Groundwater Contamination

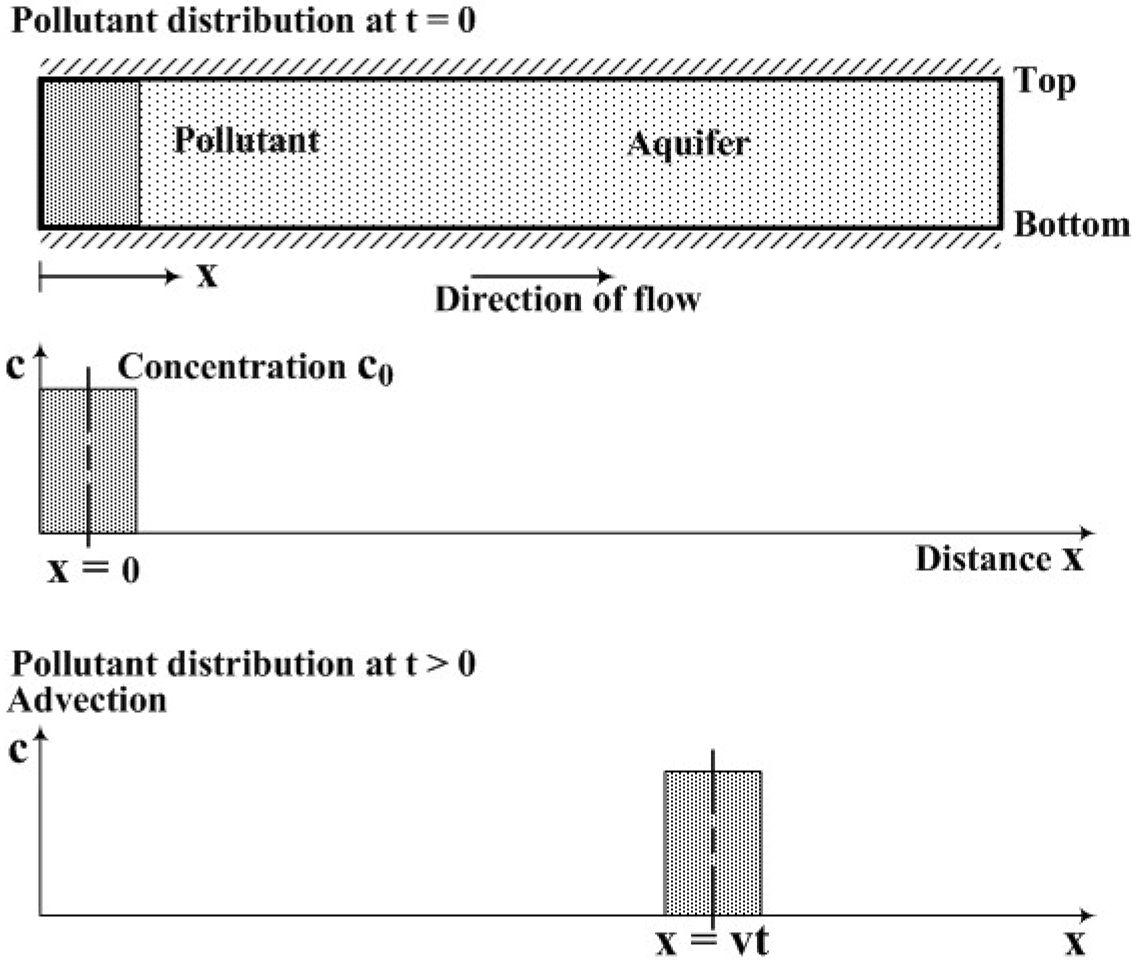
Geohydraulics| CE60113

Lecture:20

Learning Objective(s)

