Pressure drop in PBRs

We previously derived an expression:

$$aA + bB \rightarrow cC + dD$$

$$C_A = \frac{C_{A0}(1 - X_A)\pi T_0}{\pi_0 T(1+\varepsilon X_A)}$$

$$C_B = \frac{C_{A0}\left(\Theta_B - \frac{b}{a} X_A\right)\pi T_0}{\pi_0 T(1+\varepsilon X_A)}$$ & so on...

Let us still consider an isothermal case

$$\therefore \quad C_A = \frac{C_{A0}(1 - X_A)\pi}{\pi_0(1+\varepsilon X_A)}$$

Ergun's expression for pressure drop:

$$\frac{d\pi}{dz} = \frac{-G}{\rho D_p g_c}\left(\frac{1-\phi}{\phi^3}\right)\left[\underbrace{\frac{150(1-\phi)\mu}{D_p}}_{\text{dominant for laminar flow}} + \underbrace{1.75G}_{\text{dominant for turbulent flow}}\right]$$

$$\left(\text{or } \frac{dP}{dz}\right)$$

Ergun's equation is empirically derived

where:

$G \equiv$ superficial mass velocity $\left(\frac{kg}{m^2 \cdot s}\right)$
(or mass flux)
$= \rho u$ [careful in use of ρ or ρ_o]

Φ = porosity of the bed
$= \frac{\text{volume of voids}}{\text{total volume of bed}}$

g_c = conversion factor
= 1 if using metric units

D_p = particle diameter (m)

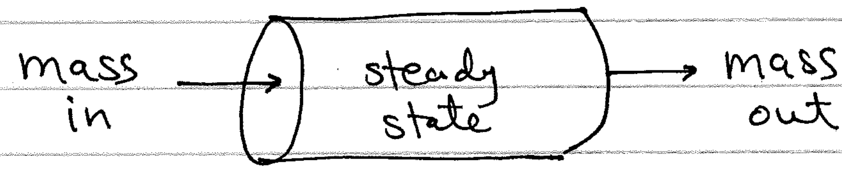
μ = viscosity of the gas $(kg/m \cdot s)$

small z → Z = length of the bed (m)

u = superficial velocity (m/s)

ρ = gas density (kg/m^3)

From the equation of continuity (which is an alternate form of conservation of mass):



$$\therefore \quad \dot{m}_0 = \dot{m} \quad \ldots\ \text{units} \left[\frac{kg}{s}\right]$$

$$\therefore \quad \rho_0 \upsilon_0 = \rho \upsilon$$

$$\therefore \quad \rho = \frac{\rho_0 \upsilon_0}{\upsilon}$$

Also, from the ideal gas law:-

$$\pi_0 \upsilon_0 = n_0 R T_0 \qquad \ldots\ n_0 \equiv F_0$$

$$\pi \upsilon = n R T$$

$$\therefore \quad \frac{\pi_0 \upsilon_0}{\pi \upsilon} = \frac{n_0 T_0}{n T}$$

$$\therefore \quad \frac{\upsilon_0}{\upsilon} = \frac{\pi n_0 T_0}{\pi_0 n T}$$

$$\therefore \; \rho = \frac{\rho_o \, \pi \, n_o T_o}{\pi_o \, n \, T}$$

Ergun's eqn:*

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

* Some peculiarities of the analysis:-

1. We don't substitute $G = \rho u$ or $\rho_o u_o$

2. The G is mass flux. However, the Ergun equation is an empirical equation. As a result, the value for G is often a fitted parameter. Never substitute $G = \rho u$ unless it has been explicitly stated.

3. Better to define G as $\boxed{\frac{\dot{m}}{A_c}}$

Subst. $\rho = \frac{\rho_o \pi n_o T_o}{\pi_o n T}$ in the Ergun eqn.

$$\therefore \; \frac{d\pi}{dZ} = \frac{-G(1-\phi)}{\rho_o g_c D_p \phi^3}\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right]\frac{\pi_o T n}{\pi T_o n_o}$$

Simplify the eqn. $\Rightarrow$ algebra!

We get: $$\frac{d\pi}{dz} = -\beta_0 \left(\frac{\pi_0}{\pi}\right)\left(\frac{T}{T_0}\right)\left(\frac{n}{n_0}\right)$$

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

Recall:

$$\frac{dX_A}{dV} = \frac{-r_A}{F_{A0}} \quad \ldots \text{ PFR}$$

$$\frac{dX_A}{dW} = \frac{-r_A'}{F_{A0}} \quad \ldots \text{ PBR}$$

For PBRs, weight of catalyst bed is more useful

$$W = \rho_{catalyst} \times V_{catalyst}$$

$$\therefore W = \rho_{catalyst} \times \underbrace{(1-\phi)}_{\text{not void}} V_{reactor}$$

$$\therefore W = \rho_{catalyst}(1-\phi) A_c Z$$

A_c: cross-sectional area

$$\therefore \quad dW = (1-\phi) A_c \rho_{catalyst} \, dZ$$

$$\therefore \quad \frac{d\pi}{dZ} = (1-\phi) A_c \rho_{catalyst} \frac{d\pi}{dW}$$

$$\therefore \quad \frac{d\pi}{dW} = \frac{-\beta_0}{(1-\phi) A_c \rho_{catalyst}} \left(\frac{\pi_0}{\pi}\right)\left(\frac{T}{T_0}\right)\left(\frac{n}{n_0}\right)$$

