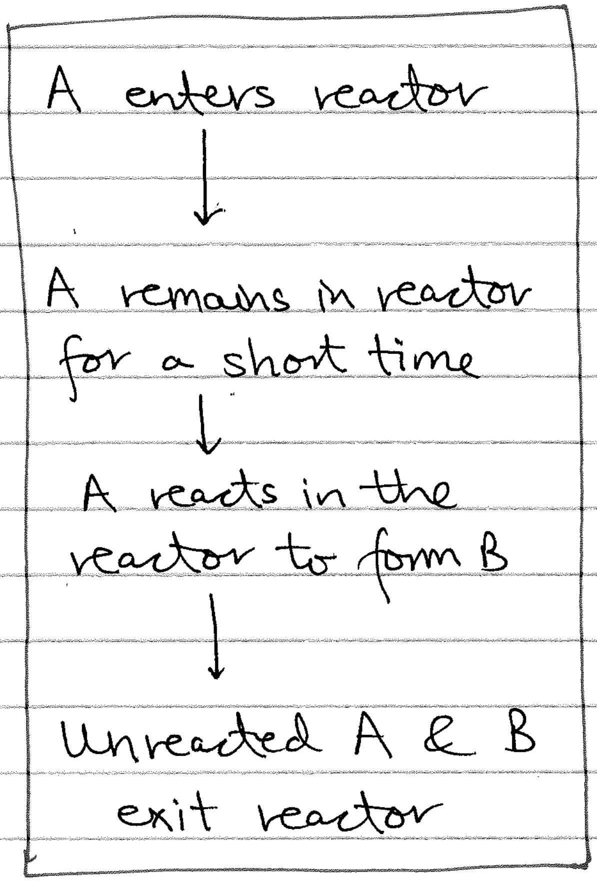


Let us write the mole balance:

$$\frac{dN_A}{dt} = F_{A_0} - F_A + \cancelto{0}{R_{gen_A}} - R_{cons_A}$$

$$\therefore \underbrace{\frac{dN_A}{dt}}_{} = F_{A_0} - F_A - R_{cons_A}$$

{When there is no accumulation of A, i.e. steady-state the reactor is called a CSTR@SS.}

At steady state, $\frac{dN_A}{dt} = 0$

__Assumptions:__ ① steady-state

② inflow rate = outflow rate

$\dot{v}_{in} = \dot{v}_{out} = \dot{v}$

$$\therefore \quad 0 = F_{A0} - F_A - R_{cons_A}$$

$$\therefore \quad R_{cons_A} = F_{A0} - F_A$$

$$\therefore \quad \underbrace{-r_A}_{\text{Remember: positive!}} V = C_{A0}\dot{v}_{in} - C_A\dot{v}_{out}$$

Fogler uses $\dot{v}_{in} = v_0$, $\dot{v}_{out} = v$

$$\boxed{\therefore \quad V = \frac{C_{A0}\dot{v}_{in} - C_A\dot{v}_{out}}{-r_A}}$$

↳ expression for volume of a CSTR, $\dot{v}_{in} = \dot{v}_{out}$

__CSTR__ means continuous stirring @ steady state

Imp. $\dot{v}_{in} = \dot{v}_{out}$ for __CSTR @ SS__

$\dot{v}_{in}$ usually $= \dot{v}_{out}$ (unless volume of mixing concept is significant)

What happens in $\underset{\text{rate}}{\text{inflow}} \neq \underset{\text{rate}}{\text{outflow}}$?

The reactor is continuously mixed but **not @ steady state.**

$$\begin{matrix}\text{continuous}\\ \text{mixing}\end{matrix} \Longrightarrow \left\{\begin{matrix}\text{conc. in}\\ \text{reactor}\end{matrix}\right\} = \left\{\begin{matrix}\text{conc. of}\\ \text{exit stream}\end{matrix}\right\}$$

In this case:

$$\frac{dN_A}{dt} = F_{A_0} - F_A + R_{gen_A} - R_{cons_A}$$

$$aA \longrightarrow bB$$

$$\therefore \frac{dN_A}{dt} = F_{A_0} - F_A - R_{cons_A}$$

$$\therefore \frac{d\,(C_A V)}{dt} = C_{A_0}\dot{v}_{in} - C_A\dot{v}_{out} - (-r_A V)$$

$$\boxed{\therefore \frac{d\,(C_A V)}{dt} = C_{A_0}\dot{v}_{in} - C_A\dot{v}_{out} - kC_A V}$$

