ERTH655/CEE623
Groundwater Modeling

Model Theory

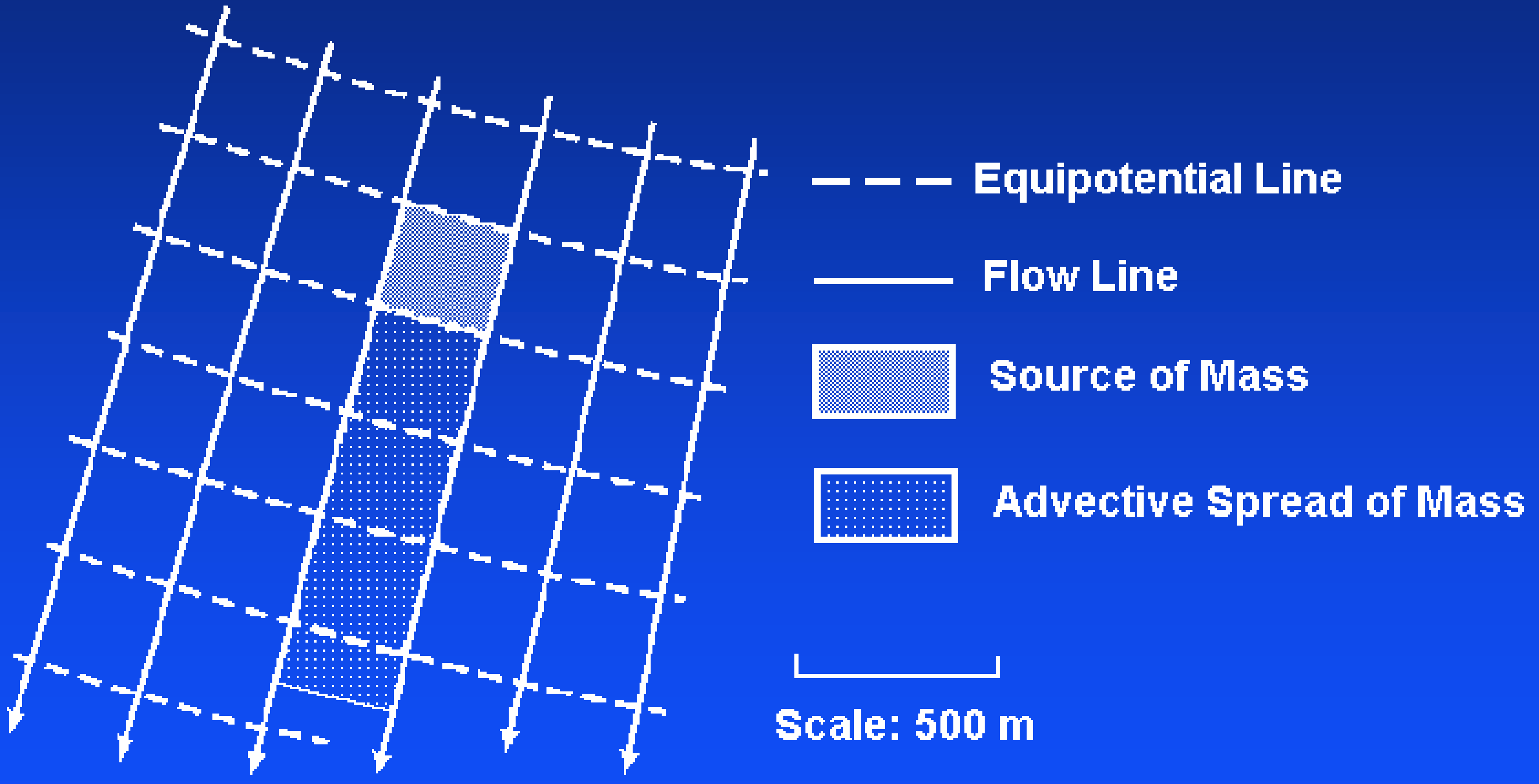
Solute Transport

Aly I. El-Kadi

Major transport/fate processes

Convection (advection)
Dispersion
Chemical reactions

Convection



Equipotential Line
Flow Line
Source of Mass
Advective Spread of Mass
Scale: 500 m

Hydrodynamic Dispersion (spreading)

