ChE 331: Kinetics and Reactor Design I

Fall: 2022-23 II **Class: MWF 9 – 10 AM in L1 (LHC)**

Syllabus:

(1) **Overview of chemical reaction engineering**: - definitions, nomenclature, notations, types of reaction, introduction to reactor design, types of reactors (batch vs flow, constant volume vs pressure)
(2) **Kinetics of homogeneous reactions**: Rate expression, temperature and concentration dependence of rate, search for a reaction mechanism.
(3) **Batch reactor**: Constant vs variable volume, interpretation of batch data for zeroth, 1st, 2^{nd} , and nth order reactions, half-life, irreversible and reversible reactions, series and parallel reactions.
(4) **Flow reactors** (Mixed flow vs plug, semi-batch reactors): Reactor design (size), performance equation, graphical representation, size comparison of reactors, multiple reactor systems (reactors in series and parallel), recycle reactor, autocatalytic reactions.
(5) **Parallel reactions**: selectivity, fractional yield, product distribution.
(6) **Series reactions**: Product distribution and maximization of yield, Denbigh reactions, qualitative description of series-parallel reactions.
(7) **Non-isothermal reactions**: Thermodynamics of a reversible reaction, equilibrium conversion vs equilibrium constant, reactor design for exothermic and endothermic reaction, optimal progression for an exothermic reaction, adiabatic and non-adiabatic operation, multiplicity
(8) **Non-ideal flow reactors**: Segregated vs non-segregated flow, residense time distribution, tank in series model, dispersion model.
(9) **Fluid-particle non-catalytic reactions:** Shrinking Core models for kinetics, diffusion (film) and ash layer control reactions, conversion vs time expressions, fluidized bed reactor
(10) **Catalytic reactions:** Characterization; Langmuir-Hinshelwood models, Diffusion and reaction in porous catalysts.

Text book: *Chemical Reaction Engineering* (**3rd ed,** Wiley) by Octave Levenspiel.
Reference books: (1*) Chemical Engineering Kinetics* (1981, McGraw) by J. M. Smith (recommended for introductory part, recycle reactors, non-ideal flow reactors, RTD)
(2) *Elements of Chemical Reaction Engineering* (2^{nd} ed, Prentice Hall) by Scott Fogler (recommended for chapters on multiplicity, non -catalytic solid-fluid reactions)

Marks distribution:
(1) Mid-term - 30
(2) End-term - 35
(3) Quizzes – 2 x 10 (only on Saturday)
(4) Homework including computer assignment: 15
(Attendance minimum 90%)