CME 504

Chemical Reaction Engineering

Credits and Contact hours: 3 credits; 2 hours 40 minutes weekly

Instructor: Tae Jin Kim (taejin.kim@stonybrook.edu, office # 218 at Old Eng. Bldg.)

Pre-requisite: Undergraduate course in chemical reactions and/or reactor engineering

Text book:
Fundamentals of Chemical Reaction Engineering, 1st Ed, M. Davis and R. Davis (2008)
Fogler, H. Scott. Elements of Chemical Reaction Engineering, 4rd Ed. Prentice Hall (2011).
Levenspiel, Octave. Chemical Reaction Engineering, 4rd Ed. Wiley (2011).
Chemical Raction Engineering: Beyond the Fundamentals, 1st Ed. CRC press (2014)

Date	Topic
Week 1	Course introduction, reaction stoichiometry; rate equations; ideal, isothermal reactors: design equations
Week 2	Ideal, isothermal reactors: batch, CSTR, PFR
Week 3	Ideal, isothermal reactors: reactors in series;
Week 4	Chemical kinetics: elementary reactions, laws of mass action
Week 5	Chemical kinetics: rate laws from reaction mechanism
Week 6	Chemical kinetics: transition state theory
Week 7	Ideal reactor design with energy balance
Week 8	**Midterm**
Week 9	Stability of nonisothermal reactors; nonlinear dynamics
Week 10	Nonideal reactors: residence-time distribution
Week 11	Diffusion-controlled reactions. Diffusion/reaction in two dimensions;
Week 12	Heterogeneous catalysis: isothermal reactions in porous catalysts
Week 13	Heterogeneous catalysis: heat transfer effects
Week 14	**Break***

Week 15	Heterogeneous catalysis: multiple reactions in porous catalysts
Week 16	**Final Exam**

*** Thanksgiving or Spring break, depending on semester offered**

Course description:

Introduce the students to the fundamental principles of reaction engineering in order to enable them to handle kinetics and kinetic-transport interactions in a variety of situations. To introduce students to the analysis of the kinetics of homogeneous chemical reactions. To apply this analysis and the concepts of material and energy conservation to the design of idealized homogeneous chemical reactors operating both in batch and continuous modes and under both isothermally and non-isothermally conditions. To introduce the analysis of non ideal flow and, using the flow model, to quantify its effect on an idealized reactor design.

Students Learning Outcomes:

1. To be able to carry out an analysis of kinetic data from most types of homogeneous reaction, to calculate the volume requirements for batch, CSTR and plug flow reactors processing simple reversible and irreversible reactions operating under both isothermal and non-isothermal conditions.
2. To understand the complexity of reactor design and to recognize their own limitations. To be able to determine from mechanisms the kinetic rate expression and its temperature and concentration dependence.
3. To be able to design and interpret rate experiments, assess the effect of transport phenomena on observed rates and determine the rate of reaction as a function of composition and temperature.
4. To be able to use appropriate reactor models to select desired reactor type and size for specified
production rate and selectivity.
5. To demonstrate the ability to use the general reaction engineering principles in different application areas such as production of fuels and chemicals, film growth, biological reaction systems, fuel cell operation, etc.