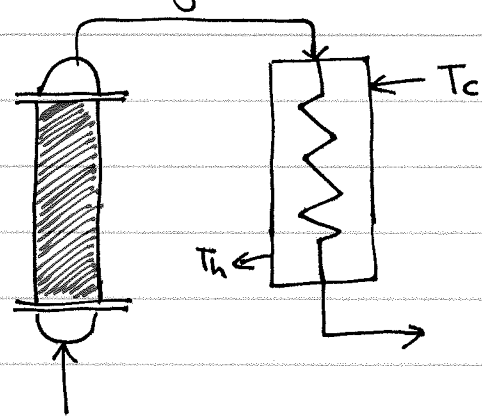
**Example:** A gas feed enters a PFR @ 720K and 1.2 atm with $C_{A0} = 100$, $C_{B0} = 150$, $C_{R0} = 50$, $C_{I0} = 100$. In the reactor, A & B combine as follows:

$$A + 3B \longrightarrow 2R$$

The exit gas passes through a cooler & leaves the system @ 300K and 1 atm with $C_A = 160$. Find $X_A$, $C_B$ & $C_R$ in the cool exit stream. Assume ideal gas behaviour.




all concs. are in $\frac{mol}{L}$

$C_{A0} = 100$
$C_{B0} = 150$
$C_{R0} = 50$
$C_{I0} = 100$
$T_0 = 720K$
$\pi_0 = 1.2\,atm$

$C_A = 160$
$C_B = ?$
$C_R = ?$
$X_A = ?$
$T = 300K$
$\pi = 1\,atm$

Remember:

$$\upsilon = \upsilon_0 \left( \frac{\pi_0 T Z}{\pi T_0 Z_0} \right) (1 + \varepsilon X_A)$$

Ideal gas $\therefore Z = Z_0 = 1$

$$\therefore \quad \upsilon = \upsilon_0 \left( \frac{\pi_0 T}{\pi T_0} \right) (1 + \varepsilon X_A)$$

What is $\varepsilon$? $\quad \varepsilon = \dfrac{n_{A0} \Delta}{n_0 a}$

A is the basis species

Also, $\quad A + 3B \rightarrow 2R$

$$\Delta = 2 + (-3) - 1 = 2 - 3 - 1$$
$$\Delta = -2$$
$$a = 1$$

$$\therefore \quad \varepsilon = \frac{-2 n_{A0}}{n_0} = -2 y_{A0}$$

Conc. $\times\, \upsilon$ = no. of moles

$\therefore$ for any inlet stream, we can calculate the mole fractions from concs.

$$C_{A0} = 100,\ C_{B0} = 150,\ C_{R0} = 50,\ C_{I0} = 100$$

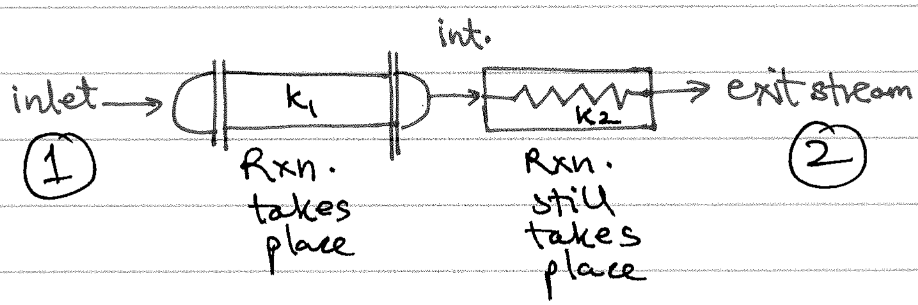
$$\therefore\ y_{A0} = \frac{C_{A0}}{C_{A0}+C_{B0}+C_{R0}+C_{I0}} = \frac{100}{400}$$

$$\therefore\ y_{A0} = \frac{1}{4}$$

$$\therefore\ \varepsilon = -2 \times \frac{1}{4} = -\frac{1}{2}$$

$$\therefore\ v = v_0 \left(\frac{\pi_0 T}{\pi T_0}\right)\left(1 - \frac{X_A}{2}\right)$$

Let's look @ the streams




But, our equation compares state 1 & 2.

