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PARTICLE CONSERVATION OF MASS (PARTICLE DIFFUSIVITY)

GOVERNING EQUATION

\[ \frac{\partial q}{\partial t} + \varepsilon_p \frac{\partial c}{\partial t} = D_{\text{eff}} \frac{\partial}{\partial r} \left( \frac{\partial c}{\partial r} \right) \]

ASSUMPTIONS

- Gas phase storage term is negligible
- \(D_{\text{eff}}\) is constant through particle
- \(D_{\text{eff}}\) is independent of loading

INITIAL CONDITIONS

\[ c(r, 0) = c_{\text{initial}} \]
\[ q(r, 0) = q_{\text{initial}} \]

BOUNDARY CONDITIONS

\[ \left( \frac{\partial c}{\partial r} \right)_{r=0} = 0 \]
\[ \left( D_{\text{eff}} \frac{\partial c}{\partial r} \right)_{r=R_i} = -K_j \left( c_B - c_R \right) \]

CONSTITUTIVE RELATIONS

- Desiccant Capacity

\[ q = q(c, T) \]
• Mass Transfer Film Coefficient

**Sherwood Number**

\[ Sh = \frac{2K_f R_s}{D_m} = 2.0 + 0.6 \text{Re}^{0.5} \text{Sc}^{0.33} \]

**Reynold Number**

\[ \text{Re} = \frac{\rho_f V 2R_s}{\mu} \]

**Schmidt Number**

\[ \text{Sc} = \frac{\mu}{\rho_f D_m} \]

• Ideal Gas Law

\[ \rho = \frac{P_v}{R_T T} \]

• Effective Diffusivity

\[ D_{eff} = \frac{D_p}{\tau} = \frac{\epsilon_p D_m}{\tau} \]

where

\[ D_m = D_{m,o} \left( \frac{P_o}{P} \right) \left( \frac{T}{T_o} \right)^{1.5} \]

**GAS STREAM CONSERVATION OF MASS**

**GOVERNING EQUATION**

\[ -\varepsilon D_e \frac{\partial^2 c}{\partial Z^2} + \frac{\partial}{\partial Z} \left( \nu c \right) + \varepsilon \frac{\partial c}{\partial t} + (1 - \varepsilon) \frac{\partial q}{\partial t} = 0 \]
ASSUMPTIONS

- Gas phase storage is neglected - \( \frac{\partial c}{\partial t} = 0 \)
- One dimensional – no gradients in radial direction
- Plug flow is assumed – \( D_L = 0 \)

INITIAL CONDITIONS

\[ c (Z, 0) = c_{initial} \]
\[ \bar{q} (Z, 0) = \bar{q}_{initial} \]

BOUNDARY CONDITIONS

\[ c (0, t) = c_{inlet} \]
\[ V (0, t) = V_{inlet} \]

CONSTITUTIVE RELATIONS

- Superficial Velocity
  \[ V = \frac{Flow_{std} \, \sigma_{std}}{c_{gas} \, A_c} \]

- Gas Concentration
  \[ c_{gas} = \frac{(P_T - P_v)}{R_{gas} \, T} \]

- Average Loading
  \[ (1 - \varepsilon) \frac{\partial \bar{q}}{\partial t} = a \, k_f \, (c_b - c_k) \]

GAS-ADSORBENT CONSERVATION OF ENERGY

GOVERNING EQUATION

\[ -\varepsilon \, K \, \frac{\partial^2 T_f}{\partial Z^2} + V \rho_f C_{p,f} \frac{\partial T_f}{\partial Z} + (1 - \varepsilon) \rho_s C_{p,s} \frac{\partial T_s}{\partial t} \]
\[ = -(1 - \varepsilon) \Delta H \frac{\partial \bar{q}}{\partial t} - \frac{4 h_v}{d_i} (T_f - T_v) \]
ASSUMPTIONS

- Conduction heat transfer is neglected
- Energy storage term in gas phase is neglected
- Thermal equilibrium between fluid and solid is assumed, i.e. $T_f(Z) = T_s(Z)$
- No radial temperature gradient in sorbent bed

INITIAL CONDITIONS

$$T_f(Z, 0) = T_s(Z, 0) = T_{\text{initial}}$$
$$\bar{q}(Z, 0) = \bar{q}_{\text{initial}}$$

BOUNDARY CONDITIONS

$$T(0, t) = T_{\text{inlet}}$$
$$V(0, t) = V_{\text{inlet}}$$

CONSTITUTIVE RELATIONS

- Film heat transfer coefficient to vessel

  \[ \text{Nusselt Number} \]
  \[ Nu = \frac{2h_f R_s}{K_f} = 2.0 + 0.369 \text{Re}^{0.64} \text{Pr}^{0.33} \]

  \[ \text{Reynold Number} \]
  \[ \text{Re} = \frac{\rho_f V 2R_s}{\mu} \]

  \[ \text{Prantl Number} \]
  \[ \text{Pr} = \frac{C_{p,f} \mu}{K_f} \]
VESSEL CONSERVATION OF ENERGY

GOVERNING EQUATION

\[ \pi d_i h_v (T - T_v) = \frac{\pi}{4} \left( d_o^2 - d_i^2 \right) \rho_v C_v \frac{dT_v}{dt} + \frac{\pi d_o}{R_d} (T_v - T_{amb}) \]

