4. The material balances for isothermal ideal reactor models

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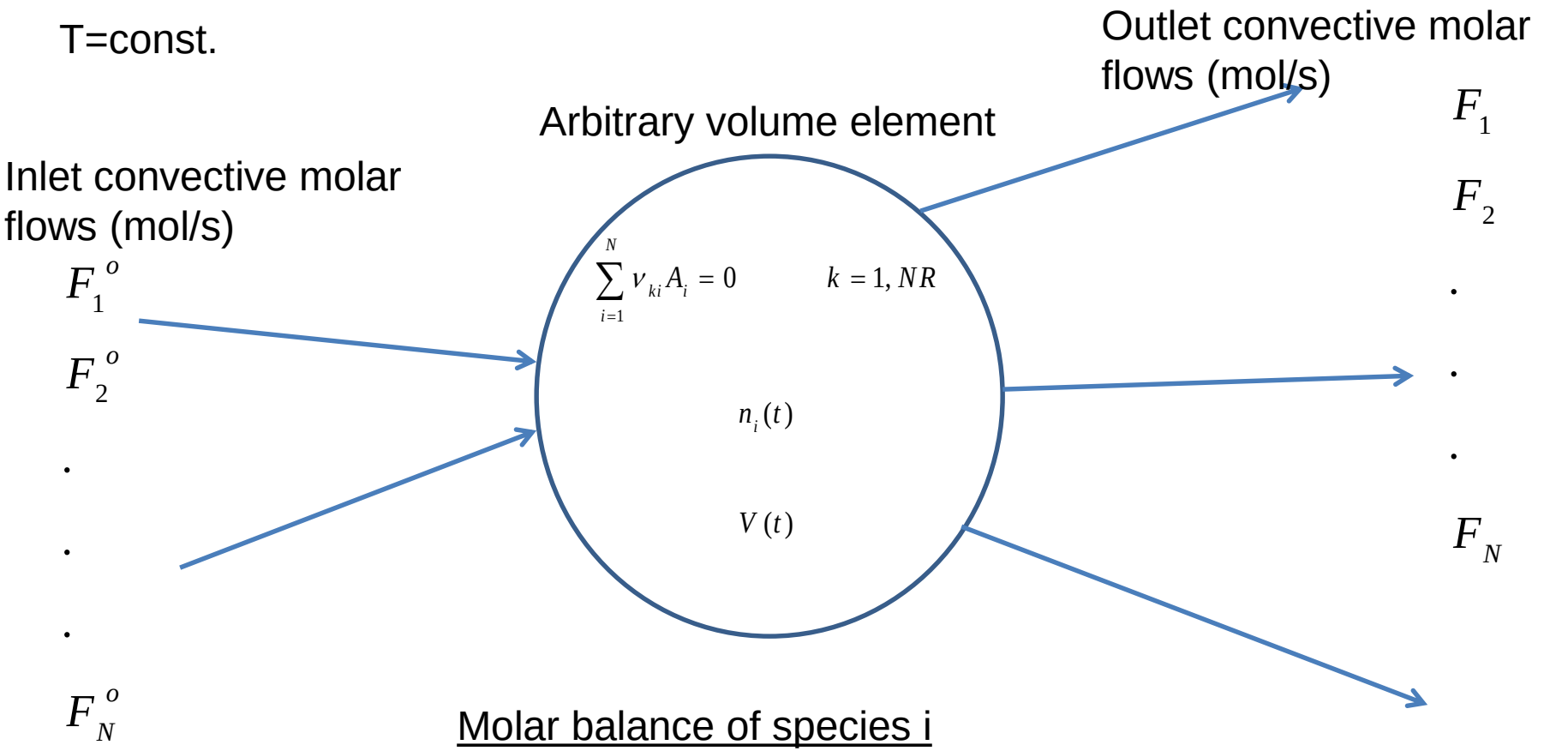
Summary

- General material balance of reacting system
- Batch reactor
- Continuous-flow reactors: CSTR (Continuous Stirred Tank Reactor)
  PFR (Plug Flow Reactor)
- Steady state of CSTR and PFR
- Design tasks : outlet (final conversion), given volume of reactor x volume of reactor, given outlet conversion

T=const.



Molar balance of species i

$$F_i^0 - F_i + \sum_{k=1}^{NR} \nu_{ki} \int_V r_{V,k}\, dV = \frac{\partial}{\partial t}\left(\int_V c_i\, dV \right) = \frac{\partial n_i}{\partial t}$$

$$\sum_{i=1}^{N} \nu_{ki} = \Delta \nu_k$$

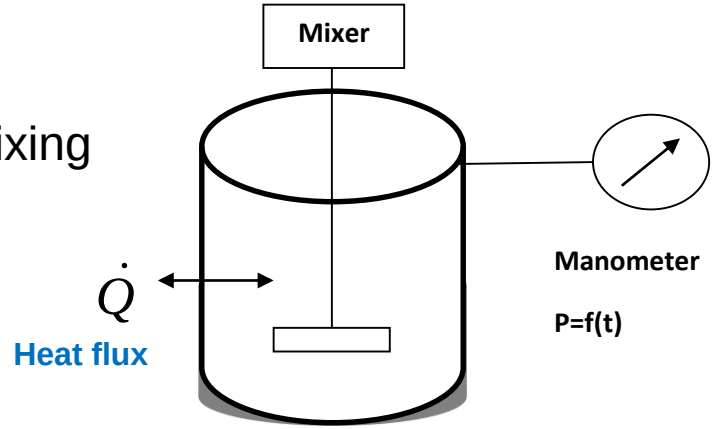
Overall molar balance

$$\sum_{i=1}^{N} \left[F_i^o - F_i \right] + \sum_{i=1}^{N} \sum_{k=1}^{NR} \nu_{ki} \int_V r_{V,k}\, dV = F^o - F + \sum_{k=1}^{NR} \Delta \nu_k \int_V r_{V,k}\, dV = \frac{\partial n}{\partial t}$$

Batch reactors

Laboratory
Pharmaceutical industry
Special chemicals
Polymers
.
.
.

