CH EN 3553 Chemical Reaction Engineering

Some Design Equations

Ideal Batch Reactor

General Design Equation:

$$-r_A V = N_{A0}\frac{dX_A}{dt}$$

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

$$t = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)} = -\int_{C_{A0}}^{C_A}\frac{dC_A}{(-r_A)} \quad \text{for} \quad \varepsilon_A = 0$$

$$t = N_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)V_0(1+\varepsilon_A X_A)} = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)} \quad \text{for any } \varepsilon_A \neq 0$$

Flow Reactors

$$\tau = \frac{V}{v_0} = \frac{C_{A0}V}{F_{A0}}$$

Ideal PFR – Steady State

$$-r_A V = F_{A0}dX_A$$

$$\tau = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)} = \frac{C_{A0}V}{F_{A0}} \quad \text{for any } \varepsilon_A$$

$$\tau = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)} = -\int_{C_{A0}}^{C_A}\frac{dC_A}{-r_A} \quad \text{for } \varepsilon_A = 0$$

Ideal CSTR – Steady State

$$\tau = \frac{V}{v_0} = \frac{VC_{A0}}{F_{A0}} = \frac{C_{A0}X_A}{-r_A} \text{ for any } \varepsilon_{\text{A}}$$

$$\tau = \frac{V}{v_0} = \frac{VC_{A0}}{F_{A0}} = \frac{C_{A0}(X_{Af} - X_{Ai})}{(-r_A)_f} \text{ for any } \varepsilon_{\text{A}} \text{ and different inlet and outlet conversions}$$

$$\tau = \frac{V}{v} = \frac{C_{A0}X_A}{-r_A} = \frac{C_{A0} - C_A}{-r_A} \text{ for } \varepsilon_A = 0$$

Batch Reactor Equations

No volume change; $\varepsilon_A = 0$

$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)} = -\int_{C_{A0}}^{C_A} \frac{dC_A}{(-r_A)} \quad \text{for} \quad \varepsilon_A = 0$$

Zero Order

$$n = 0, \quad -r_A = k$$

$$\boxed{k \cdot t = C_{A0} - C_A = C_{A0} X_A}$$

First Order

$$n = 1, \quad -r_A = k \cdot C_A$$

$$t = -\int_{C_{A0}}^{C_A} \frac{dC_A}{(-r_A)} = -\int_{C_{A0}}^{C_A} \frac{dC_A}{k \cdot C_A}$$

$$\boxed{k \cdot t = \ln \frac{C_{A0}}{C_A} = \ln \frac{1}{(1 - X_A)}}$$

Second Order

$$n = 2, \quad -r_A = k \cdot C_A^2$$

$$t = -\int_{C_{A0}}^{C_A} \frac{dC_A}{(-r_A)} = -\int_{C_{A0}}^{C_A} \frac{dC_A}{k \cdot C_A^2}$$

$$\boxed{k \cdot t = \frac{C_{A0} - C_A}{C_{A0} C_A} = \frac{X_A}{(1 - X_A)} \frac{1}{C_{A0}}}$$

n^{th} Order

$$n = n, \quad -r_A = k C_A^n$$

$$\boxed{k \cdot t \cdot (n-1) C_{A0}^{n-1} = \left(\frac{C_A}{C_{A0}} \right)^{1-n} - 1 = (1 - X_A)^{1-n} - 1}$$

First order reversible, $A \underset{k_2}{\overset{k}{\rightleftarrows}} B$, only pure A entering the reactor

First, find the equilibrium conversion

$$K_e = \frac{C_B}{C_A} = \frac{C_{A0} X_e}{C_{A0}(1-X_e)} = \frac{X_e}{1-X_e} \Rightarrow \frac{1}{K_e} + 1 = \frac{1}{X_e}$$

