Lecture # 8.2
CHE331A

▶ Mole balance → Rate Law → Stoichiometry

▶ Design and analysis of CSTRs and PFR

▶ Isothermal PBR Design accounting for pressure drop and application for the production of Ethylene Oxide

GOUTAM DEO

CHEMICAL ENGINEERING DEPARTMENT

IIT KANPUR

PBR filled with particles

$$\frac{dX}{dW} = k.\frac{C_{A0}}{\dot{v}_0}\left[\left(\frac{1-X}{1+\varepsilon X}\right)\frac{P}{P_0}\right]^2 = f(X,P)$$

$$\frac{dy}{dW} = -\frac{\alpha}{2y}(1+\varepsilon X) = g(X,P)$$

These two coupled ODEs need to be solved simultaneously

The case when $P \neq P_0$ and $\varepsilon = 0$

▶ For $\varepsilon = 0$ then $\dfrac{dy}{dW} = -\dfrac{\alpha}{2y}$ and $y^2 = 1 - \alpha.W$ $(y = 1 \;@\; W = 0)$

▶ Thus, $y = (1 - \alpha.W)^{1/2}$ → $P = P_0(1 - \alpha.W)^{1/2}$

P versus distance
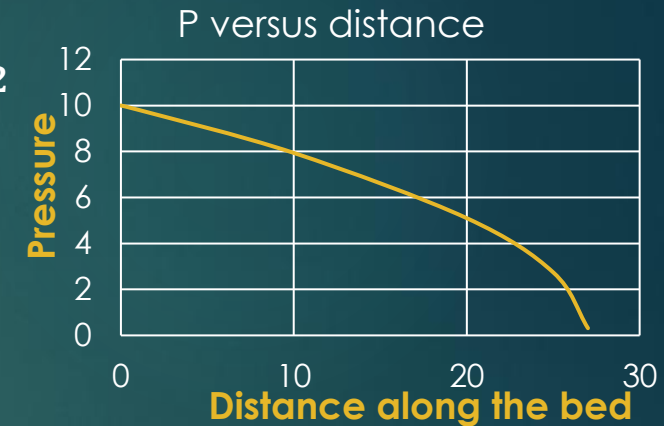
○ This is valid for isothermal operations and ideal gas

▶ Substituting in the mole balance equation:

$$\frac{dX}{dW} = k.\frac{C_{A0}}{\dot{v}_0}\left[\left(\frac{1-X}{1+\varepsilon X}\right)\frac{P}{P_0}\right]^2 = \frac{k.C_{A0}}{\dot{v}_0}[1-X]^2(1-\alpha W)$$

$$\rightarrow \quad \boxed{\frac{\dot{v}_0}{k.C_{A0}}\frac{dX}{(1-X)^2} = (1-\alpha W)dW}$$

which can be integrated from $X = 0 \;@\; W = 0$ to X @ W

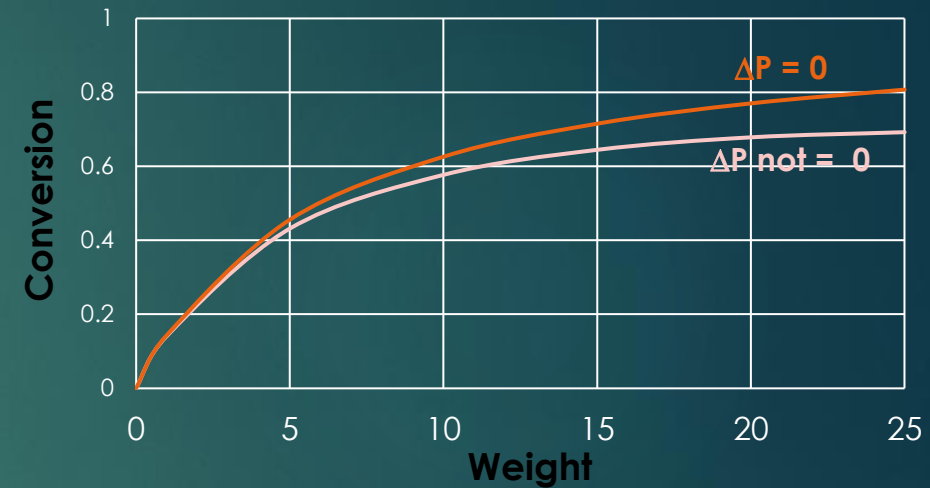# Weight of catalyst, when $P \neq P_0$, can be determined for $\varepsilon = 0$

▶ Integrating $\dfrac{\dot{v}_0}{k.C_{A0}}\dfrac{dX}{(1-X)^2} = (1-\alpha W)dW$ gives rise to

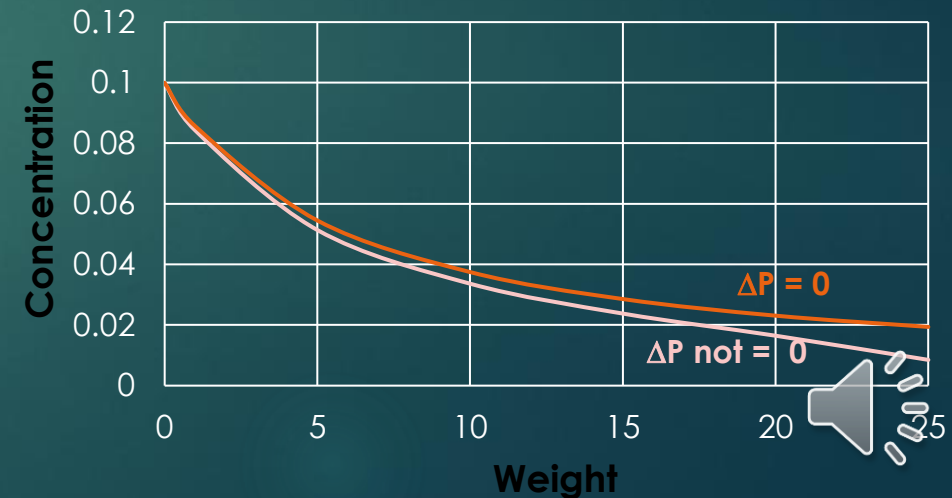$$\frac{\dot{v}_0}{k.C_{A0}}\frac{X}{(1-X)} = \left(1 - \frac{\alpha W}{2}\right)W$$