$\hookrightarrow$ equation 1 for USS CSTR

Volume expression:

$$\boxed{\frac{dV}{dt} = \dot{v}_{in} - \dot{v}_{out}}$$

$$\therefore C_A \frac{dV}{dt} + V \frac{dC_A}{dt} = C_{A_0} \dot{v}_{in} - C_A \dot{v}_{out} - k C_A V$$

$$\therefore C_A (\dot{v}_{in} - \dot{v}_{out}) + V \frac{dC_A}{dt} = C_{A_0} \dot{v}_{in} - C_A \dot{v}_{out} - k C_A V$$

$$\boxed{\therefore C_A \dot{v}_{in} + V \frac{dC_A}{dt} = C_{A_0} \dot{v}_{in} - k C_A V}$$

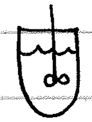
constants ≡ $\dot{v}_{in}, \dot{v}_{out}, C_{A_0}$

variables ≡ V, C_A

* One can easily solve this system of simple ODEs.

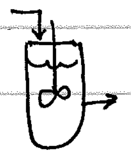
Reactors so far:

Batch reactor ≡ always @ unsteady state



need ODEs to solve system

CSTR → steady-state ≡ algebraic eqns.



→ unsteady state ≡ system of ODEs.

What if I don't want to mix?

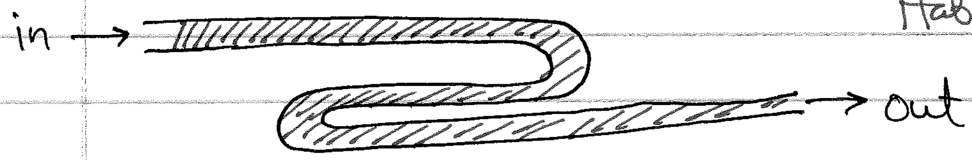
→ mixing by agitation is expensive

What if I can't mix?

→ gas-phase reactions

I can use tubes!

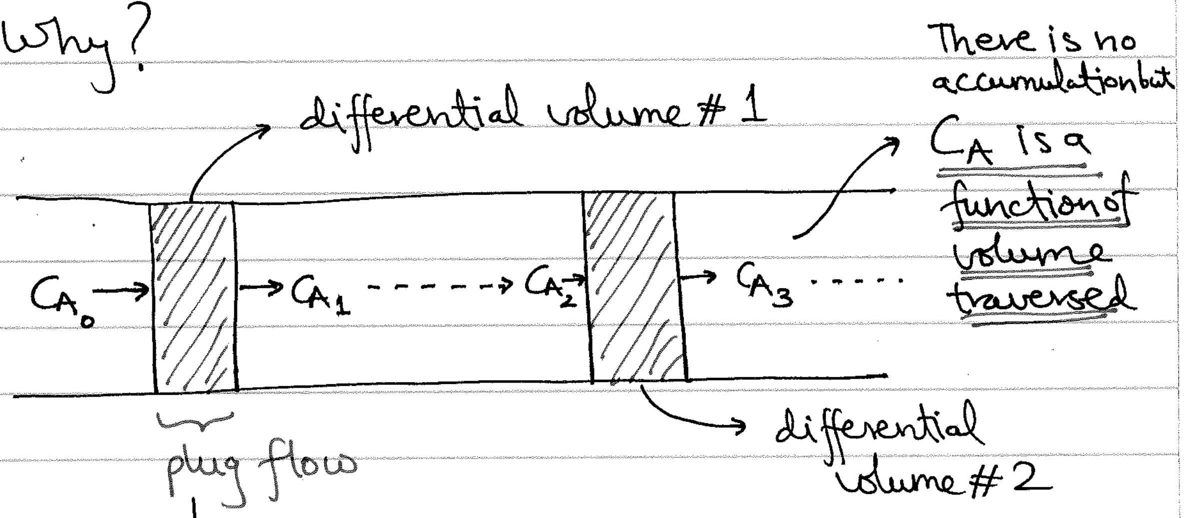
Remember Haber-Bosch!