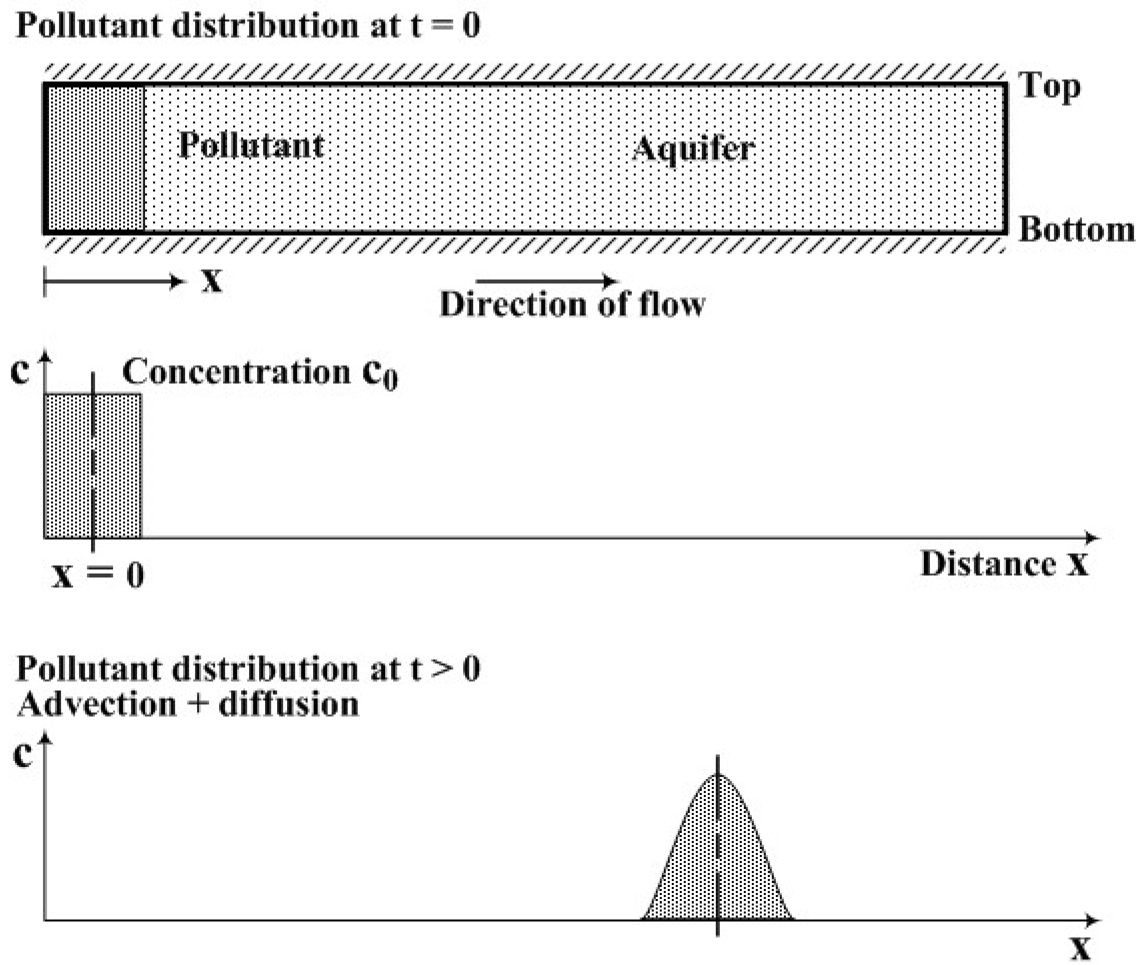
- **To conceptualize flow and transport processes**

Groundwater Contamination



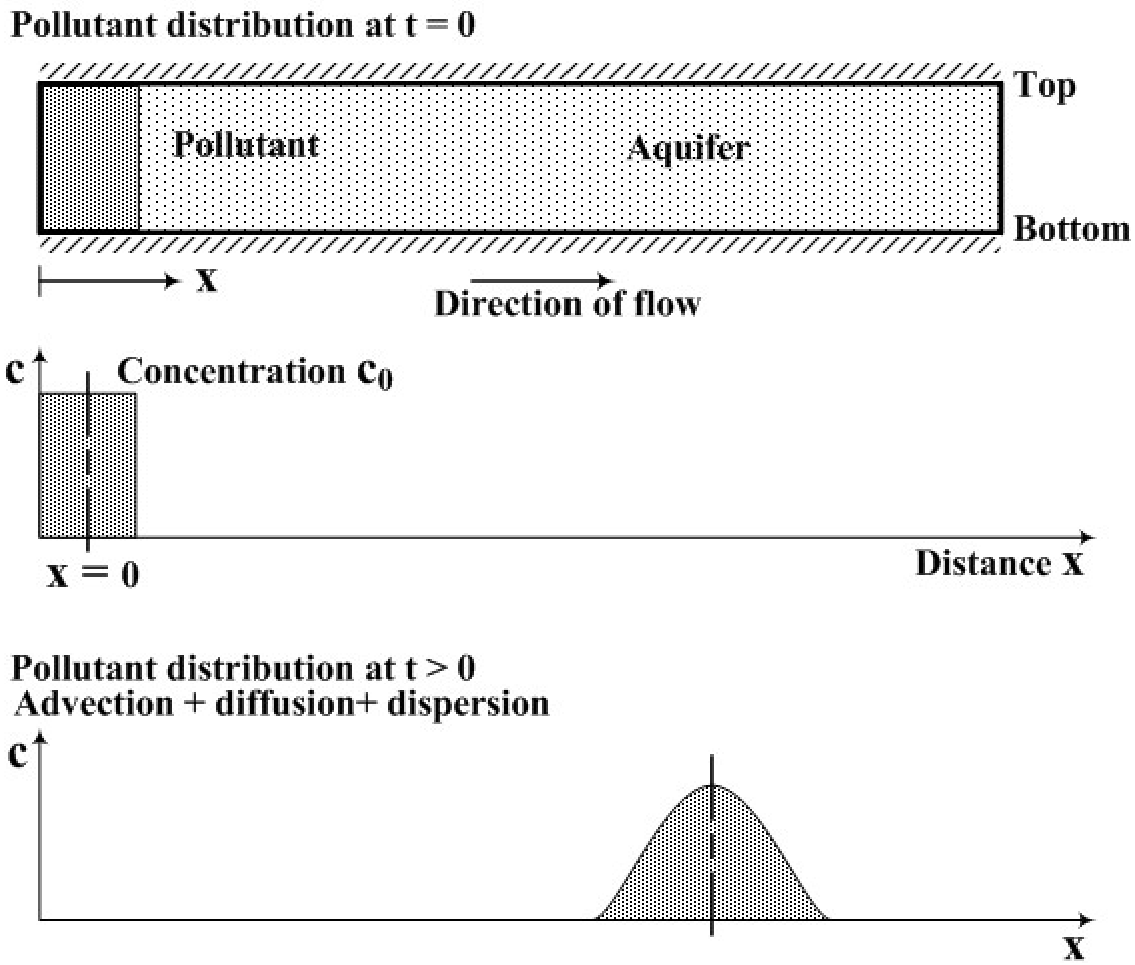
Advection: movement of solutes that are carried along with the flowing groundwater

