DEPARTAMENTO DE INGENIERÍA QUÍMICA

FACULTAD DE CIENCIAS DEL MEDIO AMBIENTE

Tema 14. Reactores químicos

Ingeniería Química

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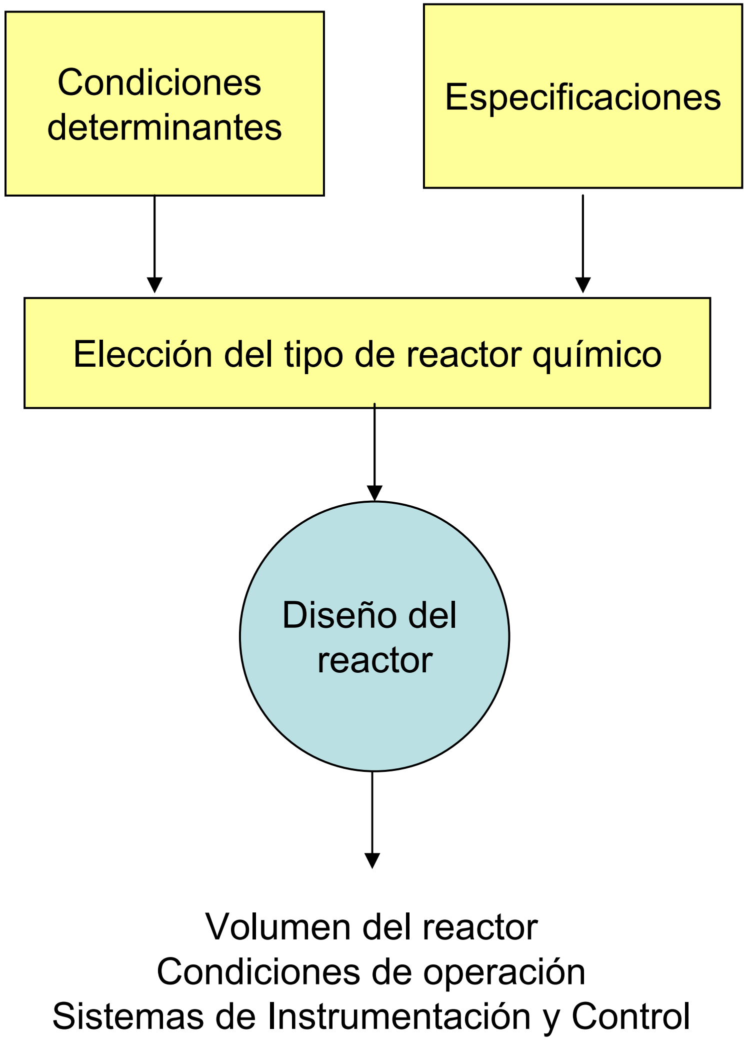
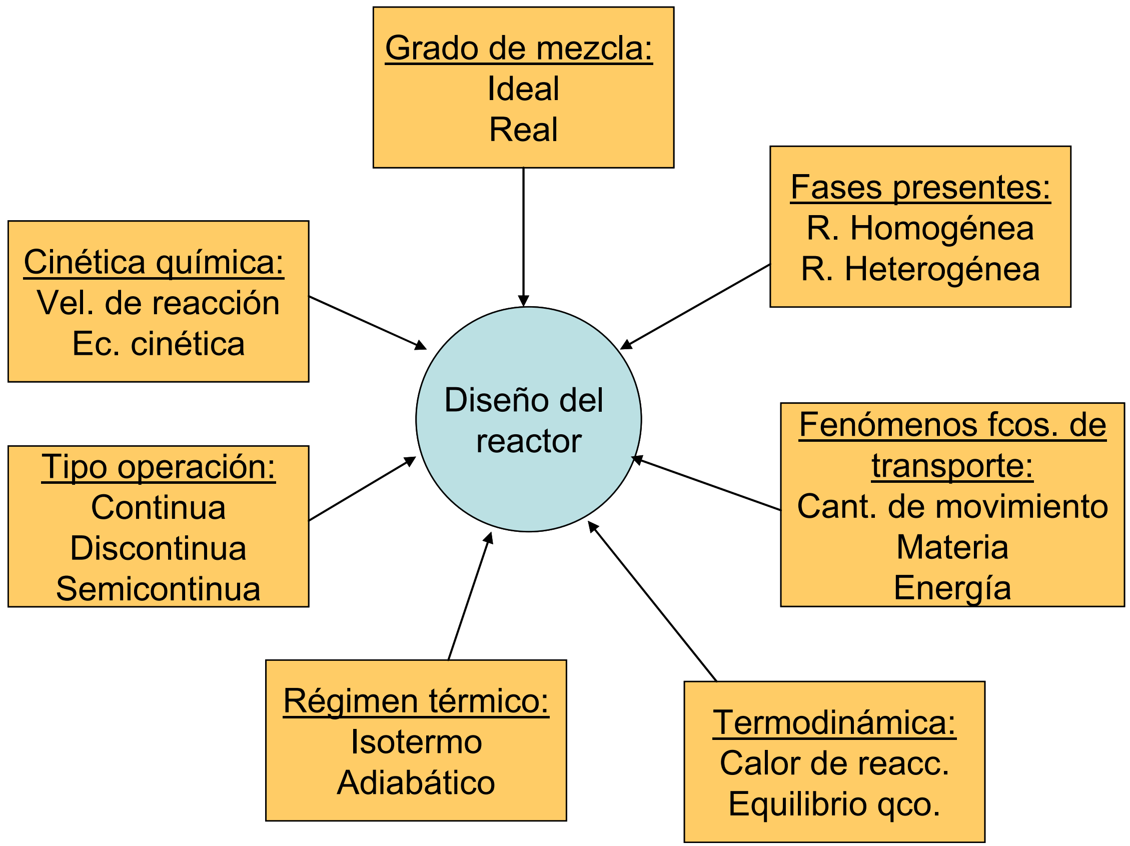
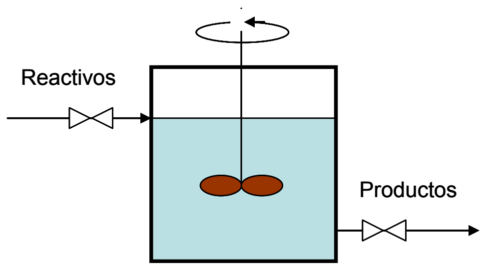
Reactores químicos