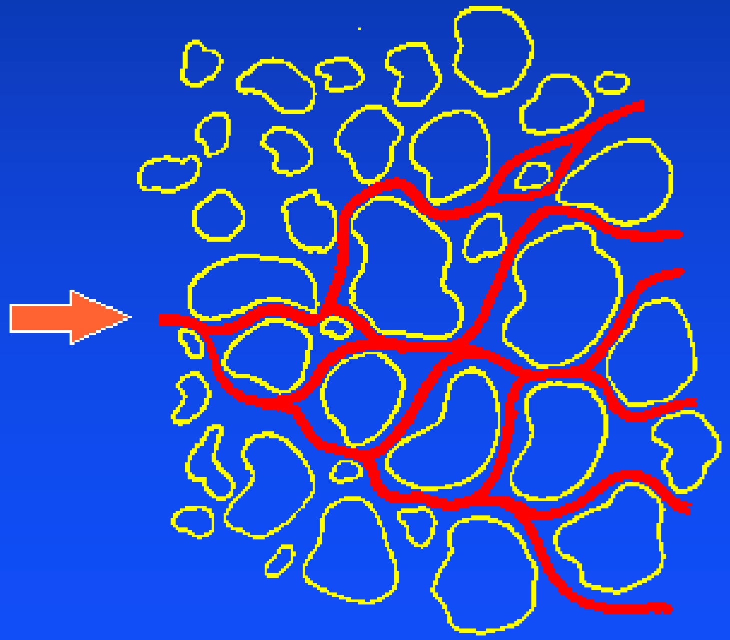
Causes solute dilution

1. mechanical mixing during advection
2. molecular diffusion due thermal – kinetic energy of solute particles

Mechanical dispersion: a microscopic process

Mechanical Dispersion

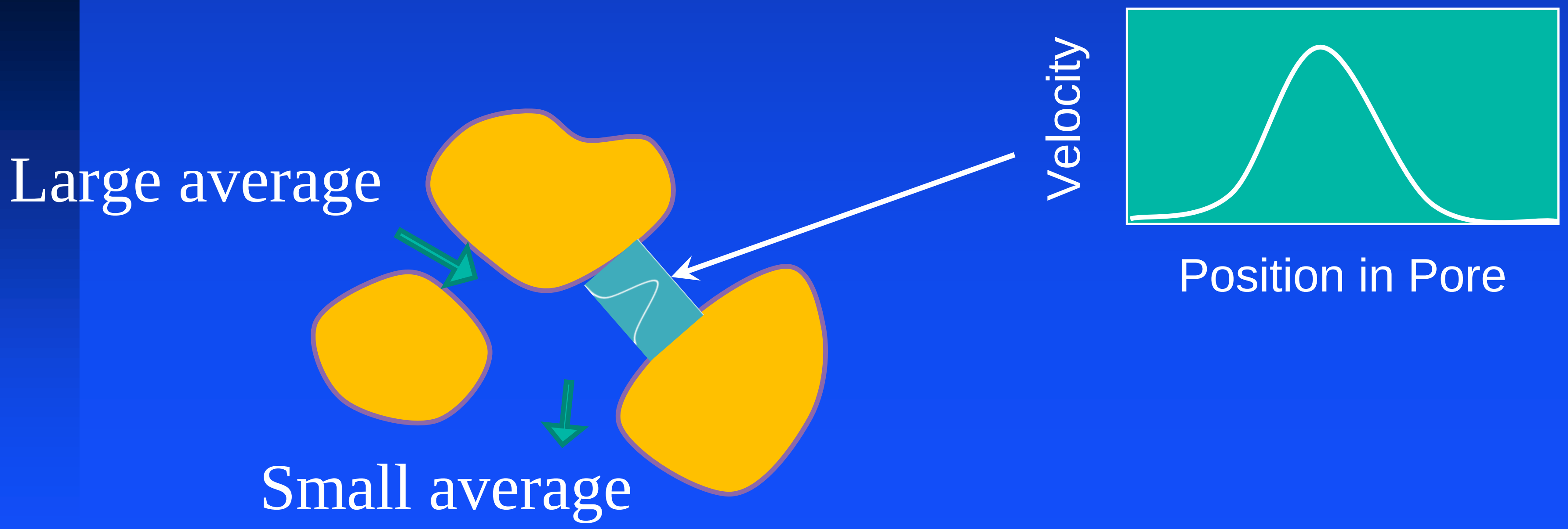
- Mechanical dispersion spreads mass within a porous medium in two ways:
  - Velocity differences within pores on a microscopic scale.
  - Path differences due to the tortuosity of the pore network.