Groundwater Contamination (Contd.)



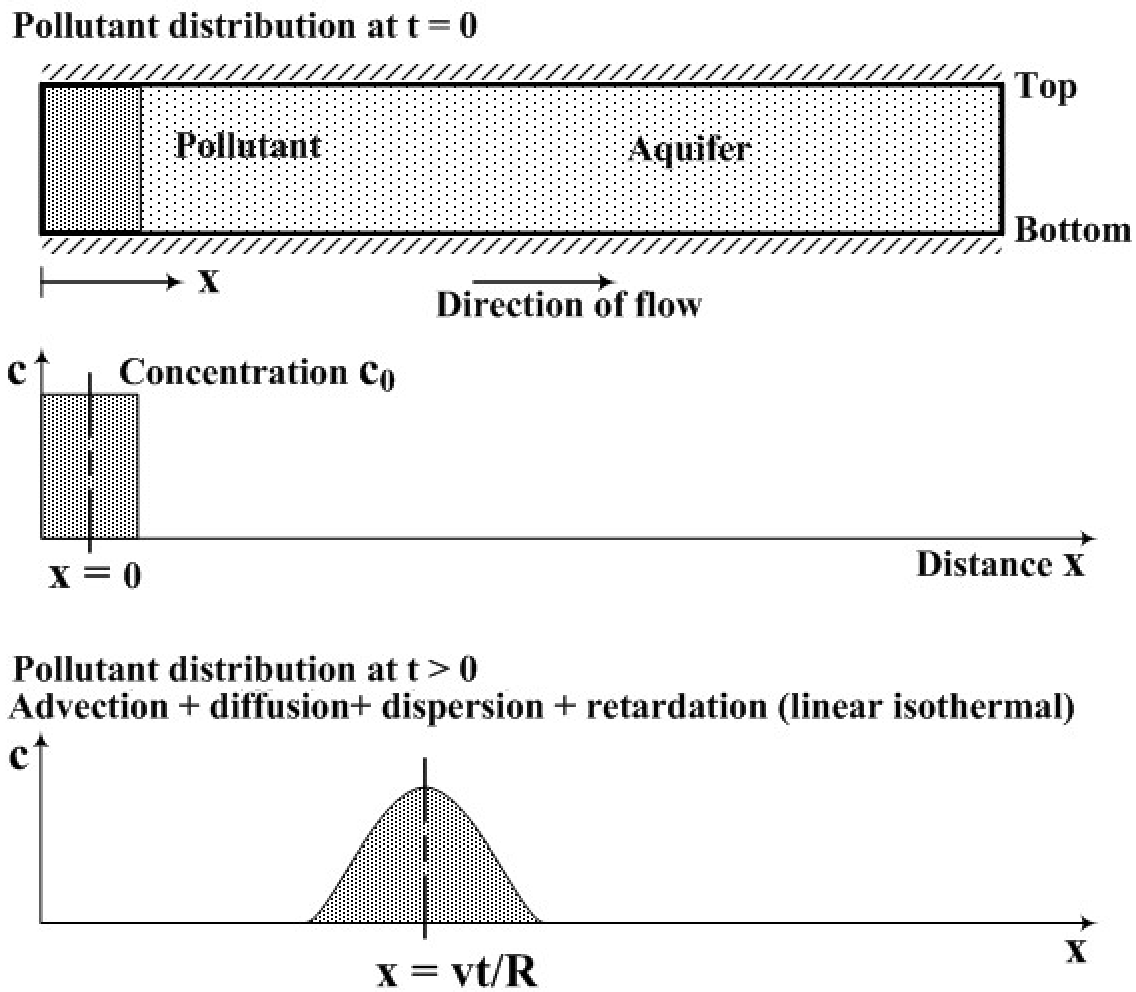
Diffusion: molecular process where constituents are spread due to differences in concentrations,

Groundwater Contamination (Contd.)