* This shows the power of conversion in sizing reactors, especially gas phase PFRs.

| Species | Initial conc. $= \frac{N_{initial}}{v_0}$ |
|---|---|
| A | $C_{A0} = N_{A0}/v_0$ |
| B | $C_{B0} = N_{B0}/v_0$ |
| R | $C_{R0} = N_{C0}/v_0$ |
| I | $C_{I0} = N_{I0}/v_0$ |

$$\Theta_B = \frac{C_{B0}}{C_{A0}} = 3/2 \Rightarrow N_{B0} = \frac{3}{2} N_{A0}$$

$$\Theta_R = \frac{C_{R0}}{C_{A0}} = 1/2 \qquad N_{R0} = \frac{1}{2} N_{A0}$$

$$\Theta_R = \frac{C_{R0}}{C_{A0}}$$

$$\Theta_I = \frac{C_{I0}}{C_{A0}} = 1 \qquad N_{I0} = N_{A0}$$

For A, change $= -N_{A0} X_A$

B, change $= -3N_{A0} X_A$

R, change $= 2N_{A0} X_A$

$$\therefore N_A = N_{A0}(1 - X_A)$$
$$N_B = N_{A0}(3/2 - 3X_A)$$
$$N_R = N_{A0}(1/2 + 2X_A)$$

$$N_I = N_{I0} = N_{A0}$$

$$C_A = \frac{N_A}{v} = \frac{N_{A0}(1-X_A)}{v_0\left(\frac{\pi_0 T}{\pi T_0}\right)\left(1-\frac{X_A}{2}\right)}$$

$$\therefore\ C_A = \frac{N_{A0}(1-X_A)}{v_0\left(\frac{\pi_0 T}{\pi T_0}\right)\left(\frac{2-X_A}{2}\right)}$$

$$\boxed{\therefore\ C_A = \frac{(2\pi T_0)\,N_{A0}(1-X_A)}{v_0\,\pi_0\,T\,(2-X_A)}}$$

iii) $$C_B = \frac{N_B}{v} = \frac{N_{A0}(3/2-3X_A)}{v_0\left(\frac{\pi_0 T}{\pi T_0}\right)\left(1-\frac{X_A}{2}\right)}$$

$$\boxed{\therefore\ C_B = \frac{(2\pi T_0)\,N_{A0}(3/2-3X_A)}{v_0\,\pi_0\,T\,(2-X_A)}}$$

& $$\boxed{C_R = \frac{(2\pi T_0)\,N_{A0}(1/2+2X_A)}{v_0\,\pi_0\,T\,(2-X_A)}}$$

Let's make the appropriate substitution:

$$C_A = \left(\frac{2\pi T_0}{\pi_0 T}\right) C_{A0}\left(\frac{1-X_A}{2-X_A}\right)$$

$$\frac{2\pi T_0}{\pi_0 T} = \frac{2\times1\times720}{1.2\times300} = 4$$

$$\therefore \frac{C_A}{C_{A_0}} = 4\left(\frac{1-X_A}{2-X_A}\right)$$

$$\therefore \frac{160}{100} = \frac{4-4X_A}{2-X_A}$$

$$16-8X_A = 20-20X_A$$

$$12X_A = 4$$

$$\boxed{X_A = 1/3}$$

$$\therefore C_B = \frac{4C_{A_0}\left(3/2-3X_A\right)}{(2-X_A)} = \frac{4\times100\times0.5\times3}{5}$$

$$\boxed{\therefore C_B = 120}$$

$$\& \; C_R = \frac{4C_{A_0}\left(1/2+2X_A\right)}{(2-X_A)} = \frac{400\left(\frac{1}{2}+\frac{2}{3}\right)\times3}{5}$$

$$\boxed{\therefore C_C = 280}$$

## Example:

mole basis

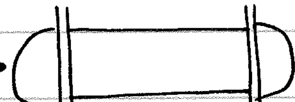
1 L/s of ozone-air 20%-80% mixture at 1.5 atm and 93°C passes through a PFR. Under these conditions, ozone undergoes the following decomposition reaction:

$$2O_3 \longrightarrow 3O_2$$

$$\& \quad -r_{O_3} = kC_{O_3}^2 \quad , \quad k = 0.05 \ \frac{L}{mol \cdot s}$$

What size of the reactor is needed for 50% decomposition of ozone? Assume ideal gas law applies here.

