- 1. Course number and name CHBE 4300 Kinetics and Reactor Design (required)
- 2. Credits and contact hours 3 credit hours, 3 lecture hours (3-0-0-3)
- 3. Instructor's or course coordinator's name Dr. Michael Filler
- 4. **Textbook, title, author, and year** Fogler, "Elements of Chemical Reaction Engineering," 5<sup>th</sup> Ed. Prentice Hall, 2016

### 5. Specific course information

- a. Catalog Description Reacting systems are analyzed in terms of reaction mechanisms, kinetics, and reactor design. Both homogeneous and heterogeneous reactions are considered.
- b. **Prerequisites or co-requisites** –CHBE 3130 Chemical Engineering Thermo II (grade "C" or better); CHBE 3200 Transport Phenomena I (grade "C" or better); CHBE 3210 Transport Phenomena II (pre-requisite with concurrency).
- c. Required, elective, or selected elective course (as per Table 5-1) Required

### 6. Specific goals for the course

## a. Specific outcomes of instruction:

- By the end of this course, a student should be able to:
  - 1) Analyze reaction mechanisms for homogeneous & heterogeneous reactions and develop kinetic rate expressions for the reactions.
  - 2) Develop microscopic and macroscopic mass and energy balances for various reactor types and identify the initial and boundary conditions
  - 3) Discern reaction kinetics by analyzing data from a variety of reactor types
  - 4) Design ideal isothermal reactors
  - 5) Design non-isothermal reactors by accounting for the heat effects (endothermic or exothermic reactions) as well as non-adiabatic reactor configurations
  - 6) Analyze RTD (residence time distribution) data to identify non-idealities in reactor configurations and utilize this information to predict reactor performance
  - 7) Analyze for the role of transport effects in isothermal heterogeneous reactions.

### b. Connection with Student Outcomes

CHBE 4300								
		Student Outcomes						
Course Outcomes	(1)	(2)	(3)	(4)	(5)	(6)	(7)	
Course Outcome 1	X							
Course Outcome 2	X							
Course Outcome 3	X					Χ		
Course Outcome 4	X	Χ						
Course Outcome 5	X	Χ						
Course Outcome 6	X	Χ				Χ		
Course Outcome 7	X	Χ				Χ		

- (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
- (5) an ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives
- (6) an ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions
- (7) an ability to acquire and apply new knowledge as needed, using appropriate learning strategies

# 7. Brief list of topics to be covered

- a. Reaction Thermodynamics
  - 1) Heat of reaction effects
  - 2) Reaction free energy and equilibrium constant
  - 3) Effect of pressure and temperature on equilibrium conversion
- b. Theories and Mechanisms of Homogeneous Reactions
  - 1) Bimolecular collision theory and Transition state theory
  - 2) Reaction intermediates and Bodenstein steady-state approximation
  - 3) Chain and non-chain reactions
  - 4) Kinetic rate expressions derived from reaction mechanisms
  - 5) Michaelis-Menten kinetics
- c. Definitions of Rate and Design Equations in Different Reactor Types
  - 1) Mass balances around ideal homogeneous reactors
  - 2) Fractional conversion as a design variable in single reactions
  - 3) Integration of kinetics into the reactor design equation
  - 4) Graphical interpretation of reactor design equations
- d. Multiple Reactions in Homogeneous Reactors
  - 1) Series vs. parallel reactions
  - 2) Yield and selectivity in multiple reactions
  - 3) Reactor design considerations
- e. Non-isothermal Homogeneous Reactor Design
  - 1) Energy balances around non-adiabatic reactors
  - 2) Numerical vs. graphical approach to reactor design
  - 3) Multiple reactions in a non-isothermal reactor
- f. Non-idealities in Homogeneous Reactors
  - 1) Residence time distribution (RTD)
  - 2) Segregated flow model
  - 3) Axial dispersion model
  - 4) CSTR's in series model
- g. Heterogeneous Reactions
  - 1) Reaction mechanisms
  - 2) Langmuir-Hinshelwood kinetics
  - 3) Catalyst structure and transport
  - 4) Single pore diffusion model
  - 5) Thiele modulus and catalyst effectiveness factor