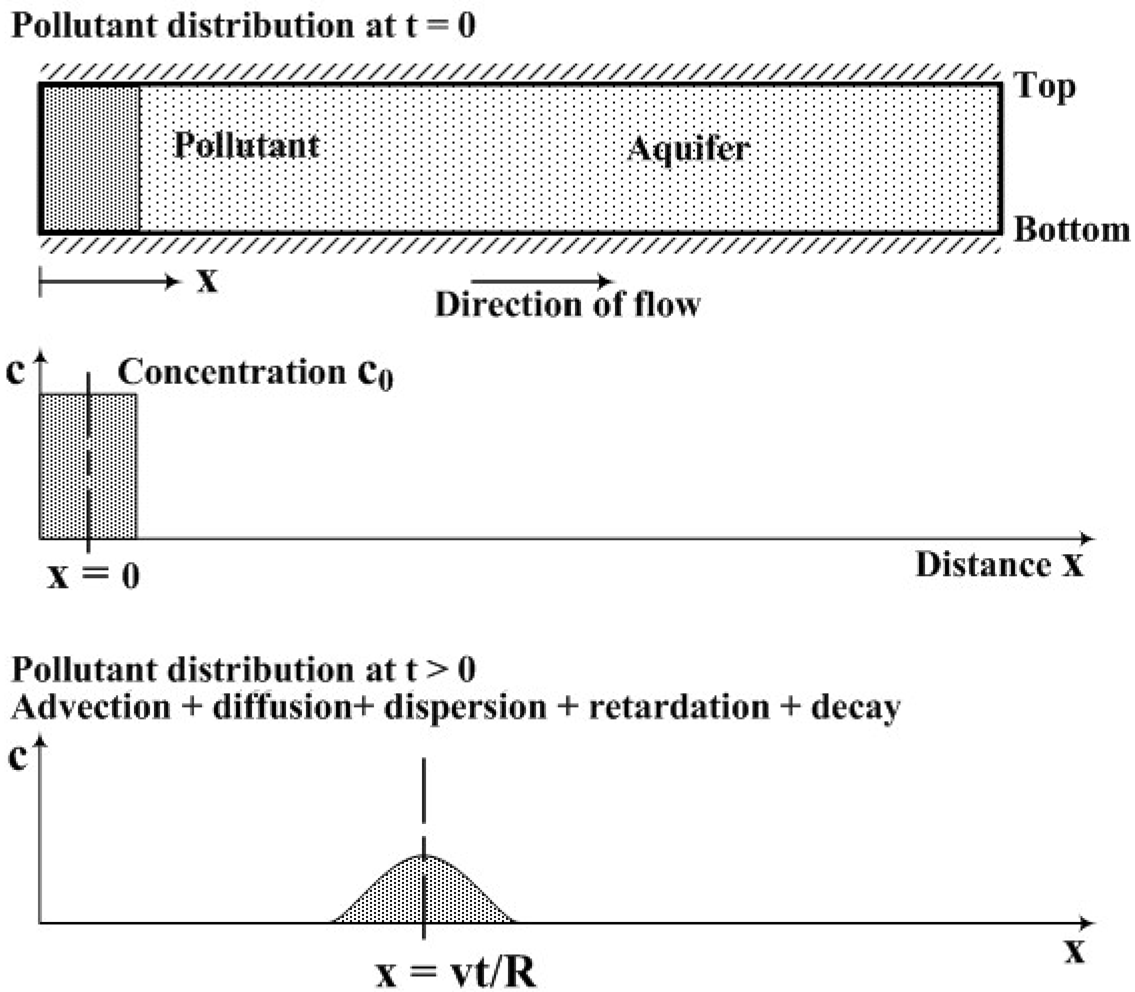
Dispersion: mixing process caused by differences in velocity (in magnitude and in direction) of water particles,

Groundwater Contamination (Contd.)



Adsorption: process where certain constituents are attached to grain material

Groundwater Contamination (Contd.)



Decay: change in concentration by biologic or radioactive decline

Groundwater Contamination (Contd.)

- Advection
  - For saturated condition

$$F_{Ax} = q_x C = \eta v_x C$$
$$F_{Ay} = q_y C = \eta v_y C$$
$$F_{Az} = q_z C = \eta v_z C$$

  - For unsaturated condition

$$F_{Ax} = q_x C = \theta v_x C$$
$$F_{Ay} = q_y C = \theta v_y C$$
$$F_{Az} = q_z C = \theta v_z C$$

- Advection mass flux vector

$$\overrightarrow{\mathbf{F}_A} = \vec{\mathbf{q}} C$$

Groundwater Contamination (Contd.)

- Molecular Diffusion: Diffusion is a net transport of molecules from a region of higher concentration to one of lower concentration by random molecular motion. Under steady-state conditions, Fick's first law describes the flux of a solute as:

$$F_{Diffx} = -\eta D^* \frac{\partial C}{\partial x} = -\eta \tau D_m \frac{\partial C}{\partial x}$$
$$F_{Diffy} = -\eta D^* \frac{\partial C}{\partial y} = -\eta \tau D_m \frac{\partial C}{\partial y}$$
$$F_{Dif} \quad = -\eta D^* \frac{\partial C}{\partial z} = -\eta \tau D_m \frac{\partial C}{\partial z}$$

D^*-> Effective molecular diffusion coefficient

D_m->Molecular diffusion coefficient in open water

τ-> Tortuosity of the porous medium (<1), Range 0.01-0.5

- Diffusive mass flux vector

$$\overrightarrow{\mathbf{F}_{Diff}} = -\eta D^* \nabla C$$

Or

$$\overrightarrow{\mathbf{F}_{Diff}} = -\theta D^* \nabla C$$

Groundwater Contamination (Contd.)