Reactions in <u>tubes</u>
- → plug flow reactors
- → packed-bed reactors

<u>Trick</u> ≡ if you see tubes, think differential volumes.

Why?



↓

assumption means → no radial gradients

→ 'the reacting mixture moves like a plug through the tube'

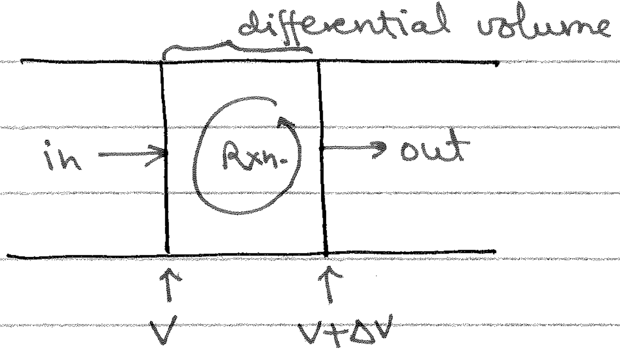
or reactor

The concentration is <u>varying across the tube</u>. In order to analyse it, we need to solve the system using <u>differential volumes</u>

The general mole balance:

$$\frac{dN_i}{dt} = F_{in}^{i} - F_{out}^{i} + R_{gen}^{i} - R_{cons}^{i}$$

The equation is 'tweaked' for analysis of differential volumes.



$$\frac{dN_i}{dt} = F_i\Big|_{V} - F_i\Big|_{V+\Delta V} + R_{gen}^{i}\Big|_{\Delta V} - R_{cons}^{i}\Big|_{\Delta}$$

observe the difference in notations

Key Assumption: All that enters, then leave

for PFRs

'no back-mixing' conditi

$\therefore$ Accumulation rate = 0

$$\therefore \quad F_i\big|_V - F_i\big|_{V+\Delta V} + R_{gen}^{i}\big|_{\Delta V} - R_{cons}^{i}\big|_{\Delta V} = 0$$

$$\left.\begin{array}{l} \text{For } A \longrightarrow \left(b/a\right) B \\ \& \quad -r_A = kC_A \end{array}\right\} \text{1st order rxn.}$$

$$F_A\big|_V - F_A\big|_{V+\Delta V} - kC_A\Delta V = 0$$

$$\therefore \quad \frac{F_A\big|_V - F_A\big|_{V+\Delta V}}{\Delta V} = kC_A$$

From calculus, $\dfrac{dy}{dx} = \dfrac{y\big|_{x+\Delta x} - y\big|_x}{\Delta x}$

$$\therefore \quad \boxed{\frac{-dF_A}{dV} = kC_A}$$

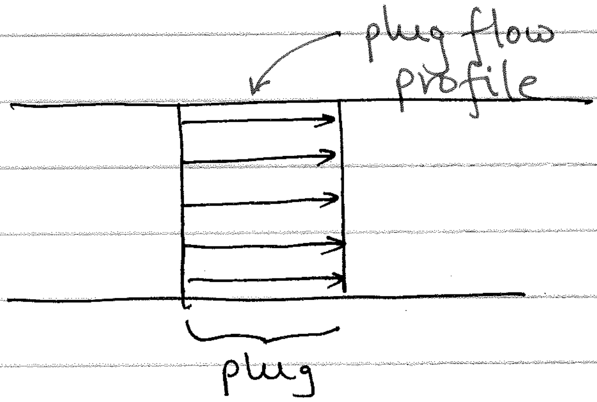
Generally, $\boxed{\dfrac{dF_A}{dV} = r_A}$ → design equation of steady state PFR

↳ or PFR with no backmixing

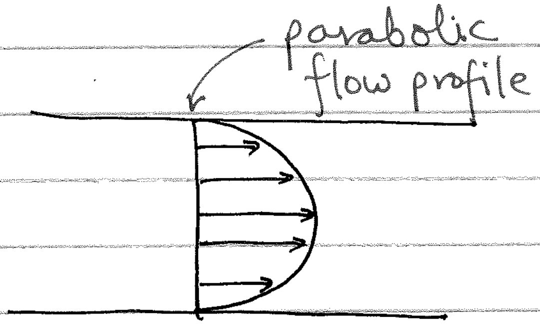
The 'no back-mixing' assumption is often synonymous with PFRs.

