Chemical Reaction Engineering I

Chapter 1
Mole Balance and Kinetics

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Chapter Description

Aims

- Formulate the rate of reactions for elementary reactions
- Define the Rate Law

Expected Outcomes

- Describe on the concepts of rate of reactions
- Explain about the chemical kinetics, emphasizing definitions and able to relate on how the reaction rate depends on the concentrations of the reacting chemicals.

References & other information

- Elements of Chemical Reaction Engineering’, by H. Scott Fogler

Subtopics

1.1 Reaction Kinetics and Data Analysis

1.2 General mole balance equations

1.3 Introduction to conceptual design

Reaction Kinetics and Data Analysis

- Rate of reaction
  - r_A → the no. of moles reacting (A) per unit time per unit volume (mol/dm^3 . s)
  - r_A' → the no. of moles A per unit time per unit catalyst mass (mol/ s . g $_{catalyst}$)
- Unit : mol/dm^3/s
- Can be expressed in terms of (sign convention):

  i. The rate of disappearance of a substance, $-r_A$

  ii. The rate of formation of the substance, r_A

Reaction Kinetics and Data Analysis

- The reaction kinetics are formulated based on experimentally proven mechanism, not an arbitrary phenomenon

- Rate law is the simplest model, for instance:

$$A \rightarrow \text{Products}$$

  The rate of transformation of A can be:-

  1. Linear function of concentration; or

$$-r_A = kC_A$$

  2. Quadratic function of concentration; or $-r_A = kC_A^2$

- Other function of concentration, such as $-r_A = k_1C_A/(1+k_2C_A)$ etc

Relation of Rate in Reaction

- For a reaction given below:

*a*A + *b*B → *c*C + *d*D

$$\frac{r_A}{-a} = \frac{r_B}{-b} = \frac{r_C}{c} = \frac{r_D}{d}$$

- Example:

$2NO + O_2 \rightarrow 2NO_2$

$$\frac{r_{NO}}{-2} = \frac{r_{O_2}}{-1} = \frac{r_{NO_2}}{2}$$

Rate Law

- Consider the following reaction:

  aA + bB → cC + dD

  The rate law may be written as : $-r_A = [k_A(T)][fn(C_A, C_B, ...)]$

  e.g; $$-r_A = kC_A^{\alpha} C_B^{\beta}$$

where k = specific reaction rate

α = order with respect to A

β = order with respect to B

α+β = overall order

- What happen if
  1. **α = a and β = b**
  2. **α ≠ a and β ≠ b**

Elementary Rate Law

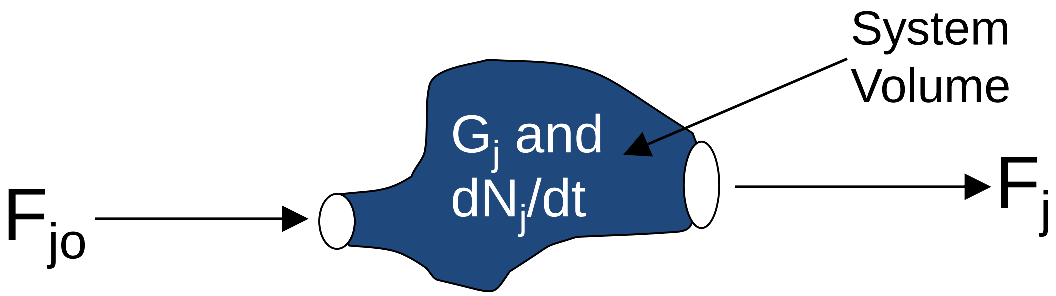
- Stoichiometry coefficients = individual reaction order of each species.
- $H_2 + I_2 \rightarrow 2HI$

  $(r_{HI}) = k\, C_{H2}\, C_{I2}$

Non-elementary Rate Law

- CO+CI2→COCI2
- This rxn is 1st order with respect to CO, 3/2 order with respect to CI2 and 5/2 order overall.

General Moles balance Equation



$$\begin{bmatrix} \text{Rate of flow} \\ \text{into the system} \end{bmatrix} - \begin{bmatrix} \text{Rate of flow} \\ \text{out of the system} \end{bmatrix} + \begin{bmatrix} \text{Rate of generation} \\ \text{by chemical reaction} \\ \text{within the system} \end{bmatrix} = \begin{bmatrix} \text{Rate of} \\ \text{accumulation} \\ \text{within the system} \end{bmatrix}$$

$$F_{jo} - F_j + G_j = \frac{dN_j}{dt}$$

Design Equation for Batch Reactor

Batch

$$\frac{dN_A}{dt} = r_A V$$

$$t = \int_{N_{AO}}^{N_j} \frac{dN_A}{(r_A)V}$$

Limiting reactant

$$X = \frac{N_{A0} - N_A}{N_{A0}}$$

$$-N_{A0}\frac{dX}{dt} = (r_A)V$$

$$t = \int_0^X \frac{N_{A0}}{V}\frac{dX}{(-r_A)}$$

Design Equation for Continuous Reactors

CSTR $V = \frac{F_{A0} - F_A}{-(r_A)}$

PFR $\frac{dF_A}{dV} = r_A V = \int_{F_{AO}}^{F_A} \frac{dF_A}{(r_A)}$

PBR $\frac{dF_A}{dW} = r'_A W = \int_{F_{AO}}^{F_A} \frac{dF_A}{(r'_A)}$

Limiting reactant →

$X = \frac{F_{A0} - F_A}{F_{A0}}$

$$V = \frac{F_{A0}X}{-r_A}$$

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}}$$

$$V = \int_0^X F_{A0} \frac{dX}{-r_A}$$

$$\frac{dX}{dW} = -\frac{r_A{}'}{F_{A0}}$$

$$W = \int_0^X F_{A0} \frac{dX}{-r_A{}'}$$

Mole Balance for Reactive Unit

- GENERAL

$$F_{j0} - F_j + r_j V = \frac{dN_j}{dt}$$

- Stirred Tank Reactor (STR)

$$F_{A0} - F_A + r_A V = \frac{dN_A}{dt}$$

→ Batch?

→ Continuous (CSTR)?

- Tubular Reactor

$$F_A\big|_V - F_A\big|_{V+\Delta V} + r_A \Delta V = \frac{dN_A}{dt}$$

→ Plug Flow?

→ Packed-Bed?

Authors Information

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