$$X = \frac{\dfrac{k.C_{A0}W}{\dot{v}_0}\left(1 - \dfrac{\alpha W}{2}\right)}{1 + \dfrac{k.C_{A0}W}{\dot{v}_0}\left(1 - \dfrac{\alpha W}{2}\right)}$$

$$W = \frac{1 - \left\{1 - \left[\dfrac{2.\dot{v}_0.\alpha}{k.C_{A0}}\right]\left[\dfrac{X}{1-X}\right]\right\}^{0.5}}{\alpha}$$

Conversion versus weight

Concentration versus weight

Pressure drop in a PBR – ethylene oxide production (Example: 4-6, Fogler)

▶ Ethylene oxide produced by partial oxidation of C_2H_4 in a PBR

$$C_2H_4 \text{ (A)} + \tfrac{1}{2} O_2 \text{ (B)} \rightarrow C_2H_4O \text{ (C)} \qquad \text{catalyst used is silver}$$

▶ Conversion desired = 0.60 $\qquad$ Feed: $C_2H_4 : O_2 = 2:1$

▶ $F_{A0} = 3 * 10^{-4}$ lbmole/s to each packed tube (PBR); pressure = 10 atm

▶ Mole balance: $W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A'} = \int_0^X \frac{F_{A0} dX}{-r_A'}$

▶ Rate law: $\quad -r_A' = k . P_A^{1/3} P_B^{2/3} \quad$ which in terms of concentration

$$-r_A' = k . RT . C_A^{1/3} C_B^{2/3}$$

During EO production there is a change in number of moles and pressure drop

▶ $\delta \neq 0$ and $P \neq P_0$ needs to be used in concentration determination

▶ $C_i = C_{A0} \left(\dfrac{\theta_i + \mu_i X}{1 + \varepsilon X} \right) \dfrac{P}{P_0} \dfrac{T_0}{T} \dfrac{Z_0}{Z}$; and for $T = T_0$ and $Z = Z_0$

$$C_A = C_{A0} \left(\frac{1 - X}{1 + \varepsilon X} \right) \frac{P}{P_0} \qquad C_B = \frac{C_{A0}}{2} \left(\frac{1 - X}{1 + \varepsilon X} \right) \frac{P}{P_0}$$

▶ With $y = \dfrac{P}{P_0}$ $\qquad P_{A0} = C_{A0} R T_0$ (ideal gas) $\qquad k' = k. P_{A0} (0.5)^{2/3}$

$$-r_A' = k. R T_0. C_A^{1/3} C_B^{2/3} = k. P_{A0} (0.5)^{2/3} \frac{1 - X}{1 + \varepsilon X} \frac{P}{P_0}$$

$$\boxed{-r_A' = k' \frac{1 - X}{1 + \varepsilon X} . y}$$

Using specific values for ethylene production

▶ Inlet flow:　　F_{A0} = 1.08 lbmol/h　　　F_{B0} = ½ F_{A0} = 0.54 lbmol/h

▶ Air is used. Thus, F_{N2} (inert) = 0.54* 0.79/21 = 2.03 lbmol/h

▶ F_{T0} = 3.65 lbmol/h; y_{A0} = 1.08/3.65 = 0.3;　$\varepsilon = 0.3 \left(1 - \frac{1}{2} - 1 \right) = -0.15$

　　P_{A0} = y_{A0}*P_0 = 3 atm　　　　$k' = k.P_{A0}(0.5)^{2/3} = 0.0266 \frac{lbmol}{lb-cat.h}$

▶ The two coupled ODE are:

$$\frac{dX}{dW} = \frac{k'}{F_{A0}} \frac{1-X}{1+\varepsilon X} . y$$ and $$\frac{dy}{dW} = -\alpha \frac{1+\varepsilon X}{2.y} . y$$

Iterations may be required to determine the weight of the catalyst for 0.60 conversion

▶ Two ODEs are obtained from the mole balance and momentum balance:
$$\frac{dX}{dW} = \frac{k'}{F_{A0}} \frac{1-X}{1+\varepsilon X} . y \quad \text{and} \quad \frac{dy}{dW} = -\alpha \frac{1+\varepsilon X}{2.y}$$

▶ The coupled ODEs need to be solved simultaneously by an ODE solver (Polymath/MatLab) for known values of the variables:
$$\frac{dX}{dW} = \frac{0.0266}{1.08} \frac{1-X}{1-0.15X} . y \quad \text{and} \quad \frac{dy}{dW} = -0.0166 \frac{1-0.15X}{2.y}$$

▶ Boundary conditions: W=0, X=0 and y=1.0 for W = 60 lbm

  ○ The value of W = 60 lbm is a guess hoping that 0.60 conversion is achieved within this weight since maximum pressure drop not given

  ○ If not than a larger weight is assumed and the calculation is redone