Plug-flow is a key assumption

Remember:



highly turbulent or plug flow



laminar flow

* No radial gradients in velocity & concentration

↓

ODEs

One achieves plug flow by ensuring high pressure.

Radial gradients in velocity & concentration

$v = f(\text{radius})$

$C = f(\text{radius, Volume})$

↓

PDEs

grad school

Back to our system:

$$A \longrightarrow \left(b/a\right) B$$

What if $\underline{\underline{b/a \neq 1}}$?

Remember: PFRs are almost always exclusively used for gas rxns.

∴ From the ideal gas law:

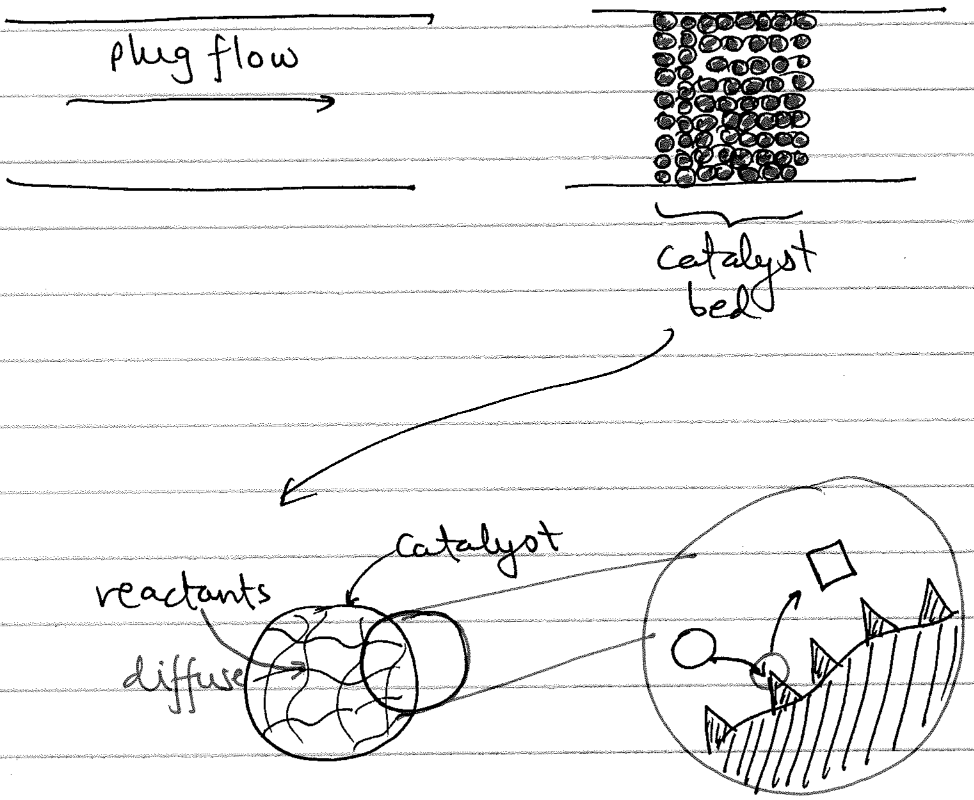
$$\underline{\underline{P\dot{V} = \dot{n}RT}}$$

When $\dot{n}$ changes over the volume of the reactor, the temperature & pressure will change.

∴ PFRs are normally operated to minimise pressure drop & keep temperature constant.

Later on in the course, we will see cases where P, T or both change.

Packed-bed reactors are special cases of Plug flow reactors.



This is a complex system:

- → multi-phase system
- → mass transfer Involved
- → adsorption / desorption
- → reaction
- → equilibrium

However, there is a reason why chemical engineers are the highest paid engineers.

$$\left\{\begin{array}{l}\text{multiphase flow}\\ \text{mass transfer}\\ \text{adsorption/desorption}\\ \text{reaction}\end{array}\right\} \xrightarrow{\text{lump}} \begin{array}{l}\text{effective}\\ \text{reaction}\\ \text{rate constant}\end{array}$$