V≠const.
T=const.
Perfect mixing



$$\sum_{i=1}^{N} \nu_{ki} A_i = 0 \qquad k = 1, NR$$

$n_i(t)$

$V_R(t)$ – Volume of reaction mixture

Molar balance of species i

$$\cancel{F_i^0} - \cancel{F_i} + \sum_{k=1}^{NR} \nu_{ki} \int_{V_R} r_{V,k}\, dV = \frac{\partial n_i}{\partial t}$$

$$\frac{dn_i}{dt} = \sum_{k=1}^{NR} \nu_{ki} r_{V,k} . V_R$$

Reactor volume constant (V_R=const.)

$$\frac{1}{V_R}\frac{dn_i}{dt} = \frac{d\left(\frac{n_i}{V_R}\right)}{dt} = \frac{dc_i}{dt} = \sum_{k=1}^{NR} \nu_{ki} r_{V,k}\left(c_1, c_2, \ldots c_N\right)$$

Reactor pressure constant (P = konst.)

$$n_i = c_i . V_R$$

$$\frac{1}{V_R}\frac{dn_i}{dt} = \frac{1}{V_R}\frac{d\left(c_i . V_R\right)}{dt} = \frac{dc_i}{dt} + c_i \frac{d \ln V_R}{dt} = \sum_{k=1}^{NR} \nu_{ki} r_{V,k}$$

$$\frac{dc_i}{dt} = \sum_{k=1}^{NR} \nu_{ki} r_{V,k} - c_i \frac{d \ln V_R}{dt}$$

To calculate $P(t)$ or $V_R(t)$

state equation f(T,P,V,composition) = 0 is needed

Example

Constant volume isothermal batch reactor, ideal gas mixture

$$P = \frac{RT}{V_R}\sum_{j=1}^{N} n_j \qquad \sum_{j=1}^{N} \nu_{kj} = \Delta\nu_k$$

$$\frac{dP}{dt} = \frac{RT}{V_R}\sum_{j=1}^{N}\frac{dn_j}{dt} = \frac{RT}{V_R}\sum_{j=1}^{N} V_R \sum_{k=1}^{NR} \nu_{kj} r_{V,k} = RT\sum_{k=1}^{NR}\Delta\nu_k r_{V,k}$$

Constant pressure isothermal batch reactor, ideal gas mixture

$$V_R = \frac{RT}{P}\sum_{j=1}^{N} n_j$$

$$\frac{dV_R}{dt} = \frac{RT}{P}\sum_{j=1}^{N}\frac{dn_j}{dt} = \frac{RT}{P}\sum_{j=1}^{N} V_R \sum_{k=1}^{NR} \nu_{kj} r_{V,k} = \frac{RTV_R}{P}\sum_{k=1}^{NR}\Delta\nu_k r_{V,k}$$

$$\frac{d\ln(V_R)}{dt} = \frac{RT}{P}\sum_{k=1}^{NR}\Delta\nu_k r_{V,k}$$

$$c_i = y_i\frac{P}{RT} \quad [*]$$

$$\frac{dc_i}{dt} = \sum_{k=1}^{NR}\nu_{ki} r_{V,k} - c_i\frac{RT}{P}\sum_{k=1}^{NR}\Delta\nu_k r_{V,k} =$$

$$= \sum_{k=1}^{NR}\nu_{ki} r_{V,k} - y_i\sum_{k=1}^{NR}\Delta\nu_k r_{V,k}$$

Example

Constant volume batch reactor, liquid mixture $\Rightarrow$ constant pressure

Second order irreversible reaction

$$A_{1(l)} + A_{2(l)} \rightarrow A_{3(l)} \qquad r_V = kc_1c_2, \qquad t = 0, c_1 = c_1^o,\ c_2 = c_2^o,\ c_3 = 0$$

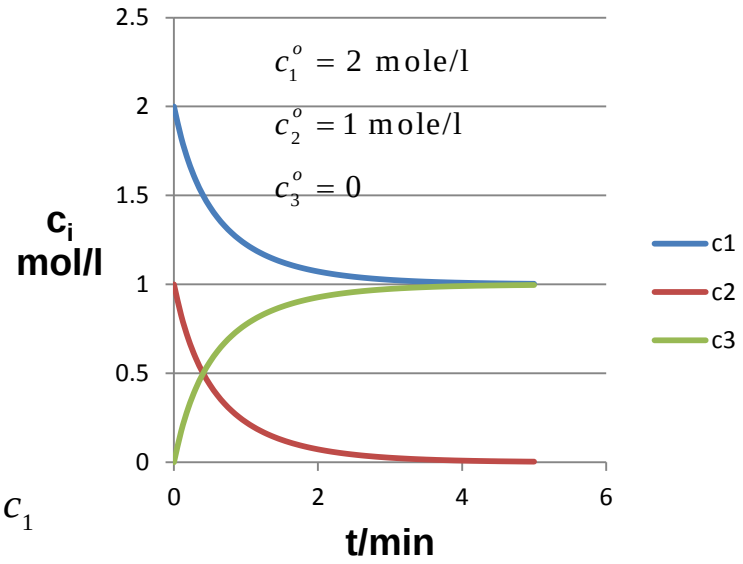
$$\frac{dc_i}{dt} = \nu_i r_V = \nu_i k c_1 c_2$$

$$\frac{dc_1}{dt} = -kc_1c_2$$

$$\frac{dc_2}{dt} = -kc_1c_2$$

$$\frac{dc_3}{dt} = kc_1c_2$$

$$c_1 - c_1^o = c_2 - c_2^o,\ c_2 = c_1 - c_1^o + c_2^o,\ c_3 = c_1^o - c_1$$

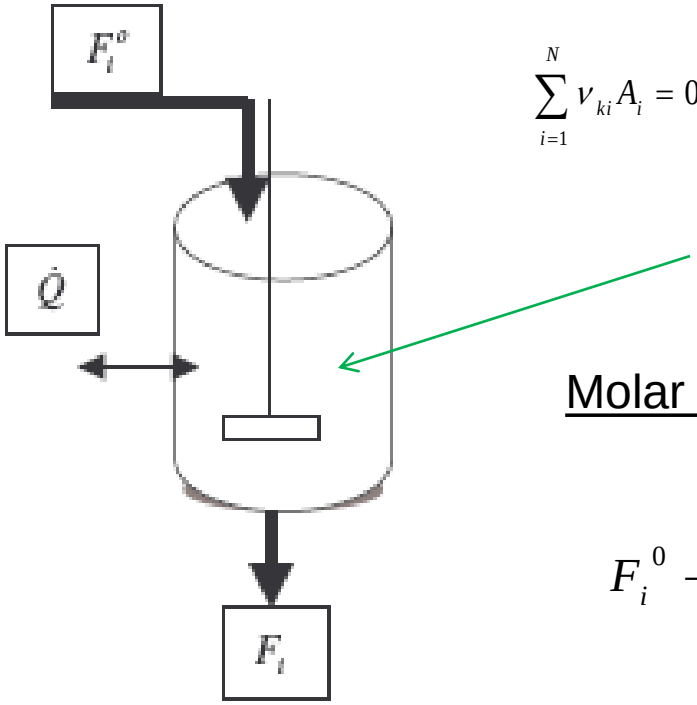


$$\frac{dc_1}{dt} = -kc_1\left(c_1 - c_1^o + c_2^o\right) \rightarrow \int_{c_1^o}^{c_1} \frac{dc_1}{c_1\left(c_1 - c_1^o + c_2^o\right)} = -k\int_0^t dt \rightarrow c_1 = \frac{\left(c_1^o - c_2^o\right)}{1 - \frac{c_2^o}{c_1^o}e^{\left(c_2^o - c_1^o\right)kt}}$$

