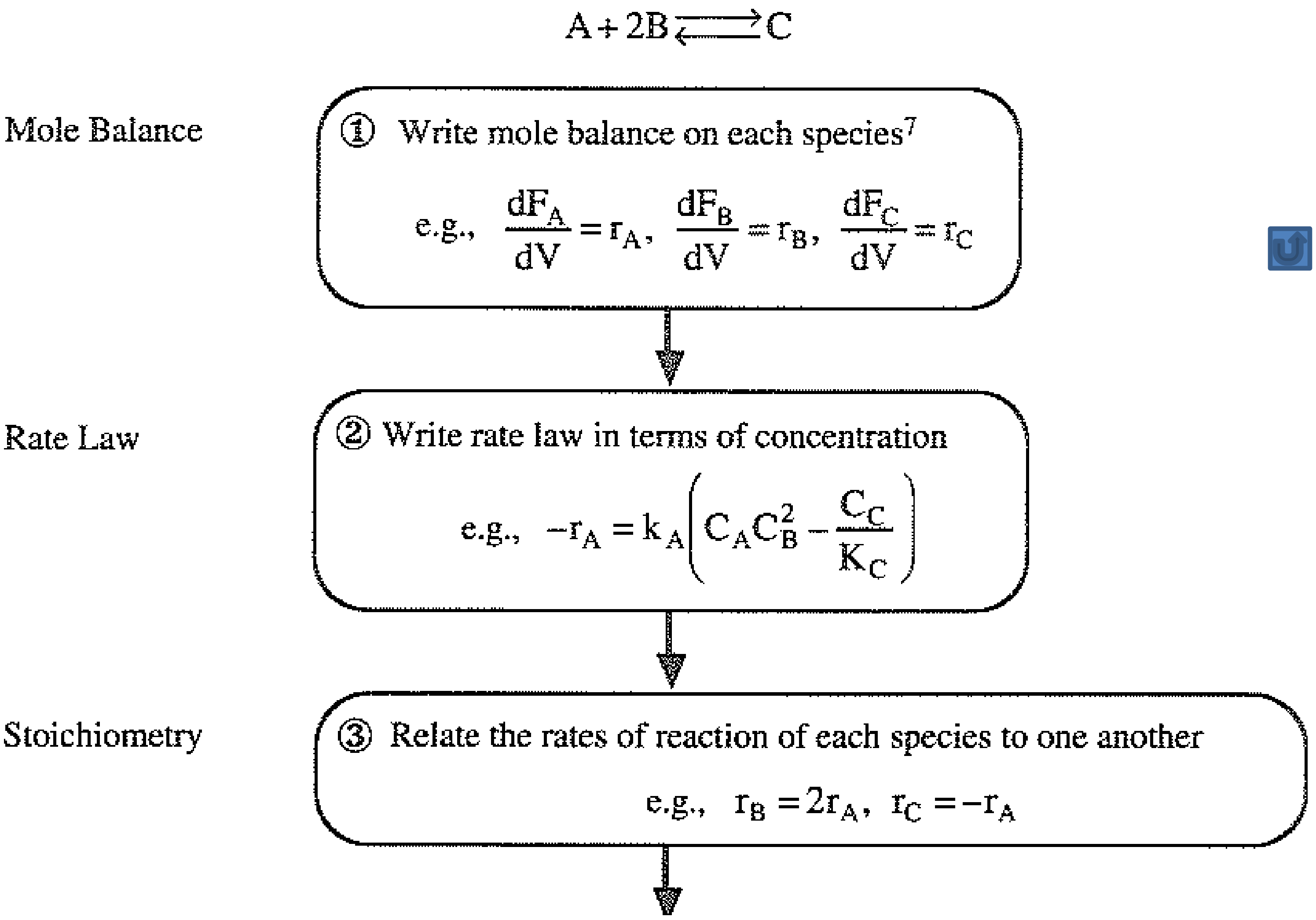
Part II, Measures Other Than Conversion I



$$A + 2B \rightleftarrows C$$

Mole Balance

① Write mole balance on each species[7]

$$\text{e.g.,}\quad \frac{dF_A}{dV} = r_A,\quad \frac{dF_B}{dV} = r_B,\quad \frac{dF_C}{dV} = r_C$$

Rate Law

② Write rate law in terms of concentration

$$\text{e.g.,}\quad -r_A = k_A\left(C_A C_B^2 - \frac{C_C}{K_C}\right)$$

Stoichiometry

③ Relate the rates of reaction of each species to one another

$$\text{e.g.,}\quad r_B = 2r_A,\quad r_C = -r_A$$

Part II, Measures Other Than Conversion II

Stoichiometry

④ (a) Write the concentrations in terms of molar flow rates for isothermal *gas-phase* reactions

$$\text{e.g.,}\quad C_A = C_{T0}\frac{F_A}{F_T}\frac{P}{P_0},\quad C_B = C_{T0}\frac{F_B}{F_T}\frac{P}{P_0}$$

$$\text{with}\quad F_T = F_A + F_B + F_C$$

(b) For *liquid-phase* reactions use concentration, e.g., C_A, C_B

Pressure Drop

⑤ Write the *gas-phase* pressure drop term in terms of molar flow rates

$$\frac{dy}{dW} = -\frac{\alpha}{2y}\frac{F_T}{F_{T_0}},\quad \text{with}\quad y = \frac{P}{P_0}$$

Combine

⑥ Use an ODE solver or a nonlinear equation solver (e.g., Polymath) to combine Steps ① through ⑤ to solve for, for example, the profiles of molar flow rates, concentration and pressure.

