

## ChE 625 Chemical Reaction Engineering Spring Semester 2011

**Instructor:** Ray Y. K. Yang (Room 441 ESB; [ryang@mail.wvu.edu](mailto:ryang@mail.wvu.edu); 304-293-9365)

**Lectures:** 9:00-10:15, M W (Room 205 MRB)

**Prerequisite:** Completion of an undergraduate course in Chemical Reaction Engineering with good grade. Preliminary experience with MATLAB is recommended but not required.

### Books Used:

1. Levenspiel, O., "Chemical Reaction Engineering", 3rd Ed., Wiley, 1999. (Recommended)
2. Fogler, H. S., "Elements of Chemical Reaction Engineering", 4<sup>th</sup> Ed., Prentice Hall, 2006. (Recommended)
3. Hahn and Valentine, *Essential MATLAB for Engineers and Scientists*, 4th Ed., Academic Press, 2010. (Recommended)

**Course Outline** (Topics may not be presented in exactly the same order as listed below):

### Part 0. Introduction to MATLAB

### Part 1. Chemical Engineering Kinetics (only key topics are listed here)

*Elements of Reaction Kinetics:* Effects of temperature and Arrhenius plot; Rate expressions and rate equations for single- and multiple-reaction systems; Non-unity stoichiometric coefficients; Rate data analysis and determination of kinetic parameters; Variable density systems; Generalized stoichiometric coefficients, extents of reaction, and generalized reaction rates; Total pressure method; Autocatalytic reactions.

*Kinetics of Heterogeneous Catalytic Reactions:* Intraparticle, interphase, and interparticle transports; Heterogeneous reaction rates; Coupled diffusion and reaction in porous and non-porous catalyst particles; Effectiveness factor and generalized Thiele modulus; Effects of strong transport resistance; Production distribution in catalyst particles.

### Part 2. Analysis and Design of Chemical Reactors (only key topics are listed here)

*Ideal Reactors:* Brief Review of Perfectly-Mixed Batch Reactor (PMBR), Continuous Stirred-Tank Reactor (CSTR), and Plug-Flow Tubular Reactor (PFTR); Ideal heterogeneous reactor models; Variable-volume reactors; Multiple-reactor systems; Product distribution in multiple-reaction systems.

*Reactor Stability:* Multiple steady states; Stability analysis of steady states.

*Non-ideal Flow and Non-ideal Reactors:* Residence time distribution (RTD); E and F curves; Micro- and Macro-fluids; Conversion directly from RTD; Models for non-ideal reactors; Fixed-bed catalytic reactors.

## **Overall Course Objective:**

To provide a rigorous and integrative treatment of a variety of subjects in chemical kinetics and chemical reactors, which are relevant to and compatible with the background of most of the first-year chemical engineering graduate students at WVU.

## **Assessment:**

- 1) Homework problems (may include projects): 20%
- 2) Two-hour mid-semester examination: 40%
- 3) Two-hour final examination: 40%

## **Other Relevant References (#1 to #7 on reserve in Evansdale Library):**

1. Aris, R., "Introduction to the Analysis of Chemical Reactors", Prentice Hall, 1965; Chapters 1-4. (5 copies on reserve)
2. Carberry, J. J., "Chemical and Catalytic Reaction Engineering", McGraw-Hill, 1976.
3. Fogler, H. S., "Elements of Chemical Reaction Engineering", 4<sup>th</sup> Ed., Prentice Hall, 2006.
4. Froment, G.F. and K. B. Bischoff, "Chemical Reactor Analysis and Design", 2nd Ed., Wiley, 1990.
5. Levenspiel, O., "Chemical Reaction Engineering", 3rd Ed., Wiley, 1999.
6. Perlmutter, D. D., "Stability of Chemical Reactors", Prentice Hall, 1972.
7. Himmelblau, D. M. and K. B. Bischoff, "Process Analysis and Simulation: Deterministic Systems", Wiley, 1968.
8. Papers from technical and professional journals (to be mentioned in relevant lectures).

## **Social Justice Statement:**

West Virginia University is committed to social justice. I concur with that commitment and expect to foster a nurturing learning environment based upon open communication, mutual respect, and non-discrimination. Our University does not discriminate on the basis of race, sex, age, disability, veteran status, religion, sexual orientation, color or national origin. Any suggestions as to how to further such a positive and open environment in this class will be appreciated and given serious consideration. If you are a person with a disability and anticipate needing any type of accommodation in order to participate in this class, please advise me and make appropriate arrangements with Disability Services.