Simulación y Optimización

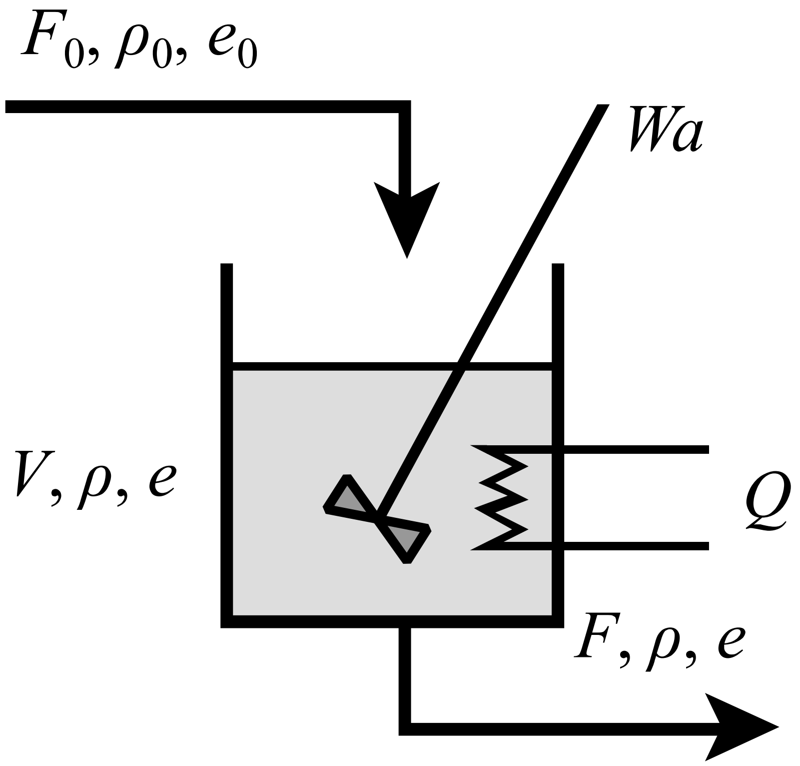
Fundamentos
Parte III

Enrique E. Tarifa, Facultad de Ingeniería, UNJu

Balance de energía

Balance de energía

- {vel. de acumulación de energía} =
  {velocidad de entrada de energía}
  -{velocidad de salida de energía}
- No existe generación.
- [energía]/[tiempo]: J/h
- Un único balance por volumen de control.

