ERQ I – Slide: Chemical Reactors

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Conteúdo

- Ideal reactors dimensioning
- Isothermic and non-isothermic operations
- Catalysts preparation and characterization

1 General equaltion of molar balance

$$\mathrm{aA + bB + \ldots \longrightarrow dD + eE + \ldots}$$

$$\boldsymbol{F_{i\,0} - F_{i\,1} + F_{i\,P} = \frac{\mathrm{d}N_i}{\mathrm{d}t}}$$

Molar balance to the limitant reagent A

$F_{A\,0}/\mathrm{mol\ (A)/L\ (0)\ h}$ input

$F_{A\,1}/\mathrm{mol\ (A)/L\ (1)\ h}$ output

$F_{A\,P}/\mathrm{mol\ (A)/L\ h}$ produced

$\frac{\mathrm{d}N_A}{\mathrm{d}t}/\mathrm{mol\ (A)/L\ h}$ Acumulated

2 Reaction rate

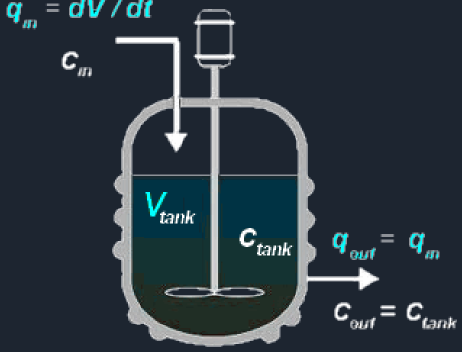
$$r_A = V^{-1} \frac{\mathrm{d}N_A}{\mathrm{d}t} \qquad r'_A = W^{-1} \frac{\mathrm{d}N_A}{\mathrm{d}t} \qquad r"_A = S^{-1} \frac{\mathrm{d}N_A}{\mathrm{d}t}$$

$$F_{A\,P} = \int_V r_A \, \mathrm{d}V$$

3 Ideal reactors

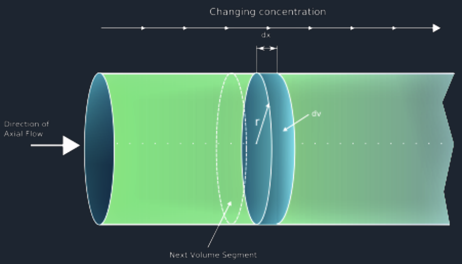
CSTR: Continuous stirred-tank reactor

Homogenous mix trought every point of the reactor



PFR: Plug flow reactor model

Homogeneous mix trought a disk section



Batch: Similar to CSTR but descontinous (no input/output)

4 How to balance each reactor

General equation

$$\boldsymbol{F}_{i\,0} - \boldsymbol{F}_{i\,1} + \boldsymbol{F}_{i\,P} = \frac{\mathrm{d}\boldsymbol{N}_i}{\mathrm{d}\boldsymbol{t}}$$

X: Conversion

$$\boldsymbol{X} = 1 - \boldsymbol{N}_{i\,1}/\boldsymbol{N}_{i\,0} = 1 - \boldsymbol{F}_{i\,1}/\boldsymbol{F}_{i\,0}$$

4.1 Continuous reactors

Steady State: Maintaining constant all functioning conditions (input current, temperature, pressure, ...), after a certain time the reactor reaches a steady state where all the output parameters (caudal, concentration, temperature, ...) become constant in time.

Spatial time:

$$\boldsymbol{\tau} = \frac{\boldsymbol{V}\text{ (reactor volume)}}{\boldsymbol{v}\text{ (volumetric caudal)}}$$

4.2 Batch balance

$$\boldsymbol{r_i\, V = \frac{\mathrm{d}N_i}{\mathrm{d}t} \iff t = C_{i\,0} \int_0^X \frac{\mathrm{d}X}{-r_A};}$$