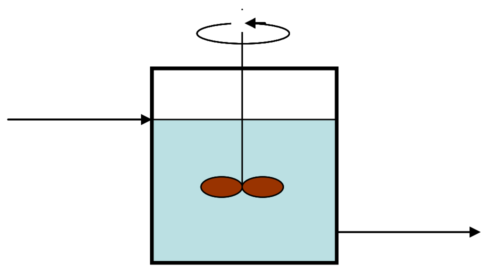
Reactores químicos



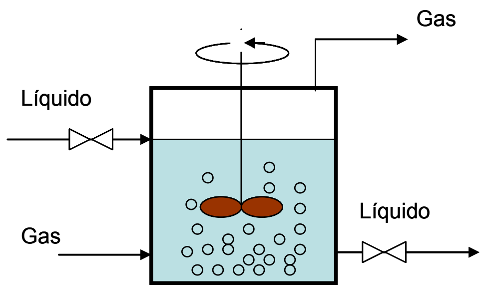
Reactores químicos



Discontinuo



Continuo de
mezcla completa



Semicontinuo

Continuo de
flujo pistón

Reactores químicos

Número de fases

- Homogéneos
- Heterogéneos

Régimen térmico

- Isotérmicos
- Adiabáticos

Tipo de operación

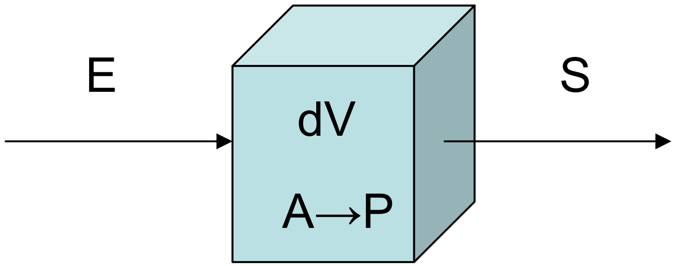
- Discontinuos
- Continuos o de flujo
  - Tubular
  - De tanque agitado
- Semicontinuos

14.1. Reactores homogéneos ideales

✓ Balance de materia

$$\begin{bmatrix} Cantidad\ de\ A \\ acumulada \\ en\ dV\ en\ dt \end{bmatrix} = \begin{bmatrix} Cantidad\ de\ A \\ que\ entra\ en \\ dV\ en\ dt \end{bmatrix} - \begin{bmatrix} Cantidad\ de\ A \\ que\ sale\ de \\ dV\ en\ dt \end{bmatrix} - \begin{bmatrix} Cantidad\ de\ A \\ que\ reacciona \\ en\ dV\ en\ dt \end{bmatrix}$$

Acumulación   *Entrada*   *Salida*   *Generación*

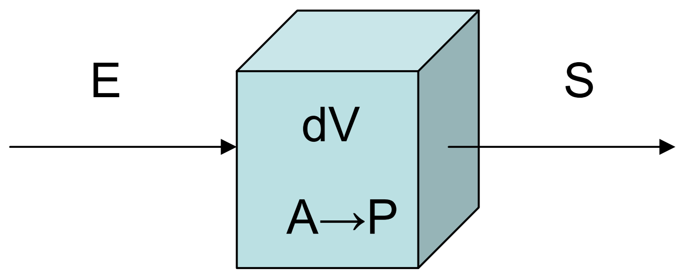


14.1. Reactores homogéneos ideales

✓ Balance de energía

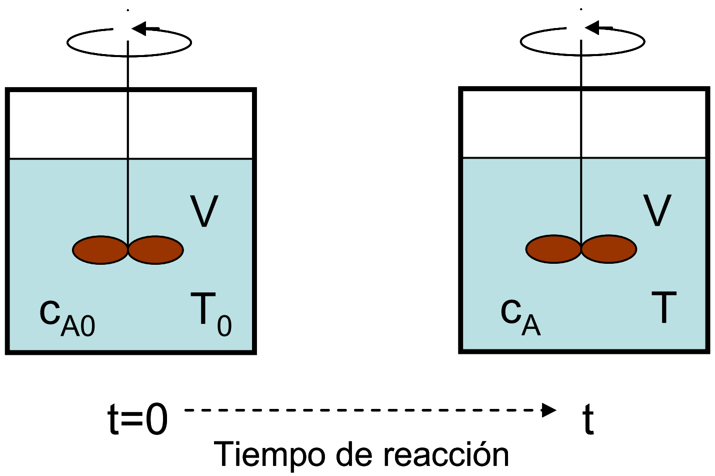
$$\begin{bmatrix} E.\text{calorífica} \\ \text{acumulada} \\ \text{en } dV \text{ en } dt \end{bmatrix} = \begin{bmatrix} E.\text{calorífica} \\ \text{que entra en} \\ dV \text{ en } dt \end{bmatrix} - \begin{bmatrix} E.\text{calorífica} \\ \text{que sale de} \\ dV \text{ en } dt \end{bmatrix} - \begin{bmatrix} E.\text{calorífica} \\ \text{que desaparece} \\ \text{por reacción} \\ \text{en } dV \text{ en } dt \end{bmatrix}$$

Acumulación *Entrada* *Salida* *Generación*



14.2. Reactores de tanque discontinuos

✓ Balance de materia



$$[Acumulación] = [Entrada] - [Salida] + [Generación]$$

$$E = 0 \qquad S = 0$$

$$\begin{bmatrix} Cantidad\ de\ A \\ acumulada\ en\ dV \\ en\ el\ tiempo\ dt \end{bmatrix} = -\begin{bmatrix} Cantidad\ de\ A \\ que\ reacciona\ en\ dV \\ en\ el\ tiempo\ dt \end{bmatrix}$$