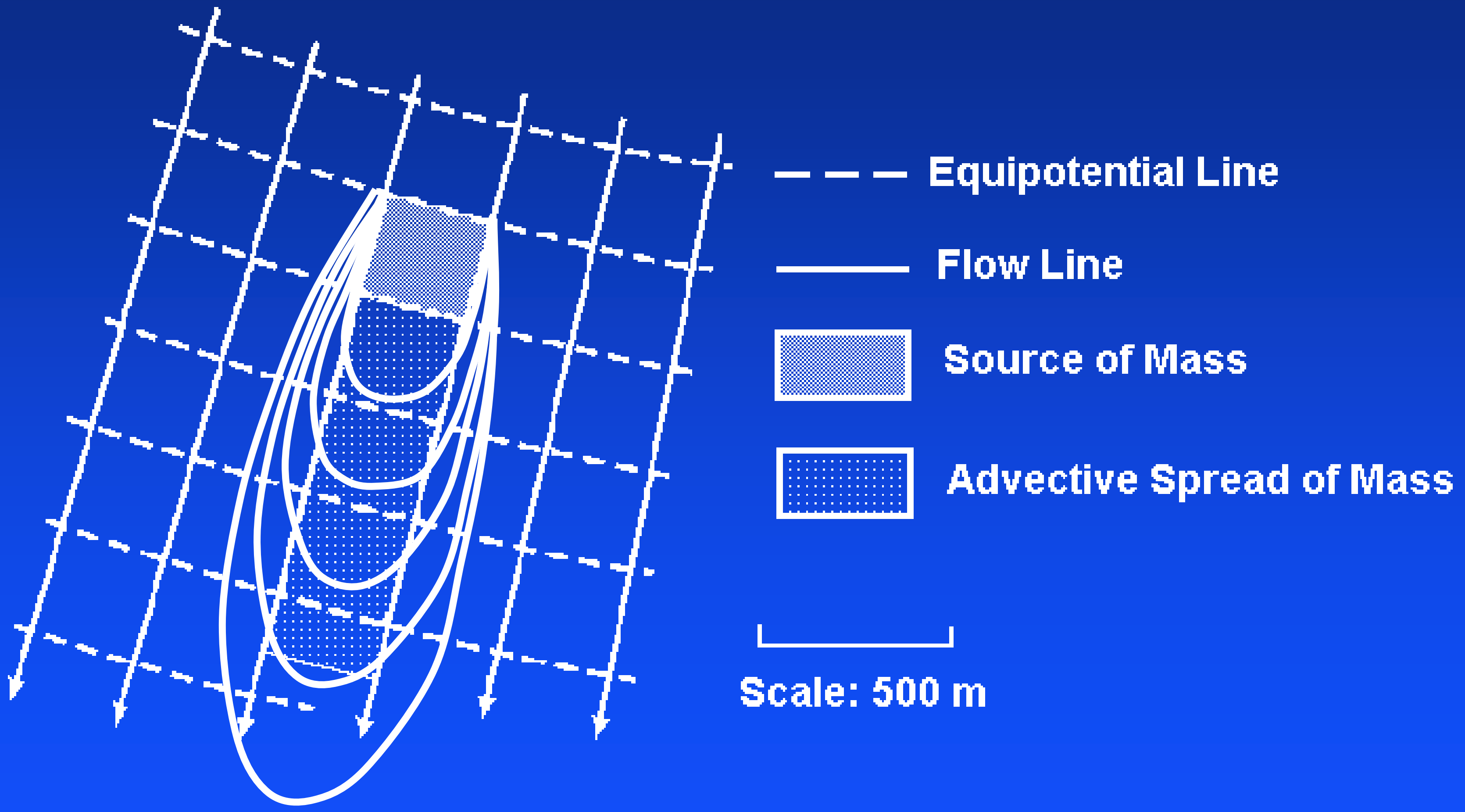


Random velocity due to

1. different velocity within same channel
2. different “average” velocity in pores

