Pressure Drop in Reactors

$C_i = \frac{F_i}{v} = \frac{F_{A0}(\Theta_i + \nu_i X)}{v_0(1+\varepsilon X)}\frac{P}{P_0}$ for isothermal reactors

For packed-bed reactors,

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

If we are considering the reaction, $A \rightarrow B$, which is first order

$$-r_A' = kC_A = \frac{kC_{A0}(1-X)}{(1+\varepsilon X)}\frac{P}{P_0}$$

$$\frac{dX}{dW} = \frac{kC_{A0}(1-X)}{(1+\varepsilon X)}\frac{P}{P_0}\frac{1}{C_{A0}v_0} = \frac{k(1-X)}{v_0(1+\varepsilon X)}\frac{P}{P_0}$$

$$\frac{dX}{dW} = f_1(X,P)$$

In this equation, conversion is a function of pressure. Hence, we need an additional relationship between pressure and conversion.

The additional relationship is obtained through the Ergun Equation

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

ϕ – Porosity

$(1-\phi)$ – Solid volume/total bed volume

ρ – Gas density

D_p – Particle diameter

μ – Viscosity of the fluid

z – Length along the reactor

u – Superficial velocity (volumetric flow/cross sectional area)

$G = \rho \cdot u =$ Mass flux = units ($\frac{\text{g}}{\text{cm}^2 - s}$)

This equation can be reduced to $\frac{dP}{dW} = f_2(X,P)$

For any flow reactor, $\dot{m}_0 = \dot{m}$

$$\rho_0 v_0 = \rho v$$

$$v = v_0 \frac{P_0}{P}\left(\frac{T}{T_0}\right)\frac{F_T}{F_{T0}} \quad \text{Ideal gas law}$$

$$\rho = \frac{\rho_0 v_0}{v} = \rho_0 \frac{P}{P_0}\left(\frac{T_0}{T}\right)\frac{F_{T0}}{F_T}$$

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

Substitute for ρ

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

Where,

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

Let $W = (1-\phi)A_C z \times \rho_c$

Bulk Density: $\rho_{\text{b}} = (1-\phi)\rho_c$

$$\frac{dP}{dW} = -\beta_0 \frac{1}{(1-\phi)A_C\rho_c}\frac{P_0}{P}\left(\frac{T}{T_0}\right)\left(\frac{F_T}{F_{T0}}\right)$$

$$\alpha \equiv \frac{2\beta_0}{(1-\phi)A_C\rho_c P_0}$$

$$\boxed{\frac{dP}{dW} = -\frac{\alpha}{2}\frac{P_0}{\left(P/P_0\right)}\left(\frac{T}{T_0}\right)\left(\frac{F_T}{F_{T0}}\right)}$$

This equation must be used for multiple reactions.

If, $y = P/P_0$

$$\frac{dP}{dW} = -\frac{\alpha}{2}\left(\frac{T}{T_0}\right)\frac{P_0}{y}\left(\frac{F_T}{F_{T0}}\right)$$

$$F_T = F_{T0} + F_{A0}\partial \bullet X = F_{T0}(1+\frac{F_{A0}}{F_{T0}}\bullet\partial\bullet X)$$

$$\frac{F_{A0}}{F_{T0}}\bullet\partial = y_{A0}\partial = \varepsilon$$

$$\frac{F_T}{F_{T0}} = 1+\varepsilon X$$

$$\frac{dP}{dW} = -\frac{\alpha}{2}\left(\frac{T}{T_0}\right)\frac{P_0}{y}(1+\varepsilon X)$$

For isothermal reactors,

$$\boxed{\frac{dP}{dW} = -\frac{\alpha}{2}\frac{P_0}{y}(1+\varepsilon X) = f_2(P,X)}$$

This is the second ODE solved for single reaction applications.

Analytical solutions are possible when $\varepsilon = 0$ or when $\varepsilon X \ll 1.$ When this is true,

$$\frac{dP}{dW} = \frac{-\alpha P_0}{2(P/P_0)}$$

$$\frac{2P}{P_0}\frac{d(P/P_0)}{dW} = -\alpha$$

$$\frac{d\left(P/P_0\right)^2}{dW} = -\alpha$$

$$\left(P/P_0\right)^2 = 1-\alpha W$$

$$\boxed{\frac{P}{P_0} = \left(1-\alpha W\right)^{1/2}} \text{ where, } \alpha = \frac{2\beta_0}{A_c(1-\varphi)\rho_c P_0}$$

$$\frac{P}{P_0} = \left(1-\frac{2\beta_0 z}{P_0}\right)^{1/2}$$

Since, $W = (1-\varphi)A_c z\rho_{c.}$