$$c_1^o = c_2^o \qquad c_1 = \left(\frac{1}{c_1^o} + kt\right)^{-1}$$

Continuous-flow reactors

Continuous Stirred Tank Reactor – CSTR



$$\sum_{i=1}^{N} \nu_{ki} A_i = 0 \qquad k = 1, NR$$

$n_i(t)$

$V_R = const$ – Volume of reactor

Molar balance of species i

$$F_i^0 - F_i + \sum_{k=1}^{NR} \nu_{ki} r_{V,k} V_R = \frac{dn_i}{dt}$$

Overall molar balance

$$F^o - F + \sum_{k=1}^{NR} \Delta\nu_k r_{V,k} V_R = \frac{dn}{dt}$$

We need suplementary information

- **state behavior of reaction mixture**
- **start-up (shut-down) molar flow rates of individual species**

Constant pressure isothermal CSTR, ideal gas mixture $RT\sum_{i=1}^{N} n_j = pV_R$

It arises from overall molar balance (volume of reactor, V_R is constant)

$$\frac{d\sum_{i=1}^{N} n_j}{dt} = \sum_{i=1}^{N} \frac{dn_i}{dt} = F^o - F + V_R \sum_{i=1}^{N}\sum_{k=1}^{NR} \nu_{ki} r_{V,k} = F^o - F + V_R \sum_{k=1}^{NR} \Delta\nu_k r_{V,k} = 0$$

$$F = F^o + V_R \sum_{k=1}^{NR} \Delta\nu_k r_{V,k}$$

and molar balance of species i becomes

$$\frac{dn_i}{dt} = F_i^o - y_i \left(F^o + V_R \sum_{k=1}^{NR} \Delta\nu_k r_{V,k} \right)_i + V_R \sum_{k=1}^{NR} \nu_{ki} r_{V,k} \qquad F_i^o = y_i^o F^o$$

$$\frac{dn_i}{dt} = \frac{PV_R}{RT}\frac{dy_i}{dt} = F^o(y_i^o - y_i) + V_R \left(\sum_{k=1}^{NR} (\nu_{ki} - y_i \Delta\nu_k) r_{V,k} \right)$$

$$\frac{dy_i}{dt} = \frac{RTF^o}{PV_R}(y_i^o - y_i) + \frac{RT}{P}\left(\sum_{k=1}^{NR} (\nu_{ki} - y_i \Delta\nu_k) r_{V,k} \right) \qquad i = 1, N$$

Inlet volumetric flow rate is

$$\frac{RTF^o}{P} = \dot{V}_o$$

Mean residence time of reaction mixture (based on inlet flow rate) is given by

$$\bar{\tau}_o = \frac{V_R}{\dot{V}_o} = \frac{PV_R}{RTF^o}$$

and molar balance of species i becomes finally

$$\frac{dy_i}{dt} = \frac{1}{\bar{\tau}_o}(y_i^o - y_i) + \frac{RT}{P}\left(\sum_{k=1}^{NR}(\nu_{ki} - y_i \Delta\nu_k) r_{V,k}\right) \qquad i = 1, N$$

If only one reaction takes place:

$$\frac{dy_i}{dt} = \frac{1}{\bar{\tau}_o}(y_i^o - y_i) + \frac{RT}{P}(\nu_i - y_i \Delta\nu) r_V \qquad i = 1, N$$

Example

Start-up of an isothermal CSTR

$$N_2O_{(g)} \rightarrow N_{2(g)} + 1/2O_{2(g)}$$

$V_R = 0.1\ \text{l} = 10^{-4}\ \text{m}^3$, $T = 320\ ^\circ\text{C}$, $P = 101\ \text{kPa}$

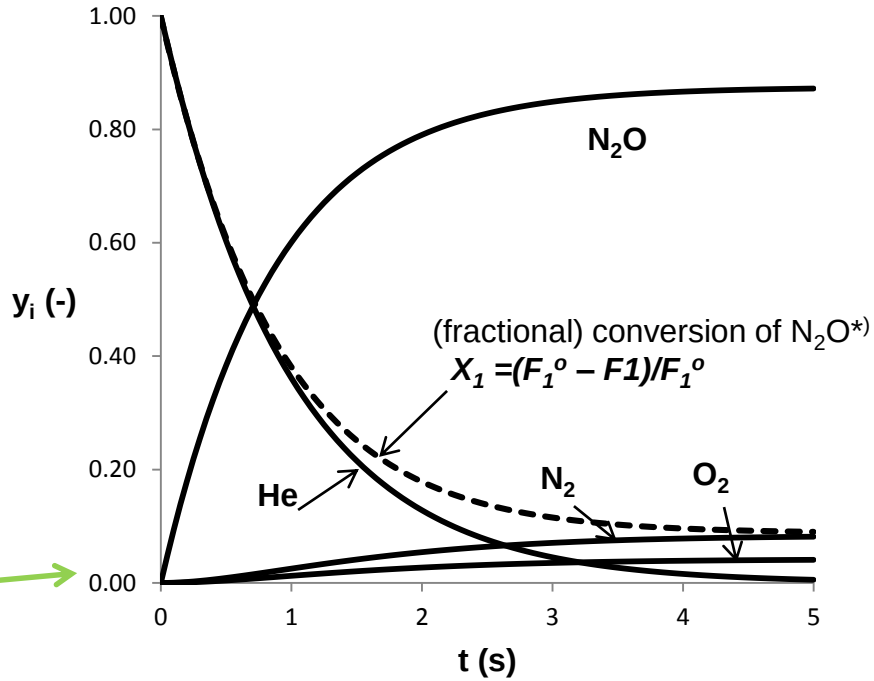
$r_V = kP_{N_2O}$, $k = 2.028 \times 10^{-5}\ \text{mole.Pa}^{-1}.\text{min}^{-1}.\text{m}^{-3}$

$y_1^o = 1, y_2^o = y_3^o = y_4^o = 0$ $\quad (1 = N_2O,\ 2 = O_2,\ 3 = N_2,\ 4 = He)$