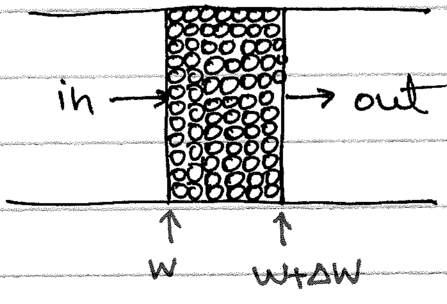
$\therefore$ the rate of rxn. in packed beds $\equiv \dfrac{\text{moles}}{\text{time} \cdot \text{mass of catalyst}}$

In the general mole balance:

$$\frac{dN_i}{dt} = F_{in}^{i} - F_{out}^{i} + \underbrace{(-R_{cons}^{i}) + R_{gen}^{i}}_{\text{rxn. terms}}$$

$$R = (-r_A')\underbrace{\Delta W}_{\substack{\text{instead of volume}\\ \text{traversed, we use}\\ \text{mass of catalyst traversed}}}$$

Let's look at this in greater detail:



$$\frac{dN_i}{dt} = F_i|_W - F_i|_{W+\Delta W} + R_{gen}'|_{\Delta W} - R_{cons}'|_{\Delta W}$$

At steady state:

$$F_i|_W - F_i|_{W+\Delta W} = R_{cons}'|_{\Delta W} - R_{gen}'|_{\Delta W}$$

For $A \rightarrow \left(b/a\right) B$:

$$F_A|_W - F_A|_{W+\Delta W} = (-r_A')\Delta W$$

$$\therefore \quad -\frac{dF_A}{dW} = -r_A'$$

$$\boxed{\frac{dF_A}{dW} = r_A'}$$ .... design equation for PBR

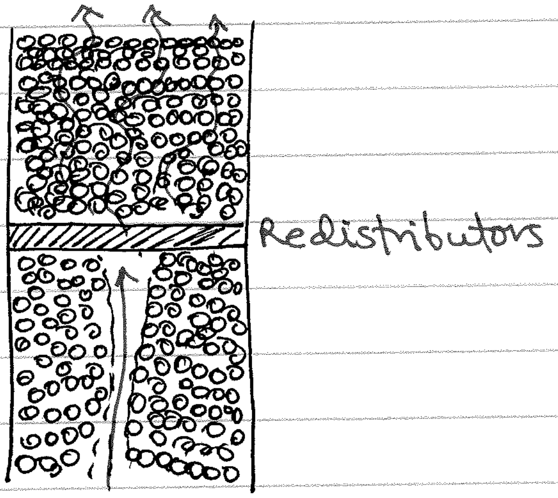
similar rules if $b/a \neq 1$ as for PFR

Note: Generally, pressure drop due to packed beds is a huge issue in the industry.

$\therefore \frac{dP}{dZ}$ is an important term in PBR design.

we will look @ some systems later

How to identify problems?



* if $\frac{dP}{dz} = 0$, you most probably have chanelling

$\downarrow$

This is bad

$$\text{As } \underset{\substack{\uparrow \\ \text{interstitial}}}{v_i} \rightarrow \underset{\substack{\uparrow \\ \text{superficial}}}{U_s}\text{, mass transfer } \underset{\substack{\downarrow \\ K_{eff} \text{ drops}}}{\text{drops}}$$

$$\boxed{\underset{\substack{\uparrow \\ \text{porosity}}}{\varepsilon} \cdot U_s = v_i}$$

Recap:

Batch : $\frac{dN_A}{dt} = r_A V$

CSTR : $F_{A0} - F_A = (-r_A) V$

PFR
PBR : $\frac{dF_A}{dV} = r_A$ $\left(\frac{dF_A}{dW} = r_A' \right)$

Conversion   Nomenclature $\equiv X$

$$X_A = \frac{\text{moles of A reacted}}{\text{moles of A fed}}$$

Why am I introducing this new term?

Non-dimensionalisation! → Chemical engineering is full of dimensionless #s.

- * Helps in scaling processes
- * Easier to gauge process efficiency

Going back to the definition:

$$X_A = \overset{\text{no flows}}{\frac{N_{A0} - N_A}{N_{A0}}} \quad \text{or} \quad \overset{\text{flows}}{\frac{F_{A0} - F_A}{F_{A0}}}$$

$$\boxed{\therefore \quad N_A = N_{A0}(1 - X_A)}$$

$\Rightarrow$ X_A ranges between 0 & 1

We can replace N_A with $N_{A0}(1-X_A)$ in the design equations of all reactors