CHBE 455: Chemical Kinetics & Reactor Design

The course covers fundamental concepts involved in the sizing and operation of batch, semibatch, continuous, plug flow and packed bed reactors. An analytical approach based on first principles is emphasized. The course is divided into 4 modules. The first module comprises introductory principles such as mole balances, stoichiometry, rate laws, thermochemistry, chemical equilibrium and derivation of rate laws. The second module introduces the different types of ideal reactors and instructs students about sizing reactors using concentrations and conversions. The third module introduces students to enzyme catalysis and elementary bioprocess engineering. The fourth module covers non-ideal reactor design and chiefly focuses on steady-state non-isothermal reactors and residence time distributions. Topics such as heat and mass transfer are also reviewed.

LEARNING OBJECTIVES

After the course, students will be able to:

- Explain the operating principles of different reactor types such as continuous stirredtank, plug-flow and batch reactors
- Derive the mathematical equations that govern the operation of different reactor types
- · Operate PFRs for gas-phase reactions
- Account for pressure drops in packed-bed reactors
- Non-dimensionalize reactor design problems through use of conversion and dimensionless numbers such as the Damköhler number
- Use numerical methods to solve system of ODEs that describe reactor performance
- Analyze reaction data to estimate rate parameters
- · Derive rate expressions for enzymes and use this information to size bioprocesses
- Model microbial growth in bioreactors
- Quantify the contribution of mass transport in reacting systems
- Account for molecular and macroscopic phenomena in the design a packed-bed reactor
- Perform energy balances on reacting systems to relate performance of the reactor to its operating temperature
- · Diagnose and model non-ideal mixing in a reactor

COURSE SCHEDULE

Lectures - 2 sessions of 80 minutes each week Tutorials - 1 session of 50 minutes each week

Week Description

- 1 History of chemical reaction engineering: The Haber-Bosch process Review of physical chemistry
- 2 Definition of reaction rate, rate constant, order Reaction stoichiometry
- 3 Mole balances Continuous-stirred tank reactors Plug-flow reactors
- 4 Conversion
 Reactors-in-series
 Levenspiel plots
- Gas-phase reactions in plug-flow reactors Pressure drops in packed-bed reactors Selectivity & yield

- **6** Analysis of rate data Numerical methods for solving reaction engineering problems
- 7 Fick's law of diffusion Convection Flux balances
- 8 Mass transport within reacting systems
 Design of a packed-bed reactor
- 9 Enzyme catalysis
 Michaelis-Menten equation
 Enzyme inhibition
- 10 Microbial growth Bioprocess design
- 11 Energy balances
 Non-isothermal reactors
- Heat exchangers and reactors Residence time distributions
- 13 Models for non-ideal mixing Course recap