

Equilibrium Dispersive Model

Equilibrium Dispersive Model (EDM) is prescribed by following partial differential equation:

$$\frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x} + D \frac{\partial^2 c}{\partial x^2} - \frac{1 - \varepsilon}{\varepsilon} \frac{\partial q^*}{\partial t}$$

Henry's isotherm

Henry's (Linear) adsorption isotherm is prescribed by following equation:

$$q^* = k_H c$$

Leading to following expression:

$$a_H \frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x} + D \frac{\partial^2 c}{\partial x^2} \quad a_H(k_H, \varepsilon) = \frac{k_H \cdot (1 - \varepsilon)}{\varepsilon} - 1$$

NOTE: a_H is constant in one optimization step. D, k_H, ε are decision variables.

Langmuir's isotherm

Langmuir's (Nonlinear) adsorption isotherm is prescribed by following equation:

$$q^* = \frac{Q \cdot k_L c}{1 + k_L c}$$

Leading to following expression:

$$a_L \frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x} + D \frac{\partial^2 c}{\partial x^2} \quad a_L(c, Q, k_L, \varepsilon) = 1 + \frac{Q \cdot k_L (1 - \varepsilon)}{(k_L c + 1)^2 \cdot \varepsilon}$$

NOTE: a_L is nonlinear function. D, Q, k_L, ε are decision variables.