2. Applications/Examples of the CRE Algorithm I

Gas Phase Elementary Reaction	Additional Information	
$2A \rightarrow B$	Only A fed	P_0 = 8.2 atm
	T_0 = 500 K	C_{A0} = 0.2 mol/dm^3
	k = 0.5 dm^3/mol·s	v_o = 2.5 dm^3/s

Solve for X = 0.9 for A is limiting

2. Applications/Examples of the CRE Algorithm II

Reactor	Mole Balance	Rate Law	Stoichiometry
Batch	$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$	$-r_A = kC_A^2$	**Gas:** **$V = V_0$**
CSTR	$V = \frac{F_{A0}X}{-r_A}$	$-r_A = kC_A^2$	**Gas:** **$T = T_0$, $P = P_0$**
PFR	$V = F_{A0}\int_0^X \frac{dX}{-r_A}$	$-r_A = kC_A^2$	**Gas:** **$T = T_0$, $P = P_0$**

2. Applications/Examples of the CRE Algorithm III

Reactor	Stoichiometry 2	
Batch	**Per mole A ?**	$C_{\mathrm{A}} = \frac{N_{\mathrm{A}}}{V} = \frac{N_{\mathrm{A0}}(1-X)}{V_0}$ $= C_{\mathrm{A0}}(1-X)$
CSTR	**Per mole A** **A $\longrightarrow$ ½B** **ε = 1.0(1- ½) = -0.5**	$C_{\mathrm{A}} = \frac{F_{\mathrm{A}}}{v} = \frac{F_{\mathrm{A0}}(1-X)}{v_0(1+\varepsilon X)}$
PFR	**Per mole A** **A $\longrightarrow$ ½B** **ε = 1.0(1- ½) = -0.5**	$= C_{\mathrm{A0}} \frac{(1-X)}{(1+\varepsilon X)}$

2. Applications/Examples of the CRE Algorithm IV

Reactor	Stoichiometry 3	
Batch	$C_{\mathrm{B}} = \frac{N_{\mathrm{B}}}{V} = \frac{N_{\mathrm{A0}}(+\frac{1}{2}X)}{V_0} = \frac{C_{\mathrm{A0}}X}{2}$	
CSTR	$C_{\mathrm{B}} = \frac{F_{\mathrm{B}}}{v} = \frac{F_{\mathrm{A0}}(+\frac{1}{2}X)}{v_0(1+\varepsilon X)}$	
PFR	$= \frac{C_{\mathrm{A0}}X}{2(1+\varepsilon X)}$	

2. Applications/Examples of the CRE Algorithm V

Reactor	Combine	Integration
Batch	$t=\frac{1}{kC_{A0}}\int_0^X\left[\frac{1}{(1-X)^2}\right]dX$	$t=\frac{1}{kC_{A0}}\left[\frac{X}{(1-X)}\right]$
CSTR	$V=\frac{F_{A0}X(1-0.5X)^2}{kC_{A0}^2(1-X)^2}$	$V=\frac{F_{A0}}{kC_{A0}^2}\left[\begin{array}{l}2\varepsilon(1+\varepsilon)\ln(1-X)\\+\varepsilon^2X+\frac{(1+\varepsilon)^2X}{1-X}\end{array}\right]$
PFR	$V=\frac{F_{A0}}{kC_{A0}^2}\int_0^X\left[\frac{(1-0.5X)^2}{(1-X)^2}\right]dX$	⇩

2. Applications/Examples of the CRE Algorithm VI

Reactor	Evaluate	For X = 0.9
Batch	$kC_{A0} = (0.5)(0.2)$ $= 0.1\ s^{-1}$	$t = 90\ s$
CSTR	$kC^2_{A0} = (0.5)(0.2)^2$ $= 0.02 mol/dm^3 \cdot s$ $F_{A0} = C_{A0} \cdot v_0$ $= (0.2)(2.5) = 0.5\ mol/s$	$V = 680.6\ dm^3$ $\tau = V/v_0 = 272.3\ s$
PFR		$V = 90.7\ dm^3$ $\tau = V/v_0 = 36.3\ s$

7. Mole Balances on 4 Basic Reactors I

- **Liquid phase** $\mathrm{A}+\frac{b}{a}\mathrm{B}\rightarrow\frac{c}{a}\mathrm{C}+\frac{d}{a}\mathrm{D}$

Batch	$\frac{dC_\mathrm{A}}{dt}=r_\mathrm{A}$	**and**	$\frac{dC_\mathrm{B}}{dt}=\frac{b}{a}r_\mathrm{A}$
CSTR	$V=\frac{v_0(C_{\mathrm{A}0}-C_\mathrm{A})}{-r_\mathrm{A}}$	**and**	$V=\frac{v_0(C_{\mathrm{B}0}-C_\mathrm{B})}{-(b/a)r_\mathrm{A}}$
PFR	$v_0\frac{dC_\mathrm{A}}{dV}=r_\mathrm{A}$	**and**	$v_0\frac{dC_\mathrm{B}}{dV}=\frac{b}{a}r_\mathrm{A}$
PBR	$v_0\frac{dC_\mathrm{A}}{dW}=r_\mathrm{A}^{'}$	**and**	$v_0\frac{dC_\mathrm{B}}{dW}=\frac{b}{a}r_\mathrm{A}^{'}$

7. Mole Balances on 4 Basic Reactors II

- **Gas phase 1**

$$v = v_0 \frac{F_{\mathrm{T0}}}{F_{\mathrm{T}}} \frac{P}{P_0} \frac{T_0}{T}$$

$$C_{\mathrm{A}} = \frac{F_{\mathrm{A}}}{v} = \frac{F_{\mathrm{A}}}{v_0} \frac{F_{\mathrm{T0}}}{F_{\mathrm{T}}} \frac{P}{P_0} \frac{T_0}{T}$$

$$C_{\mathrm{A}} = C_{\mathrm{T0}} \frac{F_{\mathrm{A}}}{v} = \left(\frac{F_{\mathrm{T0}}}{F_{\mathrm{T}}} \right) \frac{P}{P_0} \frac{T_0}{T}, \quad C_{\mathrm{T0}} = \frac{P_0}{R T_0}$$

