Simulación y Optimización

Fundamentos
Parte II

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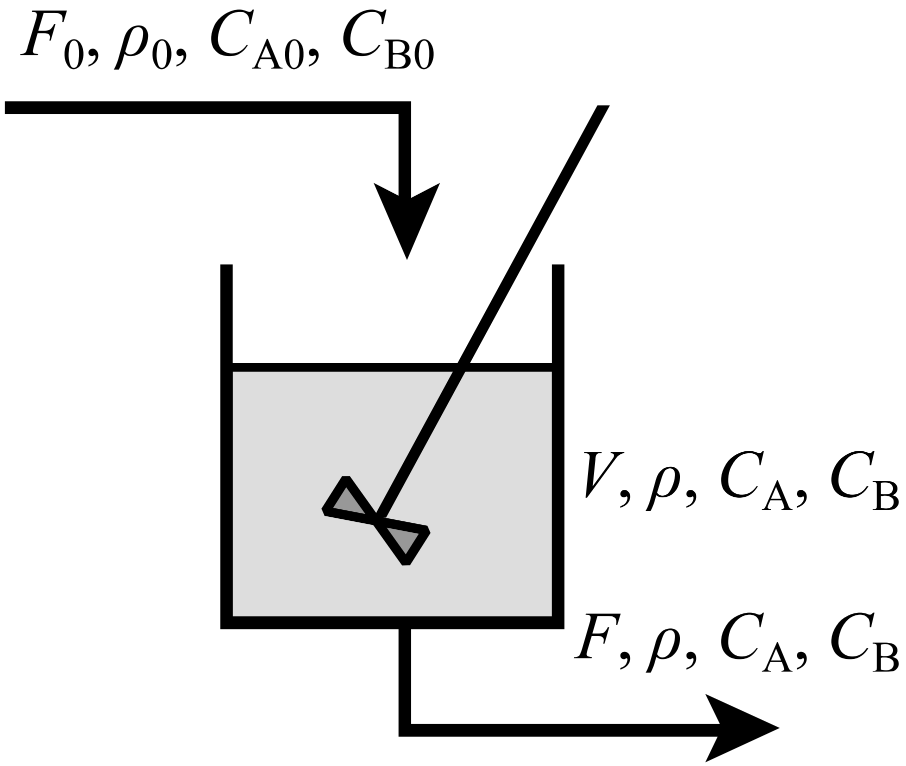
Balances de componentes en un sistema con parámetros concentrados

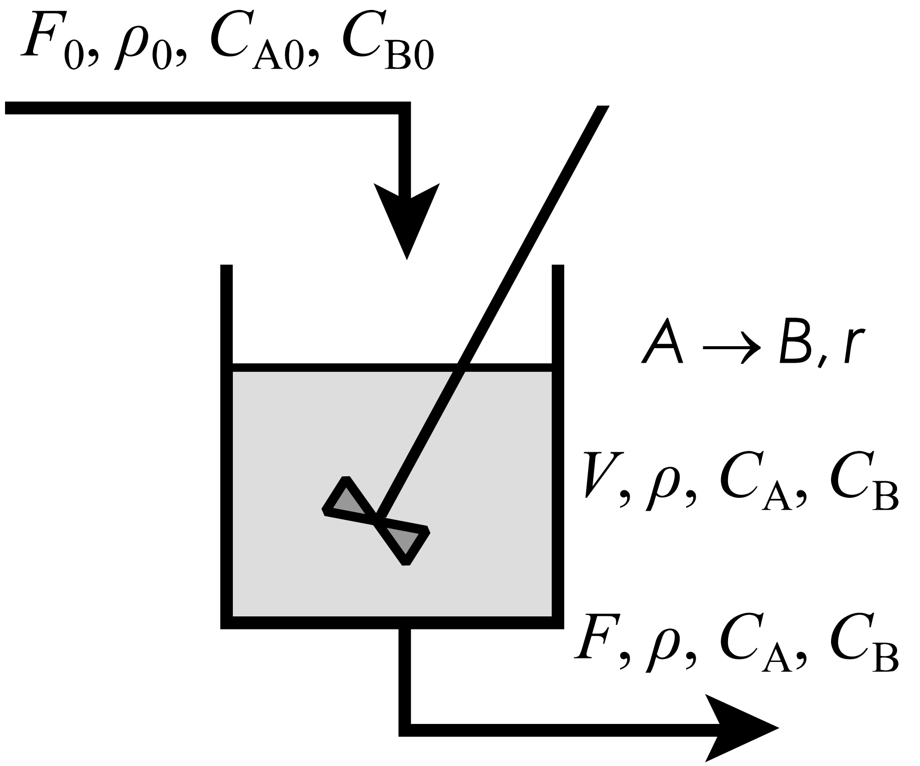
Balance de componente

- {vel. de acumulación de comp.} =
  {velocidad de entrada de comp.}
  +{velocidad de generación de comp.}
  -{velocidad de salida de comp.}
- [materia]/[tiempo]: mol/h
- *NC* o *NC*-1 y balance de materia global