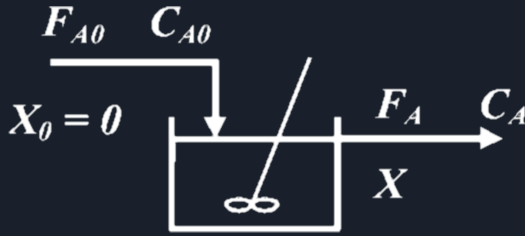
$$\left(\begin{array}{c} \boldsymbol{F_{i\,0} = F_{i\,1} = 0} \text{ (No input/output)} \\ \boldsymbol{\int_V r_i\, \mathrm{d}V = r_i\, V} \text{ (Continously agitated)} \end{array} \right)$$

$$F_{i\,0} + F_{i\,1} + F_{i\,P} = F_{i\,P} = \int_V r_i\, \mathrm{d}V = r_i \int_V \mathrm{d}V = r_i\, V = \frac{\mathrm{d}N_i}{\mathrm{d}t};$$

$$X = 1 - N_{i\,1}/N_{i\,0} \implies N_{i\,1} = N_{i\,0}\,(1 - X) \implies$$

$$\implies \frac{\mathrm{d}N_i}{\mathrm{d}t} = \frac{\mathrm{d}N_{i\,0}\,(1-X)}{\mathrm{d}t} = -N_{i\,0}\,\frac{\mathrm{d}X}{\mathrm{d}t} r_i\, V \implies$$
$$\implies \int_0^t \mathrm{d}t = t = \int_0^X \frac{-N_{i\,0}}{r_i\, V}\, \mathrm{d}X = \frac{N_{i\,0}}{V} \int_0^X \frac{\mathrm{d}X}{-r_i} = C_{i\,0} \int_0^X \frac{\mathrm{d}X}{-r_i}$$

4.3 CSTR balance

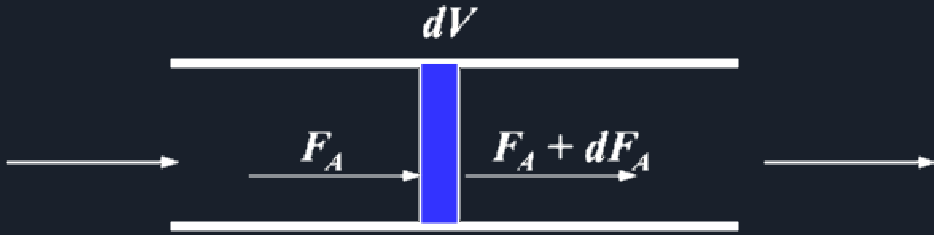


$$\boldsymbol{\tau = C_{i\,0}\,\frac{X}{-r_i};}$$

$$\left(\begin{array}{c}\dfrac{\mathrm{d}N_i}{\mathrm{d}t} = 0 \text{ (Steady state)} \\ \displaystyle\int_V r_A\,\mathrm{d}V = r_A\,V \text{ (Continously agitated)}\end{array}\right)$$

$$F_{i\,0} - F_{i\,1} + F_{i\,P} = F_{i\,0} - (F_{i\,0}(1 - X)) + (r_i\,V) = F_{i\,0}\,X + r_i\,V = (v_0\,C_{i\,0})\,X + r_i\,V =$$
$$= \frac{\mathrm{d}N_A}{\mathrm{d}t} = 0 \implies \frac{V}{v_0} = \tau = C_{i\,0}\,\frac{X}{-r_i}$$

4.4 PFR Balance



$$\boldsymbol{\tau = C_{i\,0} \int_0^X \frac{\mathrm{d}X}{-r_A};}$$

$$\text{(steady state elementar disk)}$$

$$F_{i\,j} - F_{i\,(j+1)} + F_i = F_{i\,j} - (F_{i\,j} + \mathrm{d}F_{i\,j}) + (r_i\ \mathrm{d}V) = -\,\mathrm{d}F_{i\,j} + r_i\ \mathrm{d}V =$$
$$= -\,\mathrm{d}F_{i\,0}(1 - X) + r_i\ \mathrm{d}V = F_{i\,0}\ \mathrm{d}X + r_i\ \mathrm{d}V = (C_{i\,0}\, v_0)\ \mathrm{d}X + r_i\ \mathrm{d}V =$$
$$= \frac{\mathrm{d}N_i}{\mathrm{d}t} = 0 \implies$$
$$\implies \frac{1}{v_0} \int_0^V \mathrm{d}V \frac{V}{v_0} = \tau = \int_0^X C_{i\,0} \frac{\mathrm{d}X}{-r_i} = C_{i\,0} \int_0^X \frac{\mathrm{d}X}{-r_i}$$