33 EECE 503-01: Kinetics and Reaction Engineering Principles
Spring 2015; Date 01-12-2015

Instructor:

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Reading Material for the course, that complements the lectures, will be available on the web page for the course at

http://classes.engineering.wustl.edu/eece503/

New material will be added periodically and students will be notified by e-mail of the additions to the displayed material.

Textbook:

The students are required to purchase the "Chemical Reactor Omnibook" by Professor Octave Levenspiel. It can be ordered on line from either Amazon.com or LULU. Paperback copy new is about $50, used about $40. It is an excellent source of problems to practice various reaction engineering concepts on.

COURSE DESCRIPTION

The course covers the fundamental principles of modern multi-scale reaction engineering for chemical and biochemical systems in environmentally benign and energy efficient processing. The key concepts in kinetics, the role of mass and heat transfer on kinetics at the micro and meso-scale, kinetic - transport interactions in heterogeneous systems, and the effect of mixing and contacting of phases on micro and at the reactor level are discussed. Applications of reaction engineering principles in the areas related to energy generation, pollution prevention, waste remediation, chemical and materials processing, and in biotechnology are illustrated.

Expected Outcome:

Students completing the course will demonstrate proficiency in basic concepts of reaction engineering methodology. They will be able to use these concepts to engineer reaction systems in the energy, environmental, chemical and materials processing fields.

2015 Tentative Course Outline (*to be adjusted based on class needs*)
Class in GREEN Hall L0159, Tuesday & Thursday 4:00 to 5:30 PM.

Week 1. (Jan. 13, 15)

Brief introduction to modern reaction engineering methodology.

Review of basic concepts of stoichiometry, reaction progress, heats of reaction, thermodynamics, chemical and physical equilibria.

Reading Material on Course Web Page: plus published paper + Omnibook.
"Reaction Engineering: Status and Challenges".

Week 2. (Jan. 20, 22)

Concepts of kinetic rates, activation energy, elementary reactions, reaction mechanisms, derivation of rate forms.

Transition state theory; elementary gas phase and liquid phase reactions. Diffusion limited reactions.

Reading Material on Course Web Page + Omnibook

Week 3. (Jan. 27, 29)

Compartmental models for gas – liquid systems.

Transport effects on reactions in the atmosphere.

Reading Material from Course web page)

Week 4. (Feb. 3, 5)

Ideal Reactors: Batch, Continuous Flow Stirred Tank reactor (CSTR), Plug Flow Reactor (PFR). Evaluation of rate forms from ideal reactors.

Non-ideal Flow Patterns: identification and quantification.

Reading Material on Course Web Page+ Selected chapters from Omnibook.

Week 5. (Feb. 10, 12)

Micro-mixing concepts.

Modeling of tubular flow reactors in laminar and turbulent flow.

Reading Material on Course Web Page + Omnibook

Week 6. (Feb. 17, 19)

Stirred tank reactors. Flow pattern and mixing.

General population balance model.

Interpretation of micro-mixing effects on reactions in stirred tanks.

Reading Material on Course Web Page:

Week 7. (Feb 24. 26)

Laminar and turbulent systems with instantaneous reactions.
Tubular reactors with very fast reactions.

Reading Materials on Course Web Page:

Week 8. (Mar. 3, 5)

Transport effects in heterogeneous gas-solid catalytic reactions.
Particle scale effects, packed beds and fluidized beds.

Reading Material: Selected chapters in the Omnibook
Transport effects in Heterogeneous …in ChE 471, ChE 512

Week 9. (Mar. 10, 12) ***SPRING BREAK***

Week 10. (Mar. 17, 19)

Transport effects in reactions of solids particles. Particle scale and reactor scale modeling. Aerosol reactors.
Regenerative adsorption and breakthrough curves.

Reading Material: Chapter 11 in ChE 505.
Selected supplementary material from ChE 512.

Week 11. (Mar. 24, 26)

Transport effects in gas-liquid and gas-liquid-solid systems.
Meso-scale and reactor scale considerations.

Reading Material: Selected chapters in the Omnibook.
Ch 13 on Gas Liquid Systems in ChE 505

Week 12. (Mar. 31, Apr.2)

Biochemical reaction engineering

Reading Material: Chapter 14 in ChE 505
Selected chapters in the Omnibook.

Week 13. (Apr. 7, 9)

Photochemical reaction engineering.

Reading Material: Chapter 15 in ChE 505.

Week 14. (Apr. 14, 16)

Electrochemical reaction engineering.

Reading Material: Chapter 16 in ChE 505.

Week 15. (Apr. 21, 23)

Miscellaneous topics, reviews and project presentations

Final Exam.

Wednesday, May 6, 6:00- 8:00 PM   GREEN L0159

COURSE NOTES

The course notes consist of the lectures and chapters from various sources (e.g. reaction engineering courses such asChE471, EEC 505, ChE 512, EECE 503, etc)posted on the course web page: http://classes.engineering.wustl.edu/eece503/

Homework assignments and additional materials will be posted on the site and students will be notified by e-mail of the postings.of the postings.

GRADING POLICY

Grades will be based on two exams during the semester, weekly homework, occasional quizzes, a short team project (term paper), and on the comprehensive final exam of key concepts. The project will be done in groups of two to maximum three students and will consist of a written report and an oral presentation.

The weights given to the above items towards the overall grade are as follows:

Exams 1 and 2: 25% each = 50%
Final Exam: = 25%
Homework   and quizzes = 10%
Project report (oral and written) = 15%

Dates of the exams will be announced at least a week ahead of time and will be posted on the course web site.

The students are expected (on a 100 basis) to achieve a grade of 80 or better if they aspire to a course grade of B or better.

If in the first attempt they fail to achieve 80 or better they may be given another chance! (Only two trials will be allowed).

Homework assignments will be distributed usually on Tuesday and collected on the day they are assigned for. One can expect about 10 to 12 homework assignments in the course. Homework will be graded by the TA and all questions regarding the homework grade should be directed to the TA. **Students are encouraged to work in groups on setting up the homework solutions but individual submission is required except for the term project.**

Exams must represent individual effort only.

Term paper (project) will demonstrate the students' ability to work effectively in a team and present results after a time period of finite duration assigned to the project.