Dispersion is related to average linear velocity




Equipotential Line
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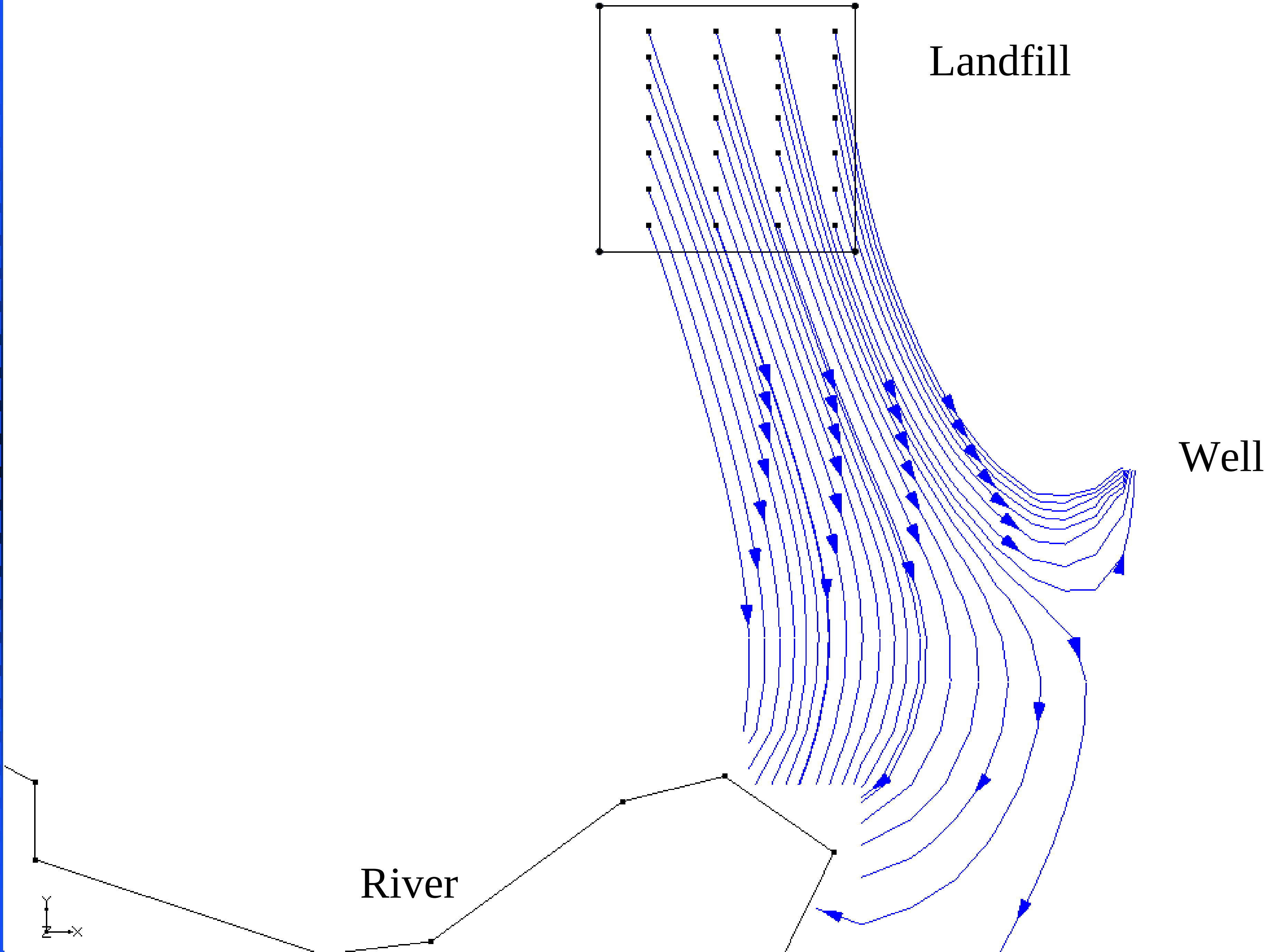
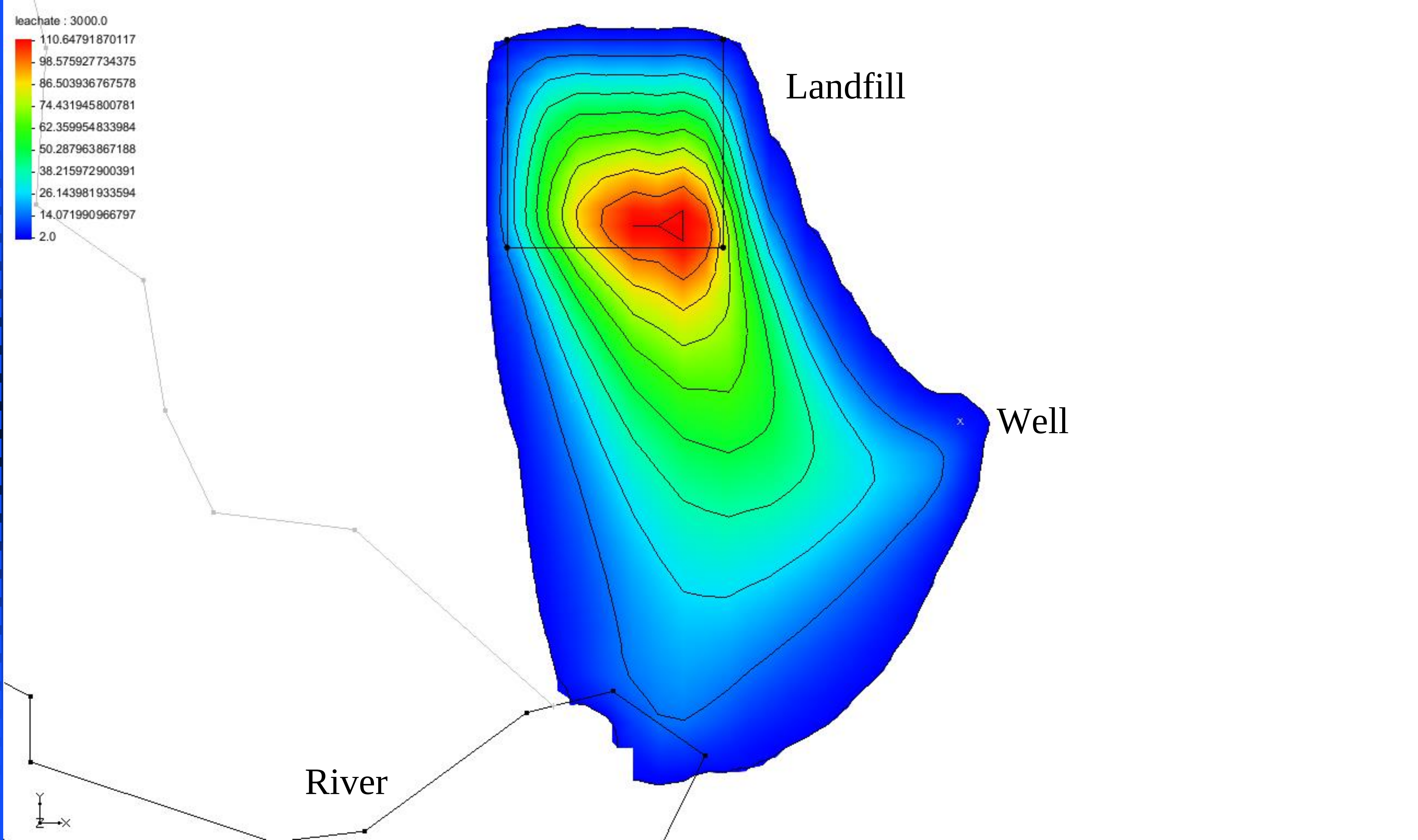