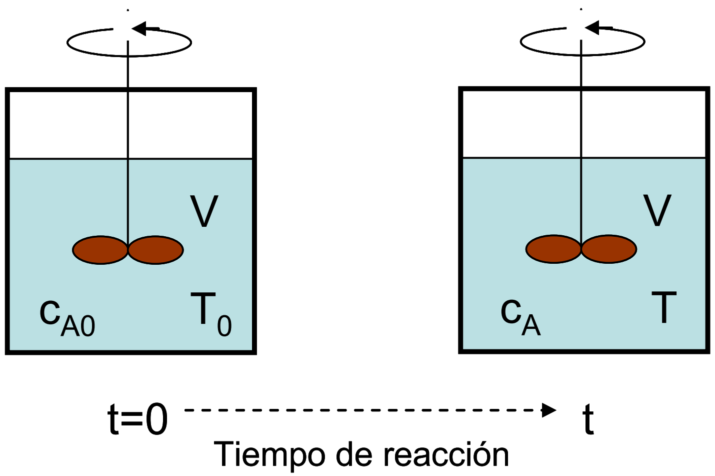
N_{A0} (moles A iniciales)
$x_{A0} = 0$

N_A (moles A)

$$x_A = \frac{N_{A0} - N_A}{N_{A0}}$$

14.2. Reactores de tanque discontinuos

✓ Balance de materia



N_{A0} (moles A iniciales)
$x_{A0} = 0$

N_A (moles A)

$$x_A = \frac{N_{A0} - N_A}{N_{A0}}$$

Acumulación

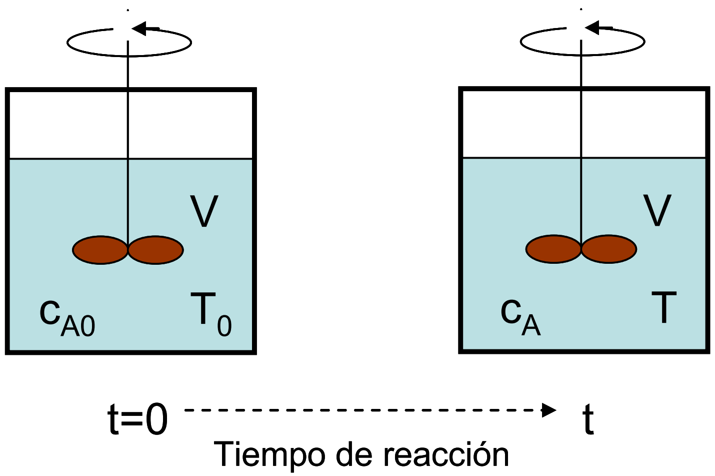
$$\frac{dN_A}{dt} = \frac{d[N_{A0}(1-x_A)]}{dt} = -N_{A0}\frac{dx_A}{dt}$$

Generación

$$(-r_A)V$$

14.2. Reactores de tanque discontinuos

✓ Balance de materia



N_{A0} (moles A iniciales)
$x_{A0} = 0$

N_A (moles A)

$$x_A = \frac{N_{A0} - N_A}{N_{A0}}$$

Diferencial

$$(-r_A)V = N_{A0}\frac{dx_A}{dt}$$

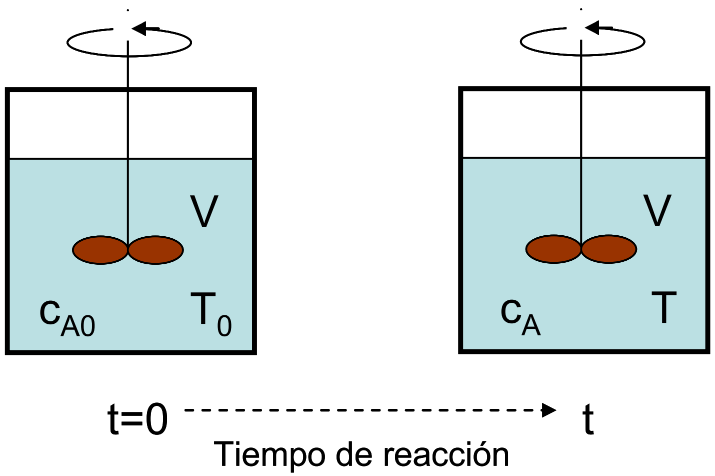
Integral

$$t = N_{A0}\int_0^{x_A}\frac{dx_A}{(-r_A)V}$$

14.2. Reactores de tanque discontinuos

✓ Ecuación cinética

$$t = \frac{N_{A0}}{V}\int_0^{x_A}\frac{dx_A}{(-r_A)} = c_{A0}\int_0^{x_A}\frac{dx_A}{(-r_A)} \quad (V = cte.)$$



$$c_A = c_{A0}(1 - x_A) \therefore dc_A = -c_{A0}\,dx_A$$

$$t = -\int_{c_{A0}}^{c_A}\frac{dc_A}{(-r_A)} \quad (V = cte.)$$

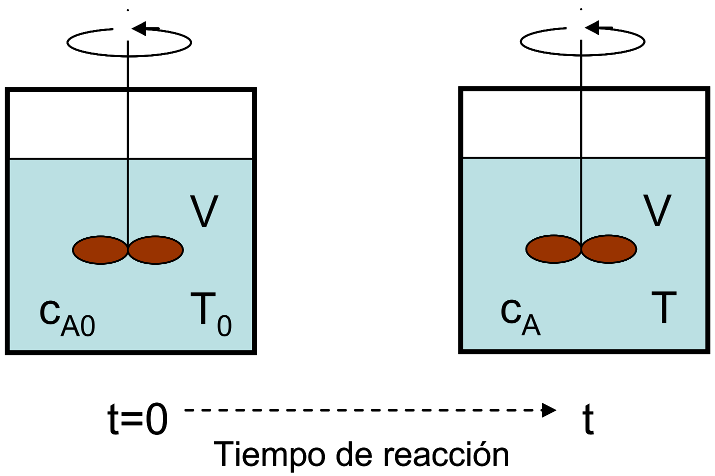
N_{A0} (moles A iniciales)
$x_{A0} = 0$

N_A (moles A)