$t = 0,\ y_1 = 0 = y_2 = y_3 = 0, y_4 = 1$

$\bar{\tau}_o = 1$

Numerical solution of balance equations



*) The equation is valid only at steady state

Steady state

$$F_i - F_i^o = V_R \sum_{k=1}^{NR} \nu_{ki} r_{V,k}, \qquad i = 1, N$$

If only one reaction takes place:

$$F_i - F_i^o = V_R \nu_i r_V, \qquad i = 1, N$$

using fractional conversion of key species j $\quad X_j = \dfrac{F_j^o - F_j}{F_j^o}$

$$F_j^o X_j = V_R \left|\nu_j\right| r_V(X_j)$$

a) The volume of reactor for given outlet conversion

$$V_R = F_j^o \frac{X_j}{\left|\nu_j\right| r_V(X_j)}$$

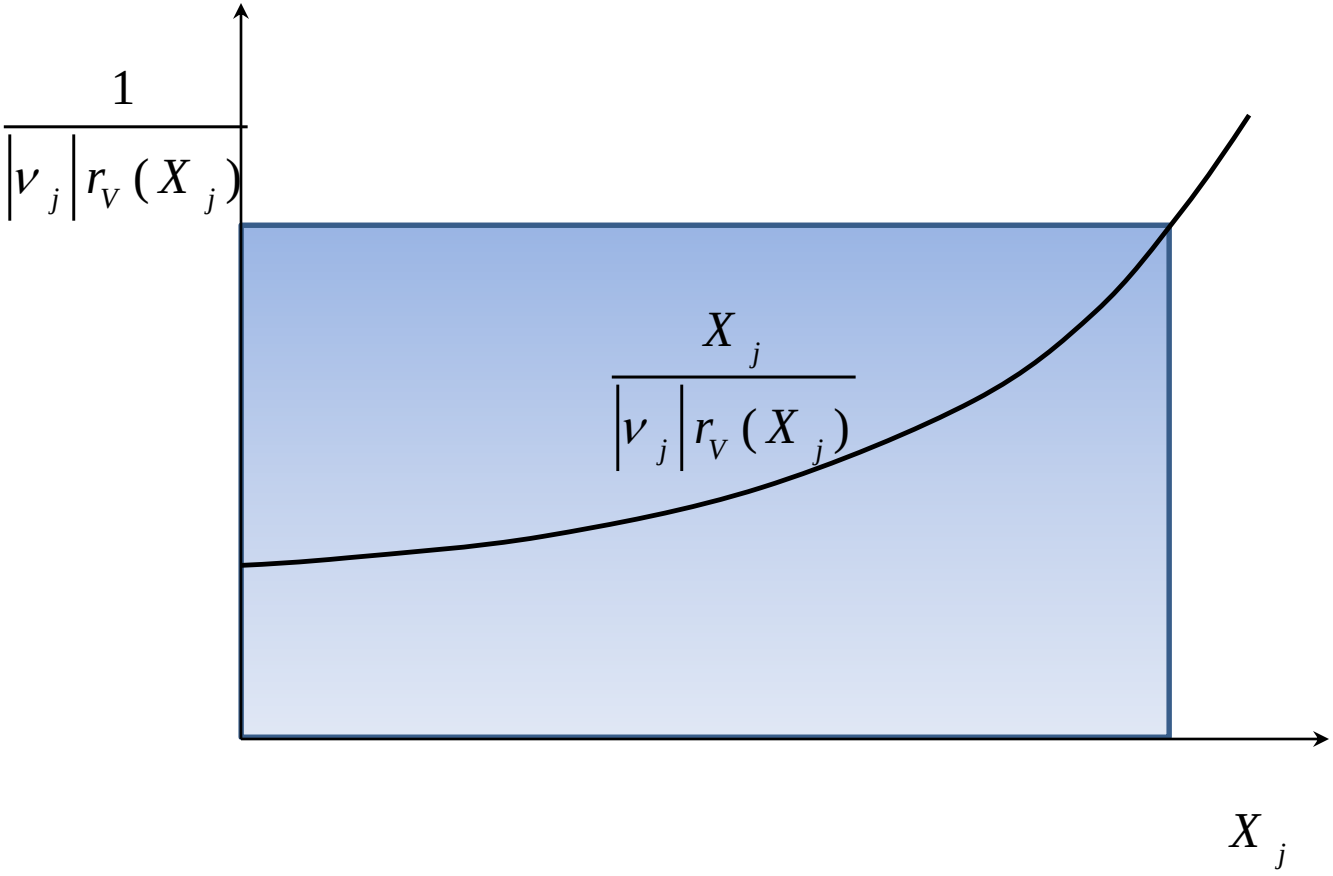
Simple substitution

b) The outlet conversion for given volume of reactor

$$\frac{F_j^o}{V_R} X_j - \left|\nu_j\right| r_V(X_j) = f(X_j) = 0$$

Graphical or numerical (iterative) solution

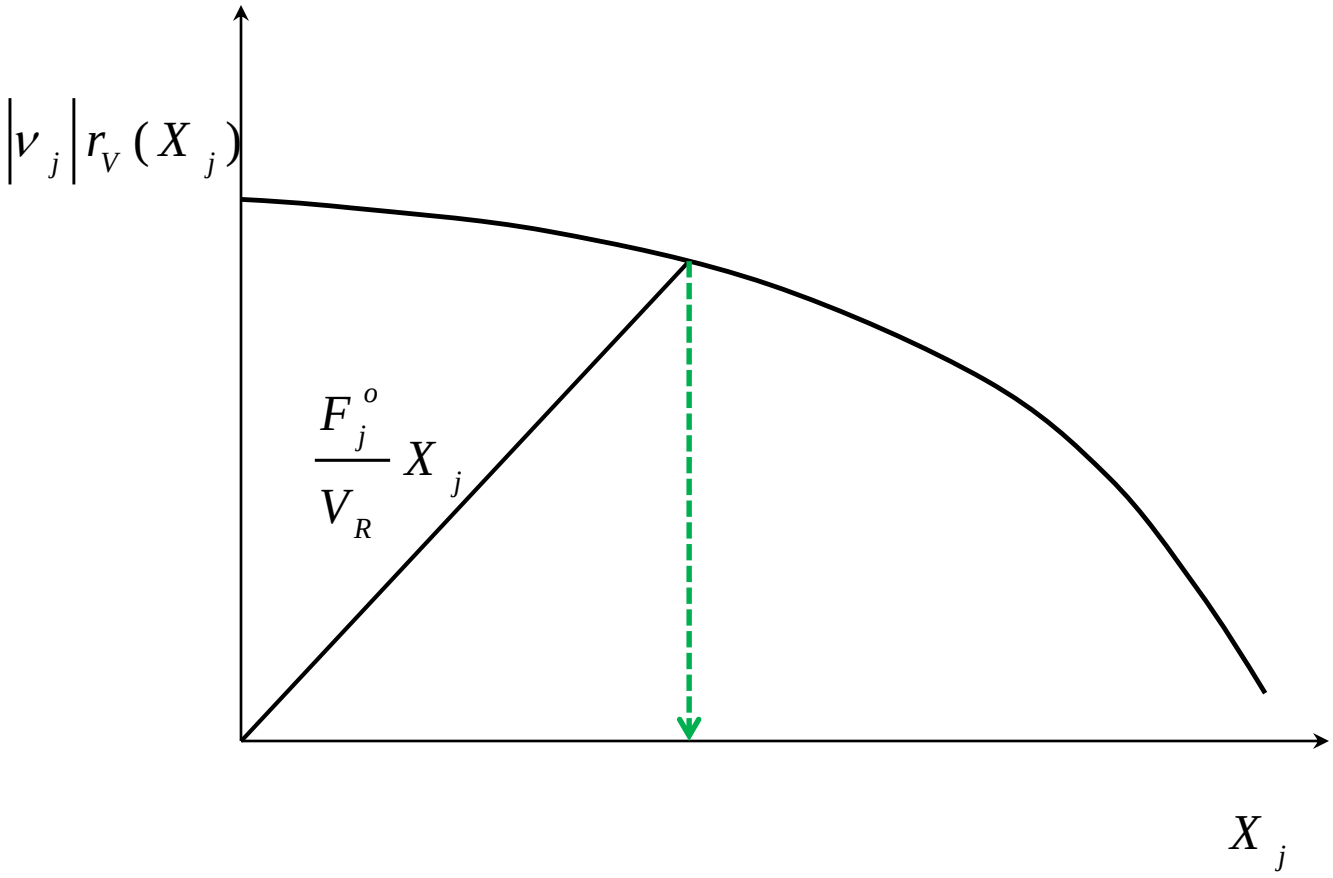
Graphical assessment of the CSTR volume



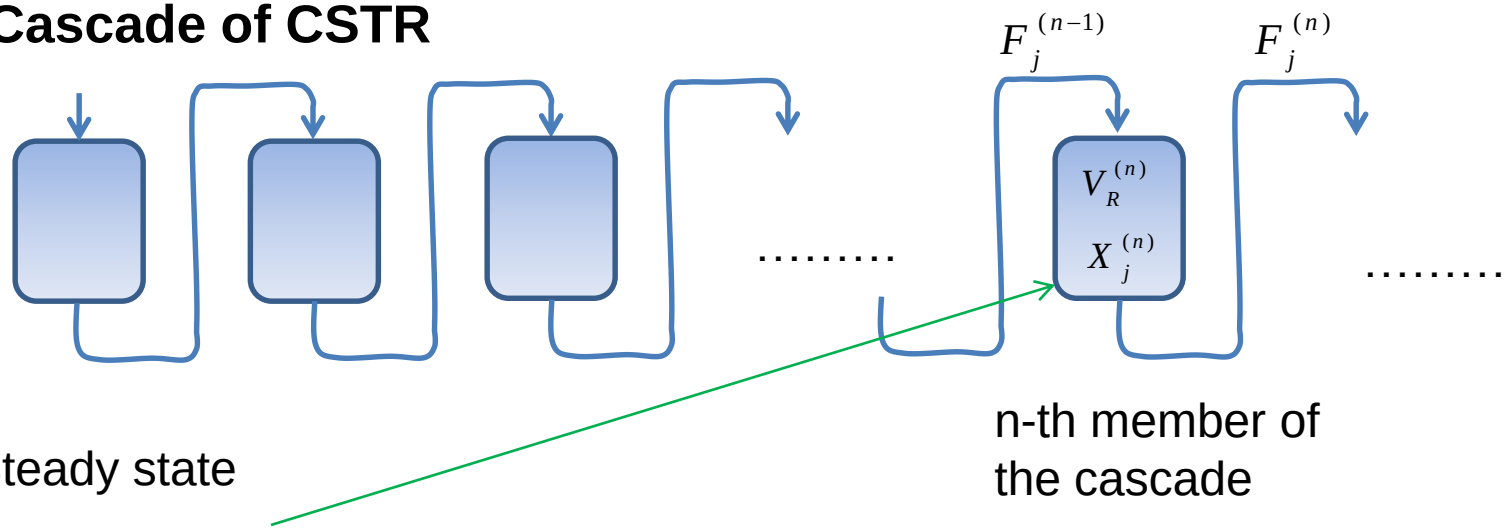
Levenspiel diagram

usually $|\nu_j| = 1$

Graphical assessment of the outlet conversion



Cascade of CSTR



$$F_i^{(n)} - F_i^{(n-1)} = V_R^{(n)} \nu_i r_V^{(n)}, \qquad i = 1, N \qquad n = 1, N_{CSTR}$$