Landfill
Well
River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38.215972900391
26.143981933594
14.071990966797
2.0
Landfill
Well
River
Y
Z
X

Derivation of Equation

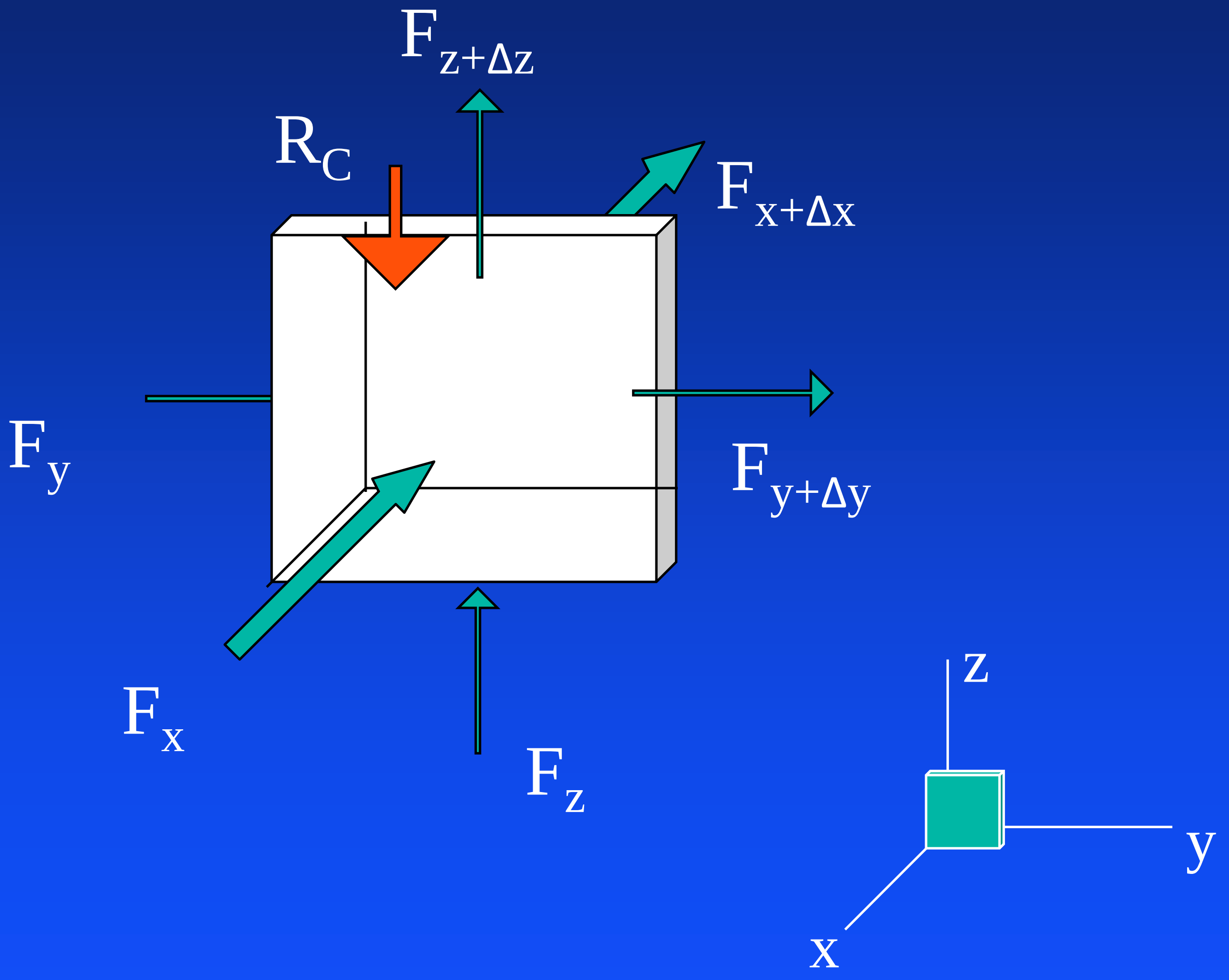
n = porosity

R_c = direct injection/discharge (M/L^3)

F = solute flux rate ($M/L^2/T$)

C = solute concentration (M/L^3)

Control volume: dimension Δx, Δy, Δz



$F_{z+\Delta z}$
R_C
$F_{x+\Delta x}$
F_y
$F_{y+\Delta y}$
F_x
F_z
z
y
x

Conservative Chemicals

$$
\left\{\begin{array}{l}
\left[F_{x+\Delta x}\Delta y\Delta z + F_{y+\Delta y}\Delta x\Delta z + F_{z+\Delta z}\Delta x\Delta y\right] - \\
\left[F_x\Delta y\Delta z + F_y\Delta x\Delta z + F_z\Delta x\Delta y + R_c\Delta x\Delta y\Delta z\right]
\end{array}\right\}\Delta t +
$$

$$
n\left[C_{t+\Delta t} - C_t\right]\Delta x\Delta y\Delta z = 0 \qquad (1)
$$

(total mass out – total mass in = mass change)

$$F_v = V_i nC \qquad (2)$$

Convection in direction i = x, y, and z

$$F_D = -nD_i \frac{\partial C}{\partial x_i} \qquad (3)$$

Dispersion in direction x_i = x, y, and z

$$F_i = V_i nC - nD_i \frac{\partial C}{\partial x_i} \qquad (4)$$

Total flux in direction x_i = x, y, and z

$$\frac{\partial F_x}{\partial x} = \lim_{\Delta x \to 0} \frac{F_{x+\Delta x} - F_x}{\Delta x}$$ (with similar expressions for y and z)