7. Mole Balances on 4 Basic Reactors III

- **Gas phase 2**

$$\mathrm{A} + \frac{b}{a}\mathrm{B} \rightarrow \frac{c}{a}\mathrm{C} + \frac{d}{a}\mathrm{D}$$

1. Mole balances Batch	CSTR	PFR
$\frac{dN_\mathrm{A}}{dt} = r_\mathrm{A}V$	$V = \frac{F_{\mathrm{A}0} - F_\mathrm{A}}{-r_\mathrm{A}}$	$\frac{dF_\mathrm{A}}{dV} = r_\mathrm{A}$
$\frac{dN_\mathrm{B}}{dt} = r_\mathrm{B}V$	$V = \frac{F_{\mathrm{B}0} - F_\mathrm{B}}{-r_\mathrm{B}}$	$\frac{dF_\mathrm{B}}{dV} = r_\mathrm{B}$
$\frac{dN_\mathrm{C}}{dt} = r_\mathrm{C}V$	$V = \frac{F_{\mathrm{C}0} - F_\mathrm{C}}{-r_\mathrm{C}}$	$\frac{dF_\mathrm{C}}{dV} = r_\mathrm{C}$
$\frac{dN_\mathrm{D}}{dt} = r_\mathrm{D}V$	$V = \frac{F_{\mathrm{D}0} - F_\mathrm{D}}{-r_\mathrm{D}}$	$\frac{dF_\mathrm{D}}{dV} = r_\mathrm{D}$

7. Mole Balances on 4 Basic Reactors IV

- Gas phase 3

2. Rate law $-r_A = k_A C_A^{\alpha} C_B^{\beta}$

3. Stoichiometry

- Relative rate

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

- Then

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

- Concentration

$$C_A = C_{T0}\left(\frac{F_A}{F_T}\right)\left(\frac{T_0}{T}\right)y \quad C_B = C_{T0}\left(\frac{F_B}{F_T}\right)\left(\frac{T_0}{T}\right)y \quad C_C = C_{T0}\left(\frac{F_C}{F_T}\right)\left(\frac{T_0}{T}\right)y$$

$$C_D = C_{T0}\left(\frac{F_D}{F_T}\right)\left(\frac{T_0}{T}\right)y \qquad \frac{dy}{dW} = \frac{-\alpha}{2y}\left(\frac{F_T}{F_{T0}}\right)\left(\frac{T}{T_0}\right), \quad y = \frac{P}{P_0}$$

7. Mole Balances on 4 Basic Reactors V

- **Gas phase 4**

- Total molar flow rate $F_{\mathrm{T}} = F_{\mathrm{A}} + F_{\mathrm{B}} + F_{\mathrm{C}} + F_{\mathrm{D}} + F_{\mathrm{I}}$

4. Combine

$$\frac{dF_{\mathrm{A}}}{dV} = -k_{\mathrm{A}} C_{\mathrm{T0}}^{\alpha+\beta} \left(\frac{F_{\mathrm{A}}}{F_{\mathrm{T}}}\right)^{\alpha} \left(\frac{F_{\mathrm{B}}}{F_{\mathrm{T}}}\right)^{\beta} \qquad \frac{dF_{\mathrm{B}}}{dV} = -\frac{b}{a} k_{\mathrm{A}} C_{\mathrm{T0}}^{\alpha+\beta} \left(\frac{F_{\mathrm{A}}}{F_{\mathrm{T}}}\right)^{\alpha} \left(\frac{F_{\mathrm{B}}}{F_{\mathrm{T}}}\right)^{\beta}$$

$$\frac{dF_{\mathrm{C}}}{dV} = \frac{c}{a} k_{\mathrm{A}} C_{\mathrm{T0}}^{\alpha+\beta} \left(\frac{F_{\mathrm{A}}}{F_{\mathrm{T}}}\right)^{\alpha} \left(\frac{F_{\mathrm{B}}}{F_{\mathrm{T}}}\right)^{\beta} \qquad \frac{dF_{\mathrm{D}}}{dV} = \frac{d}{a} k_{\mathrm{A}} C_{\mathrm{T0}}^{\alpha+\beta} \left(\frac{F_{\mathrm{A}}}{F_{\mathrm{T}}}\right)^{\alpha} \left(\frac{F_{\mathrm{B}}}{F_{\mathrm{T}}}\right)^{\beta}$$

- Specify parameter values $k_{\mathrm{A}},\ C_{\mathrm{T0}},\ \alpha,\ \beta,\ T_{0},\ a,\ b,\ c,\ d$

- Specify entering numbers $F_{A0},\ F_{B0},\ F_{C0},\ F_{D0}$

8. Microreactors I

○ Description

- High surface area-to-volume ratio in their micro structure regions
  - 100μm width, 20,000μm length (2 cm)
  - high surface area-to-volume ratio

    ☞ ca. 10,000 m^2/m^3

    reduce or eliminate heat & mass transfer resistances
  - to study intrinsic kinetics of reactions isothermally
  - production of toxic or explosive intermediates
  - shorter residence time
  - narrow residence time distribution

