ChE 471 – Chemical Reaction Engineering – Credits 3
Fall Semester – 2012
Contact Hours: 4 per week
Lectures Tuesday and Thursday 11:30 AM -1:00 PM
Required Recitation Friday either 10-11 AM or 1-2 PM

Catalog Data:
Chemical reaction engineering principles and applications in process and product development. Evaluation of reaction rates from mechanisms and experimental data, quantification of pertinent transport effects and application to reactor and product design in energy and environmental systems.

Prerequisite:
ChE 320, ChE 367, ChE 351, ChE 359

Textbook:
Class notes.

Coordinator:
M.P. Dudukovic, The Laura and William Jens Professor

Goals (Expected Outcome):
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. The students are expected to:

a) Determine from mechanisms the kinetic rate expression and its temperature and concentration dependence.
b) 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.
c) Assess the potential hazards of various reactor types in case of exothermic reactions.
d) Use appropriate reactor models to select desired reactor type and size for specified production rate and selectivity.
e) Quantify the effect of operating variables in various reactor types on product quality and purity and energy efficiency.
f) Demonstrate the ability to use the general reaction engineering principles in different application areas such as production of fuels and chemicals, CVD film growth, biological reaction systems, fuel cell operation, etc.

Prerequisites by Topic:
2. Spread sheets and Matlab or equivalent.
5. Chemical and phase equilibria.
6. Diffusion and conduction.
7. Convective transport.

**Topics Covered:**
- Reaction rate dependence on composition and temperature, mechanisms, derivation of rate forms, activation energy.
- Mass balances for ideal reactors for homogeneous systems in isothermal operation. Evaluation of rate information from data.
- Non-ideal flow patterns and their characterization. Residence time distributions.
- Transport effects in reactions on solid surfaces: surface catalyzed reactions, solid film deposition, dissolution of solids.
- Transport effects on reacting porous solids: catalytic pellet, reacting particle. Thiele modulus and effectiveness factor.
- Reactors and reactor scale models for fluid-solid reactors. Packed bed and fluidized bed.
- Extension and application of reaction engineering principles to selected examples such as: biological reactors, CVD reactors, photochemical reactors, electrochemical reactors, fuel cell. Case studies.

**Tests**
Three (3) in class exams + multiple quizzes+ final quiz.

**Computer Usage:**
Homework assignments require use of spread-sheets and MATLAB or equivalent.

**Laboratory Projects:**
- No physical laboratory. Selected virtual laboratory experiments conducted in the Computer Aided Process Engineering Laboratory.

**Prepared by:**
M.P. Dudukovic

**Date:**
8/27/2012

**ABET category content:**
Engineering Topics: 3
Che 471: Application of ABET Criterion 3. Program Outcomes and Assessment

a) ability to apply knowledge of mathematics, science, and engineering  
   - demonstrated in homeworks, quizzes, exams.

b) ability to design and conduct experiments, as well as to analyze and interpret data  
   - gained in determination of rates from experimental data and in uncovering of the magnitude of transport effects on kinetics

c) ability to design a system, component, or process to meet desired needs  
   - gained in solving HW problems.

d) ability to function on multi-disciplinary teams  
   - classroom participation plus term project

e) ability to identify, formulate, and solve engineering problems  
   - gained by open ended problems which are part of assignments and exams

f) understanding of professional and ethical responsibility  
   - gained by considering safety issues of reactor design and operation

g) ability to communicate effectively  
   - demonstrated by short presentations during Friday sessions and team project presentation at end of semester

h) the broad education necessary to understand the impact of engineering solutions in a global and societal context  
   - gained by examining the environmental impact of the reactor or process

i) a recognition of the need for, and an ability to engage in life-long learning  
   - acquired by exposure to open ended problems

j) a knowledge of contemporary issues  
   - acquired by considering alternative reactors for new energy sources, production of new materials and implementation of ‘green processing’

k) ability to use the techniques, skills, and modern engineering tools necessary for engineering practice  
   - spread-sheet and MATLAB use throughout the course