(5)

$$\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_{zz}\frac{\partial C}{\partial z}\right) - \left[\frac{\partial}{\partial x}(V_x C) + \frac{\partial}{\partial y}(V_y C) + \frac{\partial}{\partial z}(V_z C)\right] + \frac{R_c}{n} = \frac{\partial C}{\partial t}$$

(6)

$$\nabla(D \cdot \nabla C) - \nabla(VC) + \frac{R_c}{n} = \frac{\partial C}{\partial t}$$ (7)

Non-Conservative Chemicals

$$D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} - \frac{\rho_b}{n}\frac{\partial S}{\partial t} = \frac{\partial C}{\partial t} \qquad (8)$$

S = Mass adsorbed on the solids per unit mass of solids

$\frac{\partial S}{\partial t} =$ Rate at which te constituent is adsorbed

ρ_b = Bulk mass density of porous media

$\frac{\rho_b}{n}\frac{\partial S}{\partial t} =$ Change in concentration in liquid due to adsorption

Isotherm

$$S = S(C)$$

Linear isotherm

$$S = K_d C$$

$$D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} = R\frac{\partial C}{\partial t}$$

$$R = 1 + \frac{\rho K_d}{n}$$

Retardation coefficient

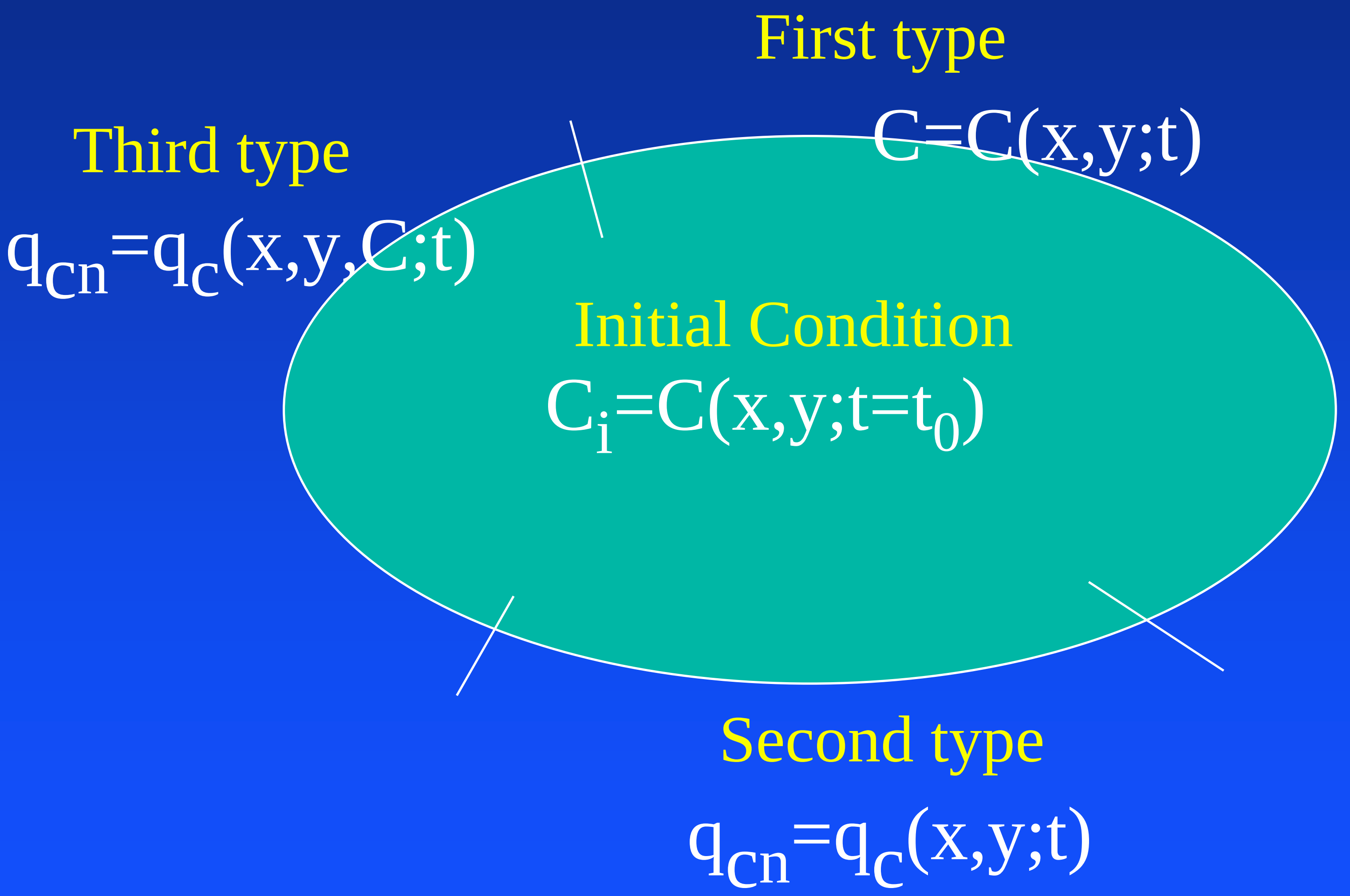
$$\frac{\partial C}{\partial t} = -\lambda C$$

