

$$D_s * \frac{\partial^2 C_s}{\partial z^2} - \frac{2 * \epsilon * km * (C_s - C_{g,pore} * S)}{r * (1 - \epsilon)} = \frac{\partial C_s}{\partial t} \quad \dots(1)$$

I.C. $t = 0, \quad C_s = C_{g1} * S$

B.C. 1 $z = 0, \quad \frac{\partial C_s}{\partial z} = 0$

B.C. 2 $z = L, \quad -D_s * \frac{\partial C_s}{\partial z} = km1 * (C_s - C_{g,bulk} * S)$

$$D_g * \frac{\partial^2 C_{g,pore}}{\partial z^2} - \frac{2 * km * (C_s - C_{g,pore} * S)}{r} = \frac{\partial C_{g,pore}}{\partial t} \quad \dots(2)$$

I.C. $t = 0, \quad C_{g,pore} = C_{g1}$

B.C. 1 $z = 0, \quad \frac{\partial C_{g,pore}}{\partial z} = 0$

B.C. 2 $z = L, \quad -D_g * \frac{\partial C_{g,pore}}{\partial z} = km2 * (C_{g,pore} - C_{g,bulk})$

$$V * \frac{dC_{g,bulk}}{dt} = -Q * C_{g,bulk} + \{(1 - \epsilon) * A_{tot} * km1 * (C_s - C_{g,bulk} * S)\} |_{z=L} + \{\epsilon * A_{tot} * km2 * (C_{g,pore} - C_{g,bulk})\} |_{z=L} \quad \dots(3)$$

I.C. $t = 0, \quad C_{g,bulk} = C_{g1}$

known = $\epsilon, A_{tot}, V, Q, C_{g1}, L$ (All are constants)

Parameters to be estimated (unknown) = $S, D_s, D_g, km, km1, km2, r$

Dependent variables = $C_s, C_{g,pore}, C_{g,bulk}$

Independent variables = z, t

We have data for $C_{g,bulk}$ w.r.t time (t). Need to fit $C_{g,bulk}$ to find the unknown parameters.