Balance de componente

- {vel. de acum.} $= \dfrac{d(VC_A)}{dt}$
- {vel. de entrada} $= F_0 C_{A0}$
- {vel. de gener.} $= V r_A = -V r$
- {vel. de salida} $= F C_A$



$$\frac{d(VC_A)}{dt} = F_0 C_{A0} - V r - F C_A = 0$$

$$\frac{d(VC_j)}{dt} = \sum_{\forall i \in E} F_i C_{i,j} + V \sum_{\forall k \in R} \alpha_{j,k} r_k - C_j \sum_{\forall i \in S} F_i$$

Dependencia lineal

Dependencia lineal

$$f(x)=0$$
$$g(x)=0$$

$\Rightarrow$

$$h(x)=af(x)+bg(x)$$

$$h(x)=\sum_{i=1}^{n} w_i f_i(x)$$

Dependencia lineal del balance de materia

$$PM_A \left\{ \frac{d(V C_A)}{dt} = F_0 C_{A0} - V r - F C_A \right\}$$

$$+PM_B \left\{ \frac{d(V C_B)}{dt} = F_0 C_{B0} + V r - F C_B \right\}$$

$$\frac{d(V \rho)}{dt} = F_0 \rho_0 - F \rho$$

$$PM_A C_A + PM_B C_B = \rho$$

$$PM_A = PM_B$$

Dependencia lineal del balance de materia

$$\sum_{\forall j \in C} PM_j \frac{d\left(V C_j\right)}{dt} = \sum_{\forall j \in C} PM_j \left(\sum_{\forall i \in E} F_i C_{i,j} + V \sum_{\forall k \in R} \alpha_{j,k} r_k - C_j \sum_{\forall i \in S} F_i \right)$$

$$\sum_{\forall j \in C} PM_j C_{i,j} = \rho_i$$

$$\frac{d\left(V \rho\right)}{dt} = \sum_{\forall i \in E} F_i \rho_i - \rho \sum_{\forall i \in S} F_i$$

$$\sum_{\forall j \in C} \alpha_{j,k} PM_j = 0$$

Variación de C

Variación de la propiedad intensiva

$$\frac{d(V C_A)}{dt} = F_0 C_{A0} - V r - F C_A$$

$$\frac{d(V \rho)}{dt} = F_0 \rho_0 - F \rho$$

$$V \frac{dC_A}{dt} + C_A \frac{dV}{dt} = F_0 C_{A0} - V r - F C_A$$

$$-\frac{C_A}{\rho}\left\{V \frac{d\rho}{dt} + \rho \frac{dV}{dt} = F_0 \rho_0 - F \rho\right\}$$

$$V \frac{dC_A}{dt} - V \frac{C_A}{\rho}\frac{d\rho}{dt} = F_0\left(C_{A0} - C_A \frac{\rho_0}{\rho}\right) - V r$$

$$\rho_0 = \rho$$

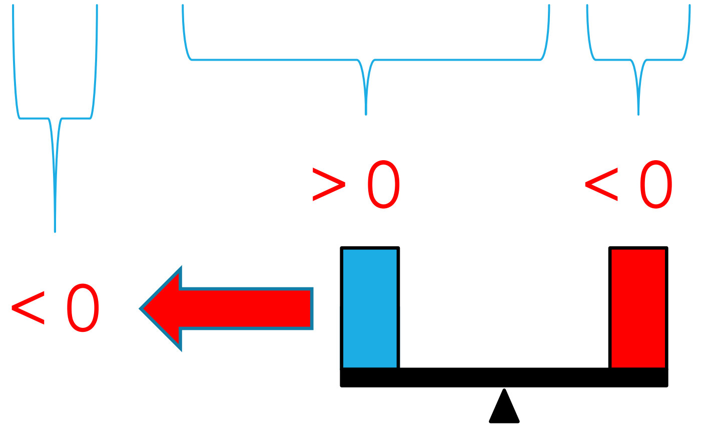
$$\frac{d\rho}{dt} = 0$$

$$V \frac{dC_A}{dt} = F_0 (C_{A0} - C_A) - V r$$

Análisis dinámico cualitativo

- Estado estacionario:
  - $dC_A/dt = 0$
- Disminuye F:
  - No cambia C_A.
- Disminuye F_0:
  - Disminuye C_A.
- Propagación rápida en AEs.
- Propagación lenta en ODEs y PDEs.

