

Lecture # 20 CHE331A

Introduction:
Importance of
CRE and Definition
of rate

Design equation for
Ideal Reactors,
Levenspiel plots, and
multiple reactors

Basic concepts in
Chemical Kinetics:
Types of reactions,
rate and equilibrium
constants

Isothermal Reactor Design:
Batch, Mixed flow, PFR/PBR,
in terms of conversion,
concentration and molar
flowrates

Collection and Analysis of
Rate Data: Constant and
variable volume; differential
and integral methods; half-
life and initial rates;
differential reactors

Design of isothermal
reactors for multiple
reactors: selectivity/yield;
series/parallel/complex
reactions; best operating
conditions

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Basic Design/Analysis steps of reactors

- ▶ Mole Balance Equation for the specific reactor
- ▶ Rate Law for the reaction(s)
- ▶ Use collection and analysis of rate data for determining rate law and its constants
- ▶ Reaction stoichiometry – single and multiple
- ▶ Form design/analysis equation in terms of conversion, concentration or molar flow rates
- ▶ Solve differential equation(s) to design/analyze reactors



Summary of Week 6

- ▶ Non elementary reactions and non-integer rate laws
- ▶ Reaction mechanisms of some non-elementary reactions
 - Active Intermediate
 - Pseudo-Steady-State-Hypothesis (PSSH)
- ▶ Chain Reactions
 - Thermal cracking of ethane
- ▶ Enzymatic Reactions
 - Michaelis-Menten Kinetics
 - Constants K_M and V_{\max}



Post Mid-Sem Course contents

- ▶ Non – Isothermal reactors 6 lectures
- ▶ Non – Ideal flow 4 lectures
- ▶ Catalysis 2 lectures
- ▶ Kinetics of Catalytic Reactions 3 lectures
- ▶ Diffusion and Reaction in Porous Catalysts 5 lectures
- ▶ 20 lecture and 6 weeks!
- ▶ Reduce the portion and make it to 17-18



Non-isothermal reactors

- ▶ Energy balances for reactors
 - Batch
 - Mixed flow
 - PFR/PBR
- ▶ Adiabatic reactors
- ▶ Non-adiabatic reactors
- ▶ Multiple reactors and inter-stage cooling
- ▶ Multiple steady-states



Most reactions are not carried out isothermally

► For example, an adiabatic liquid-phase reaction $A \rightarrow P$ in a PFR

► $F_{A0} \frac{dX}{dV} = -r_A$ first order reaction: $-r_A = kC_A$ and $C_A = C_{A0}(1 - X)$

$$\frac{dX}{dV} = \frac{kC_A}{\dot{v}_0 C_{A0}} = \frac{k}{\dot{v}_0} (1 - X)$$

► $k = A \cdot \exp\left(-\frac{E}{RT}\right)$ OR $k = k_1 \cdot \exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$

$$\frac{dX}{dV} = \frac{kC_A}{\dot{v}_0 C_{A0}} = \frac{k}{\dot{v}_0} (1 - X) \rightarrow \frac{dX}{dV} = \frac{k_1}{\dot{v}_0} (1 - X) \exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$$

► To determine ' V ' the relationship $T = T(X)$ or $T = T(V)$ is required

► These relationships are provided by Energy Balance



Energy balance done as per ESO201A

- ▶ $\sum_{inlet} \dot{E} - \sum_{outlet} \dot{E} + \dot{Q} - \dot{W} = \frac{d(E)_{CV}}{dt}$ $\dot{E} = \frac{\text{Enthalpy}}{\text{per unit time}} = \dot{H}$
- ▶ Further, \dot{W} is not often significant in Chemical Processes and $\dot{W} = 0$
- ▶ Steady state and adiabatic operation, $\frac{d(E)_{CV}}{dt} = 0$ and $\dot{Q} = 0$
- ▶ Thus, $\sum_{inlet} \dot{H} - \sum_{outlet} \dot{H} = 0$
- ▶ For this reaction we will see that: $T = T_0 + \frac{-\Delta H_{Rxn} \cdot X}{C_{PA}}$ which is $T = T(X)$
- ▶ This along with the mol balance equation can then be used to determine the volume of the reactor to achieve a particular conversion

