A First Course on Kinetics and Reaction Engineering

Class 22 on Unit 21

Where We're Going

- Part I - Chemical Reactions
- Part II - Chemical Reaction Kinetics
- Part III - Chemical Reaction Engineering
  - A. Ideal Reactors
  - B. Perfectly Mixed Batch Reactors
  - C. Continuous Flow Stirred Tank Reactors
    - 21. Reaction Engineering of CSTRs
    - 22. Analysis of Steady State CSTRs
    - 23. Analysis of Transient CSTRs
    - 24. Multiple Steady States in CSTRs
  - D. Plug Flow Reactors
  - E. Matching Reactors to Reactions
- Part IV - Non-Ideal Reactions and Reactors

Reaction Engineering with CSTRs

- Typically CSTRs are designed to operate most of the time at steady state
- Transient operation occurs whenever a reactor variable is changed
  - Start up and shut down are examples of transient operation
- Factors that favor CSTRs
  - Liquid phase reaction
  - Large quantities of reactant to be processed
  - Exothermic reactions
  - Reactions with “unusual” kinetics
    - Reactant inhibited reactions
    - Auto-catalytic reactions
  - Cold feed and exothermic reaction (auto-thermal operation)
    - Feed is heated due to being mixed directly into the hot reactor contents; no need for a separate heat exchanger
- Disadvantages
  - For reactions with “typical” kinetics, the rate of reaction is low throughout the process
    - Due to mixing, reactant concentration is low and product concentration is high
    - Need larger reactor volume (compared to batch or plug flow reactor)
  - Not well-suited to gas phase reactions because gases are hard to “stir.”

Qualitative Analysis of CSTRs

- Steady state CSTRs are fundamentally different from batch reactors
  - The composition and temperature change during the time that reaction occurs in a batch reactor
    - The amount of time reaction occurs is controlled directly
  - The composition and temperature are constant during the time that reaction occurs in a steady state CSTR
    - The amount of time reaction occurs is controlled by changing the flow rate
    - On average, the reaction occurs for a time equal to the space time, τ
      - $\tau = \frac{V_{fluid}}{\dot{V}^0}$
- Qualitative analysis of CSTR
  - Conversion, concentration, temperature and other profiles as a function of space time behave similar to profiles for batch reactors as a function of processing time
  - When comparing to batch reactors at processing times equal to the CSTR space time
    - Concentrations and temperature change during the time the fluid is reacting in a batch reactor
    - Concentrations and temperature are constant during the time the fluid is reacting in a CSTR
      - Their values are the final values; i. e. the reactant concentration is low and the product concentration is high
      - In an adiabatic reactor, the temperature is the final value; higher for exothermic reactions and lower for endothermic reactions

Questions?

Activity 21.1

- The handout for Activity 21.1 lists 10 problems, each involving a CSTR
- Read through each problem and
  - Determine whether it calls for the analysis of a steady state CSTR or a transient CSTR
  - If you decide a problem involves a transient analysis, justify your response by identifying at least one reactor variable that will change over time

Activity 21.1

- Question 1: steady state
- Question 2: transient
  - The outlet cell mass, among other things, will vary over time
- Question 3: transient
  - The outlet concentrations of all reagents will vary over time
- Question 4: steady state
- Question 5: steady state
- Question 6: transient
  - The reactant concentrations leaving the reactor will vary over time
- Question 7: steady state
  - The outlet concentration of Z will not vary with time
- Question 8: steady state
- Question 9: transient
  - The outlet concentrations of reactants and products will vary over time
- Question 10: transient
  - The outlet temperature will vary over time

Predicting Qualitative CSTR Behavior

- Open the Adiabatic CSTR Simulator
  - Without changing any of the inlet settings, click start experiment and then add experiment to data set to create a base case
- Go through the inlet settings one by one
  - Predict how the outlet temperature and concentration will change if the setting is increased/ decreased
  - Then run the simulator to check your prediction
  - If your prediction was incorrect, make sure you understand why

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