- Dispersion or Mechanical Dispersion

$$F_{Dis} = -\eta D_{xx}\frac{\partial C}{\partial x} - \eta D_{xy}\frac{\partial C}{\partial y} - \eta D_{xz}\frac{\partial C}{\partial z}$$
$$F_{Dispy} = -\eta D_{yx}\frac{\partial C}{\partial x} - \eta D_{yy}\frac{\partial C}{\partial y} - \eta D_{yz}\frac{\partial C}{\partial z}$$
$$F_{Disp} = -\eta D_{zx}\frac{\partial C}{\partial x} - \eta D_{zy}\frac{\partial C}{\partial y} - \eta D_{zz}\frac{\partial C}{\partial z}$$

- Physical mechanisms responsible for "Mechanical Dispersion"
  - The particles nearest the walls of the pore channel move more slowly than those near the channel center
  - The variations of pore dimensions along the pore axes cause the particles to move at different relative speeds
  - Adjacent particles in one channel can follow different streamlines that lead to different channels. These particles may later come together in another channel or they may continue to move farther apart.
  - Solute molecules move at different speeds (even when the hydraulic gradient is uniform) due to heterogeneous hydraulic conductivity field.

Groundwater Contamination (Contd.)

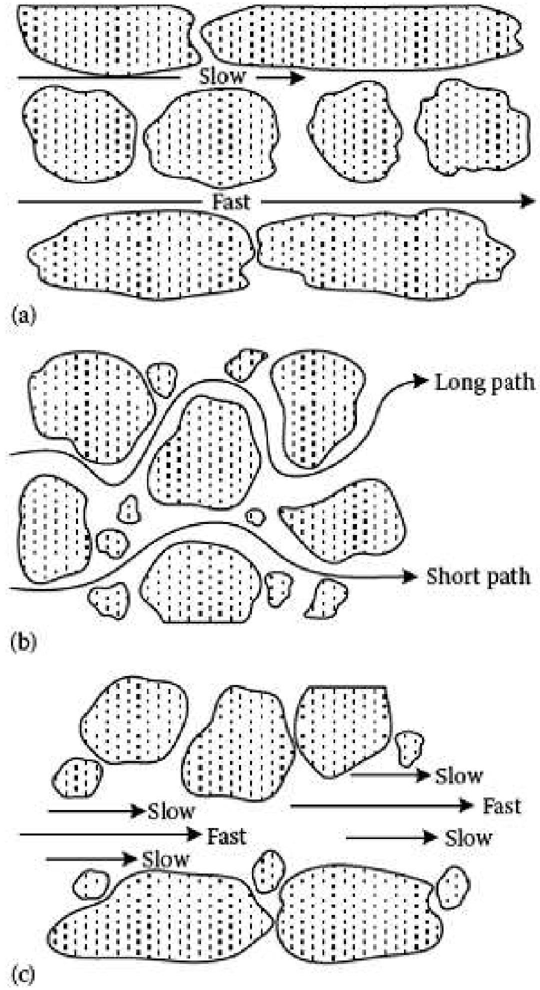


FIGURE 5.7 Main factors that cause longitudinal dispersion in subsurface area. (a) Larger pores let fluid move faster, (b) travel time through longer paths is more than shorter ones, and (c) fluid moves faster through the center of the pore.

Groundwater Contamination (Contd.)

- Longitudinal dispersion occurs based on the following reasons:
  - Fluid moves faster through the center of the pore than along the edges.
  - Some portions of the fluid travel in longer pathways than other portions.
  - The movement of fluid through larger pores travels faster than that in smaller pores.
  - Heterogeneity of the aquifer causes the groundwater to move faster in some layers and slower in some others.

Groundwater Contamination (Contd.)