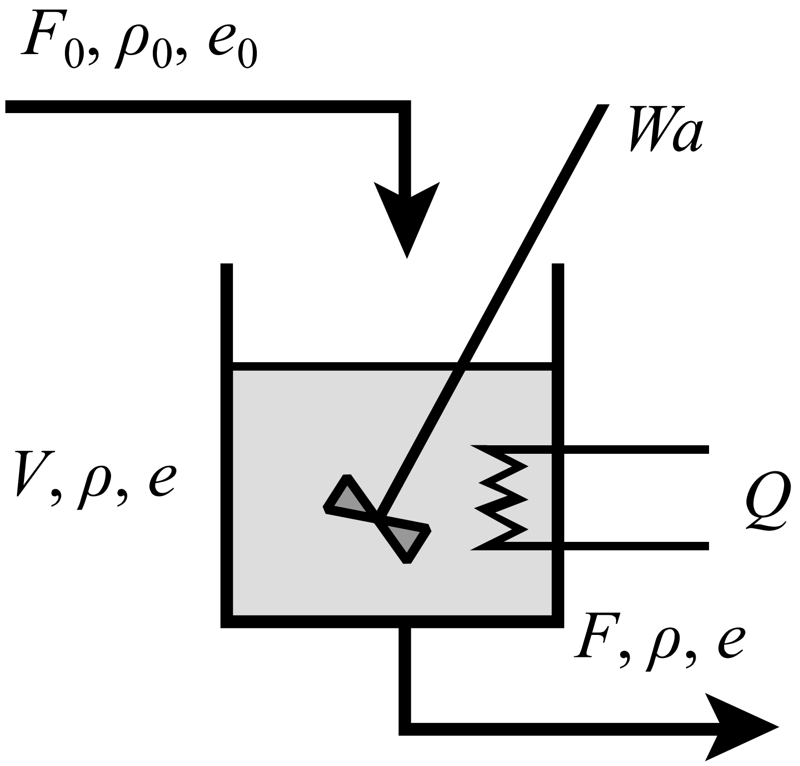


Balance de energía

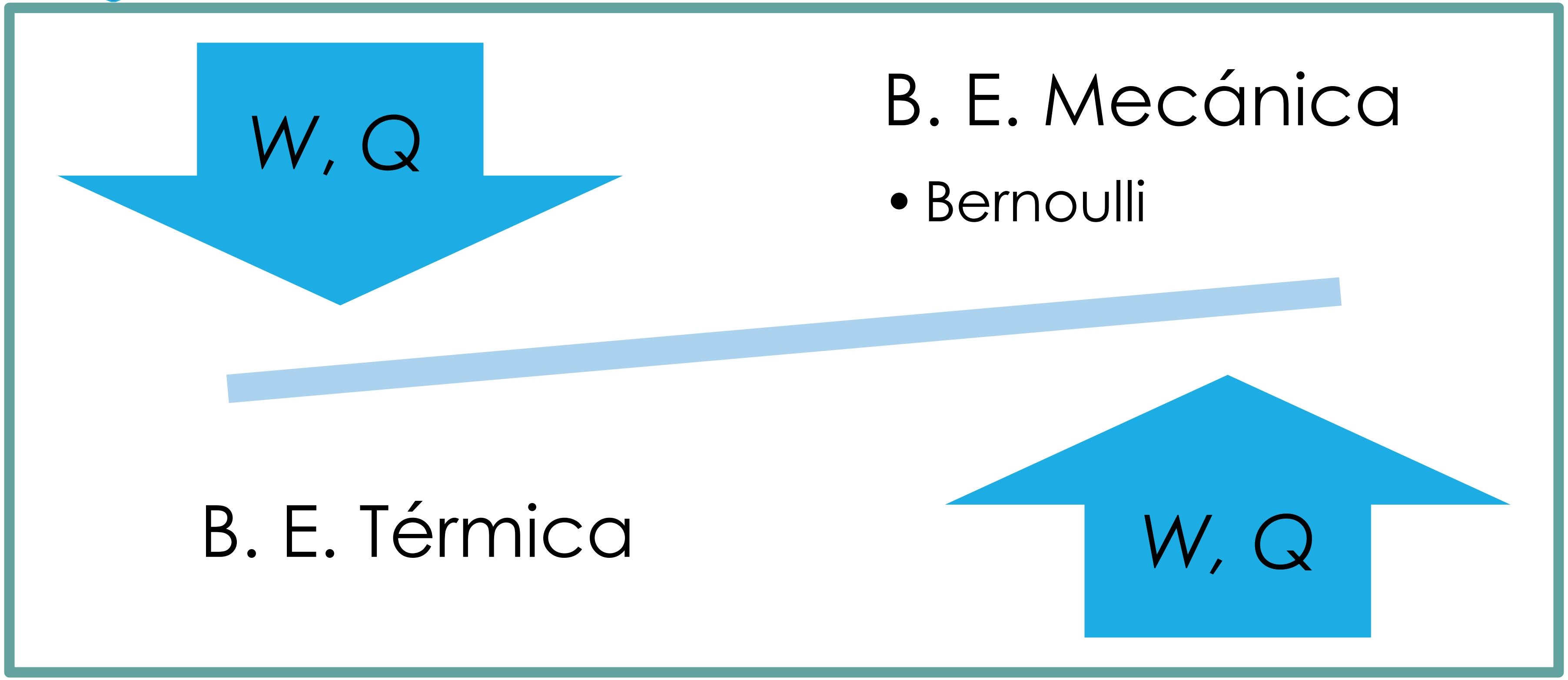
- {vel. de acum.} $= \dfrac{d(V\rho e)}{dt}$
- {vel. de entrada} $= F_0\,\rho_0\,e_0 + Q + Wn$
- {vel. de salida} $= F\rho e$