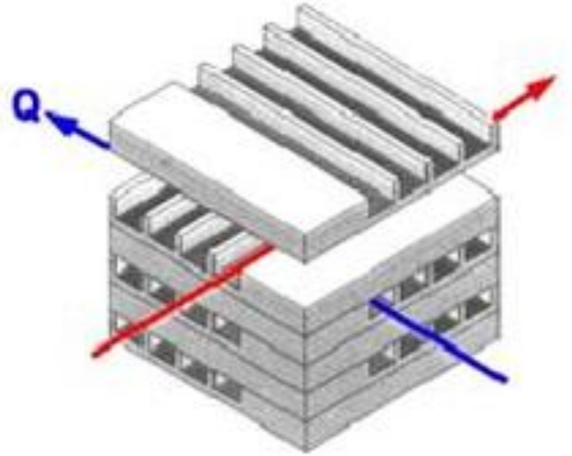
8. Microreactors II

- **Example**

$$R-CH_2OH+1/2O_2 \xrightarrow[Ag]{} R-CHO+H_2O$$

- 32 microreaction system in parallel produce 2000 t/yr

- Lab-on-a-chip



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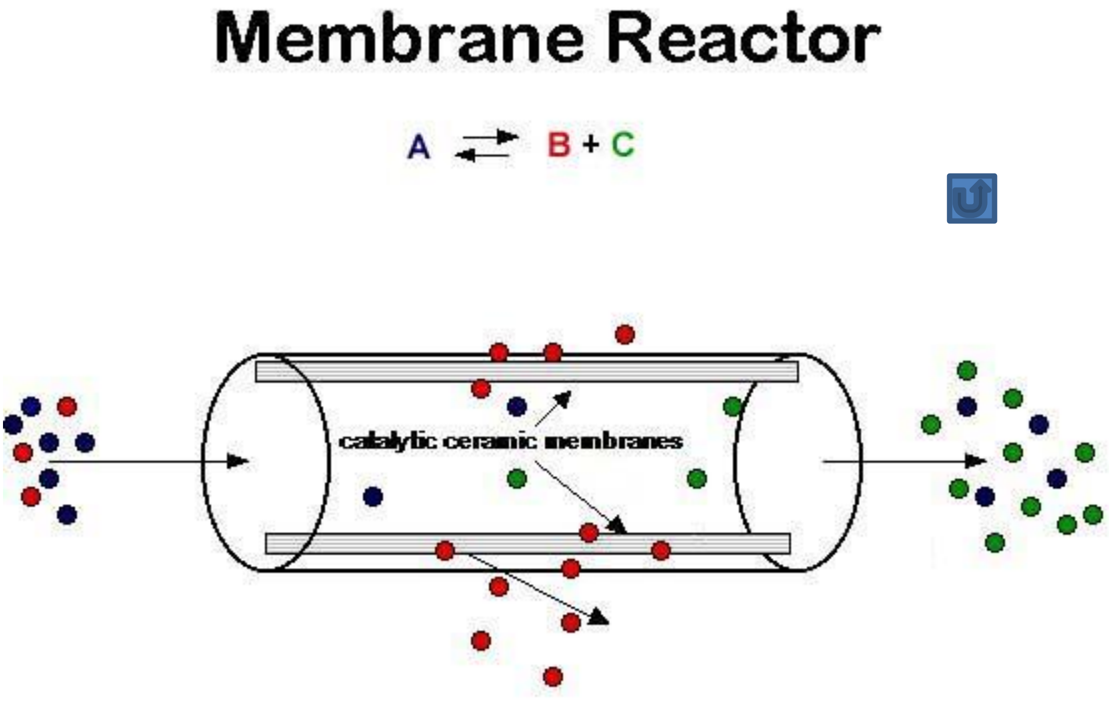
9. Membrane Reactors I

- ○ Description
  - \- Really just a plug-flow reactor
    - contains an additional cylinder of some porous material within it, kind of like the tube within the shell of a shell-and-tube heat exchanger
    - this porous inner cylinder is the membrane that gives the membrane reactor its name
  - \- The membrane is a barrier that only allows certain components to pass through it
    - selectivity of the membrane is controlled by its pore diameter, which can be on the order of Angstroms, for microporous layers, or on the order of microns for macroporous layers

9. Membrane Reactors II

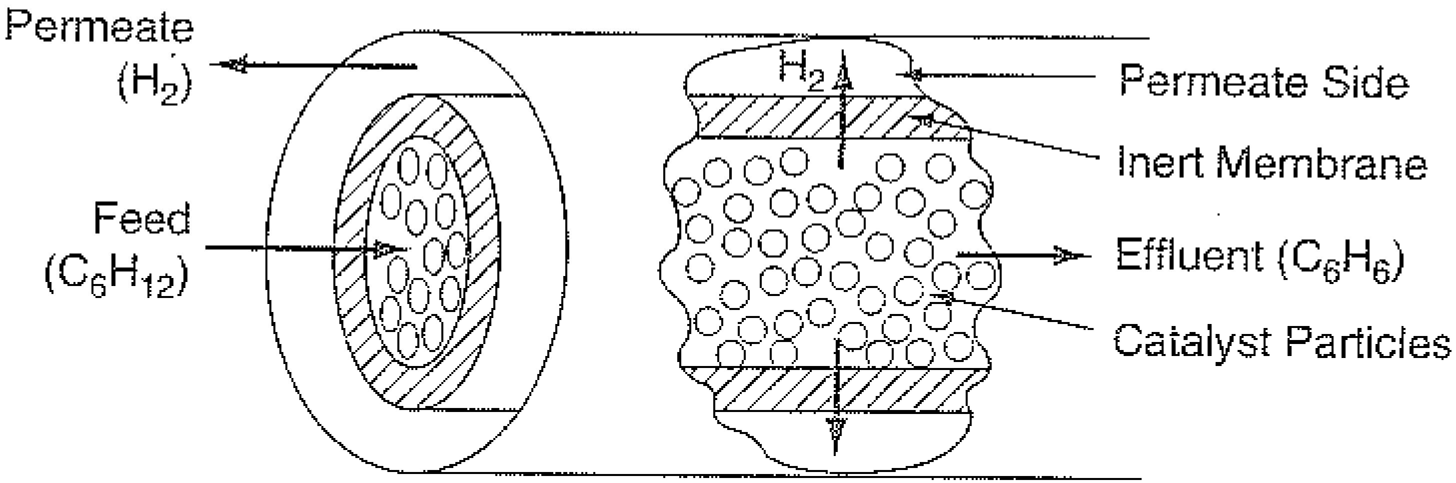
- **What is it?**
  - **Combine reaction with separation to increase conversion and/or selectivity**



A mixed feed of A and B enters the membrane reactor. C is produced in the reactor, and B diffuses out through the membrane pores. There are multiple ceramic membranes, but only two are shown for simplicity.

