Modeling and simulation of fixed bed adsorption column: effect of velocity variation

situation z→0, net rate of accumulation or depletion is given as

$$-D_L\frac{\partial^2 C_b}{\partial z^2}+V\frac{\partial C_b}{\partial z}+C_b\frac{\partial V}{\partial z}+\frac{\partial C_b}{\partial t}+\rho_p\left(\frac{1-\varepsilon}{\varepsilon}\right)\frac{\partial q_p}{\partial t}=0$$

(1)

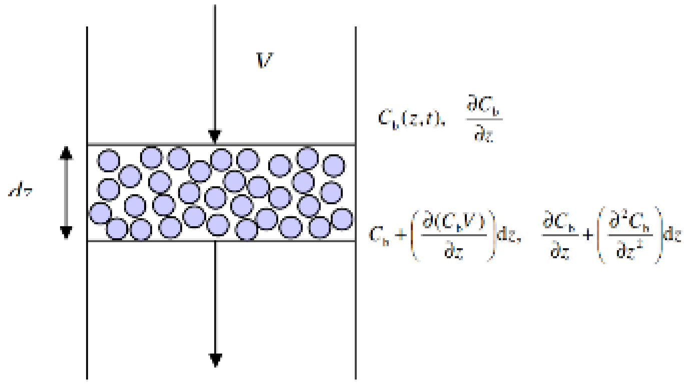

Figure 1: Mass balance in element of fixed bed

The following initial condition is considered

$$C_b = C_{bo} \qquad z=0,\ t=0 \tag{2}$$

$$C_b = 0 \qquad 0<z\le L,\ t=0 \tag{3}$$

The contour conditions at both ends of the column are given by the following equations

$$D_L\frac{\partial C_b}{\partial z} = -V_0(C_{bo}-C_b), \quad z=0,\ t>0 \tag{4}$$

$$\frac{\partial C_b}{\partial z}=0, \qquad z=L,\ t\ge 0 \tag{5}$$

The superficial velocity, V in fixed-bed adsorption is not constant because of adsorption. The following equation was used to estimate (dV/dz), the variation of velocity of bulk fluid along the axial direction of the bed. For liquid adsorption, assuming the liquid density to be constant, then the total mass balance gives

$$\rho_l\frac{\partial V}{\partial z} = -(1-\varepsilon)\rho_s\frac{\partial q_p}{\partial t} \tag{6}$$

Velocity boundary conditions

$$V=V_0, \qquad z=0,\ t>0 \tag{7}$$

$$\frac{\partial V}{\partial t}=0, \qquad z=L,\ t>0 \tag{8}$$

The inter-phase mass transfer rate may be expressed as

$$\rho_s \frac{\partial q_p}{\partial t} = \frac{3k_f}{a_p}(C_b - C_s) \tag{9}$$

The intra-pellet mass transfer is due to the diffusion of adsorbate molecules through the pore. The macroscopic conservation equation is given as

$$\varepsilon_p \frac{\partial c}{\partial t} + (1-\varepsilon_p)\rho_p \frac{\partial q}{\partial t} = D_p\left(\frac{\partial^2 c}{\partial r^2} + \frac{2}{r}\frac{\partial c}{\partial r}\right) \tag{10}$$

The following initial condition is considered

$$c = 0, \quad q = 0, \qquad 0 < r < a_p,\ t = 0 \tag{13}$$

The symmetry condition at the center of the particles and continuity condition on the external surface of the adsorbent bed are expressed as

$$\frac{\partial c}{\partial r} = 0, \qquad r = 0,\ t > 0 \tag{14}$$

$$k_f(C_b - C_s) = D_p \frac{\partial c}{\partial r}, \qquad r = a_p, t > 0 \tag{15}$$

The adsorption isotherm was favorable and nonlinear, and it described by Langmuir isotherm

$$q = \frac{q_m bc}{1 + bc} \tag{16}$$