$$x_A = \frac{N_{A0} - N_A}{N_{A0}}$$

14.2. Reactores de tanque discontinuos

✓ Ecuación cinética



N_{A0} (moles A iniciales)
$x_{A0} = 0$

N_A (moles A)

$$x_A = \frac{N_{A0} - N_A}{N_{A0}}$$

Volumen variable

$$V = V_0 (1 + \varepsilon_A x_A) \qquad \varepsilon_A = \frac{V_{conv.completa} - V_{\sin conv.}}{V_{\sin conv.}}$$

$$t = N_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A) V_0 (1 + \varepsilon_A x_A)} = c_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)(1 + \varepsilon_A x_A)}$$

$$c_A = \frac{N_A}{V} = \frac{N_{A0}(1 - x_A)}{V_0 (1 + \varepsilon_A x_A)} = c_{A0} \frac{(1 - x_A)}{(1 + \varepsilon_A x_A)}$$

14.2. Reactores de tanque discontinuos

Reacción	Ecuación de velocidad	Forma integrada
a) Reacciones irreversibles (volumen variable)		
Orden cero	$(-r_A) = k$	$\frac{c_{A0}}{\varepsilon_A}\ln(1+\varepsilon_A x_A) = kt$
Primer orden	$(-r_A) = k\frac{c_{A0}(1-x_A)}{(1+\varepsilon_A x_A)}$	$-\ln(1-x_A) = kt$
Segundo orden	$(-r_A) = \frac{kc_{A0}^2(1-x_A)^2}{(1+\varepsilon_A x_A)^2}$	$\frac{(1+\varepsilon_A)x_A}{(1-x_A)} + \varepsilon_A \ln(1-x_A) = kc_{A0}t$
b) Reacciones irreversibles (volumen constante)		
Orden cero	$(-r_A) = k$	$c_{A0}x_A = kt$
Primer orden	$(-r_A) = k\,c_A$	$-\ln(1-x_A) = kt$
Segundo orden	$(-r_A) = k\,c_A^2$	$\frac{1}{c_{A0}}\frac{x_A}{1-x_A} = kt$

Ejemplo 1

- ✓ Reactor discontinuo de volumen variable
- ✓ T=350 ºC y P=1 atm
- ✓ A (g) → B (g) + C (g)
- ✓ Cinética de primer orden
- ✓ $k = 2{,}5 \cdot 10^{-5}\ s^{-1}$
- ✓ x_A (t=1 h)?

Ejemplo 1

- ✓ Reacción primer orden

$$-\ln(1-x_A) = kt \therefore (1-x_A) = e^{-kt}$$
$$x_A = 1-\exp(-2{,}5 \cdot 10^{-5} \cdot 3600) = 0{,}086 \therefore$$
$$\therefore 8{,}6\%\, de\, A\, descompuesto$$

- ✓ Volumen constante $c_A = c_{A0}(1-x_A)$

- ✓ Volumen variable $c_A = c_{A0}\dfrac{(1-x_A)}{(1+\varepsilon_A x_A)}$

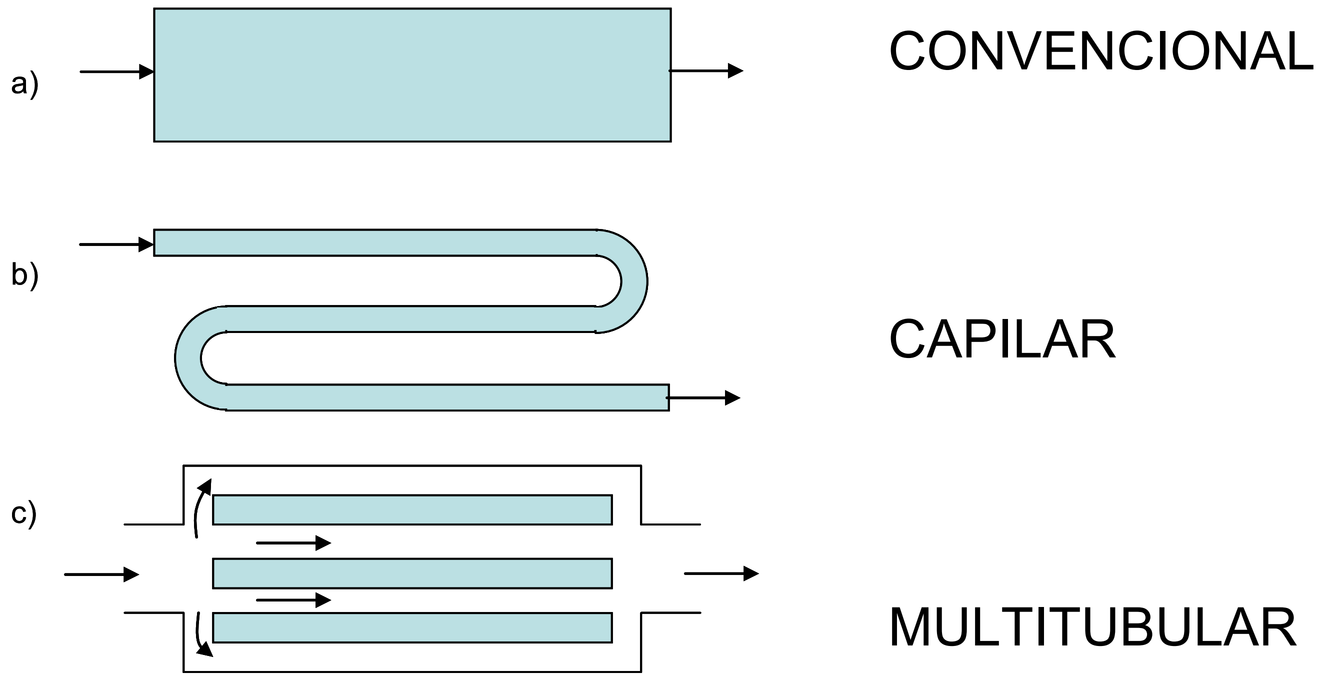
Ejemplo 1

$$c_{A0} = \frac{P_{A0}}{RT} = \frac{1(atm)}{0,082(atm\cdot l/mol\cdot K)623(K)} = 0,019(mol/l)$$