Decay

General equation with adsorption and decay

$$\nabla(\nabla \cdot DC) - \nabla(VC) + \frac{R_c}{n} - \lambda C = R\frac{\partial C}{\partial t}$$

Boundary and Initial Conditions



Glossary

- Absorption - dissolving or mixing of a substance in gaseous, liquid, or solid form with groundwater.
- Adsorption - adherence of molecules in solution to the surface of solids.
- Adsorption Isotherm - the graphical representation of the relationship between the solute concentration and the mass of the solute species adsorbed on the aquifer sediment or rock.
- Advection - the process by which solutes are transported by moving groundwater. This is also called convective transport.

- Contaminant Transport Velocity - the rate in which contamination moves through an aquifer.
- Diffusion - process by which ions or molecules move in a random manner, because of their thermal kinetic energy, from areas of high solute concentrations to areas of low concentration in the direction of the solute concentration gradient. Also referred to as molecular diffusion.
- Dispersivity - a scale dependent property of an aquifer that determines the degree to which a dissolved constituent will spread in flowing groundwater. Dispersivity is comprised of three directional components - longitudinal, transverse, and vertical.

- Dispersion - process by which some of the water molecules and solute molecules travel more rapidly than the average linear velocity and some travel more slowly; spreading of the solute in the direction of the groundwater flow (longitudinal dispersion) or direction perpendicular to groundwater flow (transverse or vertical dispersion).
- Dispersion Coefficient - (1) a measure of the spreading of a flowing substance due to the nature of the porous medium, with its interconnected channels distributed at random in all directions; (2) the sum of the coefficients of mechanical dispersion and molecular diffusion in a porous medium.
- Distribution Coefficient - the quantity of the solute, chemical, or radionuclide sorbed by the solid per unit weight of solid divided by the quantity dissolved in the water per unit volume of water.

- Flow Path - the subsurface course a water molecule or solute would follow in a given groundwater velocity field.
- Porosity, Total - the ratio of the volume of void spaces in a rock or sediment to the total volume of the rock or sediment.
- Porosity, Effective - (1) the ratio, usually expressed as a percentage of the total volume of voids available for field transmission to the total volume of the porous medium; (2) the ratio of the volume of the voids of a soil or rock mass that can be drained by gravity to the total volume of the mass; (3) the amount of interconnected pore space and fracture openings available for the transmission of fluids, expressed as the ratio of the volume of interconnected pores and openings to the volume of rock.

- Retardation Factor - used to simulate the resistance of the contamination to move through the groundwater aquifer. A factor of one (1) represents the no resistance while increasing values show increasing resistance.
- Source of Contaminants - the physical location (and spatial extent) of the source contaminating the aquifer; in order to model fate and transport of a contaminant, the characteristics of the contaminant source must be know or assumed.