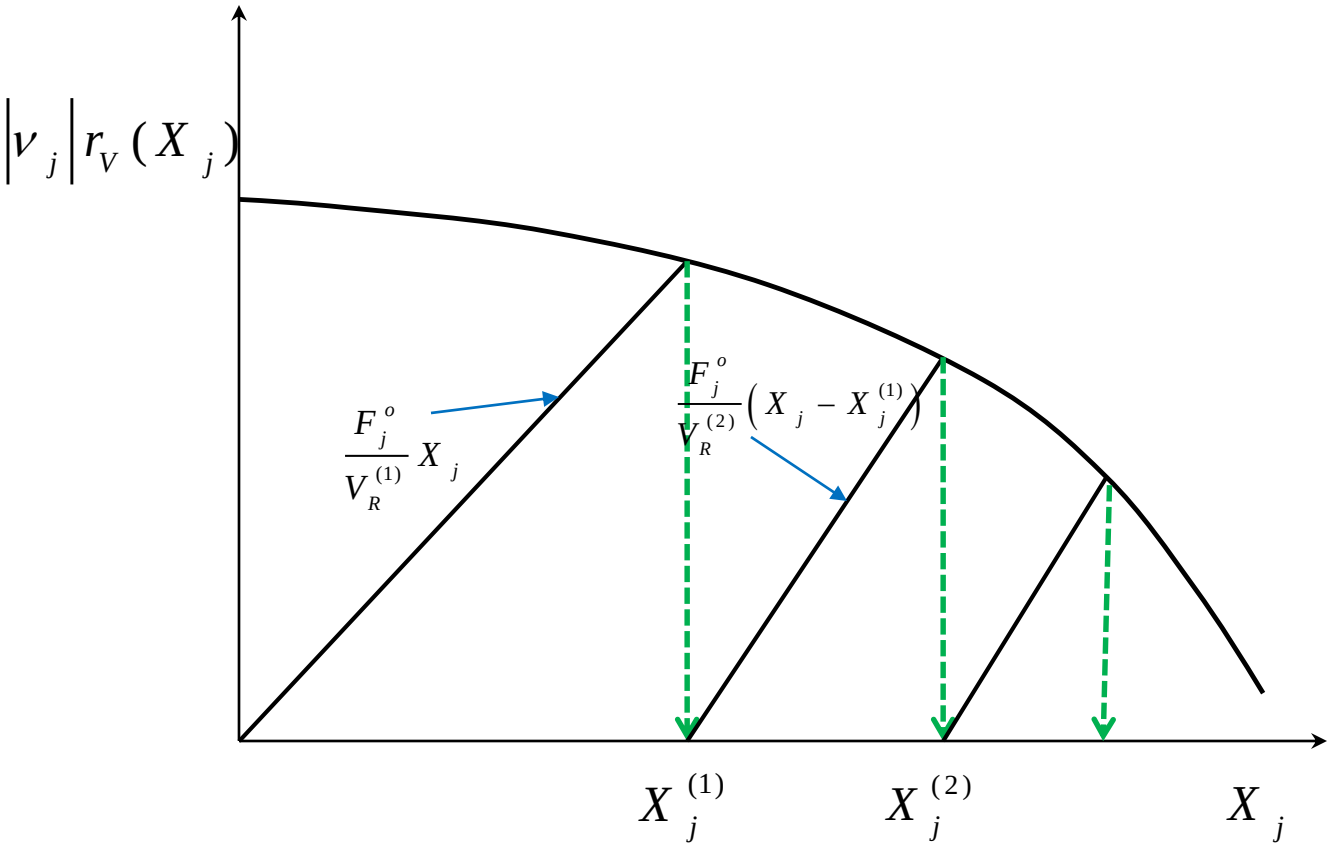
$$X_j^{(n)} = \frac{F_j^{o} - F_j^{(n)}}{F_j^{o}}$$

$$F_j^{(n)} = F_j^{o}(1 - X_j^{(n)})$$

$$F_i^{(n)} = F_i^{o} - \frac{\nu_i}{\nu_j} F_j^{o} X_j^{(n)}$$

$$\frac{F_j^{o}}{V_R^{(n)}}\left(X_j^{(n)} - X_j^{(n-1)}\right) = \left|\nu_j\right| r_V(X_j^{(n)}), \qquad n = 1, N_{CSTR}$$

Graphical assessment of the outlet conversion in the cascade of CSTR



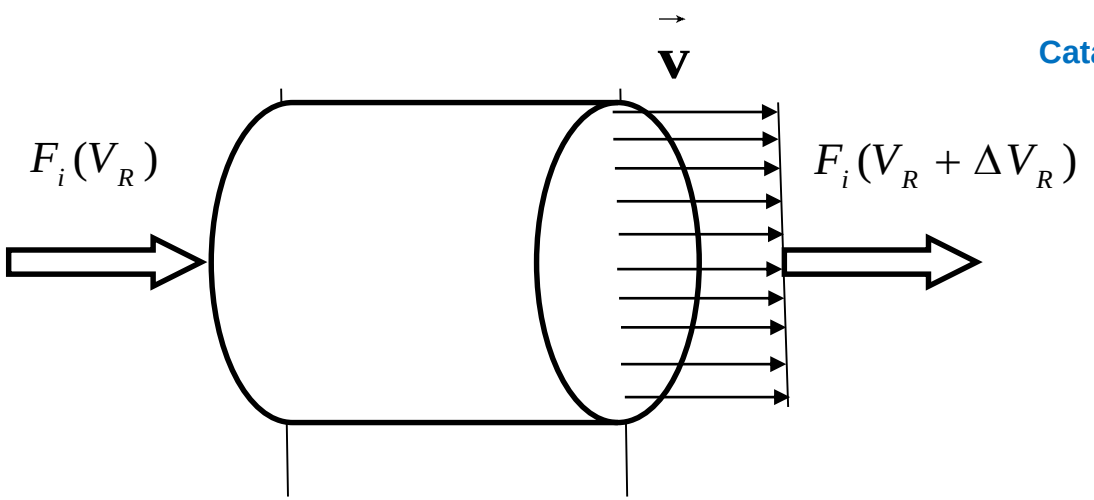
Homework 6

Prove that $X_j^{(n)} = 1 - (1 + k\bar{\tau}_o)^{-n}, \bar{\tau}_o = \frac{V_R^{(n)}}{V_o}$ for first order constant-volume reaction.

In the limit $\lim_{n \to \infty} X_j^{(n)} = 1 - e^{-k\bar{\tau}_{oR}}, \bar{\tau}_{oR} = \frac{nV_R^{(n)}}{V_o}$

Plug Flow reactor – PFR

Tubular reactors
High production capacity
Catalytic reactors (e.g. ammonia synthesis)



z ***z + Δz*** $V_R = S_R z$

V_R $V_R + \Delta V_R$

Molar balance of species i

$$\frac{\partial c_i(t,z)}{\partial t} = -\frac{1}{S_R}\frac{\partial F_i(t,z)}{\partial z} + \sum_{k=1}^{NR} \nu_{ki} r_{V,k}(t,z) \qquad i = 1, N$$

Steady state

$$\frac{dF_i}{dV_R} = \sum_{k=1}^{NR} \nu_{ki} r_{V,k} \qquad i = 1, N$$

If only one reaction takes place:

$$\frac{dF_i}{dV_R} = \nu_i r_V \qquad i = 1, N$$

using fractional conversion of key species j $\quad X_j = \dfrac{F_j^o - F_j}{F_j^o}$

$$F_j^o \frac{dX_j}{dV_R} = \left|\nu_j\right| r_V(X_j)$$

$$F_j^o \int_{X_j(1)}^{X_j(2)} \frac{dX_j}{\left|\nu_j\right| r_V(X_j)} = V_R$$

useful relations:

$$y_i = \frac{F_i}{\sum_{j=1}^{N} F_j}, c_i = \frac{F_i}{V_m \sum_{j=1}^{N} F_j} = \frac{y_i}{V_m} = \frac{F_i}{\dot{V}}$$