$$\frac{d(V\rho e)}{dt} = F_0\,\rho_0\,e_0 + Q + Wn - F\rho e$$

$$e = u + \cancel{ek + ep} \qquad ek = \tfrac{1}{2}v^2,\;\; ep = g\,y$$



Energía mecánica y térmica



Balance de energía total

Balance de energía

$$Wn = F_0 P_0 + Wa - F P$$

$$f\,v = P\,A\,v = P\,F$$

$$h = u + \frac{P}{\rho}$$

$$\frac{d(VP)}{dt} = V\cancel{\frac{dP}{dt}} + P\cancel{\frac{dV}{dt}}$$

$$\frac{d(V\rho u)}{dt} = F_0\,\rho_0\,u_0 + Q + Wn - F\,\rho u$$

$$\frac{d(V\rho u)}{dt} = F_0\,\rho_0\left(u_0 + \frac{P_0}{\rho_0}\right) + Q + Wa - F\,\rho\left(u + \frac{P}{\rho}\right)$$

$$\frac{d(V\rho h)}{dt} - \frac{d(VP)}{dt} = F_0\,\rho_0\,h_0 + Q + Wa - F\,\rho\,h$$

$$\boxed{\frac{d(V\rho h)}{dt} = F_0\,\rho_0\,h_0 + Q + Wa - F\,\rho\,h}$$

Estado de referencia

$$\frac{d(V\rho h)}{dt}=F_0\rho_0 h_0+Q+Wa-F\rho h$$

$$V\rho\frac{dh}{dt}+h\frac{d(V\rho)}{dt}=F_0\rho_0 h_0+Q+Wa-F\rho h$$

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

$$h_1-h_0=\int_{T_0}^{T_1}Cp(T)\,dT$$

$$V\rho\frac{dh}{dt}+(h-hr)\frac{d(V\rho)}{dt}=F_0\rho_0(h_0-hr)+Q+Wa-F\rho(h-hr)$$

$$hr=h$$

$$\boxed{V\rho\frac{dh}{dt}=F_0\rho_0(h_0-h)+Q+Wa}$$

$$\boxed{V\rho Cp\frac{dT}{dt}=F_0\rho_0 Cp_0(T_0-T)+Q+Wa}$$

Análisis dinámico cualitativo

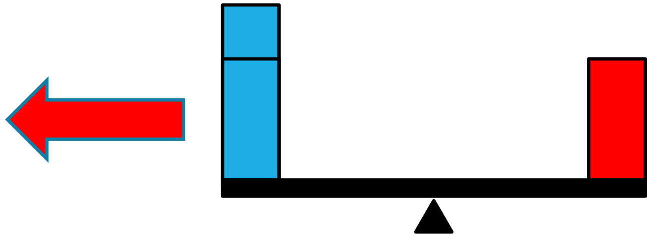
- Estado estacionario:
  - $dT/dt = 0$
- Disminuye F_0:
  - Aumenta $T(+)$.

$$V\rho Cp \underbrace{\frac{dT}{dt}}_{>0} = \underbrace{F_0\,\rho_0\,Cp_0\left(T_0 - T\right)}_{<0} + \underbrace{Q + Wa}_{>0} = 0$$

Análisis dinámico cualitativo

- Estado estacionario:
  - $dT/dt = 0$
- Aumenta x, dado $F_0 = kx$:
  - Disminuye T(-).

$$V\rho Cp \underbrace{\frac{dT}{dt}}_{<0} = \underbrace{F_0\,\rho_0\,Cp_0\left(T_0 - T\right)}_{<0} + \underbrace{Q + Wa}_{>0} = 0$$



Análisis dinámico cualitativo

- Estado estacionario:
  - $dT/dt = 0$
- Disminuye F, dado $\frac{dV}{dt} = F_0 - F$:
  - No cambia $T(0)$.

$$V\rho Cp\underbrace{\frac{dT}{dt}}_{=0} = \underbrace{F_0\rho_0 Cp_0\left(T_0 - T\right)}_{<0} + \underbrace{Q + Wa}_{>0} = 0$$

