# CHE 527: Advanced Chemical Reaction Engineering

## Spring 2022 Course Syllabus

**Instructor**

Prof. Meenesh R. Singh
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Office Hours – W 4:15 pm – 5:15 pm

**Course Email Address**

All the questions, and concerns related to the course can be sent directly to the instructor with the subject line starting with [CHE 527]

**Lectures**

M W, 03:00 – 04:15 PM on Blackboard Collaborate

**Course Description**

Chemical reaction engineering, almost exclusively the domain of chemical engineers, has been an area of particularly vigorous research activity. It comprises a complex medley of different disciplines and there is little wonder that widely varying treatments are available of the subject. Broadly, however, the behavior of chemical reactors is intimately related to the interplay of physical and chemical rate processes in various reactor settings. The investigation of chemical reactors involves a *synthesis* of information pertaining to the chemical reacting system such as kinetics (reaction rate expressions), thermodynamics (equilibrium compositions, heat of reaction etc.) and those relating to pertinent physical rate processes (momentum, heat and mass transfer). The basic conservation principles (conservation of mass, momentum and energy) appended by appropriate phenomenological descriptions of physical processes (e.g., Fourier's law of heat conduction) and economic considerations will govern suitable mathematical models often admixed with some empiricism and by profuse applications of relevant mathematical techniques.

A unified treatment of chemical reaction engineering is complicated by at least two sources of divergent behavior. Naturally, the diversity of chemically reacting systems would be inherited by the reactors in which reactions are carried out. Furthermore, reaction equipment in themselves cover a wide variety such as stirred tank, packed bed, moving bed, fluidized bed, trickle bed and other types of reactors in which the relative role of physical and chemical rate processes may be profoundly different. In the face of such diversity, it should be evident that *general* results on reactor behavior or design prescriptions are not to be found. However, the divergent features of chemical reaction engineering have been presented in a proper perspective by Aris. The student is urged to develop an appreciation for this "morphological view" of the subject to understand clearly the roles and relationships of the different forms of activity in reaction engineering.

**Recommended Text**:

There has been an increasing number of books on reaction engineering analysis in recent times with widely varying directions of emphasis. This course will use my Class Notes in which we will refer to research articles and various sections in the following books**:**

1. ***Chemical Reaction Engineering***, by D. Ramkrishna (**DR**) (Unpublished Book)
2. ***Chemical Reactor Analysis and Design,*** by G. Froment, K. B. Bischoff, Juray De Wilde, 3rd Edition: John Wiley & Sons, 2010. **(FBD):** *This book presents a wide range of topics in reactor analysis***.** *While primary reliance is made on my lecture notes, I will try to relate lecture material to reading assignments from appropriate sections in the text book FBD*.
3. ***Chemical Reactor Theory. A Review,*** Edited by L. Lapidus and N. R. Amundson, Prentice-Hall, 1977. **(LA)**: *This contains several articles on various aspects of reaction engineering.*
4. ***Elementary Chemical Reactor Analysis****,* by R. Aris, Dover Publications, 2000 (**RA**) This book contains an excellent treatment of stoichiometry and the implications of the law of mass action to the algebraic treatment of chemical reactions, stability and sensitivity of continuous reactors, and optimization problems connected with reactor design.

The following outline of the course is tentative but generally represents the direction of emphasis. Numbers in parenthesis refer to related sections in the books mentioned above. Other references will be provided as we progress in the course.

**Topics to be Covered**

1. Basic Concepts in Chemical Kinetics (Notes)
2. Kinematics of Reaction (DR, RA- Ch. 2, 3)
3. Dynamic Modeling of Chemical Reactors (DR, FBD- 7.1, 7.2)
4. Biochemical Reaction (DR, FBD 1.5)
5. Enzyme-Substrate Kinetics (DR, FBD 1.5)
6. Polymerization Kinetics (DR, LA 9)
7. DeDonder Analysis of Reaction Mechanism (Article)
8. Microkinetic Modeling and Reduction of Mechanism (Notes)
9. Lumping of Rate Expressions (DR)
10. Fundamental Theories of Chemical Reactions (FBD- 1.7)
11. Experimental Estimation of Rate Parameters (DR, FBD, Notes)
12. Review of Experimental Methods to Measure Rate Parameters (Notes)
13. Microscopic Balances, Transport Effects in Hetrogeneous Catalysis (DR)
14. Transport Effects in Non-Catalytic Reactors- Solid-Gas and Gas-Liquid Reactors (DR)
15. Averaged Macrscopic Balances of Chemical Reactors (DR)
16. Residence Time Analysis (DR)
17. Stability Analysis of Chemical Reactors (DR)
18. Advanced Reactor Modeling
    a. Multiphase Reactors- Precipitation Reactors (Notes)
    b. Electrochemical Reactors (Notes)
    c. Fluidized Bed Reactor (Notes)

**Grading Scheme:**

The course grade will be evaluated based on the performance in homework assignments, mid-semester examination, computer exam, and final examination. The weightage for each component towards your final score is-

***i) Homework Assignments* - 20%**: There will be a total of 6 homework assignments in this course.

***ii) Weekly Quiz* - 10%**: There will be no more than 15 weekly quizzes in this course.

***iii) Active Participation - 5%:*** Turn ON your camera pointing at your face (during virtual classes) and be physically present (during in-person classes) to receive active participation points.

***ii) Mid-semester Exam-1* – 20%**: This will be an open book, and open notes exam. Scheduled on ***Wednesday, March 2nd.***

***iii) Mid-Semester Exam-2* – 20%*:*** This will be an open book, and open notes exam. Scheduled on ***Monday, April 4tht.***

***iv) Final Exam* – 25%**: This will be an open book, and open notes exam. Scheduled on ***TBD.***

The minimum points required for different grades are-

**Grade A**: > 80

**Grade B**: > 70

**Grade C:** > 60

**Grade D**: < 60