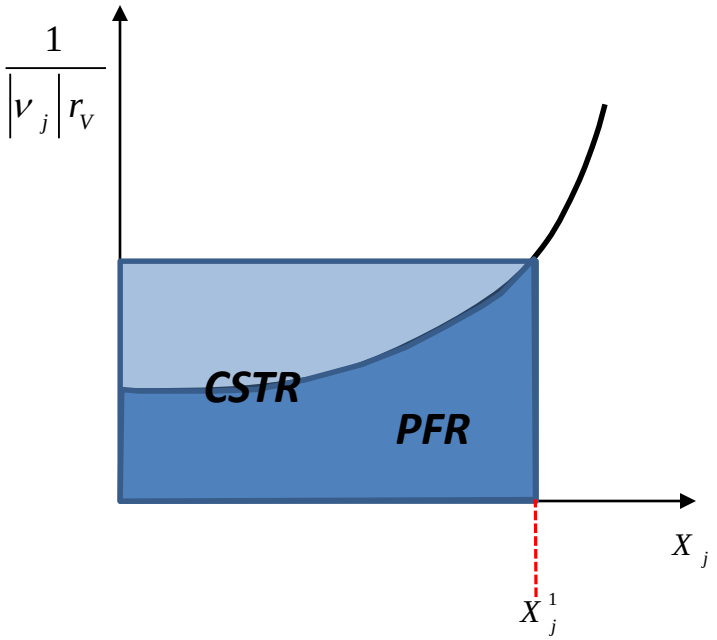
V_m – molar volume $(\mathrm{m}^3\mathrm{mole}^{-1})$

BATCH, CSTR, PFR (PBCR), one reaction, fractional conversion of key component

BATCH

$$-\frac{n_j^o}{\nu_j V_R}\int_0^{X_j^1}\frac{dX_j}{r_V(X_j)}=\int_0^{t_R}dt=t_R$$

$$\frac{c_j^o}{|\nu_j|}\int_0^{X_j^1}\frac{dX_j}{r_V(X_j)}=\int_0^{t_R}dt=t_R$$



CSTR

$$V_R=-\frac{F_j^o}{\nu_j}\frac{X_j^1}{r_V(X_j^1)}=\frac{F_j^o}{|\nu_j|}\frac{X_j^1}{r_V(X_j^1)}$$

PBCR

Packed Bed Catalytic Reactor

PFR

$$V_R=-\frac{F_j^o}{\nu_j}\int_0^{X_j^1}\frac{dX_j}{r_V(X_j)}=\frac{F_j^o}{|\nu_j|}\int_0^{X_j^1}\frac{dX_j}{r_V(X_j)}$$

$$W=-\frac{F_j^o}{\nu_j}\int_0^{X_j^1}\frac{dX_j}{r_M}=\frac{F_j^o}{|\nu_j|}\int_0^{X_j^1}\frac{dX_j}{r_M(X_j)}$$

Mean residence time

$$\bar{\tau} = \frac{V_R}{\dot{V}}$$

BATCH, PFR

$$\frac{c_j^o}{|\nu_j|} \int_0^{X_j^1} \frac{dX_j}{r_V(X_j)} = \bar{\tau}_o$$

CSTR

$$\frac{c_j^o}{|\nu_j|} \frac{X_j^1}{r_V(X_j^1)} = \bar{\tau}_o$$

$$\bar{\tau}_o = \frac{V_R}{\dot{V}_o}$$

$\dot{V}_o$ volumetric flow rate (m^3/s) of reaction mixture at inlet conditions

Gas Hourly Space Velocity

$$GHSV = \frac{\text{Gas volumetric flow rate}(m^3/hr)}{\text{Volume of reactor } (m^3)}$$

Liquid Hourly Space Velocity

$$LHSV = \frac{\text{Liquid volumetric flow rate } (m^3/hr)}{\text{Volume of reactor } (m^3)}$$

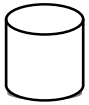
Tasks

1. Calculate the volume of reactor (mass of catalyst) (CSTR, PFR, PBCR) or time of reaction (BATCH) to obtain given conversion.

2. Calculate the outlet conversion for given volume of reactor.

3. Calculate the reaction rate in laboratory reactor to obtain kinetic law and estimate the kinetic parameters.

NR = 1 $\sum_{i=1}^{N} \nu_i A_i = 0$ $\Delta\nu = \sum_{i=1}^{N} \nu_i$ ***j – subscript of key component***

BATCH 	**FLOW** 
$n_i = n_i^o + \nu_i \xi = n_i^o - \frac{\nu_i}{\nu_j} n_j^o . X_j$	$F_i = F_i^o + \nu_i \int r_V . dV_R = F_i^o - \frac{\nu_i}{\nu_j} F_j^o . X_j$
$n = \sum_{i=1}^{N} n_i^o + \xi \sum_{i=1}^{N} \nu_i = n^o + \xi . \Delta\nu = n^o - \frac{\Delta\nu}{\nu_j} n_j^o . X_j$	$F = F^o - \frac{\Delta\nu}{\nu_j} F_j^o . X_j$
$x_i = \frac{n_i}{n} = \frac{n_i^o - \frac{\nu_i}{\nu_j} n_j^o . X_j}{n^o - \frac{\Delta\nu}{\nu_j} n_j^o . X_j} = \frac{x_i^o - \frac{\nu_i}{\nu_k} x_j^o . X_j}{1 - \frac{\Delta\nu}{\nu_j} x_j^o . X_j}$	$x_i = \frac{F_i}{F} = \frac{F_i^o - \frac{\nu_i}{\nu_j} F_j^o . X_j}{F^o - \frac{\Delta\nu}{\nu_j} F_j^o . X_j} = \frac{x_i^o - \frac{\nu_i}{\nu_j} x_j^o . X_j}{1 - \frac{\Delta\nu}{\nu_j} x_j^o . X_j}$
$c_i = \frac{n_i}{V} = \frac{n_i}{n . V_m} = \frac{x_i}{V_m} = \frac{1}{V_m} \frac{x_i^o - \frac{\nu_i}{\nu_j} x_j^o . X_j}{1 - \frac{\Delta\nu}{\nu_j} x_j^o . X_j}$ V_m - molar volume of reaction mixture (m^3/mol)	$c_i = \frac{F_i}{\dot{V}} = \frac{F_i}{F . V_m} = \frac{x_i}{V_m} = \frac{1}{V_m} \frac{x_i^o - \frac{\nu_i}{\nu_j} x_j^o . X_j}{1 - \frac{\Delta\nu}{\nu_j} x_j^o . X_j}$

