6. Isothermal reactor design: molar flow rates

→ In many instances it is easier to work with molar flow rates / no. of moles than conversion.

molar flowrates are necessary } ⇒ membrane reactor
⇒ multiple reactions in gas phase

Molar flow rate balance algorithm:

→ We must write a mole balance for each and every species as opposed to just one species (in the conversion algorithm)

steps:

1. write mole balance on all the species
2. write rate law
3. relate mole balances to one another through relative rates
4. relate conc. in rate laws to ~~flow rates (molar)~~ molar flow rates through stoichiometry and pressure drop
5. combine and solve using ODE solver.

Notes on
Elements of chemical reaction engineering, H. Scott Fogler
- Ranjeet Utikar

Mole balances on CSTRs, PFRs, PBRs and batch reactors

Liquid phase:

$V = V_0$ .... constant volume

$\upsilon = \upsilon_0$ ... no change in volumetric flow rate

$$aA + bB \longrightarrow cC + dD$$

Mole balances

	Species A	Species B
Batch	$\frac{dC_A}{dt} = r_A$	$\frac{dC_B}{dt} = \frac{b}{a} r_A$
CSTR	$V = \frac{\upsilon_0 (C_{A0} - C_A)}{-r_A}$	$V = \frac{\upsilon_0 (C_{B0} - C_B)}{-(b/a) r_A}$
PFR	$\upsilon_0 \frac{dC_A}{dV} = r_A$	$\upsilon_0 \frac{dC_B}{dV} = \frac{b}{a} r_A$
PBR	$\upsilon_0 \frac{dC_A}{dW} = r'_A$	$\upsilon_0 \frac{dC_B}{dW} = \frac{b}{a} r'_A$

$$\frac{r_A}{-a} = \frac{r_B}{-b} = \frac{r_C}{c} = \frac{r_D}{d}$$

⇒ We have only to specify the parameter values for the system $C_{A0}, C_{B0}, \upsilon_0, \dots$ and rate law parameters $k_A, \alpha, \beta, \dots$

Gas phase

→ The molar flow rates for each species F_j are obtained by mole balance on each species.

$$aA + bB \longrightarrow cC + dD$$

Mole balances:

	CSTR	PFR	PBR
A)	$V = \frac{F_{A0} - F_A}{-r_A}$	$\frac{dF_A}{dV} = r_A$	$\frac{dF_A}{dW} = r'_A$
B)	$V = \frac{F_{B0} - F_B}{-r_B}$	$\frac{dF_B}{dV} = r_B$	$\frac{dF_B}{dW} = r'_B$
C)	$V = \frac{F_{C0} - F_C}{-r_C}$	$\frac{dF_C}{dV} = r_C$	$\frac{dF_C}{dW} = r'_C$
D)	$V = \frac{F_{D0} - F_D}{-r_D}$	$\frac{dF_D}{dV} = r_D$	$\frac{dF_D}{dW} = r'_D$

Rates: ... For PBR

rate law: $-r'_A = k_A C_A^{\alpha} C_B^{\beta}$

$$\frac{r'_A}{-a} = \frac{r'_B}{-b} = \frac{r'_C}{c} = \frac{r'_D}{d}$$

$$r'_B = \frac{b}{a} r'_A$$

$$r'_C = \frac{-c}{a} r'_A$$

$$r'_D = \frac{-d}{a} r'_A$$

Stoichiometry

$$C_A = C_{T0} \frac{F_A}{F_T} \frac{T_0}{T} P/P_0$$

$$C_B = C_{T0} \frac{F_B}{F_T} \frac{T_0}{T} P/P_0$$

$$C_C = C_{T0} \frac{F_C}{F_T} \frac{T_0}{T} P/P_0$$

$$C_D = C_{T0} \frac{F_D}{F_T} \frac{T_0}{T} P/P_0$$

Pressure:

$$\frac{dp}{dW} = \frac{-\alpha}{2p} \frac{F_T}{F_{T0}} \frac{T}{T_0} \qquad p = \frac{P}{P_0}$$

Total molar flow rate

$$F_T = \sum_{i=1}^{N} F_i = F_A + F_B + F_C + F_D + F_I$$