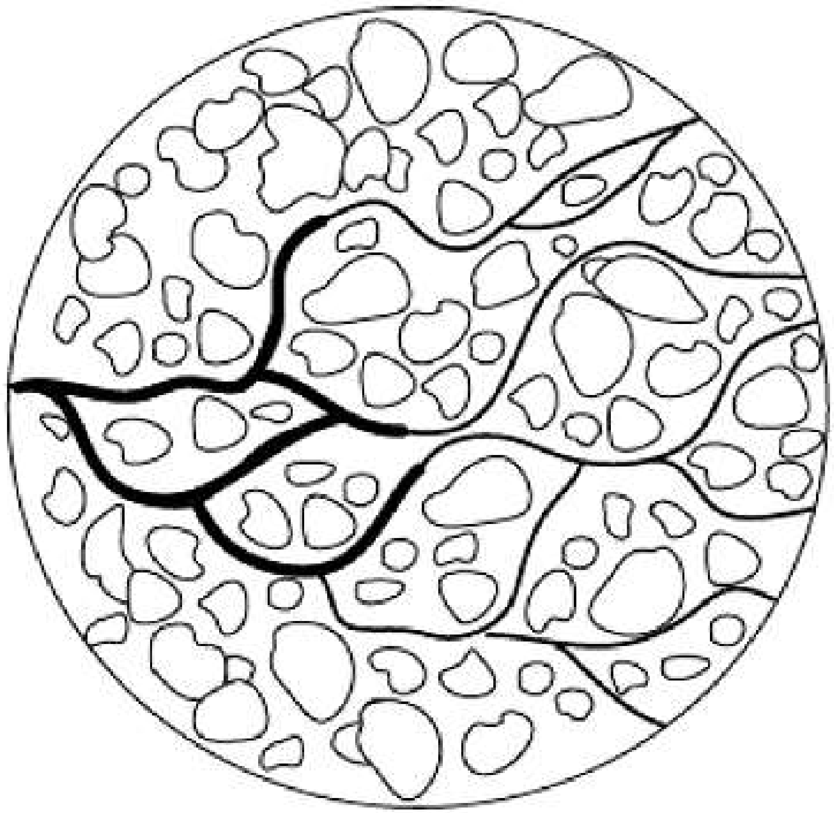


FIGURE 5.8 Flow paths in the porous medium causing transverse dispersion.

Groundwater Contamination (Contd.)

- Dispersive mass flux vector

$$\overrightarrow{\mathbf{F}_{\boldsymbol{Disp}}} = -\eta \mathbf{D}\, \boldsymbol{\nabla} C$$

Or

$$\overrightarrow{\mathbf{F}_{\boldsymbol{Disp}}} = -\theta \mathbf{D}\, \boldsymbol{\nabla} C$$

$$D_{xx} = \alpha_L \frac{v_x^2}{|\mathbf{v}|} + \alpha_{TH} \frac{v_y^2}{|\mathbf{v}|} + \alpha_{TV} \frac{v_z^2}{|\mathbf{v}|} + D^*$$

$$D_{yy} = \alpha_L \frac{v_y^2}{|\mathbf{v}|} + \alpha_{TV} \frac{v_z^2}{|\mathbf{v}|} + \alpha_{TH} \frac{v_x^2}{|\mathbf{v}|} + D^*$$

$$D_{zz} = \alpha_L \frac{v_z^2}{|\mathbf{v}|} + \alpha_{TV} \frac{v_x^2}{|\mathbf{v}|} + \alpha_{TV} \frac{v_y^2}{|\mathbf{v}|} + D^*$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_{TH}) \frac{v_x v_y}{|\mathbf{v}|}$$

$$D_{xz} = D_{zx} = (\alpha_L - \alpha_{TV}) \frac{v_x v_z}{|\mathbf{v}|}$$

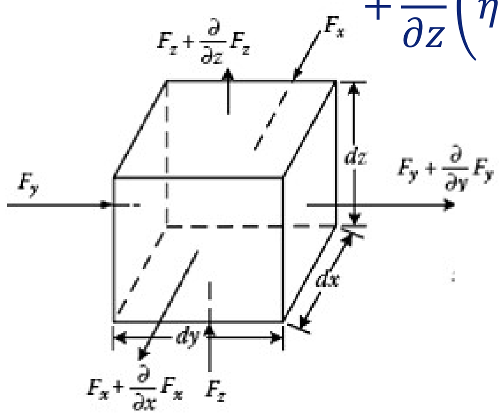
$$D_{yz} = D_{zy} = (\alpha_L - \alpha_{TV}) \frac{v_y v_z}{|\mathbf{v}|}$$

- Longitudinal and transverse dispersivities (unit of length)

Groundwater Contamination (Contd.)

$$\left(F_x + \frac{\partial F_x}{\partial x}\Delta x\right)\Delta z\Delta y - F_x\Delta z\Delta y + \left(F_y + \frac{\partial F_y}{\partial y}\Delta y\right)\Delta z\Delta x - F_y\Delta z\Delta x$$
$$+\left(F_z + \frac{\partial F_z}{\partial z}\Delta z\right)\Delta x\Delta y - F_z\Delta x\Delta y = -\frac{\partial(\eta C)}{\partial t}\Delta x\Delta y\Delta z$$

$$\frac{\partial}{\partial t}(\eta C) = \frac{\partial}{\partial x}\left(\eta D_{xx}\frac{\partial C}{\partial x} + \eta D_{xy}\frac{\partial C}{\partial y} + \eta D_{xz}\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial x}(q_x C)$$
$$+\frac{\partial}{\partial y}\left(\eta D_{yx}\frac{\partial C}{\partial x} + \eta D_{yy}\frac{\partial C}{\partial y} + \eta D_{yz}\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial y}(q_y C)$$
$$+\frac{\partial}{\partial z}\left(\eta D_{zx}\frac{\partial C}{\partial x} + \eta D_{zy}\frac{\partial C}{\partial y} + \eta D_{zz}\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial z}(q_z C) + q_s C_s + \sum_{n=1}^{N} R_n$$



Groundwater Contamination (Contd.)