9. Membrane Reactors III

- **Typical reactors 1**
  - **IMRCF (Inert Membrane Reactor with Catalyst Pellets on the Feed Side)**

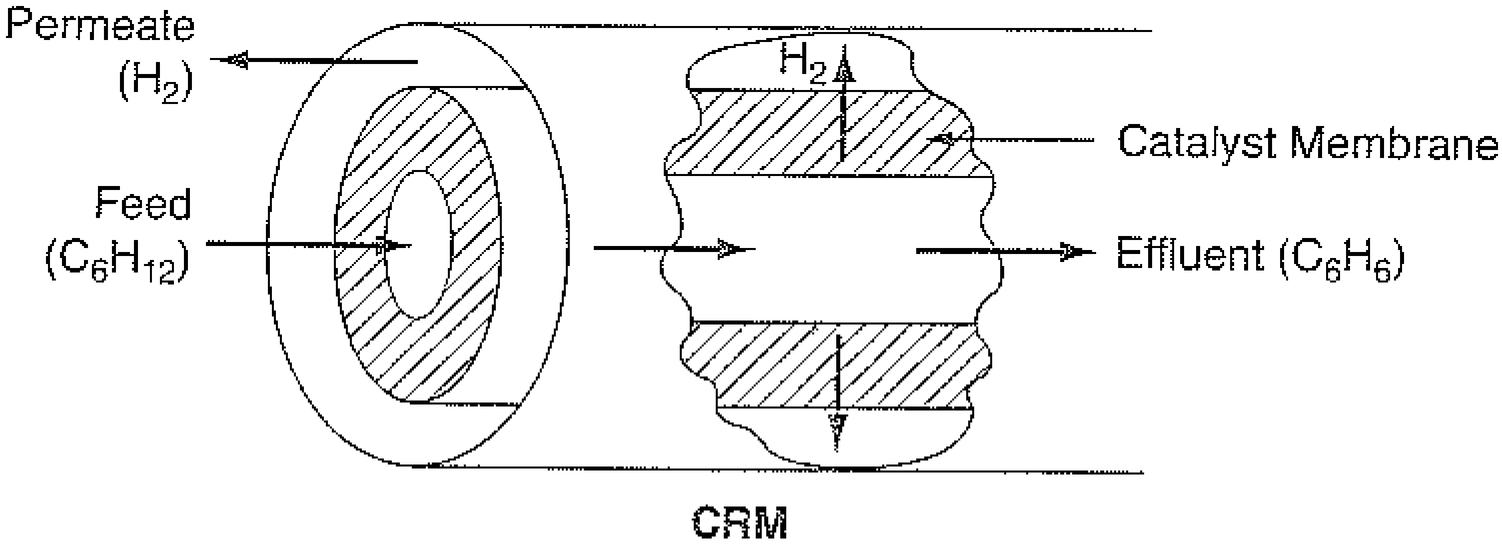


IMRCF

9. Membrane Reactors IV

○ **Typical reactors 2**

- CMR (Catalytic Membrane Reactor)