Rate: $-r = k(C_A - \frac{C_B}{K_e}) = kC_{A0}\left((1-X) - \frac{X}{K_e}\right) = kC_{A0}\left(1 - X(1+\frac{1}{K_e})\right)$

$$-r = kC_{A0}\left(1 - \frac{X}{X_e}\right)$$

$$t = C_{A0}\int_0^{X_A} \frac{dX}{(-r)} = C_{A0}\int_0^{X} \frac{dX}{kC_{A0}(1-\frac{X}{X_e})}$$

$$kt = \int_0^{X} \frac{dX}{(1-\frac{X}{X_e})}$$

Use the integral

$$\int \frac{dx}{1-ax} = -\frac{1}{a}\ln(ax-1)$$

$$\boxed{k \cdot t == X_{Ae} \ln\left(\frac{X_e}{X_e - X}\right) = \left(1 - \frac{C_{Ae}}{C_{A0}}\right)\ln\left(\frac{C_{A0} - C_{Ae}}{C_A - C_{Ae}}\right)}$$

Plug Flow Reactor

No volume change; $\varepsilon_A = 0$

$$n = 0, \quad -r_A = k$$

$$k \cdot \tau = C_{A0} - C_A = C_{A0} X_A$$

$$n = 1, \quad -r_A = k \cdot C_A$$

$$k \cdot \tau = \ln \frac{C_{A0}}{C_A} = \ln \frac{1}{(1 - X_A)}$$

$$n = 2, \quad -r_A = k \cdot C_A^2$$

$$k \cdot \tau = \frac{C_{A0} - C_A}{C_{A0} C_A} = \frac{X_A}{(1 - X_A)} \frac{1}{C_{A0}}$$

$$n = n, \quad -r_A = k C_A^n$$

$$k \cdot \tau \cdot (n-1) C_{A0}^{n-1} = \left(\frac{C_A}{C_{A0}} \right)^{1-n} - 1 = (1 - X_A)^{1-n} - 1$$

First order reversible, $A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B$, only pure A entering the reactor

$$k_1 \cdot \tau = \left(1 - \frac{C_{Ae}}{C_{A0}} \right) \ln \left(\frac{C_{A0} - C_{Ae}}{C_A - C_{Ae}} \right) = X_{Ae} \ln \left(\frac{X_{Ae}}{X_{Ae} - X_A} \right)$$

CSTR

No volume change; $\varepsilon_A = 0$

$n = 0, \quad -r_A = k$

$$k \cdot \tau = C_{A0} - C_A = C_{A0} X_A$$

$n = 1, \quad -r_A = k \cdot C_A$

$$k \cdot \tau = \frac{C_{A0} - C_A}{C_A} = \frac{X_A}{(1 - X_A)}$$

$n = 2, \quad -r_A = k \cdot C_A^2$

$$k \cdot \tau = \frac{C_{A0} - C_A}{C_A^2} = \frac{X_A}{(1 - X_A)^2} \frac{1}{C_{A0}}$$

$n = n, \quad -r_A = kC_A^n$

$$k \cdot \tau = \frac{C_{A0} - C_A}{C_A^n} = \frac{X_A}{(1 - X_A)^n} \frac{1}{C_{A0}^{n-1}}$$

First order reversible, $A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B$, only pure A entering the reactor

$$k_1 \cdot \tau = \left(\frac{(C_{A0} - C_A)(C_{A0} - C_{Ae})}{C_{A0}(C_A - C_{Ae})} \right) = \left(\frac{X_A X_{Ae}}{X_{Ae} - X_A} \right)$$

Volume Change Equations for Batch and PFR Same or Different?

Batch:

$$N_A = N_{A0}(1-X); \quad V = V_0(1+\varepsilon X)$$

$$-r_A V = N_{A0}\frac{dX_A}{dt}; -r_A = kC_A = k\frac{N_A}{V} = k\frac{N_{A0}(1-X)}{V_0(1+\varepsilon X)}$$

Substitute the rate expression:

$$k\frac{N_{A0}(1-X)}{V_0(1+\varepsilon X)}V_0(1+\varepsilon X) = N_{A0}\frac{dX_A}{dt}$$

Integrate

$$\underline{\underline{-\ln(1-X) = kt}}$$

Plug Flow Reactor

$$F_A = F_{A0}(1-X)$$

$$v = v_0(1+\varepsilon X)$$

$$F_{A0}dX = (-r_A)dV$$

$$F_{A0}dX = kC_{A0}\frac{(1-X)}{(1+\varepsilon X)}dV$$

$$\int_0^X \frac{(1-X)}{(1+\varepsilon X)}dX = k\frac{C_{A0}}{F_{A0}}V$$

$$(1+\varepsilon)\ln\frac{1}{(1-X)} - \varepsilon X = k\tau$$