- Sorption: adsorption and absorption

- *Freundlich Isotherm* can be described by

$$\bar{C} = K_f C^a = K_d C$$

- Slope of the isotherm

$$\frac{\partial \bar{C}}{\partial C} = K_f a C^{a-1} = K_d$$

Sorbed concentration must be changing at a rate $\frac{\partial \bar{C}}{\partial t}$,

$$\frac{\partial \bar{C}}{\partial t} = \frac{\partial \bar{C}}{\partial C}\frac{\partial C}{\partial t} = K_d \frac{\partial C}{\partial t}$$

Chemical source/sink term

$$\sum_{n=1}^{N} R_n = -\rho_b \frac{\partial \bar{C}}{\partial t}$$

Groundwater Contamination (Contd.)

- Decay: Chemical reaction

$$A \rightarrow B$$

reactant A is transformed into product B

$$-\frac{\partial C_A}{\partial t} = \frac{\partial C_B}{\partial t} = \lambda C_A$$

both of which equal the concentration of A multiplied by the proportionality constant

Under first order, irreversible condition (biodegradation, radioactive decay)

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

Chemical source/sink term

$$\sum_{n=1}^{N} R_n = -\lambda \eta C$$

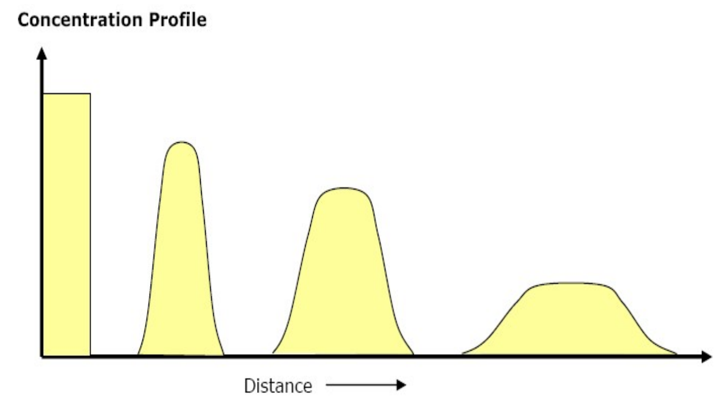
Groundwater Contamination (Contd.)

$$\frac{\partial}{\partial t}(\eta C) = \frac{\partial}{\partial x}\left(\eta D_{xx}\frac{\partial C}{\partial x} + \eta D_{xy}\frac{\partial C}{\partial y} + \eta D_{xz}\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial x}(q_x C)$$
$$+ \frac{\partial}{\partial y}\left(\eta D_{yx}\frac{\partial C}{\partial x} + \eta D_{yy}\frac{\partial C}{\partial y} + \eta D_{yz}\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial y}(q_y C)$$
$$+ \frac{\partial}{\partial z}\left(\eta D_{zx}\frac{\partial C}{\partial x} + \eta D_{zy}\frac{\partial C}{\partial y} + \eta D_{zz}\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial z}(q_z C) + q_s C_s - \rho_b K_d \frac{\partial C}{\partial t} - \lambda \eta C$$

$$\eta R \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(\eta D_{xx}\frac{\partial C}{\partial x} + \eta D_{xy}\frac{\partial C}{\partial y} + \eta D_{xz}\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial x}(q_x C)$$
$$+ \frac{\partial}{\partial y}\left(\eta D_{yx}\frac{\partial C}{\partial x} + \eta D_{yy}\frac{\partial C}{\partial y} + \eta D_{yz}\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial y}(q_y C)$$
$$+ \frac{\partial}{\partial z}\left(\eta D_{zx}\frac{\partial C}{\partial x} + \eta D_{zy}\frac{\partial C}{\partial y} + \eta D_{zz}\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial z}(q_z C) + q_s C_s - \lambda \eta C$$
$$R = 1 + \frac{\rho_b}{\eta} K_d$$

R-> Retardation factor

Groundwater Contamination (Contd.)