Let $y = \frac{\pi}{\pi_0}$ ..... pressure drop term

$$\therefore \quad dy = \frac{1}{\pi_0} d\pi$$

$$\therefore \quad \frac{dy}{dW} = \frac{-\beta_0}{(1-\phi) A_c \rho_{cat}} \left(\frac{1}{\pi}\right)\left(\frac{T}{T_0}\right)\left(\frac{n}{n_0}\right)$$

$$\therefore \quad \frac{dy}{dW} = \frac{-\beta_0}{(1-\phi) A_c \rho_{cat}} \left(\frac{1}{y}\right)\left(\frac{T n}{\pi_0 T_0 n_0}\right)$$

$$\therefore \quad \frac{dy}{dW} = \left[\frac{-\beta_0}{(1-\phi) A_c \rho_{cat} \pi_0}\right] \left(\frac{1}{y}\right)\left(\frac{T}{T_0}\right)\left(\frac{n}{n_0}\right)$$

Foglar defines this as:

Let $\alpha = \dfrac{2\beta_0}{A_c \rho_{cat}(1-\phi)P_0}$ .... you can use any convention you like

$$\therefore \frac{dy}{dW} = -\frac{\alpha}{2}\left(\frac{1}{y}\right)\left(\frac{T}{T_0}\right)\left(\frac{n}{n_0}\right)$$

Recollect: $\dfrac{n}{n_0} = 1 + \varepsilon X_A$

$$\therefore \frac{dy}{dW} = \frac{-\alpha}{2y}\left(\frac{T}{T_0}\right)\left(1+\varepsilon X_A\right)$$

For isothermal case,

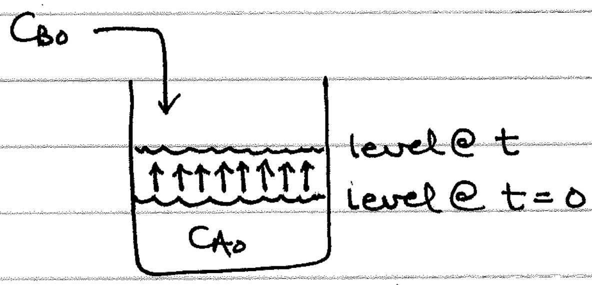
$$\boxed{\frac{dy}{dW} = \frac{-\alpha}{2y}\left(1+\varepsilon X_A\right)}$$

When not isothermal:

Energy balance: $\dfrac{dT}{dW}$

$\therefore$ We will have eqns. for $\underbrace{\dfrac{dX_A}{dW}, \dfrac{dP}{dW} \,\&\, \dfrac{dT}{dW}}_{\text{numerical solutions!}}$

Fed-batch reactors



* B enters the reactor
* A already present

The volume of the reactor is constantly changing

Fed-batch reactors are @ unsteady state.

The limiting reactant is typically filled inside first.

The limiting reactant ≡ Basis species

Consider the following reaction:

$$aA + bB \longrightarrow cC \quad , \quad -r_A = k C_A C_B$$

At time $t=0$, volume of reacting mix $= V_0$

$$C_A(t=0) = C_{A0}$$

Let us assume the volumetric flow rate inside is v

$$\therefore \frac{dV}{dt} = v \quad \text{.... volume balance}$$

rate of change in volume

flow in.

$$\therefore V = vt + \alpha$$

At $t = 0$, $V = V_0 \Rightarrow \alpha = V_0$

$$\therefore V = V_0 + vt \longrightarrow (1)$$

Let us write a mole balance for A:

$$\frac{dN_A}{dt} = -kC_AC_BV \quad \text{.... A only reacts in the system}$$

$$\frac{dN_B}{dt} = vC_{B0} - kC_AC_BV\left(\frac{b}{a}\right)$$

$$\therefore \frac{d(C_AV)}{dt} = -kC_AC_BV$$

$$\therefore C_A\frac{dV}{dt} = -\frac{VdC_A}{dt} - kC_AC_BV$$

$$\therefore\ C_A v + (V_0 + vt)\frac{dC_A}{dt} + k C_A C_B V = 0$$

Similarly,

$$C_B v + (V_0 + vt)\frac{dC_B}{dt} + \left(\frac{kb}{a}\right) C_A C_B V = 0$$

This is a system of ODEs.

If $C_A = x$ & $C_B = y$

& $\frac{dC_A}{dt} = \frac{dx}{dt} = \dot{x}$ & $\frac{dC_B}{dt} = \dot{y}$

$$xv + (V_0 + vt)\dot{x} + kxy(V_0 + vt) = 0$$

$$yv + (V_0 + vt)\dot{y} + \frac{kb}{a}xy(V_0 + vt) = 0$$

$$\boxed{\begin{aligned} \therefore\ \frac{xv}{V_0 + vt} + \dot{x} + kxy &= 0 \\ \frac{yv}{V_0 + vt} + \dot{y} + \frac{kb}{a}xy &= 0 \end{aligned}} \Longrightarrow$$

needs to be solved numerically