$$V\frac{dC_A}{dt} = F_0\left(C_{A0} - C_A\right) - Vr \quad = 0$$



Variable de estado

Variable de estado n_A

$$\frac{d\left(V C_A\right)}{dt} = F_0 C_{A0} - V r - F C_A$$

$$\frac{dn_A}{dt} = F_0 C_{A0} - V r - F C_A$$

$$C_A = \frac{n_A}{V}$$

Variable de estado C_A

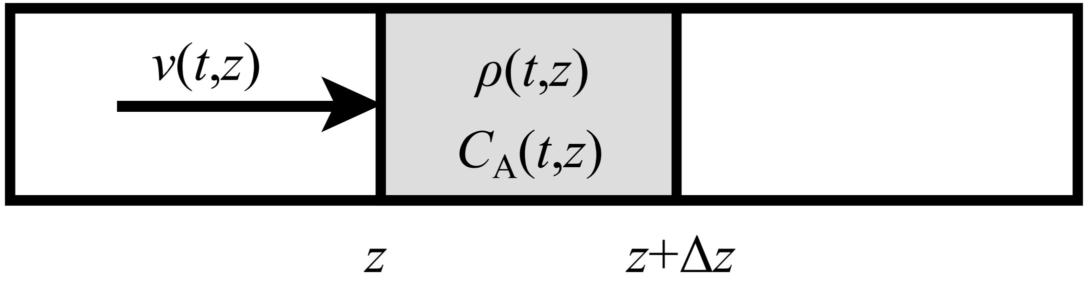
$$V \frac{dC_A}{dt} = F_0 \left(C_{A0} - C_A\right) - V r$$

$$V \frac{dC_j}{dt} = \sum_{\forall i \in E} F_i \left(C_{i,j} - C_j\right) + V \sum_{\forall k \in R} \alpha_{j,k} r_k$$

Balances de componentes en un sistema con parámetros distribuidos

Balance por componente

- {vel. de acum.} $= \dfrac{\partial\left(\Delta z\, A\, C_A\right)}{\partial t}$
- {vel. de entrada} $= v\, A\, C_A\big|_z$
- {vel. de gener.} $= r_A\, A\, \Delta z = -r\, A\, \Delta z$
- {vel. de salida} $= v\, A\, C_A\big|_{z+\Delta z}$



$$\frac{\partial\left(\Delta z\, A\, C_A\right)}{\partial t} = v\, A\, C_A\big|_z - r\, A\, \Delta z - v\, A\, C_A\big|_{z+\Delta z}$$

$$\Delta z \frac{\partial C_A}{\partial t} = v\, C_A\big|_z - r\, \Delta z - v\, C_A\big|_{z+\Delta z}$$

$$\frac{\partial C_A}{\partial t} = -\frac{v\, C_A\big|_{z+\Delta z} - v\, C_A\big|_z}{\Delta z} - r$$

$$\frac{\partial C_A}{\partial t} = -\frac{\partial\left(v\, C_A\right)}{\partial z} - r = 0$$

Variación de la propiedad intensiva

$$\frac{\partial C_A}{\partial t} = -\frac{\partial (v C_A)}{\partial z} - r$$

$$\frac{\partial \rho}{\partial t} = -\frac{\partial (v \rho)}{\partial z}$$

$$\frac{\partial \rho}{\partial z} = 0$$

$$\frac{\partial \rho}{\partial t} = 0$$

$$\frac{\partial C_A}{\partial t} = -v \frac{\partial C_A}{\partial z} - C_A \frac{\partial v}{\partial z} - r$$

$$-\frac{C_A}{\rho} \left\{ \frac{\partial \rho}{\partial t} = -v \frac{\partial \rho}{\partial z} - \rho \frac{\partial v}{\partial z} \right\}$$