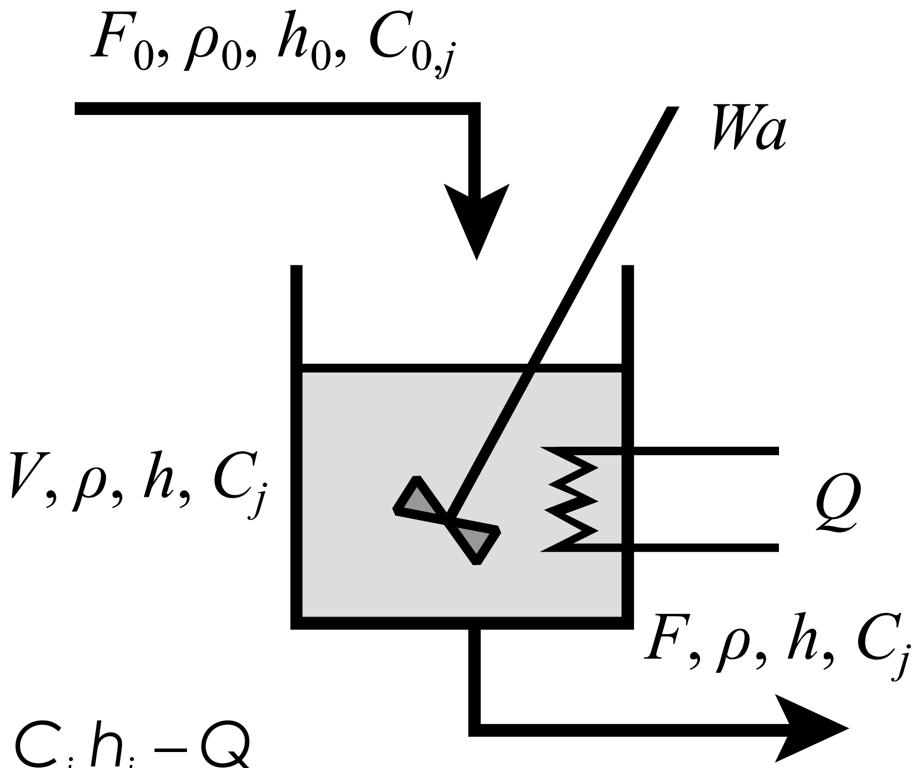
Calor de reacción en un sistema con parámetros concentrados

Solución ideal

- {vel. de acum.} $= \dfrac{d}{dt}\left(V C_A h_A + V C_B h_B\right)$
- {Vel. de acum.} $= \dfrac{d}{dt}\left(V\left(C_A h_A + C_B h_B\right)\right)$
- {Vel. de acum.} $= \dfrac{d}{dt}\left(V \sum_{j=1}^{NC} C_j h_j\right)$

Calor de reacción

- {vel. de acum.} $= \frac{d}{dt}\left(V\sum_{j=1}^{NC} C_j h_j\right)$
- {vel. de entrada} $= F_0 \sum_{j=1}^{NC} C_{0,j} h_{0,j} + Wa$
- {vel. de salida} $= F \sum_{j=1}^{NC} C_j h_j + Q$



$$\frac{d}{dt}\left(V\sum_{j=1}^{NC} C_j h_j\right) = F_0 \sum_{j=1}^{NC} C_{0,j} h_{0,j} + Wa - F \sum_{j=1}^{NC} C_j h_j - Q$$

Derivada de un producto

$$\frac{d}{dt}\left(V\sum_{j=1}^{NC} C_j h_j\right)$$

$$=\frac{d}{dt}\left(\sum_{j=1}^{NC} V C_j h_j\right)$$

$$=\sum_{j=1}^{NC} V C_j \frac{dh_j}{dt}+\sum_{j=1}^{NC} h_j \frac{d\left(V C_j\right)}{dt}$$

$$=V\sum_{j=1}^{NC} C_j \frac{dh_j}{dt}+\sum_{j=1}^{NC} h_j \frac{d\left(V C_j\right)}{dt}$$

$$\frac{d}{dt}\left(V\left(C_A h_A + C_B h_B\right)\right)$$

$$=\frac{d}{dt}\left(V C_A h_A + V C_B h_B\right)$$

$$=\left(V C_A \frac{dh_A}{dt}+h_A\frac{d\left(V C_A\right)}{dt}\right)+\left(V C_B \frac{dh_B}{dt}+h_B\frac{d\left(V C_B\right)}{dt}\right)$$

$$=V\left(C_A \frac{dh_A}{dt}+C_B\frac{dh_B}{dt}\right)+\left(h_A\frac{d\left(V C_A\right)}{dt}+h_B\frac{d\left(V C_B\right)}{dt}\right)$$

