PEDCO Adsorptive Gas-Dryer Simulation Software

Conservation Equations, Assumptions, Initial Conditions, Boundary Conditions, and Constitutive Relations

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PARTICLE CONSERVATION OF MASS (PARTICLE DIFFUSIVITY)

GOVERNING EQUATION

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

ASSUMPTIONS

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

INITIAL CONDITIONS

$$c(r,0) = c_{initial}$$
$$q(r,0) = q_{initial}$$

BOUNDARY CONDITIONS

$$\left(\frac{\partial c}{\partial r}\right)_{r=0} = 0$$
$$\left(D_{eff} \frac{\partial c}{\partial r}\right)_{r=R_s} = -K_f\,(c_B - c_R)$$

CONSTITUTIVE RELATIONS

- Desiccant Capacity

$$q = q(c,T)$$

• Mass Transfer Film Coefficient

Sherwood Number

$$Sh = \frac{2K_f R_s}{D_m} = 2.0 + 0.6\,\mathrm{Re}^{0.5}\ Sc^{0.33}$$

Reynold Number

$$\mathrm{Re} = \frac{\rho_f V\ 2R_s}{\mu}$$

Schmidt Number

$$Sc = \frac{\mu}{\rho_f D_m}$$

• Ideal Gas Law

$$c = \frac{P_v}{R_v T}$$

• Effective Diffusivity

$$D_{eff} = \varepsilon_p\ D_p = \frac{\varepsilon_p\ D_m}{\tau}$$

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

$$-\varepsilon\ D_L \frac{\partial^2 c}{\partial Z^2} + \frac{\partial}{\partial Z}(Vc) + \varepsilon \frac{\partial c}{\partial t} + (1-\varepsilon)\frac{\partial \bar{q}}{\partial t} = 0$$

ASSUMPTIONS

- Gas phase storage is neglected - $\partial c / \partial t = 0$
- One dimensional – no gradients in radial direction
- Plug flow is assumed – $D_L = 0$

INITIAL CONDITIONS

$$c\left(Z,0\right)=c_{initial}$$
$$\bar{q}\left(Z,0\right)=\bar{q}_{initial}$$

BOUNDARY CONDITIONS

$$c\left(0,t\right)=c_{inlet}$$
$$V\left(0,t\right)=V_{inlet}$$

CONSTITUTIVE RELATIONS

- Superficial Velocity

$$V=\frac{Flow_{std}\;\sigma_{std}}{c_{gas}A_c}$$

- Gas Concentration

$$c_{gas}=\frac{\left(P_T-P_v\right)}{R_{gas}\;T}$$

- Average Loading

$$\left(1-\varepsilon\right)\frac{\partial\bar{q}}{\partial t}=a\,k_f\;\left(c_b-c_R\right)$$

GAS-ADSORBENT CONSERVATION OF ENERGY

GOVERNING EQUATION

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

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

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

BOUNDARY CONDITIONS

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

CONSTITUTIVE RELATIONS

- Film heat transfer coeficient to vessel

Nusselt Number

$$Nu = \frac{2h_v R_s}{K_f} = 2.0 + 0.369\ \mathrm{Re}^{0.64}\ \mathrm{Pr}^{0.33}$$

Reynold Number

$$\mathrm{Re} = \frac{\rho_f V\ 2R_s}{\mu}$$

Prantl Number

$$\mathrm{Pr} = \frac{C_{P,f}\,\mu}{K_f}$$

VESSEL CONSERVATION OF ENERGY

GOVERNING EQUATION

$$\pi\, d_i\, h_v\, (T - T_v) = \frac{\pi}{4}\left(d_o^2 - d_i^2\right)\rho_v C_v\, \frac{\partial T_v}{\partial t} + \frac{\pi\, d_o}{R_a}\left(T_v - T_{amb}\right)$$

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

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

NOMENCLATURE

- a – sorbent external surface area [ft^2/ft^3]
- A_c – Bed cross sectional area [ft^2]
- c – gas phase concentration [$lb_{H2O}/ft^3{}_g$]
- c_B – gas phase concentration in bulk stream [$lb_{H2O}/ft^3{}_g$]
- c_{gas} – concentration of gas (density) [lb/ft^3]
- $c_{initial}$ – initial gas phase concentration [$lb_{H2O}/ft^3{}_g$]
- c_{inlet} – gas phase concentration at bed inlet [$lb_{H2O}/ft^3{}_g$]
- $C_{P,f}$ – 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 [$lb_{H2O}/ft^3{}_g$]
- 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_f/ft^2]
- P_{inlet} –pressure at bed inlet [lb_f/ft^2]
- P_o – standard pressure [lb_f/ft^2]
- P_T – total gas pressure [lb_f/ft^2]
- P_v – sorbate vapor pressure [lb_f/ft^2]
- q – solid phase concentration [$lb_{H2O}/ft^3{}_s$]
- $\bar{q}$ - average solid phase concentration [$lb_{H2O}/ft^3{}_s$]
- $q_{initial}$ – initial solid phase concentration [$lb_{H2O}/ft^3{}_s$]
- $\bar{q}_{initial}$ – 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_f/lb_m-R]
- R_s – adsorbent particle radius [ft]
- R_v – gas constant of sorbate [ft-lb_f/lb_m-R]
- t – time [min]
- T – temperature [R]
- T_{amb} – ambient temperature [R]
- T_f – fluid temperature [R]

T_{inlet} – temperatue 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]
- ΔH – heat of adsorption [Btu/lb]
- ε - voidage of sorbent bed [ft^3/ft^3]
- ε_p – porosity of adsorbent particle [ft^3/ft^3]
- ρ_f – fluid density [lb/ft^3]
- ρ_s – sorbent density [lb/ft^3]
- ρ_{std} – fluid density at standard pressure and temperature [lb/scf]
- ρ_v – vessel density [lb/ft^3]
- τ - tortuosity [ft/ft]
- μ - viscosity [lb_m/ft-min]