PDE System and Related Equations for PSA

Dimensionless variables

$\overline{P} = \frac{P}{P_0}, \overline{T} = \frac{T}{T_0}, x_i = \frac{q_i}{q_s}, \overline{u}_z = \frac{u_z}{u_0}, \tau = \frac{tu_0}{L}, Z = \frac{z}{L}$

Component mass balance

$\frac{\partial y_i}{\partial \tau} = \frac{1}{Pe}\left(\frac{\partial^2 y_i}{\partial Z^2} + \frac{1}{\overline{P}}\frac{\partial \overline{P}}{\partial Z}\frac{\partial y_i}{\partial Z} - \frac{1}{\overline{T}}\frac{\partial \overline{T}}{\partial Z}\frac{\partial y_i}{\partial Z}\right) - \overline{u}_z\frac{\partial y_i}{\partial Z} + \frac{\psi\overline{T}}{\overline{P}}\rho_s\left(\left(y_i - 1\right)\frac{\partial x_i}{\partial \tau} + y_i\sum_{j,j\neq i}\frac{\partial x_j}{\partial \tau}\right)$

$Pe = \frac{u_0 L}{D_L}$

$D_L = 0.7D_m + r_p u_0$

$\psi = \frac{(1-\varepsilon)}{\varepsilon}\frac{RT_0 q_S}{P_0}$

Overall mass balance

$\frac{\partial \overline{P}}{\partial \tau} = \left(-\overline{P}\frac{\partial \overline{u}_z}{\partial Z} - \overline{u}_z\frac{\partial \overline{P}}{\partial Z} + \overline{u}_z\frac{\overline{P}}{\overline{T}}\frac{\partial \overline{T}}{\partial Z}\right) - \psi\overline{T}\sum_i\frac{\partial x_i}{\partial \tau} + \frac{\overline{P}}{\overline{T}}\frac{\partial \overline{T}}{\partial \tau}$

Energy balance

$\frac{\partial \overline{T}}{\partial \tau} = \pi_1\frac{\partial^2 \overline{T}}{\partial Z^2} - \pi_2\overline{u}_z\frac{\partial \overline{T}}{\partial Z} + \sum_i \pi_{3i}\frac{\partial x_i}{\partial \tau}$

$\pi_1 = \frac{1}{\varepsilon C_{pg}\rho_g + (1-\varepsilon)(C_{ps}\rho_s + C_{pa}q_s)}\frac{K_z}{u_0 L}$

$\pi_2 = \frac{1}{\varepsilon C_{pg}\rho_g + (1-\varepsilon)(C_{ps}\rho_s + C_{pa}q_s)}\varepsilon C_{pg}\rho_g$

$\pi_3 = \frac{1}{\varepsilon C_{pg}\rho_g + (1-\varepsilon)(C_{ps}\rho_s + C_{pa}q_s)}\frac{(1-\varepsilon)(-\Delta H_i)q_s\rho_s}{T_0}$

$\rho_g = \frac{\overline{P}P_0}{R\overline{T}T_0}$

$\Delta H_i = \Delta U_i - R\overline{T}T_0$

Linear driving force

$\frac{\partial x_i}{\partial \tau} = \frac{k_i L}{u_0}(x_i^* - x_i)$

Ergun equation

$-\frac{\partial \overline{P}}{\partial Z} = \frac{150\mu(1-\varepsilon)^2 L u_0}{4{r_p}^2\varepsilon^3 P_0}\overline{u}_z + \frac{1.75(1-\varepsilon)L{u_0}^2}{2r_p\varepsilon^3 P_0}\left(\sum_i MW_i y_i \rho_g\right)x_i|x_i|$

Dual-site Langmuir isotherm

$$q_i = \frac{q_{b,i} B_i y_i P}{1+\sum_i B_i y_i P} + \frac{q_{d,i} D_i y_i P}{1+\sum_i D_i y_i P}$$

$$B_i = b_i e^{-\frac{\Delta U_{b,i}}{RT}}$$

$$D_i = d_i e^{-\frac{\Delta U_{d,i}}{RT}}$$

Weighted Essentially Non-Oscillatory (WENO) scheme

Backward:

$$f_{j+0.5} = \frac{\alpha_{0,j}}{\alpha_{0,j}+\alpha_{1,j}}\left[\frac{1}{2}\left(f_j + f_{j+1}\right)\right] + \frac{\alpha_{1,j}}{\alpha_{0,j}+\alpha_{1,j}}\left(\frac{3}{2} f_j - \frac{1}{2} f_{j+1}\right)$$

$$\alpha_{0,j} = \frac{2}{3}\frac{1}{\left(f_{j+1}-f_j+\delta\right)^4}$$

$$\alpha_{1,j} = \frac{1}{3}\frac{1}{\left(f_j-f_{j-1}+\delta\right)^4}$$

Forward:

$$f_{j+0.5} = \frac{\alpha_{0,j}}{\alpha_{0,j}+\alpha_{1,j}}\left[\frac{1}{2}\left(f_j + f_{j+1}\right)\right] + \frac{\alpha_{1,j}}{\alpha_{0,j}+\alpha_{1,j}}\left(\frac{3}{2} f_{j+1} - \frac{1}{2} f_{j+2}\right)$$

$$\alpha_{0,j} = \frac{2}{3}\frac{1}{\left(f_j-f_{j+1}+\delta\right)^4}$$

$$\alpha_{1,j} = \frac{1}{3}\frac{1}{\left(f_{j+1}-f_{j+2}+\delta\right)^4}$$

Reference

[1] K.T. Leperi, R.Q. Snurr, F. You. Optimization of two-stage pressure/vacuum swing adsorption with variable dehydration level for postcombustion carbon capture. *Industrial & Engineering Chemistry Research*, 2016, 55(12), 3338-3350.

[2] D. Yancy-Caballero, K.T. Leperi, B.J. Bucior, et al. Process-level modelling and optimization to evaluate metal–organic frameworks for post-combustion capture of CO2. *Molecular Systems Design & Engineering*, 2020, 5(7), 1205-1218.

[3] GitHub repository: https://github.com/PEESEgroup/PSA