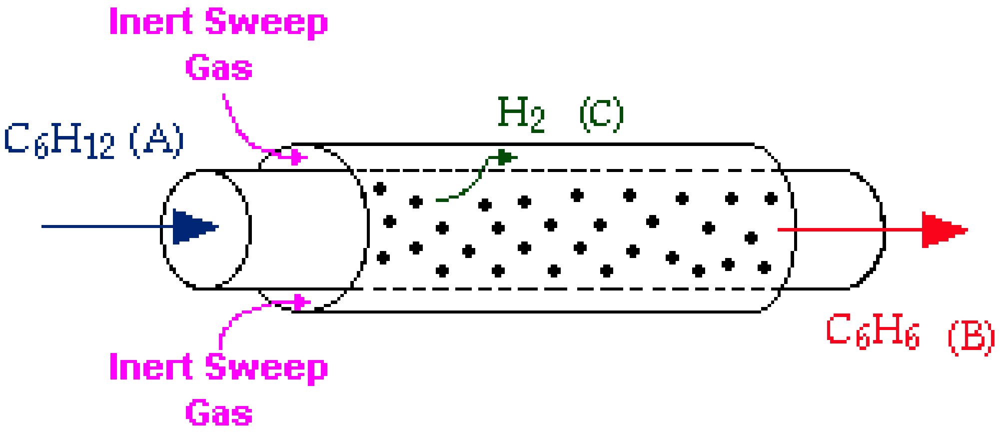
9. Membrane Reactors V

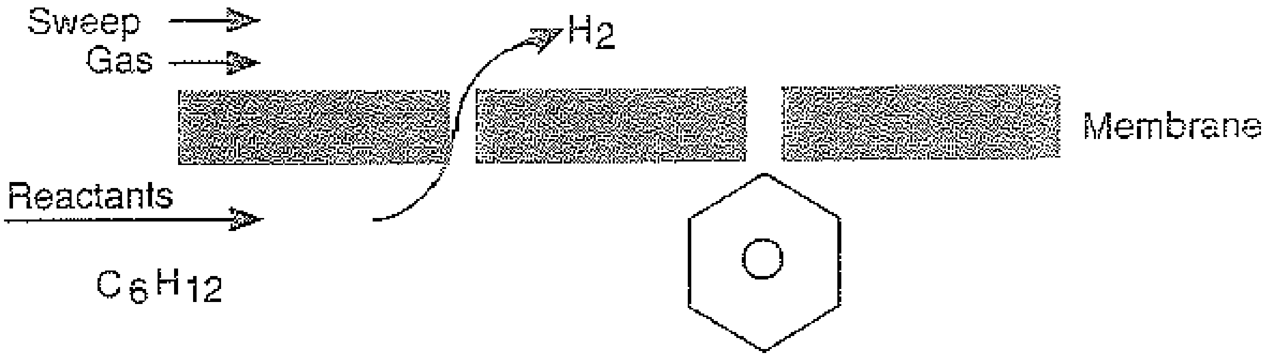
○ Modeling 1

- IMRCF

$$C_6H_{12} \Leftrightarrow C_6H_6 + 3H_2$$

$$A \Leftrightarrow B + 3C$$





9. Membrane Reactors VI

○ Modeling 2

- Change the algorithm a little, $V \rightarrow W\ (= \rho_b V)$

- mole balance for A $\boxed{\dfrac{dF_A}{dV} = r_A}$

- mole balance for C $\boxed{\dfrac{dF_C}{dV} = r_C}$

- mole balance for B

$$\boxed{\frac{dF_B}{dV} = r_B - R_B}$$

$$\begin{bmatrix}\text{In}\\ \text{by flow}\end{bmatrix} - \begin{bmatrix}\text{Out}\\ \text{by flow}\end{bmatrix} - \begin{bmatrix}\text{Out by}\\ \text{Diffusion}\end{bmatrix} + [\text{Gen.}] = [\text{Accu.}]$$

$$\overbrace{F_{B|_V}} \quad - \quad \overbrace{F_{B|_{V+\Delta V}}} \quad - \quad \overbrace{R_B \Delta V} \quad \overbrace{R_B \Delta V} \ = 0$$

9. Membrane Reactors VII

○ **Modeling 3**

- **Rate of molar flux B out through the membrane**

$$W_{\mathrm{B}} = k_{\mathrm{C}}^{'}(C_{\mathrm{B}} - C_{\mathrm{BS}})$$

- **Rate of transport B out through the membrane**

$$R_{\mathrm{B}} = W_{\mathrm{B}}a = k_{\mathrm{C}}^{'}a(C_{\mathrm{B}} - C_{\mathrm{BS}})$$

$$a = \frac{\text{Area}}{\text{Volume}} = \frac{\pi D L}{\frac{\pi D^2}{4} L} = \frac{4}{D}$$

- **Let $k_{\mathrm{C}} = k'_{C}a$ and $C_{\mathrm{BS}} \approx 0$,** $\boxed{R_{\mathrm{B}} = k_{\mathrm{C}}C_{\mathrm{B}}}$

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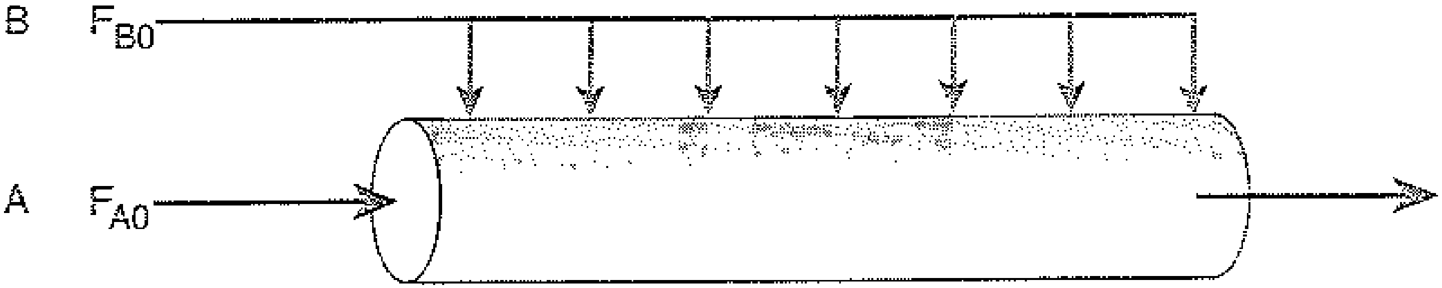
9. Membrane Reactors VIII

- **Enhance selectivity**
  - **Fed species to the reactor through the sides of membrane**



$$\frac{dF_B}{dV} = r_B + R_B$$

10. Unsteady-State Operation of Stirred Reactors I

- **Startup of a CSTR 1**

- Mole balance equation

$$F_{A0} - F_A + r_A V = \frac{dN_A}{dt}$$

- For batch reactor, conversion means little

$$C_{A0} - C_A + r_A \tau = \tau \frac{dC_A}{dt}$$

- 1st order rxn

$$\frac{dC_A}{dt} + \frac{1+\tau k}{\tau} C_A = \frac{C_{A0}}{\tau}$$

- With initial conditions $C_A = 0$ at $t = 0$

$$C_A = \frac{C_{A0}}{1+\tau k}\left\{1 - \exp\left[-(1+\tau k)\frac{\mathrm{t}}{\tau}\right]\right\}$$

