Tut 1.4 2019

PBR

$2A \rightarrow B$ PBR

- → Gas phase
- → Elementary reaction
- → isothermal
- → feed is pure A
- → $P_0 = 5 atm$
- → $P = 20 atm$
- → $X = 0,3$

Basis: 1kmol feed per second

	Initial	Δ	Final
A:	1	$-X$	$1-X$
B:	0	$+\frac{1}{2}X$	$\frac{1}{2}X$
	$F_{T0} = 1$	$-\frac{1}{2}X$	$F_T = 1-0,5X$

$\therefore F_{A0} = 1$

$F_{B0} = 0$

$F_{T0} = 1$

$F_A = 1-X$

$F_B = 0,5X$

$F_T = 1-0,5X$

$Q_0 = 1$ @ T_0

$$\therefore \quad r_A' = -k' C_A^2$$

But $C_A = \dfrac{F_A}{Q}$ and $Q = Q_0 \dfrac{F_T}{F_{T0}} \dfrac{P_0}{P} \cancel{\dfrac{Z T}{Z_0 T_0}}$

$$Q = F_T \frac{P_0}{P}$$

2,

$$\therefore \quad r_A' = -k'\left(\frac{F_A}{Q}\right)^2$$

$$= -k'\left(\frac{F_A}{F_T}\frac{P}{P_0}\right)^2$$

$$\Rightarrow r_A' = -k'\left(\frac{1-X}{1-0{,}5X}\right)^2\left(\frac{P}{P_0}\right)^2 \quad --- \quad (1)$$

$$r_B' = -\frac{1}{2} r_A' \quad -- \quad (2)$$

$$\frac{dF_A}{dW} = -F_{A0}\frac{dX}{dW} = r_A'$$

$$\frac{dX}{dW} = \frac{-r_A'}{1} \quad -- \quad (3)$$

$$\frac{dP}{dW} = -k\left(\frac{F_T}{F_{T0}}\right)\left(\frac{P_0}{P}\right)$$

$$\frac{dP}{dW} = -k\,(1-0{,}5X)\left(\frac{P_0}{P}\right) \quad --- \quad (4)$$

$$\therefore \quad k' = 0{,}695 \ \frac{m^6}{mol.s}$$

$$k = 10{,}431 \ \frac{\cancel{atm}\ Pa}{kg}$$

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a) CSTR

$W = 1\,kg$

$P_0 = P = 20\,atm$

mole balance: $r_A' = \frac{F_A - F_{A0}}{W}$

$= \frac{(1-X) - 1}{1}$

$r_A' = -X$

rate law: $r_A' = -k'\left(\frac{1-X}{1-0{,}5X}\right)^2$

$\therefore\ X = k'\left(\frac{1-X}{1-0{,}5X}\right)^2$

Using fsolve, $X = 0{,}4$

b) $k_1' = 0{,}695$

If $\dot{m}$ doubles, then F_{A0} doubles

Since $r_A' = -k_1'\left(\frac{F_A}{Q}\right)^2$

new ~~flow~~ rate, $r_{A_1}' = -k_1'\left(2\frac{F_A}{Q}\right)^2 = -4k_1'\left(\frac{F_A}{Q}\right)^2$

$\therefore\ k_2' = 4k_1'$

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for the ergun k_1 in:

$$\frac{dP}{dz} = -k_1 \left(\frac{F_T}{F_{T0}}\right)\left(\frac{P_0}{P}\right)$$

where $K_1 = \frac{G}{\rho_0 D_p} \frac{(1-\varepsilon)}{\varepsilon^3}\left[\cancel{\left(\frac{150(1-\varepsilon)\mu}{D_p}\right)} + 1.75G\right] \times \left(\frac{1}{A_c(1-\varepsilon)\rho_c}\right)$

for turbulent flow

let the constant, $\alpha_1 = \frac{G^2}{D_p}$

where mass flow rate decreases by factor of 4 and particle size doubles, the new constant is:

$$\alpha_2 = \frac{(G/4)^2}{2D_p}$$

So k_1 changes by a factor of:

$$\frac{\alpha_2}{\alpha_1} = \frac{(G/4)^2}{2D_p} \cdot \frac{D_p}{G^2} = \frac{1}{32}$$

$\therefore$ new $k_2 = \frac{k_1}{32}$

new $X = 0{,}845$ (Python)