Lecture 8: The Plug Flow Reactor

$$r_A = -k[A]^2$$

$$X_A F_{Ao} = -r_A V$$

$$V_{CSTR} = \frac{X_A F_{Ao}}{k[A]_0^2 (1-X_A)^2}$$ (2nd order reaction)

$$t_{react.} = \frac{X_A}{k[A]_0 (1-X_A)}$$

$$V_{Batch}\left([A]_0\right) = ?$$

$$F_{Ao} = \frac{\text{moles A}}{\text{time}} = \frac{V_{Batch}[A]_0}{t_{react} + t_d}$$

$$V_{Batch} = \frac{F_{Ao}}{[A]_0}\left[t_d + \frac{X_A}{k[A]_0 (1-X_A)}\right]$$

Assume $X_A = 90\%$

If $t_{react} > t_d$ then

$$V_{Batch} = \frac{2F_{Ao}\cdot 0.9}{[A]_0 k[A]_0 (1-0.9)}$$

$$V_{CSTR} = \frac{0.9F_{Ao}}{k[A]_0^2} \le \frac{1.8F_{Ao}}{k[A]_0^2}$$

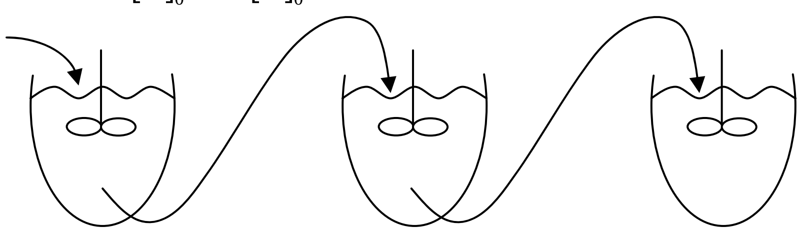


Figure 1. Three tanks in series.

$$[A]_{CSTR} = [A]_{in} + r_A \frac{V}{v_0}$$

If $r_A = -k[A]$

$$[A]_{out} = \frac{[A]_{in}}{1+Da} = \frac{[A]_{in}}{1+\frac{kV}{v_0}}$$

If n CSTRs are in series:

each volume $= \frac{V}{n}$

$$[A]_{out} = \frac{[A]_{in}}{1+\left(\frac{kV}{nv_0}\right)^n}$$

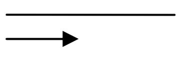
→improves productivity:
concentration of A in 1st one is higher than would be in one large CSTR

$$[A]_{out\atop Batch} = [A]_0 e^{\frac{-kV}{v_0}}$$

$$\frac{kV}{v_0} = 3 \Rightarrow 95\% \text{ conversions}$$

$$[A]_{out\atop CSTR\ series} = \frac{[A]_0}{\left(1+\frac{3}{n}\right)^n}$$

N	X_A
1	.75
10	.93
100	.948



PFR

Figure 2. Diagram of a plug flow reactor.

Plug Flow Reactor (behaves like an infinite number of infinitely small CSTRs)

$$F_{Ain} - F_{Aout} + r_A(\Delta V) = 0 \quad \text{CSTR}$$

$$\left(\frac{F_{Ain} - F_{Aout}}{\Delta V}\right) = -r_A$$

$$\frac{dF_A}{dV} = -r_A \quad \text{design equation for PFR}$$

$$\frac{dF_A}{dV} = r(C_A, C_B, \ldots)$$

$$= -kC_AC_B \quad \text{(for example)}$$

$$F_A = C_A v_0$$

$$\frac{dF_A}{dV} = -k\frac{F_A}{v_0}\frac{F_B}{v_0}$$

This can be expressed as: $\frac{d\underline{Y}}{dt} = F(t, \underline{Y})$ where t is replaced by V.

Example:

$$A + B \underset{k_{rev}}{\overset{k}{\rightleftharpoons}} C$$

$$\frac{d}{dV}\underbrace{\begin{pmatrix} F_A \\ F_B \\ F_C \end{pmatrix}}_{\underline{Y}} = \underbrace{\begin{pmatrix} -\frac{kF_AF_B}{v_0^2}+\frac{k_{rev}F_C}{v_0} \\ -\frac{kF_AF_B}{v_0^2}+\frac{k_{rev}F_C}{v_0} \\ +\frac{kF_AF_B}{v_0^2}-\frac{k_{rev}F_C}{v_0} \end{pmatrix}}_{F(t,\underline{Y})}$$

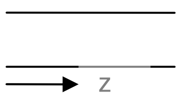


Figure 3. Diagram of a plug flow reactor showing flow in the z-direction.

$$dV = area \cdot dz$$

Mass flow rate is constant

$$(v\rho A) = const.$$

$$\rho = \sum C_i W_i$$

For a liquid, $\frac{d\rho}{dz} = 0$

$$\frac{d(v\rho A)}{dz} = \rho A \frac{dv}{dz} + \rho v \frac{dA}{dz} + Av\frac{d\rho}{dz} = 0$$

Rearrange:

$$\frac{dv}{dz} = -v\left(\frac{1}{A}\frac{dA}{dz} + \frac{1}{\rho}\frac{d\rho}{dz}\right)$$

For a normal pipe $\frac{dA}{dz} = 0$ and for a liquid $\frac{d\rho}{dz} = 0$

Therefore: $\frac{dv}{dz} = 0 \Rightarrow v = v_0$

(We can't assume this for gases!)

For a PFR:

$$\frac{dF_A}{dV} = r_A$$

$$F_A = v[A]$$

$$\frac{d(vC_A)}{dV} = r_A$$

For liquids, v is constant so we can take it out of the differential.

$$r_A = \frac{v}{area}\frac{dC_A}{dz}$$, for liquids

$$\frac{dC_A}{dz} = \frac{area}{v_0} r_A$$

Instead of t_{react} we have z_{react}!

$$t_{pipe} = \frac{area \cdot length}{v_0}$$

$$t_{PFR} = \frac{area \cdot z}{v_0} = \frac{X_A}{k\left[A\right]_0 \left(1 - X_A\right)}$$

Flow is driven by the pressure drop across the pipe.

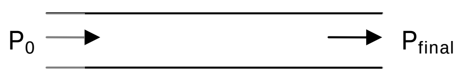


Figure 4. Diagram of a pipe showing pressure upstream and downstream.

$$PV = NRT$$

$$\sum C_i = \frac{P}{RT}$$

$$\left. C_i = \frac{P}{RT}\frac{F_i}{\sum_n F_n} \right\}$$ turns F's into concentrations

$\rho = \sum C_i W_i$, W_i is molecular weight of i.

$$v = \frac{\text{mass flowrate}^{\leftarrow const.}}{\rho\left(z\right)}$$