10. Unsteady-State Operation of Stirred Reactors II

○ **Startup of a CSTR 2**

- Steady state analysis

- **assume time to reach 99% of st-st conc., C_{AS}**

$$C_{AS} = \frac{C_{A0}}{1+\tau k}$$

- **$C_{A0} = 0.99C_{AS}$**

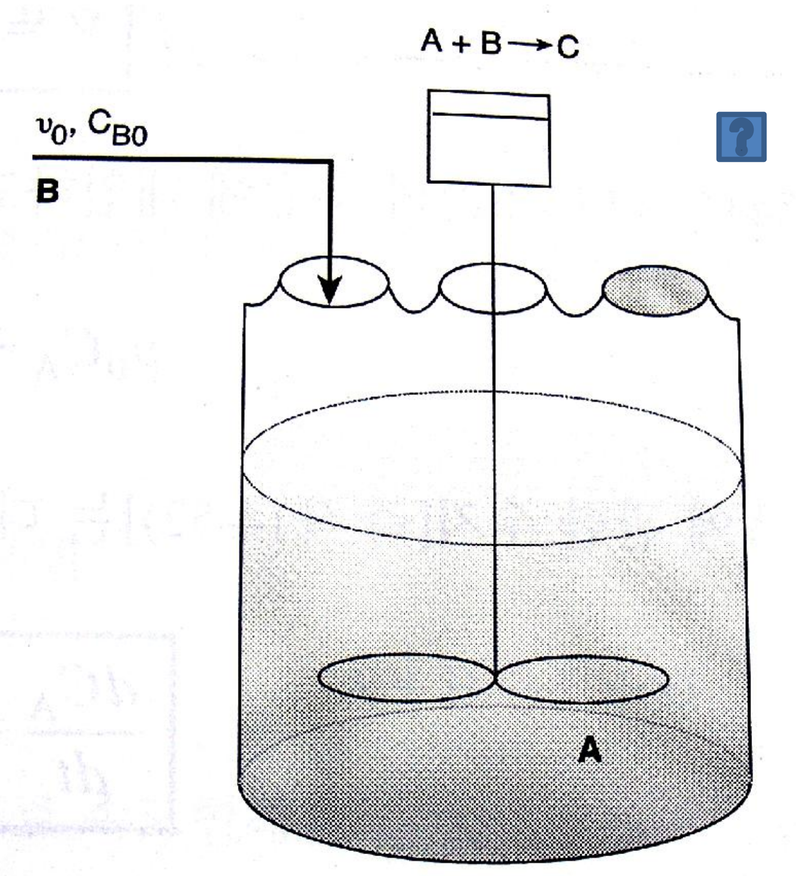
$$t_S = 4.6\frac{\tau}{1+\tau k}$$

- **for slow rxn with small k ($1 \gg \tau k$)** $\boxed{t_S = 4.6\tau}$
- **for rapid rxn with large k ($1 \ll \tau k$)** $\boxed{t_S = 4.6/k}$

☞ **most 1st-order system, st-st achieved in 3 ~ 4 space time**

10. Unsteady-State Operation of Stirred Reactors III

- Semibatch reactor 1
  - Motivation
    - to obtain high selectivity
    - maintain A at high conc.
    - feed B as low as possible



10. Unsteady-State Operation of Stirred Reactors IV

- **Semibatch reactor 2**

- Mole balance equation 1

$$\begin{bmatrix}\text{Rate}\\ \text{in}\end{bmatrix} - \begin{bmatrix}\text{Rate}\\ \text{out}\end{bmatrix} + \begin{bmatrix}\text{Rate of}\\ \text{Generation}\end{bmatrix} = \begin{bmatrix}\text{Rate of}\\ \text{Accum}\end{bmatrix}$$

$$\overbrace{0} \quad - \quad \overbrace{0} \quad - \quad \overbrace{r_A V(t)} \quad = \quad \overbrace{\frac{dN_A}{dt}}$$

$$r_A V = \frac{d(C_A V)}{dt} = \frac{V dC_A}{dt} + C_A \frac{dV}{dt}$$

10. Unsteady-State Operation of Stirred Reactors V

- **Semibatch reactor 3**

- Mole balance equation 2

$$r_A V = \frac{d(C_A V)}{dt} = \frac{V dC_A}{dt} + C_A \frac{dV}{dt}$$

- Since the reactor is being filled, V varies

$$\begin{bmatrix}\text{Rate}\\ \text{in}\end{bmatrix} - \begin{bmatrix}\text{Rate}\\ \text{out}\end{bmatrix} + \begin{bmatrix}\text{Rate of}\\ \text{Generation}\end{bmatrix} = \begin{bmatrix}\text{Rate of}\\ \text{Accum}\end{bmatrix}$$

$$\overbrace{\rho_0 v_0} \quad - \quad \overbrace{0} \quad - \quad \overbrace{0} \quad = \quad \overbrace{\frac{d(\rho V)}{dt}}$$

10. Unsteady-State Operation of Stirred Reactors VI

- Semibatch reactor 4

  - Constant density
    $$\frac{dV}{dt} = v_0$$

  - With initial condition $V = V_0$ at $t = 0$
    $$\boxed{V = V_0 + v_0 t}$$

  - Balance on A can be rewritten as
    $$\boxed{\frac{dC_A}{dt} = r_A - \frac{v_0}{V} C_A}$$

  - For B, we have generation term, $r_B V$
    - balance on B can be
      $$\boxed{\frac{dC_B}{dt} = r_B + \frac{v_0 (C_{B0} - C_B)}{V}}$$

10. Unsteady-State Operation of Stirred Reactors VII

○ **Semibatch reactor 5** $\mathrm{A + B \rightleftarrows C + D}$

- Design equations in terms of conversion 1

- **for species A**

$$\begin{bmatrix}\text{\# of moles}\\ \text{of A in the vat}\\ \text{at time } t\end{bmatrix} = \begin{bmatrix}\text{\# of moles}\\ \text{of A in the vat}\\ \text{initially}\end{bmatrix} - \begin{bmatrix}\text{\# of moles}\\ \text{of A reacted}\\ \text{up to time } t\end{bmatrix}$$

$$\overbrace{N_{\mathrm{A}}} = \overbrace{N_{\mathrm{A0}}} - \overbrace{N_{\mathrm{A0}}X}$$

- **for species B**

$$\begin{bmatrix}\text{\# of moles}\\ \text{of B in the vat}\\ \text{at time } t\end{bmatrix} = \begin{bmatrix}\text{\# of moles}\\ \text{of B in the vat}\\ \text{initially}\end{bmatrix} + \begin{bmatrix}\text{\# of moles}\\ \text{of B added}\\ \text{to the vat}\end{bmatrix} - \begin{bmatrix}\text{\# of moles}\\ \text{of B reacted}\\ \text{up to time } t\end{bmatrix}$$

$$\overbrace{N_{\mathrm{B}}} = \overbrace{N_{\mathrm{B}i}} + \overbrace{\int_0^t F_{B0}\,dt} - \overbrace{N_{\mathrm{A0}}X}$$

