Outcomes	Program Learning Objectives*				
	A	B	C	D	E
Perform mass and energy balances on reacting systems					
Interpret kinetic data to determine rate law parameters					
Select from among different types of ideal reactors and contacting schemes to meet specific process objectives					
Utilize ideal models for the design of reactors for homogeneous systems					
Apply the concepts of chemical kinetics and transport phenomena in determining the overall kinetic equations of heterogeneous reactions					
Formulate a basic design of heterogeneous packed-bed reactors for desired process requirements					

* **A** Equip students with strong technical education in chemical engineering necessary to succeed in their chosen careers and to become responsive citizens.
B Develop the students' ability to effectively communicate technical information to any audience.
C Train students to function in multidisciplinary teams, manage projects, and take leadership roles in their respective fields.
D Engage students in research, innovation, and life-long learning to identify opportunities, and address issues and challenges in their respective spheres of influence.
E Instill in students a strong commitment to the ethical practice of their profession; to health, safety, and environment; and to service to society.

2. Course Content

Lecture Topics	No. of Hours
Overview of chemical reaction engineering 1. What is chemical reaction engineering? 2. Stoichiometry and mole balances in reacting systems 3. Characterization of reactor performance a. Conversion b. Yield c. Selectivity	2
Kinetics of homogeneous reactions 1. Fundamental concepts in chemical kinetics 2. Writing rate laws for elementary reactions 3. Rate laws for non-elementary reactions a. Quasi-equilibrium approximation (QEA) b. Steady-state approximation (SSA) c. Obtaining kinetic data for liquids and gases 4. Kinetic data interpretation and analysis for batch and flow reactors a. Integral method b. Differential method c. Fractional life method	8

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Lecture Topics	No. of Hours
d. Initial rates method e. Isolation method f. Analysis of total pressure data	
Long Examination 1	
Isothermal reactor design for homogeneous systems 1. Design for single reactions a. Performance equation for batch, CSTR, and PFR b. Size comparison of single reactors c. Combinations of reactors (series and parallel) d. Recycle reactor	10
Long Examination 2	
2. Design for multiple reactions a. Optimum contacting patterns b. Kinetics of a network of reactions from batch experiment c. Reaction-based design equations for batch, CSTR, and PFR i. Parallel and series reactions ii. Other multiple reactions	6
Pressure effects for flow reactors	2
Long Examination 3	
Non-isothermal reactor design for homogeneous systems 1. Temperature and energy effects in reactors 2. Contacting patterns for non-isothermal cases 3. Energy balances for ideal reactors a. Adiabatic operation b. Non-isothermal operation 4. Stability analysis in CSTR 5. Runaway temperature in PFR	6
Reactor Design Problem 1	
Heterogeneous systems 1. Global rate of reaction 2. Review of adsorption 3. Heterogeneous catalysts	8
Kinetics of solid-fluid catalytic reactions 1. Rates of adsorption, surface reaction, and desorption 2. Rate equations in terms of concentrations in the fluid phase at the catalyst surface 3. Qualitative analysis of rate equations 4. Quantitative interpretation of kinetic data	6
Long Examination 4	
External transport process in heterogeneous reactions 1. The effect of physical processes on observed rates of reaction 2. Calculation of external concentration and temperature differences	6
Internal transport process in heterogeneous reactions 1. Intrapellet mass transfer 2. Intrapellet heat transfer 3. Mass transfer with reaction 4. Mass and heat transfer with reaction	6
Design of an isothermal fixed-bed reactor 1. Calculation of the global rate of reaction 2. Design equations for isothermal catalytic fixed-bed reactor	4
Reactor Design Problem 2	
Total number of hours	**64**

3. Course Coverage

Week	CO	TOPIC	ESSENTIAL/ KEY QUESTIONS	Suggested Teaching and Learning Activities	Suggested Assessment Tools
1	1,2	**Overview of chemical reaction engineering** 1. What is chemical reaction engineering? 2. Stoichiometry and mole balances in reacting systems 3. Characterization of reactor performance a. Conversion b. Yield c. Selectivity	What is the scope of chemical reaction engineering? What are the different variables needed in reactor design and performance analysis?	lecture, classwork	problem set/quiz
1-3	2	**Kinetics of homogeneous reactions** 1. Fundamental concepts in chemical kinetics 2. Writing rate laws for elementary reactions 3. Rate laws for non-elementary reactions a. Quasi-equilibrium approximation (QEA) b. Steady-state approximation (SSA) c. Obtaining kinetic data for liquids and gases 4. Kinetic data interpretation and analysis for batch and flow reactors a. Integral method b. Differential method c. Fractional life method d. Initial rates method e. Isolation method f. Analysis of total pressure data	How are rate laws determined for different homogenous chemical reactions? What are the different methods of analyzing kinetic data from experiments?	lecture, classwork	problem set/quiz
					Long Examination 1

