Week 13

Contaminant Transport Modeling

12.1. Solute and Particle Transport

Advection

$$J_i = v_x C n$$

Particle Transport

Basic Concepts of Dispersion

$$D_L = \frac{\sigma_L^2}{2t} = \frac{\sigma_L^2 v}{2x}$$

Diffusion

$$J = -D_d \, grad(C * n)$$

12.2. The Mathematics of Mass Transport

Mass Transport Equations

Mass inflow rate - mass outflow rate = change in mass storage with time

$$-divJ = net - mass - outflow - rat - per - unit - volume$$

$$-divJ = \frac{\partial(C * n)}{\partial t}$$

The Diffusion Equation

$$-div[D_d^* \, ngrad(C)] = \frac{\partial(Cn)}{\partial t}$$

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} = \nabla^2 C = (\frac{1}{D_d^*}) \frac{\partial C}{\partial t}$$

Laplace's equation when the left hand side=0.

The Advection-Diffusion Equation

$$J_x = -nD_d^*(\frac{\partial C}{\partial t}) + v_x Cn$$

$$J_y = -nD_d^*(\frac{\partial C}{\partial t}) + v_y Cn$$

$$J_z = -nD_d^*(\frac{\partial C}{\partial t}) + v_z Cn$$

For isotropic conditions,

$$J = -nD_d^* grad(C) + vCn$$

$$\nabla.(nD_d^* \nabla C) - \nabla.vCn = \frac{\partial (Cn)}{\partial t}$$

The one-dimensional form

$$D_d^* \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}$$

The Advection-Dispersion Equation

$$\nabla.(nD_d^* \nabla C) - nv\nabla C - nC\nabla v = \frac{\partial (Cn)}{\partial t}$$

Mass Transport with Reaction

Mass inflow rate - mass outflow rate +/- mass production rate = change in mass storage with time

$$D\frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} + /- \frac{r}{n} = \frac{\partial C}{\partial t}$$

Boundary and Initial Conditions

Constant concentration	Fixed concentration
Pulse-type loading with constant concentration	Fixed concentration
Exponential decay with source centration>0	Fixed concentration
Exponential decay with source centration>Ca	Fixed concentration
Constant flux with constant input concentration	Variable flux
Pulse-type loading with constant input concentration	Variable flux