$$\frac{\partial C_A}{\partial t} - \frac{C_A}{\rho} \frac{\partial \rho}{\partial t} = -v \frac{\partial C_A}{\partial z} - r + v \frac{C_A}{\rho} \frac{\partial \rho}{\partial z}$$

$$\frac{\partial C_A}{\partial t} = -v \frac{\partial C_A}{\partial z} - r$$

Medidas de concentración

Medidas de concentración

- Densidad de la solución [masa]/[volumen]: $\rho = \sum_{j=1}^{NC} \rho_j$
- Concentración de masa del componente *j*: $\rho_j = C_j PM_j$
- Fracción másica de *j*: $w_j = \frac{\rho_j}{\rho}$

Medidas de concentración

- Densidad molar [mol]/[volumen]: $C = \sum_{j=1}^{NC} C_j$
- Concentración molar de *j*: $C_j = \dfrac{\rho_j}{PM_j}$
- Fracción molar de *j*: $x_j = \dfrac{C_j}{C}$
- Peso molecular medio: $PM = \dfrac{\rho}{C}$

Relaciones útiles

1. $$\sum_{j=1}^{NC} x_j = 1$$

2. $$\sum_{j=1}^{NC} w_j = 1$$

3. $$\sum_{j=1}^{NC} x_j PM_j = PM$$

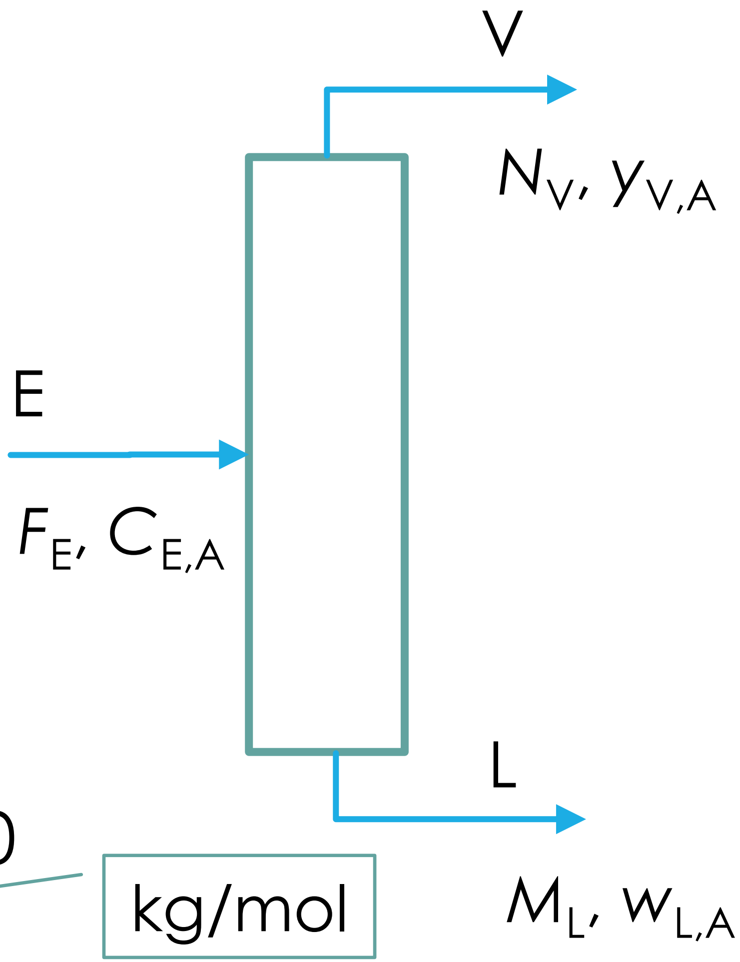
4. $$\sum_{j=1}^{NC} \frac{w_j}{PM_j} = \frac{1}{PM}$$

5. $$x_j = PM \frac{w_j}{PM_j}$$

6. $$w_j = \frac{x_j PM_j}{PM}$$

Balance en estado estacionario de A

- *F*: flujo volumétrico (m³/h)
- C: concentración molar (mol/m³)
- *N*: flujo molar (mol/h)
- *y*: fracción molar
- *M*: flujo másico (kg/h)
- w: fracción másica



$$F_E C_{E,A} - F_V C_{V,A} - F_L C_{L,A} = 0$$

$$F_E C_{E,A} - N_V y_{V,A} - \frac{M_L w_{L,A}}{PM_A} = 0$$

kg/mol