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Week	CO	TOPIC	ESSENTIAL/ KEY QUESTIONS	Suggested Teaching and Learning Activities	Suggested Assessment Tools
3-7	1,3	**Isothermal reactor design for homogeneous systems** 1. Design for single reactions a. Performance equation for batch, CSTR, and PFR b. Size comparison of single reactors c. Combinations of reactors (series and parallel) d. Recycle reactor	What are the different types of reactors? How are performance equations for different types of reactors derived from mass and energy balances? What are the criteria for selecting the appropriate type of reactor to use, taking into account performance, safety, and economic considerations?	lecture, classwork	problem set/quiz
					Long Examination 2
		2. Design for multiple reactions a. Optimum contacting patterns b. Kinetics of a network of reactions from batch experiment c. Reaction-based design equations for batch, CSTR, and PFR i. Parallel and series reactions ii. Other multiple reactions			
7	1,3,4	**Pressure effects for flow reactors**	How does pressure drop across a tubular reactor affect its efficiency?	lecture, classwork	problem set/quiz
					Long Examination 3
8-9	1,3,4	**Non-isothermal reactor design for homogeneous systems** 1. Temperature and energy effects in reactors 2. Contacting patterns for non-isothermal cases 3. Energy balances for ideal reactors a. Adiabatic operation b. Non-isothermal operation 4. Stability analysis in CSTR	How are non-isothermal reactors designed? What considerations are needed for designing heat effects for reactors?	lecture, classwork	problem set/quiz

Week	CO	TOPIC	ESSENTIAL/ KEY QUESTIONS	Suggested Teaching and Learning Activities	Suggested Assessment Tools
		5. Runaway temperature in PFR			quiz
					Design Problem 1
9-11	5	**Heterogeneous systems** 1. Global rate of reaction 2. Review of adsorption 3. Heterogeneous catalysts	What are the salient distinction points between homogeneous and heterogeneous reactions? What is catalysis?	lecture, classwork	problem set/quiz
11-13	2,5	**Kinetics of solid-fluid catalytic reactions** 1. Rates of adsorption, surface reaction, and desorption 2. Rate equations in terms of concentrations in the fluid phase at the catalyst surface 3. Qualitative analysis of rate equations 4. Quantitative interpretation of kinetic data	How are rate laws determined for different heterogenous chemical reactions? How does adsorption affect the rate of reaction on the surface of a solid catalyst? What are the different methods of analyzing kinetic data from experiments?	lecture, classwork	problem set/quiz
					Long Examination 4
13-14	1,5,6	**External transport process in heterogeneous reactions** 1. The effect of physical processes on observed rates of reaction 2. Calculation of external concentration and temperature differences	How does mass transfer from bulk fluid to solid surface define the rate of a catalyzed reaction?	lecture, classwork	problem set, quiz
14-15	1,5,6	**Internal transport process in heterogeneous reactions** 1. Intrapellet mass transfer 2. Intrapellet heat transfer 3. Mass transfer with reaction 4. Mass and heat transfer with reaction	How does diffusion from solid surface to the pores define the rate of a catalyzed reaction?	lecture, classwork	problem set, quiz
16	1,5,6	**Design of an isothermal fixed-bed reactor** 1. Calculation of the global rate of reaction 2. Design equations for isothermal catalytic fixed-bed reactor	How are transport effects accounted in the calculation of the global rate of reaction?	lecture, classwork	problem set/quiz
					Design Problem 2

4. Course Requirements

1. Long examinations (4)
2. Design problems (2)
3. Problem set
4. Quizzes

REFERENCES:

Cesar, H. D. and Somera, J. J. (2014). Ethylbenzene Production through benzene alkylation with FCC off-gas over platinum-containing zeolite bifunctional catalyst (Plant design report). University of the Philippines Diliman.

Fogler, H. S. (2016). *Elements of Chemical Reaction Engineering* 5th Ed. NJ: Pearson Education, Inc.

Froment, G. F., Bischoff, K. B. and De Wilde, J. (2011). *Chemical Reactor Analysis and Design* 3rd Ed. NJ: John Wiley and Sons, Inc.

Hill, C. (2014). *An Introduction to Chemical Engineering Kinetics and Reactor Design* 2nd Ed. NJ: John Wiley and Sons, Inc.

Mann, U. (2009). *Principles of Chemical Reactor Analysis and Design* 2nd Ed. NJ: John Wiley and Sons Inc.