Gas phase - Ideal state behavior

$$V_m = \frac{RT}{P}$$

$$c_i = \frac{x_i}{\frac{RT}{P}} = \frac{P_i}{RT} = \frac{P}{RT}\frac{x_i^o - \frac{\nu_i}{\nu_j}x_j^o.X_j}{1-\frac{\Delta\nu}{\nu_j}x_j^o.X_j}$$

$$c_i = \frac{F_i}{\dot{V}} = \frac{F_i}{F.\frac{RT}{P}} = \frac{P_i}{RT} = \frac{P}{RT}\frac{x_i^o - \frac{\nu_i}{\nu_j}x_j^o.X_j}{1-\frac{\Delta\nu}{\nu_j}x_j^o.X_j}$$

$$c_i = \frac{n_i}{V} = \frac{n_i}{V_o\frac{T}{T_o}\frac{P_o}{P}(1-\frac{\Delta\nu}{\nu_j}x_j^oX_j)} =$$

$$= \frac{T_o}{T}\frac{P}{P_o}\frac{1}{V_o}\left(\frac{n_i^o - \frac{\nu_i}{\nu_j}n_j^o.X_j}{1-\frac{\Delta\nu}{\nu_j}x_j^oX_j}\right) = \frac{T_o}{T}\frac{P}{P_o}\left(\frac{c_i^o - \frac{\nu_i}{\nu_j}c_j^o.X_j}{1-\frac{\Delta\nu}{\nu_j}x_j^oX_j}\right)$$

$$c_i = \frac{F_i}{\dot{V}} = \frac{F_i}{\dot{V}_o\frac{T}{T_o}\frac{P_o}{P}\left(1-\frac{\Delta\nu}{\nu_j}x_j^oX_j\right)} =$$

$$= \frac{T_o}{T}\frac{P}{P_o}\frac{1}{\dot{V}_o}\left(\frac{F_i^o - \frac{\nu_i}{\nu_j}F_j^o.X_j}{1-\frac{\Delta\nu}{\nu_j}x_j^oX_j}\right) = \frac{T_o}{T}\frac{P}{P_o}\left(\frac{c_i^o - \frac{\nu_i}{\nu_j}c_j^o.X_j}{1-\frac{\Delta\nu}{\nu_j}x_j^oX_j}\right)$$

Homework 7

Calculate volume of PFR to produce 150 kt ethylen/year. Reaction of the 1st order

$$C_2H_{6(g)} \rightarrow C_2H_{4(g)} + H_{2(g)}$$

takes place at 1100 K and 0,6 Mpa. Final conversion of ethan is 80 %. Reaction rate is given by

$$r_V = k.\, c_A$$

k (1000 K) = 0,072 s^{-1} E = 343,6 kJ/mol

Pure ethan is fed into the reactor.

Assumptions:
Ideal gas, molar weight of ethylen is 28,054 kg/kmol.

K. J. Laidler and B. W. Wojciechowski: Kinetics and Mechanisms of the Thermal Decomposition of Ethane. I. The Uninhibited Reaction, Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, Vol. 260, No. 1300 pp. 91-102

Homework 4 (due after Chapter 4)

Calculate volumes of CSTR a PFR working at 150 ^{o}C and 300 kPa to produce 1 t $COCl_2$/day with CO conversion equal to 95 %. A mixture of CO and Cl_2 (molar ratio 1:1) is fed at 300 kPa and 150 ^{o}C.

Data

***k*(423 K) = 0.07 $(m^3mol^{-1})^{3/2}.s^{-1}$**

M_{COCl2} = 98.92 kg/kmol.

Answer:

V_{CSTR} = 0.053 m^3 **V_{PFR} = 0.0021 m^3**

$$CO_{(g)} + Cl_{2(g)} \rightarrow COCl_{2(g)}$$

$F_i^o \rightarrow$ [ ] $\rightarrow F_i$ $\quad F_i = F_i^o - \frac{\nu_i}{\nu_j} F_j^o X_j$

steady state; j - key component

	IN	OUT
CO (1)	F_1^o	$F_1 = F_1^o (1 - X_1)$
Cl_2 (2)	F_1^o	$F_2 = F_1^o (1 - X_1)$
$COCl_2$ (3)	0	$F_3 = F_1^o X_1$
Σ	$F^o = 2F_1^o$	$F = F_1^o (2 - X_1)$

$$\text{ideal gas} \Rightarrow V_m = \frac{RT}{P} \quad [\text{m}^3/\text{mol}]$$

$$c_{CO} = c_1 = \frac{F_1}{\dot{V}} = \frac{F_1}{V_m F} = \frac{P}{RT}\frac{F_1}{F} = \frac{P}{RT}\frac{F_1^o\left(1-X_1\right)}{F_1^o\left(2-X_1\right)} = \frac{P}{RT}\frac{\left(1-X_1\right)}{\left(2-X_1\right)} = c_{Cl_2} = c_2 \quad [\text{mol/m}^3]$$

$$r_V = kc_{CO}c_{Cl_2}^{3/2} = k\left(\frac{P}{RT}\right)^{5/2}\left(\frac{1-X_1}{2-X_1}\right)^{5/2} \quad [\text{mol/m}^3/\text{s}]$$

$$F_1^o = \frac{F_3}{X_1^1} = \frac{1\times10^6 / 98.92 / \left(24\times3600\right)}{0.95} = 0.123163 \text{ mol/s}$$

$$V_{CSTR} = \frac{F_1^o}{\left|\nu_1\right|}\frac{X_1^1}{r_V\left(X_1^1\right)} = \frac{F_1^o}{\left|-1\right|}\frac{X_1^1}{k\left(\frac{P}{RT}\right)^{5/2}\left(\frac{1-X_1^1}{2-X_1^1}\right)^{5/2}} = \frac{0.123163\times0.95}{0.07\times\left(\frac{300\times10^3}{8.3145\times423}\right)^{5/2}\left(\frac{1-0.95}{2-0.95}\right)^{5/2}} =$$

$$= 0.0503 \text{ m}^3$$

$$V_{PFR} = \frac{F_j^o}{|\nu_j|}\int_0^{X_j^1}\frac{dX_j}{r_V(X_j)} = \frac{F_1^o}{|-1|}\int_0^{0.95}\frac{dX_1}{k\left(\frac{P}{RT}\right)^{5/2}\left(\frac{1-X_1}{2-X_1}\right)^{5/2}} = \frac{F_1^o}{k}\left(\frac{RT}{P}\right)^{5/2}\int_0^{0.95}\left(\frac{2-X_1}{1-X_1}\right)^{5/2}dX_1 =$$

$$= \frac{0.123163}{0.07}\times\left(\frac{8.3145\times 423}{300\times 10^3}\right)^{5/2}\times 79.42692225 = 2.08\times 10^{-3}\ \mathrm{m}^3$$

Summary

- General material balance of reacting system
- Batch reactor
- Continuous-flow reactors: CSTR (Continuous Stirred Tank Reactor)
  PFR (Plug Flow Reactor)
- Steady state of CSTR and PFR
- Design tasks : outlet (final conversion), given volume of reactor x volume of reactor, given outlet conversion