ASSUMPTIONS

• No radial temperature gradient through vessel
• No axial conduction through vessel

INITIAL CONDITIONS

\[ T_v (Z, 0) = T_{v, initial} \]

BOUNDARY CONDITIONS

\[ T_{amb} (t) = T_{amb} \]

CONSTITUTIVE RELATIONS – none

GAS CONSERVATION OF MOMENTUM

GOVERNING EQUATION

\[ \frac{\partial P}{\partial Z} = f \left( \frac{\sigma V^2}{2R_s} \right) \]

ASSUMPTIONS – none

INITIAL CONDITIONS – none

BOUNDARY CONDITIONS

\[ P(0, t) = P_{inlet} \]

CONSTITUTIVE RELATION

• Ergun friction factor

\[ f = \left( \frac{1 - \varepsilon}{\varepsilon^3} \right) \left[ \frac{150(1 - \varepsilon)}{Re} + 1.75 \right] \]
NOMENCLATURE

- $a$ – sorbent external surface area [ft$^2$/ft$^3$]
- $A_c$ – Bed cross sectional area [ft$^2$]
- $c$ – gas phase concentration [lb$_{H2O}$/ft$^3$]
- $c_B$ – gas phase concentration in bulk stream [lb$_{H2O}$/ft$^3$]
- $c_{gas}$ – concentration of gas (density) [lb/ft$^3$]
- $c_{initial}$ – initial gas phase concentration [lb$_{H2O}$/ft$^3$]
- $c_{inlet}$ – gas phase concentration at bed inlet [lb$_{H2O}$/ft$^3$]
- $C_{P,f}$ – fluid specific heat [Btu/lb-R]
- $C_{P,s}$ – sorbent specific heat [Btu/lb-R]
- $C_v$ – vessel specific heat [Btu/lb-R]
- $c_R$ – gas phase concentration at sorbent particle surface [lb$_{H2O}$/ft$^3$]
- $D_{eff}$ – effective diffusivity through adsorbent particle [ft$^2$/min]
- $d_i$ – vessel inside diameter [ft]
- $D_L$ – axial dispersion coefficient – [ft$^2$/min]
- $D_m$ – molecular diffusivity [ft$^2$/min]
- $D_{m,o}$ – molecular diffusivity at standard temperature and pressure [ft$^2$/min]
- $d_o$ – vessel outside diameter [ft]
- $D_p$ – sorbate pore diffusivity [ft$^2$/min]
- $Flow_{std}$ – flow referenced to standard temperature and pressure [scfm]
- $K$ – thermal conductivity of sorbent bed [Btu/min-ft-R]
- $K_f$ – external fluid film mass transfer coefficient [ft/min]
- $h_v$ – film coefficient to vessel [Btu/min-ft$^2$-R]
- $P$ – pressure [lb/ft$^2$]
- $P_{inlet}$ – pressure at bed inlet [lb/ft$^2$]
- $P_o$ – standard pressure [lb/ft$^2$]
- $P_T$ – total gas pressure [lb/ft$^2$]
- $P_v$ – sorbate vapor pressure [lb/ft$^2$]
- $q$ – solid phase concentration [lb$_{H2O}$/ft$^3$]
- $q_{average}$ – average solid phase concentration [lb$_{H2O}$/ft$^3$]
- $q_{initial}$ – initial solid phase concentration [lb$_{H2O}$/ft$^3$]
- $q_{initial}$ – average initial solid phase concentration [lb$_{H2O}$/ft$^3$]
- $r$ – radial coordinate for adsorbent [ft]
- $R_a$ – resistance to ambient heat loss from vessel [min-ft$^2$-R/Btu]
- $R_{gas}$ – gas constant of bulk gas [ft-lb/lb$_m$-R]
- $R_s$ – adsorbent particle radius [ft]
- $R_v$ – gas constant of sorbate [ft-lb/lb$_m$-R]
- $t$ – time [min]
- $T$ – temperature [R]
- $T_{amb}$ – ambient temperature [R]
- $T_f$ – fluid temperature [R]
- $T_{inlet}$ – temperature of inlet fluid [R]
• $T_o$ – standard temperature [R]
• $T_s$ – sorbent temperature [R]
• $T_v$ – vessel temperature [R]
• $T_{v,initial}$ – initial vessel temperature [R]
• $V$ – superficial velocity [ft/min]
• $V_{inlet}$ – superficial velocity at bed inlet [ft/min]
• $Z$ – axial coordinate [ft]
• $\Delta H$ – heat of adsorption [Btu/lb]
• $\varepsilon$ - voidage of sorbent bed [ft$^3$/ft$^3$]
• $\varepsilon_p$ – porosity of adsorbent particle [ft$^3$/ft$^3$]
• $\rho_f$ – fluid density [lb/ft$^3$]
• $\rho_s$ – sorbent density [lb/ft$^3$]
• $\rho_{std}$ – fluid density at standard pressure and temperature [lb/scf]
• $\rho_v$ – vessel density [lb/ft$^3$]
• $\tau$ - tortuosity [ft/ft]
• $\mu$ - viscosity [lbm/ft-min]