Calor de reacción

$$\frac{d}{dt}\left(V\sum_{j=1}^{NC} C_j\, h_j\right) = F_0 \sum_{j=1}^{NC} C_{0,j}\, h_{0,j} + Wa - F\sum_{j=1}^{NC} C_j\, h_j - Q$$

$$V\sum_{j=1}^{NC} C_j \frac{dh_j}{dt} + \sum_{j=1}^{NC} h_j \frac{d\left(V C_j\right)}{dt} = F_0 \sum_{j=1}^{NC} C_{0,j}\, h_{0,j} + Wa - F\sum_{j=1}^{NC} C_j\, h_j - Q$$

$$\sum_{j=1}^{NC} h_j \left\{ \frac{d\left(V C_j\right)}{dt} = F_0\, C_{0,j} + \alpha_j\, r\, V - F\, C_j \right\}$$

$$-\left\{ \sum_{j=1}^{NC} h_j \frac{d\left(V C_j\right)}{dt} = F_0 \sum_{j=1}^{NC} h_j\, C_{0,j} + V\, r \sum_{j=1}^{NC} \alpha_j\, h_j - F\sum_{j=1}^{NC} h_j\, C_j \right\}$$

$$\Delta H = \sum_{j=1}^{NC} \alpha_j\, h_j$$

$$V\sum_{j=1}^{NC} C_j \frac{dh_j}{dt} = F_0 \sum_{j=1}^{NC} C_{0,j}\left(h_{0,j} - h_j\right) + V\, r\left(-\Delta H\right) + Wa - Q$$

$$\Delta H = \Delta Hr + \int_{Tr}^{T} \Delta Cp\left(\xi\right) d\xi \qquad \Delta Cp\left(T\right) = \sum_{j=1}^{NC} \alpha_j\, Cp_j\left(T\right)$$

Ley de Kirchhoff

Calor de reacción

$$V\sum_{j=1}^{NC} C_j \frac{dh_j}{dt} = F_0 \sum_{j=1}^{NC} C_{0,j}\left(h_{0,j} - h_j\right) + V\,r\left(-\Delta H\right) + Wa - Q$$

$$h_1 - h_0 = \int_{T_0}^{T_1} Cp(T)\,dT$$

$$V\sum_{j=1}^{NC} C_j\,Cp_j \frac{dT}{dt} = F_0 \sum_{j=1}^{NC} C_{0,j}\,Cp_j\left(T_0 - T\right) + V\,r\left(-\Delta H\right) + Wa - Q$$

$$Cp = \sum_{j=1}^{NC} x_j\,Cp_j$$

Regla de mezcla

$$V\,C\,Cp\frac{dT}{dt} = F_0\,C_0\,Cp_0\left(T_0 - T\right) + V\,r\left(-\Delta H\right) + Wa - Q$$