$v_0 = 1 \ L/s \longrightarrow$



$\longrightarrow X_{O_3} = 0.5$

$\pi_0 = 1.5 atm$

$T_0 = 93°C$

$y_{O_3} = 0.2$

$\boxed{\text{Isothermal} \quad \text{Isobaric}}$

Let us re-write ozone as A

$\therefore$ The reaction is $2A \rightarrow 3B$

The inlet stream is a 20%-80% ozone-air mixture.

mole basis

But air is 78% $N_2$, 21% $O_2$ & 1% others

For this system, air = 79% inerts, 21% $O_2$

For a 100 mole inlet stream:

ozone = 20 moles
inerts = 63.2 moles
oxygen = 16.8 moles

$$\left.\begin{aligned} \therefore \quad y_{A_0} &= 0.2 \\ y_{B_0} &= 0.168 \\ y_{I_0} &= 0.632 \end{aligned}\right\} \longrightarrow \text{inlet composition}$$

Now, $\Delta = 3-2 = 1$ & $\underline{A \equiv \text{basis}}$

$$\therefore \quad \varepsilon = \frac{y_{A_0}\Delta}{a} = \frac{0.2 \times 1}{2} = 0.1$$

$$\therefore \quad \varepsilon = 0.1$$

$$\boxed{\text{Remember:} \quad v = v_0 \left(\frac{\pi_0 T Z}{\pi T_0 Z_0}\right)(1+\varepsilon X_A)}$$

Let us commence our analysis of the system:

What is the expression for volume of a PFR?

Recollect: $$dV_{PFR} = \left(\frac{F_{A0}}{-r_A}\right) dX_A$$

Here, $-r_A = k C_A^2$

<u>Stoichiometric table:</u>

| Species | Initial | Change | Final |
|---|---|---|---|
| A | $N_{A0}$ | $-N_{A0}X_A$ | $N_{A0}(1-X_A)$ |
| B | $\Theta_B N_{A0}$ | $3/2\, N_{A0}X_A$ | $N_{A0}(\Theta_B + 3/2\, X_A)$ |
| I | $\Theta_I N_{A0}$ | $0$ | $N_{A0}\Theta_I$ |

$$\therefore C_A = \frac{N_A}{v} = \frac{N_{A0}(1-X_A)}{v_0\left(\frac{\pi_0 T Z}{\pi T_0 Z_0}\right)(1+\varepsilon X_A)}$$

Since it is an ideal gas, $Z = Z_0 = 1$

$$\therefore C_A = \frac{N_{A0}(1-X_A)\pi T_0}{v_0 \pi_0 T (1+\varepsilon X_A)}$$

The process is isothermal & isobaric.

$$\therefore \pi = \pi_0 \quad \& \quad T = T_0$$

$$\therefore \quad C_A = \frac{N_{A0}(1-X_A)}{v_0(1+\varepsilon X_A)}$$

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

$$\therefore \quad -r_A = kC_A^2 = kC_{A0}^2\left(\frac{1-X_A}{1+\varepsilon X_A}\right)^2$$

$$\therefore \quad dV_{PFR} = \left(\frac{F_{A0}}{-r_A}\right) dX_A$$

$$\therefore \quad dV_{PFR} = \frac{C_{A0}v_0}{kC_{A0}^2}\left(\frac{1+\varepsilon X_A}{1-X_A}\right)^2 dX_A$$

$$\therefore \quad dV_{PFR} = \frac{v_0}{kC_{A0}}\left(\frac{1+\varepsilon X_A}{1-X_A}\right)^2 dX_A$$

$$\therefore \quad V_{PFR} = \frac{v_0}{kC_{A0}}\int_0^{0.5}\left(\frac{1+\varepsilon X_A}{1-X_A}\right)^2 dX_A$$

Either look up the solution in App. A

(OR, if you like challenges in life, solve this using your knowledge of integral calculus)

From App. A:

$$\int_0^x \left(\frac{1+\varepsilon X}{1-X}\right)^2 dX = 2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 x + \frac{(1+\varepsilon)^2 X}{1-X}$$

How will you solve this?

$$\int\left(\frac{1+\varepsilon X}{1-X}\right)^2 dX = \int \frac{1+2\varepsilon X+\varepsilon^2 X^2}{(1-X)^2}\,dX$$

$$= \int\frac{1}{(1-X)^2}\,dX + \int\frac{2\varepsilon X}{(1-X)^2}\,dX + \int\frac{\varepsilon^2 X^2}{(1-X)^2}\,dX$$

$$= \int\frac{1}{(1-X)^2}\,dX + 2\varepsilon\int\frac{X+1-1}{(1-X)^2}\,dX + \varepsilon^2\int\frac{X^2+1-1}{(1-X)^2}\,dX$$

$$= \int\frac{1}{(1-X)^2}\,dX + 2\varepsilon\left[\int\frac{1}{(1-X)^2}\,dX - \int\frac{1}{1-X}\,dX\right] + \varepsilon^2\int\frac{X^2-1}{(1-X)^2}\,dX + \varepsilon^2\int\frac{1}{(1-X)^2}\,dX$$

