ChemE 3900 - Chemical Kinetics & Reactor Design

Chemical Engineers design and analyze processes and products based on chemical change.

The chemical reaction is the essence of any chemical product.
The chemical reactor is the essence of any chemical process.

Reactor Design is the core of Process Design. Other units serve the reactor and/or treat the reactor output. The reactor dictates the type and size of other process units.

**Part 1 - Chemical Kinetics**

Reaction Coordinate Energy Level Diagrams
  - Thermodynamics vs. Kinetics

Rate Equations from Experimental Data
  - Method of Initial Rates
  - Saturation Methods
  - Method of Half Lives

Rate Constants and Activation Energies from Experimental Data
  - Arrhenius Plots

Rate Equations from Mechanisms of Elementary Reactions
  - Reactive Intermediates - the usual suspects
  - Steady-State Approximation
  - Pre-equilibrium Approximation
  - Rate-Limiting Step

Special Classes of Reactions
  - Chain Reactions
  - Photo-initiated Reactions
  - Polymerization
  - Homogeneous Catalysis - Enzymes
  - Heterogeneous Catalysis - Solid Acids and Transition Metals
  - Autocatalysis (if time permits)
  - Reactions in Solutions (if time permits)
Part 2 - Reactor Design

Thermodynamics of Chemical Reactions
  heat of reaction
  chemical equilibrium

Isothermal Reactors
  one chemical reaction
  multiple chemical reactions

Non-isothermal Reactors

Non-ideal Reactors

Multiphase Reactors

Ancillary Skills

Mathematical Modeling & Graphical Modeling
  How to translate a chemical description into equations and graphs

Approximation
  How to identify dominant effects and estimate the consequences of neglecting secondary effects.

Evaluation
  How to test assumptions and assess predictions.

Numerical Methods
  Numerical Integration
  Statistical methods - linear regression and least-squares fits
  Finite elements

Analytical Concepts
  Rate constants and time constants
  Residence times and residence time distributions
Weekly Quizzes?

**Advantages**

- Promotes steady learning.
- Decreases the weighting of evening exams.
- Prefaces Prelim Problems.
- Promotes attendance in Calculation Sessions.

**Disadvantages**

- Requires attendance in Calculation Sessions.
  - Quizzes are inherently abhorrent.
Quizzes or No Quizzes?

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<th>Option A</th>
<th>Option B</th>
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<td>Quizzes</td>
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<td>Computing Modules</td>
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- You may choose Option A or Option B.
  You must choose Monday, 1/30.
  The default is Option B - take Quizzes.

- Calculation Session will begin with a Question & Answer period. **Questions must be submitted in advance.**

- After all questions are answered, the quiz will be distributed.

- Quizzes will be designed for a mean of 8 out of 10.