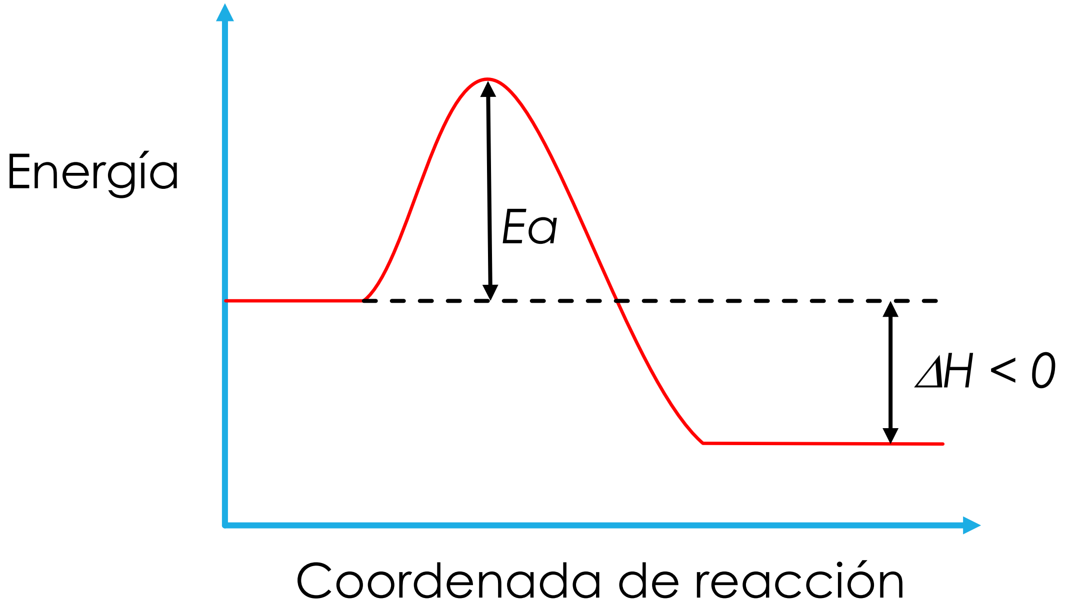
$$V\,\rho\,Cp\frac{dT}{dt} = F_0\,\rho_0\,Cp_0\left(T_0 - T\right) + V\,r\left(-\Delta H\right) + Wa - Q$$

$$C_j = x_j\,C$$

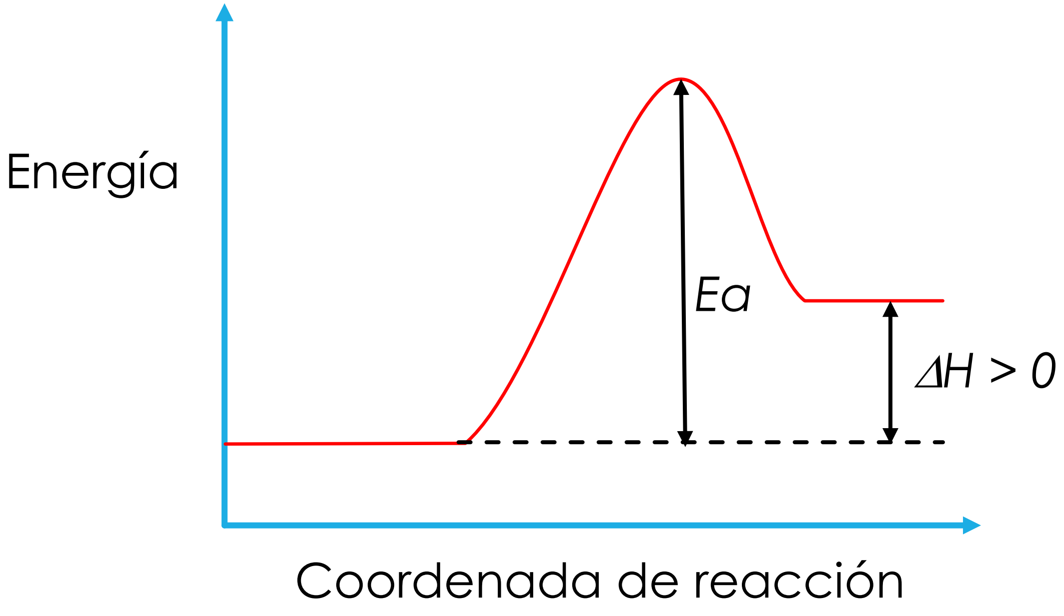
$$\boxed{V\,\rho\,Cp\frac{dT}{dt} = \sum_{\forall i\in E} F_i\,\rho_i\,Cp_i\left(T_i - T\right) + V\sum_{\forall k\in R} r_k\left(-\Delta H_k\right) + Wa - Q}$$

Calor de reacción

$$V\,\rho\,Cp\,\frac{dT}{dt}=\sum_{\forall i\in E}F_i\,\rho_i\,Cp_i\left(T_i-T\right)+V\sum_{\forall k\in R}r_k\left(-\Delta H_k\right)+Wa-Q$$