10. Unsteady-State Operation of Stirred Reactors VIII

- Semibatch reactor 6 $\quad A + B \rightleftarrows C + D$

  - Design equations in terms of conversion 2

    - for a constant molar feed rate & no B initially

$$N_{\mathrm{B}} = F_{\mathrm{B0}}t - N_{\mathrm{A0}}X$$

- mole balance on species A

$$r_{\mathrm{A}}V = \frac{dN_{\mathrm{A}}}{dt} = -N_{\mathrm{A0}}\frac{dX}{dt}$$

- for a reversible 2nd order rxn

$$-r_{\mathrm{A}} = k\left(C_{\mathrm{A}}C_{\mathrm{B}} - \frac{C_{\mathrm{C}}C_{\mathrm{D}}}{K_{\mathrm{C}}}\right)$$

- recalling $V = V_0 + v_0 t$

$$C_{\mathrm{A}} = \frac{N_{\mathrm{A}}}{V} = \frac{N_{\mathrm{A0}}(1-X)}{V_0 + v_0 t} \qquad C_{\mathrm{B}} = \frac{N_{\mathrm{B}}}{V} = \frac{N_{\mathrm{B}i} + F_{\mathrm{B0}}t - N_{\mathrm{A0}}X}{V_0 + v_0 t} \qquad C_{\mathrm{C}} = \frac{N_{\mathrm{A0}}X}{V_0 + v_0 t}$$

$$C_{\mathrm{D}} = \frac{N_{\mathrm{A0}}X}{V_0 + v_0 t}$$

$$\boxed{\frac{dX}{dt} = \frac{k\left[(1-X)(N_{\mathrm{B}i} + F_{\mathrm{B0}}t - N_{\mathrm{A0}}X) - (N_{\mathrm{A0}}X^2/K_{\mathrm{C}})\right]}{V_0 + v_0 t}}$$

10. Unsteady-State Operation of Stirred Reactors IX

- Semibatch reactor 7 $\quad \mathrm{A + B \rightleftarrows C + D}$

- Equilibrium conversion 1

- at time *t*, equilibrium conversion

$$K_\mathrm{C}=\frac{C_{\mathrm{C}e}C_{\mathrm{D}e}}{C_{\mathrm{A}e}C_{\mathrm{B}e}}=\frac{\left(\frac{N_{\mathrm{C}e}}{V}\right)\left(\frac{N_{\mathrm{D}e}}{V}\right)}{\left(\frac{N_{\mathrm{A}e}}{V}\right)\left(\frac{N_{\mathrm{B}e}}{V}\right)}=\frac{N_{\mathrm{C}e}N_{\mathrm{D}e}}{N_{\mathrm{A}e}N_{\mathrm{B}e}}$$

- for $N_B = F_{B0}t - N_{A0}X$

$$K_\mathrm{C}=\frac{(N_{\mathrm{A0}}X_e)(N_{\mathrm{A0}}X_e)}{N_{\mathrm{A0}}(1-X_e)(F_{\mathrm{B0}}t-N_{\mathrm{A0}}X_e)}=\frac{N_{\mathrm{A0}}X_e^2}{(1-X_e)(F_{\mathrm{B0}}t-N_{\mathrm{A0}}X_e)}$$

$$\text{then,}\quad t=\frac{N_{\mathrm{A0}}}{K_\mathrm{C}F_{\mathrm{B0}}}\left(K_\mathrm{C}X_e+\frac{X_e^2}{1-X_e}\right)$$

10. Unsteady-State Operation of Stirred Reactors X

- Semibatch reactor 8 $A + B \rightleftharpoons C + D$
  - \- Equilibrium conversion 2
    - at a semibatch reactor

$$X_e = \frac{K_C\left(1+\frac{F_{B0}t}{N_{A0}}\right) - \sqrt{\left[K_C\left(1+\frac{F_{B0}t}{N_{A0}}\right)\right]^2 - 4(K_C - 1)K_C\frac{tF_{B0}}{N_{A0}}}}{2(K_C - 1)}$$

10. Unsteady-State Operation of Stirred Reactors XI

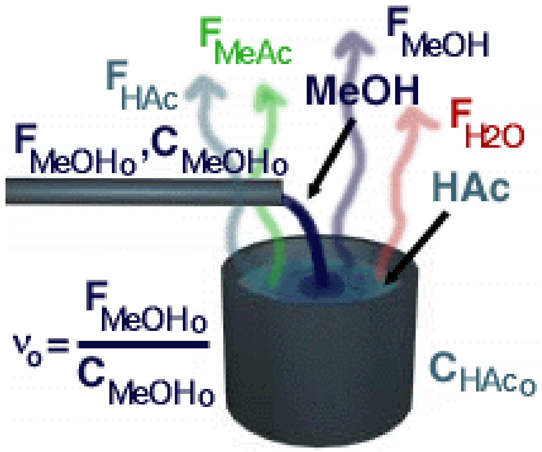
- **Reactive distillation**

  - Applicable to reversible, liquid phase reactions

$CH_3COOH + CH_3OH \rightleftharpoons CH_3COOCH_3 + H_2O$

Acetic Acid Methanol Methyl Acetate Water

$A + B \rightleftharpoons C + D$



- **the equilibrium point lies far to the left and little product is formed**

$A + B \leftharpoondown\!\!\rightharpoonup C + D$

- **if one or more of the products are removed more of the product will be formed because of Le Chatlier's Principle**

$A + B \rightleftharpoons C + D\uparrow$