$$\varepsilon_A = \frac{2-1}{1} = 1$$

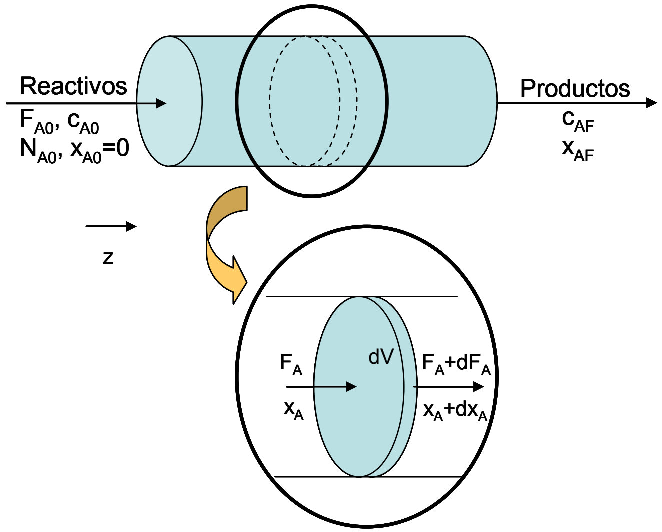
V = cte: cA = 0,0179 (mol/l)
V ≠ cte: cA = 0,0165 (mol/l)

14.3. Reactores tubulares continuos



14.3. Reactores tubulares continuos

✓ Balance de materia



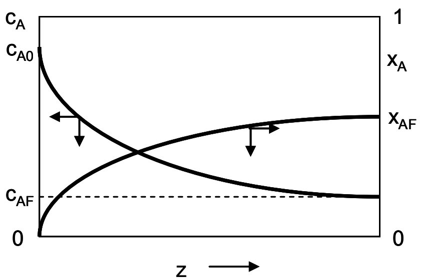
$$[Acumulación] = [Entrada] - [Salida] + [Generación]$$

$$0 \quad = \quad F_A \quad - (F_A + dF_A) \quad - (-r_A)dV$$

$$\therefore \ -dF_A = (-r_A)dV \quad (molA/s)$$

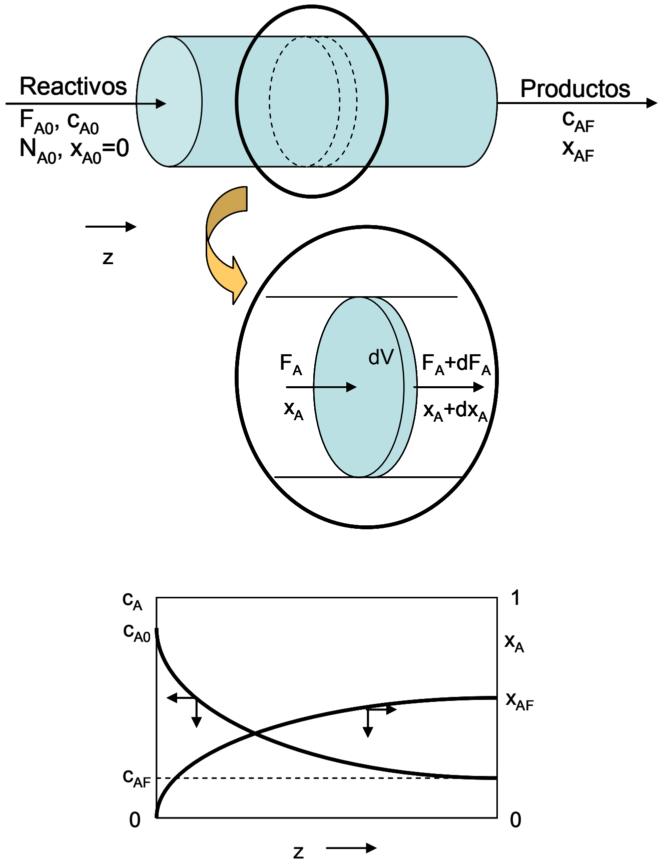
$$F_A = F_{A0}(1 - x_A) \therefore \ dF_A = -F_{A0}dx_A$$

$$F_{A0}dx_A = (-r_A)dV$$



14.3. Reactores tubulares continuos

✓ Ecuación cinética



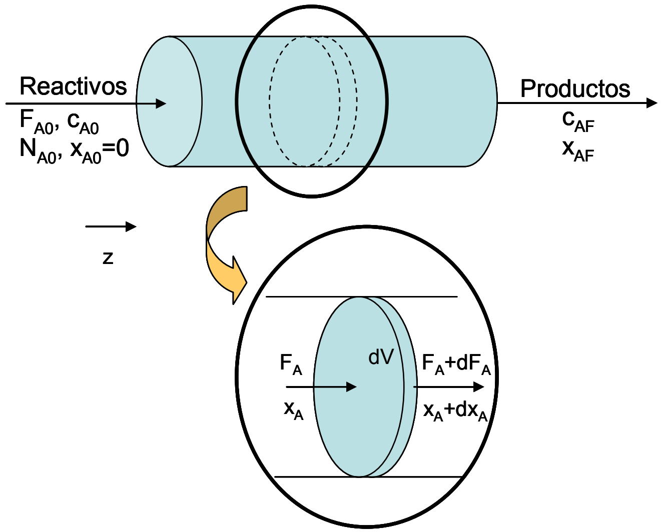
$$\frac{V}{F_{A0}} = \int_0^{x_{AF}} \frac{dx_A}{(-r_A)}$$