Exotérmica

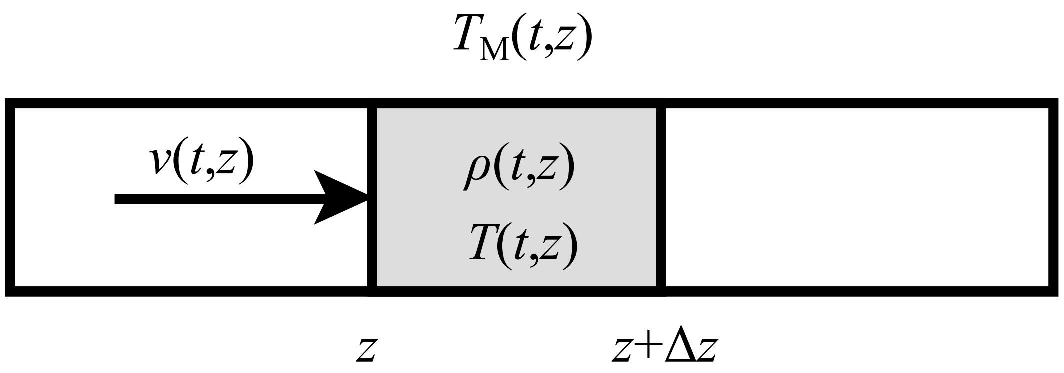


Endotérmica

Balance de energía en un sistema con parámetros distribuidos

Balance de energía

- {vel. de acum.} $= \dfrac{\partial\left(A\,\Delta z\,\rho h\right)}{\partial t}$
- {vel. de entrada} $= v A \rho h\big|_z + A q\big|_z + \Delta Q$
- {vel. de salida} $= v A \rho h\big|_{z+\Delta z} + A q\big|_{z+\Delta z}$



$$\frac{\partial\left(A\,\Delta z\,\rho h\right)}{\partial t} = v A \rho h\big|_z + A q\big|_z + \Delta Q - v A \rho h\big|_{z+\Delta z} - A q\big|_{z+\Delta z}$$

$$\frac{\partial\left(\rho h\right)}{\partial t} = -\frac{v \rho h\big|_{z+\Delta z} - v \rho h\big|_z}{\Delta z} - \frac{q\big|_{z+\Delta z} - q\big|_z}{\Delta z} + \frac{1}{A}\frac{\Delta Q}{\Delta z}$$

$$\Delta z \frac{\partial\left(\rho h\right)}{\partial t} = v \rho h\big|_z + q\big|_z + \frac{1}{A}\Delta Q - v \rho h\big|_{z+\Delta z} - q\big|_{z+\Delta z}$$

$$\boxed{\cancel{\frac{\partial\left(\rho h\right)}{\partial t}} = -\frac{\partial\left(v \rho h\right)}{\partial z} - \frac{\partial q}{\partial z} + \frac{1}{A}\frac{\partial Q}{\partial z} = 0}$$

Variación de la propiedad intensiva

$$\frac{\partial(\rho h)}{\partial t} = -\frac{\partial(v\rho h)}{\partial z} - \frac{\partial q}{\partial z} + \frac{1}{A}\frac{\partial Q}{\partial z}$$

$$\rho\frac{\partial h}{\partial t} + h\frac{\partial \rho}{\partial t} = -h\frac{\partial(v\rho)}{\partial z} - v\rho\frac{\partial h}{\partial z} - \frac{\partial q}{\partial z} + \frac{1}{A}\frac{\partial Q}{\partial z}$$

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

$$\boxed{\rho\frac{\partial h}{\partial t} = -v\rho\frac{\partial h}{\partial z} - \frac{\partial q}{\partial z} + \frac{1}{A}\frac{\partial Q}{\partial z}}$$

$$\frac{dh}{dt} = \left(\frac{\partial h}{\partial T}\right)_P \frac{dT}{dt} = Cp\frac{dT}{dt}$$

$$\boxed{\rho Cp\frac{\partial T}{\partial t} = -v\rho Cp\frac{\partial T}{\partial z} - \frac{\partial q}{\partial z} + \frac{1}{A}\frac{\partial Q}{\partial z}}$$