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Chemical Reaction Engineering I

Chapter 4
Isothermal Reactor Design

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Chapter Description

Synopsis

This chapter describes the chemical reaction engineering algorithm for isothermal reactor design in order to solve chemical reaction engineering problems.

Expected Outcomes

- Describe the CRE algorithm that can be used to solve chemical reaction engineering problems through logic rather than memorization.
- To be able to do sizing of batch reactors, semi-batch reactors and other continuous reactors; CSTRs, PFRs and PBRs for isothermal operation given the rate law and feed conditions.

References & other information

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

Subtopics

- 4.1 CRE Design Algorithm
- 4.2 PBR with Pressure Drop
- 4.3 Unsteady State Operation of Reactors
- 4.4 Algebraic Formulation in Conceptual Design

Useful Definitions

Reaction: $A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$

1. Parameter Θ

$$\Theta_i = \frac{N_{i0}}{N_{A0}} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}}$$

2. Net mole change for the reaction

$$\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$$

3. Relationship between 'δ' and initial mole fraction of A

$$\varepsilon = \frac{\text{Change in total number of moles when complete conversion of A is attained}}{\text{Total number of moles of all species fed to the reactor}}$$

$$\varepsilon = \frac{N_{AO}}{N_{TO}}\delta = y_{A0} \cdot \delta$$

$\Rightarrow$

$$\frac{N_T}{N_{TO}} = \frac{N_{T0} + \delta \cdot X \cdot N_{A0}}{N_{T0}} = 1 + \varepsilon \cdot X$$

Pressure Drop in Reactor

- P/P_0 = f(Volume, V) or f(catalyst weight, W)
- Majority gas phase reactions happened in a packed bed reactors (packed with catalyst particles). The pressure drop can be calculated using Ergun Eqn.:

$$\frac{dP}{dz} = -\frac{G}{\rho g_C D_P}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)\mu}{D_P} + 1.75G\right]$$

$$\rho = \rho_0 \frac{P}{P_0}\left(\frac{T_0}{T}\right)\frac{F_{T0}}{F_T}$$

$$\frac{dP}{dz} = -\frac{G}{\rho_0 g_C D_P}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)\mu}{D_P} + 1.75G\right]\frac{P_0}{P}\left(\frac{T}{T_0}\right)\frac{F_T}{F_{T0}}$$

Pressure Drop in Reactor

- Analyze the second order gas phase reaction occurring isothermally in a PBR: A → B

- Define the mole balance

- Rate law, $$-r_A' = kC_A^2$$

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

- Combine, $$C_A = C_{A0}\left(\frac{1-X}{1+\varepsilon X}\right)\frac{P}{P_o}$$

Need to find (P/P_0) as a function of W (or V if you have a PFR).

$$\frac{dX}{dW} = \frac{kC_{A0}^2}{F_{A0}}\frac{(1-X)^2}{(1+\varepsilon X)^2}\left(\frac{P}{P_0}\right)^2$$

Pressure Drop in Reactor

$$\text{Given } \beta_0 = \frac{G(1-\phi)}{\rho_0 g_c D_P \phi^3}\left[\frac{150(1-\phi)\mu}{D_P} + 1.75G\right]$$

$$\frac{dP}{dz} = -\beta_0 \frac{P_0}{P}\left(\frac{T}{T_0}\right)\frac{F_T}{F_{T0}}$$

ρ_b= bulk density
ρ_c= solid catalyst density
ϕ = porosity (void fraction)

- $W = (1-\phi)A_c z \rho_c$
- $y = P / P_0$
- $\alpha = \frac{2\beta_0}{A_c \rho_c (1-\phi) P_0}$

$$\frac{dy}{dW} = -\frac{\alpha}{2y}\frac{T}{T_0}\frac{F_T}{F_{T0}}$$

Pressure Drop in Reactor

- Further simplification yields:

$$\frac{dy}{dW} = -\frac{\alpha}{2y}\frac{T}{T_0}\frac{F_T}{F_{T0}}$$

Above Eqn. is for multiple reactions and reaction in a membrane reactor.

- For single reaction: $$\frac{dP}{dW} = -\frac{\alpha}{2}\frac{T}{T_o}\frac{P_o}{P/P_o}(1+\varepsilon X)$$

- For isothermal operation, T=T0 with ε = 0;

$$y = \frac{P}{P_0} = (1-\alpha W)^{\frac{1}{2}}$$

Unsteady State Operation of Reactors

<u>Start-up of a CSTR</u>

- Always begin with the general mole balance equation:

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

- For 1st-order reaction in liquid phase with constant overflow:

$$\frac{dC_A}{dt} + \frac{1+\tau k}{\tau} C_A = \frac{C_{A0}}{\tau}$$

- which solves to

$$C_A = \frac{C_{A0}}{1+\tau k}\left\{1 - \exp\left[-(1+\tau k)\frac{t}{\tau}\right]\right\}$$

Unsteady State Operation of Reactors

- Letting t_s be time necessary to achieve 99% of the steady-state concentration:

$$C_{AS} = \frac{C_{A0}}{1+\tau k}$$

- For slow reactions:

$$t_s = 4.6\tau$$

- For rapid reactions:

$$t_s = \frac{4.6}{k}$$

Authors Information

Credit to the authors:

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