$$= \int\frac{1}{(1-X)^2}\,dX + 2\varepsilon\int\frac{1}{(1-X)^2}\,dX + \varepsilon^2\int\frac{1}{(1-X)^2}\,dX - 2\varepsilon\int\frac{1}{1-X}\,dX + \varepsilon^2\int\frac{(X+1)(X-1)}{(1-X)^2}\,dX$$

$$= \left(1+2\varepsilon+\varepsilon^2\right)\int \frac{1}{(1-X)^2}\,dX - 2\varepsilon\int \frac{1}{(1-X)}\,dX + \varepsilon^2\left[\int \frac{-(X+1)\,dX}{(1-X)}\right]$$

$$= (1+\varepsilon)^2\int \frac{1}{(1-X)^2}\,dX - 2\varepsilon\int \frac{1}{(1-X)}\,dX - \varepsilon^2\left[\int \frac{1}{1-X}\,dX + \int \frac{X}{1-X}\,dX\right]$$

$$= (1+\varepsilon)^2\int \frac{1}{(1-X)^2}\,dX - \left(2\varepsilon+\varepsilon^2\right)\int \frac{1}{1-X}\,dX - \varepsilon^2\int \frac{X+1-1}{1-X}\,dX$$

$$= (1+\varepsilon)^2\int \frac{1}{(1-X)^2}\,dX - \left(2\varepsilon+\varepsilon^2\right)\int \frac{1}{1-X}\,dX - \varepsilon^2\left[\int \frac{1}{1-X}\,dX - \int dX\right]$$

$$= (1+\varepsilon)^2\int \frac{1}{(1-X)^2}\,dX - \left(2\varepsilon+2\varepsilon^2\right)\int \frac{1}{1-X}\,dX + \varepsilon^2\int dX$$

$$= \frac{(1+\varepsilon)^2}{-1}\,\frac{(1-X)^{-2+1}}{(-2+1)} + \left(2\varepsilon+2\varepsilon^2\right)\ln(1-X) + \varepsilon^2 X$$

$$= \frac{(1+\varepsilon)^2}{(1-X)} + 2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X$$

Take limits from 0 to $X_A$

$$\therefore \text{ Integral} = \left[\frac{(1+\varepsilon)^2}{1-X_A} - (1+\varepsilon)^2\right] + 2\varepsilon(1+\varepsilon)\left\{\ln(1-X_A) - \ln(1)\right\} + \varepsilon^2 X_A$$

$$\therefore \text{Integral} = (1+\varepsilon)^2\left[\frac{1}{1-X_A} - 1\right] + 2\varepsilon(1+\varepsilon)\ln(1-X_A) + \varepsilon^2 X_A$$

$$\boxed{\therefore \text{Integral} = \frac{(1+\varepsilon)^2 X_A}{(1-X_A)} + 2\varepsilon(1+\varepsilon)\ln(1-X_A) + \varepsilon^2 X_A}$$

$$\therefore V_{PFR} = \frac{\upsilon_0}{kC_{A0}}\left[\frac{(1+\varepsilon)^2 X_A}{(1-X_A)} + 2\varepsilon(1+\varepsilon)\ln(1-X_A) + \varepsilon^2 X_A\right]$$

$\varepsilon = \dfrac{y_{A0}\Delta}{a}$, $X_A$ given $\Rightarrow$ solve by subst

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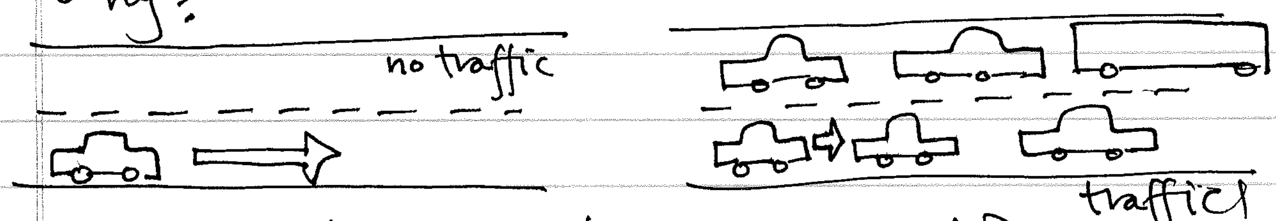
Now, imagine this rxn. takes place in a packed bed reactor.

In the previous, we assumed constant P & T.

Generally, PBRs can be operated isothermally

However, they will encounter pressure drops

why?




What happens to your speed?