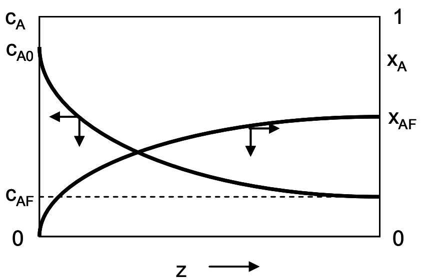
$$x_A = \frac{c_{A0} - c_A}{c_{A0}} \therefore dx_A = -\frac{dc_A}{c_{A0}}$$

$$\frac{V}{F_{A0}} = -\frac{1}{c_{A0}} \int_{c_{A0}}^{c_{AF}} \frac{dc_A}{(-r_A)}$$

14.3. Reactores tubulares continuos

✓ Ecuación cinética



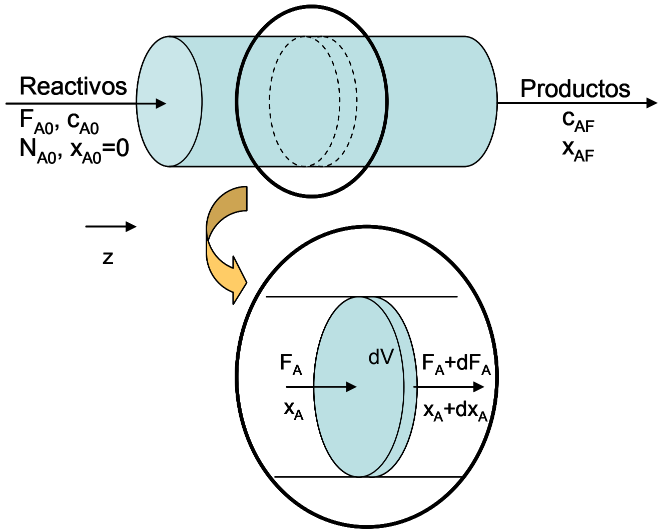


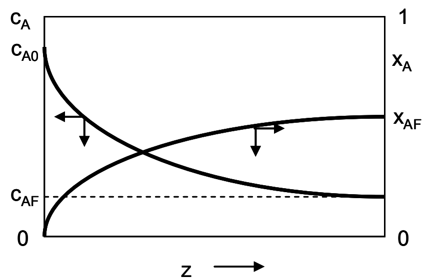
$$\tau = \frac{V}{Q_V} = c_{A0} \int_0^{x_{AF}} \frac{dx_A}{(-r_A)}$$

$$\tau = \frac{V}{Q_V} = -\int_{c_{A0}}^{c_{AF}} \frac{dc_A}{(-r_A)}$$

14.3. Reactores tubulares continuos

✓ Ecuación cinética





Orden cero

$$k\tau = c_{A0} - c_A = c_{A0} x_A$$

Orden uno

$$k\tau = -(1+\varepsilon_A)\ln(1-x_A) - \varepsilon_A x_A$$

Orden dos (2A→P)

$$c_{A0} k\tau = 2\varepsilon_A (1+\varepsilon_A)\ln(1-x_A) + \varepsilon_A^2 x_A + (1+\varepsilon_A)^2 \frac{x_A}{1-x_A}$$

Ejemplo 2

- ✓ Reactor de flujo pistón de V?
- ✓ T=400 ºC y P=1atm
- ✓ $CH_3CHO \rightarrow CH_4 + CO$
- ✓ Cinética de segundo orden
- ✓ k = 0,30 l/(mol·s)
- ✓ $x_A = 0,4$
- ✓ $F_A = 1.200$ mol/h

Ejemplo 2

✓ Ecuación de diseño

$$\frac{V}{F_{A0}} = \int_0^{x_A} \frac{dx_A}{(-r_A)}$$

✓ Variación de volumen (ε_A=1)

$$c_A = c_{A0}\frac{(1-x_A)}{(1+\varepsilon_A x_A)} \qquad (-r_A) = kc_A^2 = kc_{A0}^2\frac{(1-x_A)^2}{(1+x_A)^2}$$

Ejemplo 2

✓ Ecuación de diseño

$$\frac{V}{F_{Ao}} = \frac{1}{kc_{A0}^2} \int_{c_{A0}}^{c_{AF}} \frac{(1+x_A)^2}{(1-x_A)^2} dx_A$$

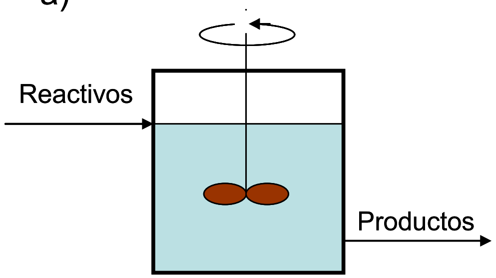
$$V = \frac{F_{A0}}{kc_{A0}^2} \left[\frac{4}{1-x_A} + 4\ln(1-x_A) + x_A - 4 \right]$$

F_{A0} = 1.200/3.600 = 0,333 (mol/s)
k = 0,30 (l/mol·s)
c_{A0} = P_{A0}/RT = 0,018 (mol/l)
x_A = 0,4

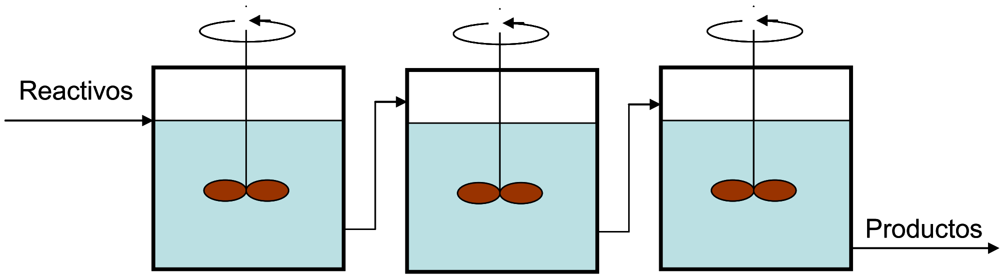
V = 3.505 (l)

