

Chemical Reaction Engineering I

Chapter 4 Isothermal Reactor Design

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Isothermal Reactor Design by Sureena

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

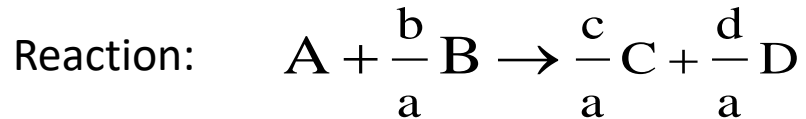
4.2 PBR with Pressure Drop

4.3 Unsteady State Operation of Reactors

4.4 Algebraic Formulation in Conceptual Design



Useful Definitions



1. Parameter Θ

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

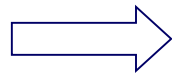
2. Net mole change for the reaction

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

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

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

$$\varepsilon = \frac{N_{A0}}{N_{T0}} \delta = y_{A0} \cdot \delta$$



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



Pressure Drop in Reactor

- $P/P_0 = f(\text{Volume}, V)$ or $f(\text{catalyst weight}, W)$
- 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: $A \rightarrow B$

- Define the mole balance

$$-r'_A = kC_A^2$$

- Rate law,

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

- Stoichiometry,

- Combine,

$$C_A = C_{A0} \left(\frac{1-X}{1+\epsilon X} \right) \frac{P}{P_0}$$

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

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

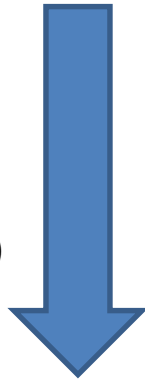


Pressure Drop in Reactor

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

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

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:

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

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

- For single reaction:
$$\frac{dP}{dW} = -\frac{\alpha T}{2 T_0} \frac{P_0}{P/P_0} (1 + \varepsilon X)$$

- For isothermal operation, $T=T_0$ with $\varepsilon = 0$;

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



Unsteady State Operation of Reactors

Start-up of a CSTR

- 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

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