14.4. Reactores de tanque continuos

a)

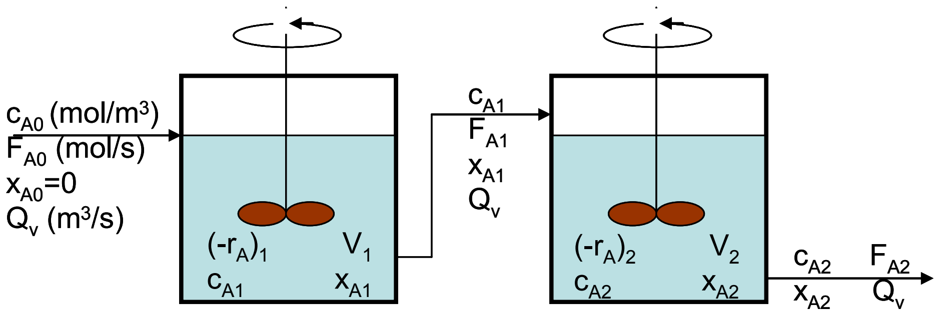


b)



14.4. Reactores de tanque continuos

✓ Balance de materia



$$[Acumul.] = [Entrada] - [Salida] + [Generación]$$

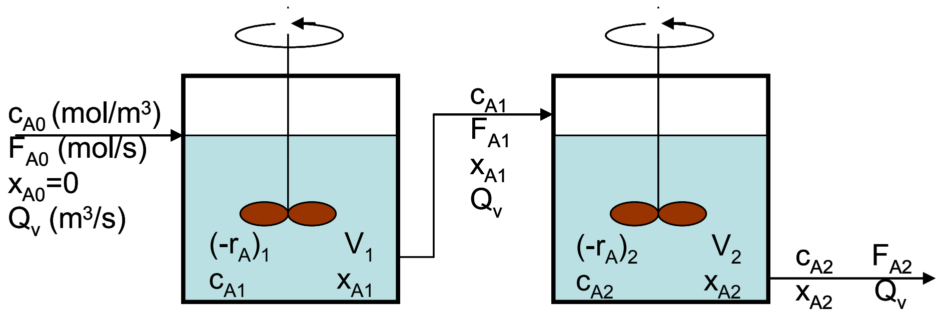
$$0 \quad = \quad F_{A0} \quad - F_{A0}(1 - x_{A1}) - \quad (-r_{A1})V_1$$

$$\therefore \; F_{A0}x_{A1} = (-r_A)_1 V_1 \quad (mol\, A/s)$$

$$\therefore \frac{V_1}{F_{A0}} = \frac{x_{A1}}{(-r_A)_1} (m^3 s/mol\, A)$$

14.4. Reactores de tanque continuos

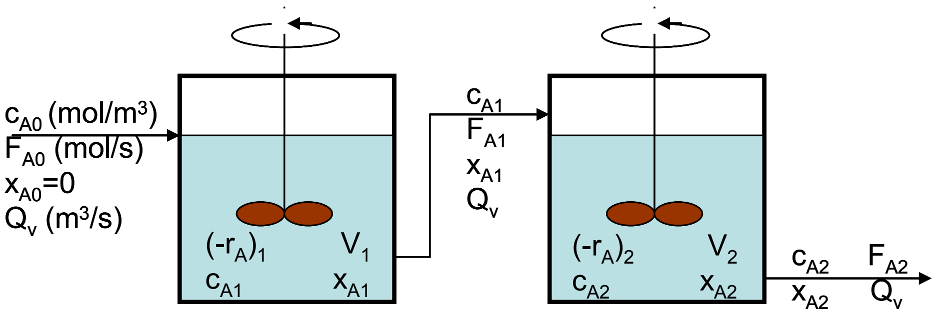
✓ Balance de materia



$$\frac{V_1 c_{A0}}{F_{A0}} = \frac{c_{A0} - c_{A1}}{(-r_A)_1} \qquad \tau_1 = \frac{V_1}{Q_v} = \frac{V_1 c_{A0}}{F_{A0}} = \frac{c_{A0} - c_{A1}}{(-r_A)_1} \ (s)$$

14.4. Reactores de tanque continuos

✓ Balance de materia



$$\frac{V_2}{F_{A1}} = \frac{x_{A2}}{(-r_A)_2}$$

$$\tau_2 = \frac{V_2\, c_{A1}}{F_{A1}} = \frac{c_{A1} - c_{A2}}{(-r_A)_2} = \frac{c_{A1} x_{A2}}{(-r_A)_2}$$

Ejemplo 3

- ✓ 3 reactores de m. completa en serie
- ✓ $V_1 = 60 \text{ l} = 2\ V_2 = 6\ V_3$
- ✓ F = 1.000 l/h
- ✓ $c_{A0} = 2$ mol/l
- ✓ $x_{A1} = 0{,}5 \quad x_{A2} = 0{,}33 \quad x_{A3} = 0{,}14$
- ✓ Ecuación cinética?

Ejemplo 3

- ✓ Reactor 1

$$\tau_1 = \frac{V_1}{Q_v} = \frac{c_{A0} x_{A1}}{(-r_A)_1}$$

- ✓ Reactores 2 y 3

$$\tau_2 = \frac{V_2}{Q_v} = \frac{c_{A1} x_{A2}}{(-r_A)_2} \qquad \tau_3 = \frac{V_3}{Q_v} = \frac{c_{A2} x_{A3}}{(-r_A)_3}$$

Ejemplo 3

- ✓ Concentraciones

$$c_{A1} = c_{A0}(1 - x_{A1}); c_{A2} = c_{A1}(1 - x_{A2}); c_{A3} = c_{A2}(1 - x_{A3})$$

c_{A1}=1 mol/l, c_{A2} = 0,67 mol/l y c_{A3}=0,576 mol/l

$$\tau_1 = \frac{60}{1.000/60} = 3,6\,(\text{min})$$

$$\tau_2 = \frac{30}{1.000/60} = 1,8\,(\text{min})$$

$$\tau_3 = \frac{10}{1.000/60} = 0,6\,(\text{min})$$

Ejemplo 3

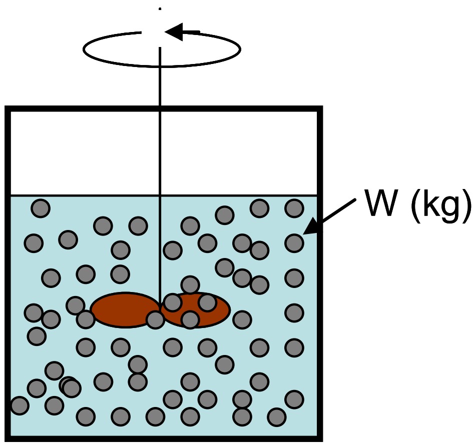
- ✓ Velocidades de reacción

$$(-r_A)_1 = 0{,}277\,(mol/l\cdot\text{min})$$
$$(-r_A)_2 = 0{,}183\,(mol/l\cdot\text{min})$$
$$(-r_A)_3 = 0{,}156\,(mol/l\cdot\text{min})$$

$(-r_A)/c_A = k = 0{,}274\ \text{min}^{-1}$

14.5. Reactores heterogénos

✓ Reactor por cargas



t=0, $c_A=c_{A0}$

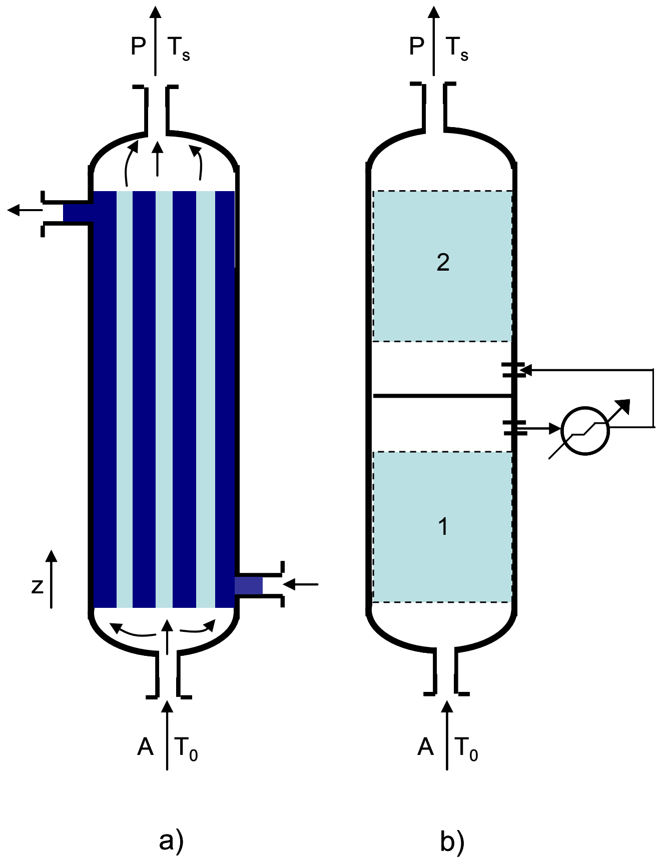
$$(-r_A) = -\frac{1}{W}\frac{dN_A}{dt} = f(c_A) \;\; (mol/kg \cdot s)$$

$$(-r_A)W = c_{A0}V\frac{dx_A}{dt}$$

$$t = \frac{c_{A0}V}{W}\int_0^{x_A}\frac{dx_A}{(-r_A)}$$

14.5. Reactores heterogénos

✓ Reactor de lecho fijo



$$F_{A0}dx_A = (-r_A)dW$$

$$\frac{W}{F_{A0}} = \int_0^{x_{AF}} \frac{dx_A}{(-r_A)}$$

Ejemplo 4

- ✓ Reactor de lecho fijo con catalizador
- ✓ A (g) → 2B (g)
- ✓ T = 500 ºC y P = 6 atm
- ✓ F_A = 2 mol/h

Conversión x_A (%)	Catalizador W (kg)
5	0,020
10	0,043
25	0,127
40	0,242
75	0,789

W ?

F_A = 1.000 mol/h

x_A = 0,5

Ejemplo 4

✓ Ecuación cinética

$$(-r_A) = k\frac{c_{A0}(1-x_A)}{(1+\varepsilon_A x_A)}$$

$$\frac{W}{F_{A0}} = \int_0^{x_{AF}} \frac{dx_A}{(-r_A)} = \frac{1}{kc_{A0}} \int_0^{x_{AF}} \frac{(1+\varepsilon_A x_A)}{(1-x_A)} dx_A$$

$$\frac{Wc_{A0}}{F_{A0}}k = (1+\varepsilon_A)\ln\frac{1}{(1-x_A)} - \varepsilon_A x_A$$

Ejemplo 4

c_{A0}=P_{A0}/RT=6/(0,082·773)=0,095 (mol/l)
F_{A0}=2/3.600=5,55·10^{-4} (mol/s)
ε_A=1

$$(171{,}17)Wk = 2\ln\frac{1}{(1-x_A)} - x_A \qquad k = 1{,}497\cdot 10^{-2}\, l/kg\, de\, cat\cdot s$$

Ejemplo 4

$$W = \frac{F_{A0}}{kc_{A0}}\left[(1+\varepsilon_A)\ln\frac{1}{(1-x_A)} - \varepsilon_A x_A\right] = \frac{(1.000/3.600)}{(1{,}497\cdot 10^{-2})(0{,}095)}(0{,}886) = 173\ kg$$

14.5. Reactores heterogéneos

✓ Reactor de lecho fluidizado