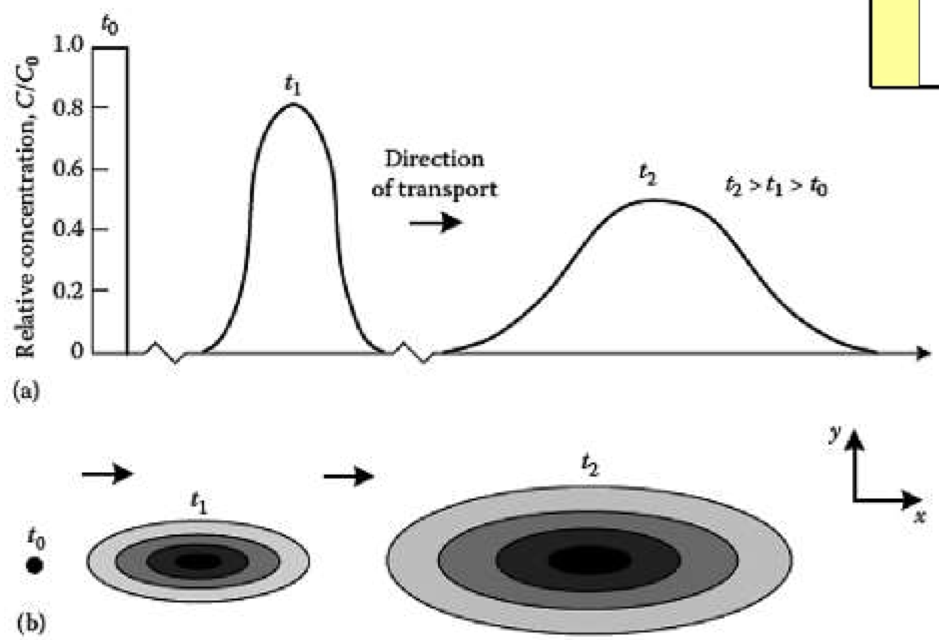


FIGURE 5.6 An instantaneous (pulse) source in a flow field creates a plume that spreads as it moves down-gradient: (a) in 1D and (b) in 2Ds (darker colors mean higher concentrations). (From Bedient, P.B. et al., *Ground Water Contamination: Transport and Remediation*, Prentice-Hall Publishing, Englewood Cliffs, NJ, 560, 1994.)

Groundwater Contamination (Contd.)

- General continuity: The pore space is filled by the sum of the fluids

$$\eta = \theta_w + \theta_a + \theta_o$$

- The constituent mass density or bulk concentration, m (mass of constituent per bulk volume), can be represented as

$$m = \theta_w c_w + \theta_a c_a + \theta_o c_o + \theta_b c_s$$

- Continuity Equation can be written as

$$\frac{\partial m}{\partial t} + \nabla \cdot \vec{\mathbf{F}} = S^+$$

Groundwater Contamination (Contd.)

- Ogata and Banks (1961) analytical solution: It solves the ADE equation for a *Continuous Source of Infinite Duration* and a 1D domain:

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

with the following boundary and initial conditions:

$$C(0,t) = C_0; t \geq 0$$
$$C(\infty,t) = 0; t \geq 0$$
$$C(x,0) = 0; x \geq 0$$

where C is the concentration [ML^{-3}], x is the distance [L], R is the retardation factor [−], D is the effective dispersion/diffusion [L^2T^{-1}], v is the flow velocity [LT^{-1}] and C_0 is the concentration at the upstream boundary [ML^{-3}].

- The analytical solution is

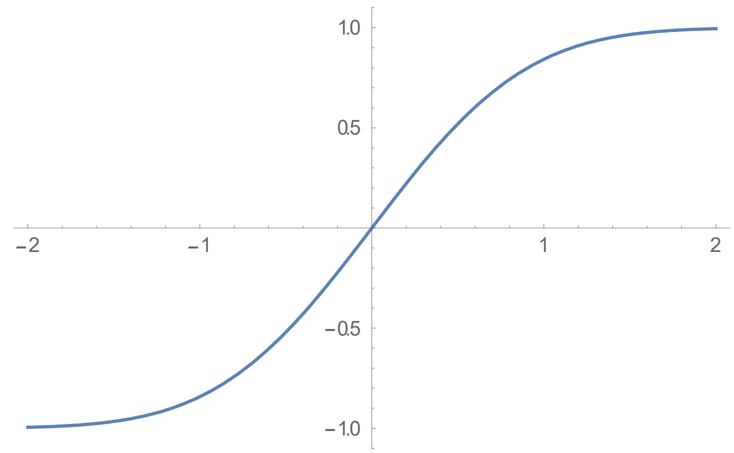
$$C(x,t) = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x - vt/R}{2\sqrt{Dt/R}}\right) + \exp\left(\frac{vx}{D}\right)\operatorname{erfc}\left(\frac{x + vt/R}{2\sqrt{Dt/R}}\right)\right]$$

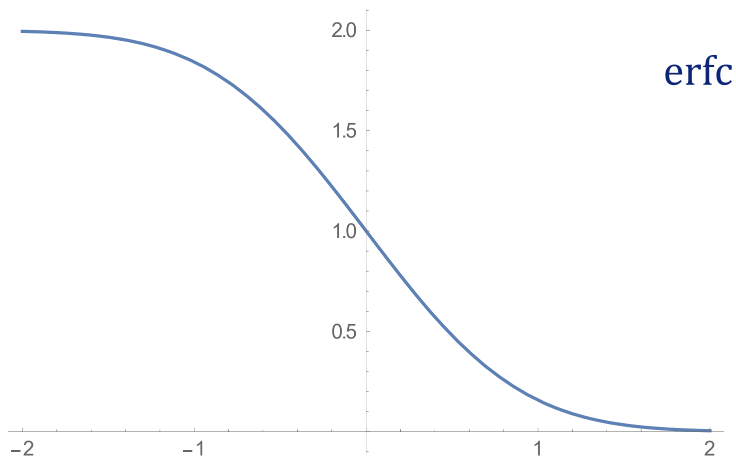
$$\operatorname{erf}(\varphi) = \frac{2}{\sqrt{\pi}}\int_0^{\varphi} e^{-\omega^2}\,d\omega$$

$$\operatorname{erfc}(\varphi) = 1 - \operatorname{erf}(\varphi)$$

Groundwater Contamination (Contd.)

$$\mathrm{erf}(\varphi) = \frac{2}{\sqrt{\pi}} \int_0^{\varphi} e^{-\omega^2} d\omega$$





$$\mathrm{erfc}(\varphi) = 1 - \mathrm{erf}(\varphi)$$

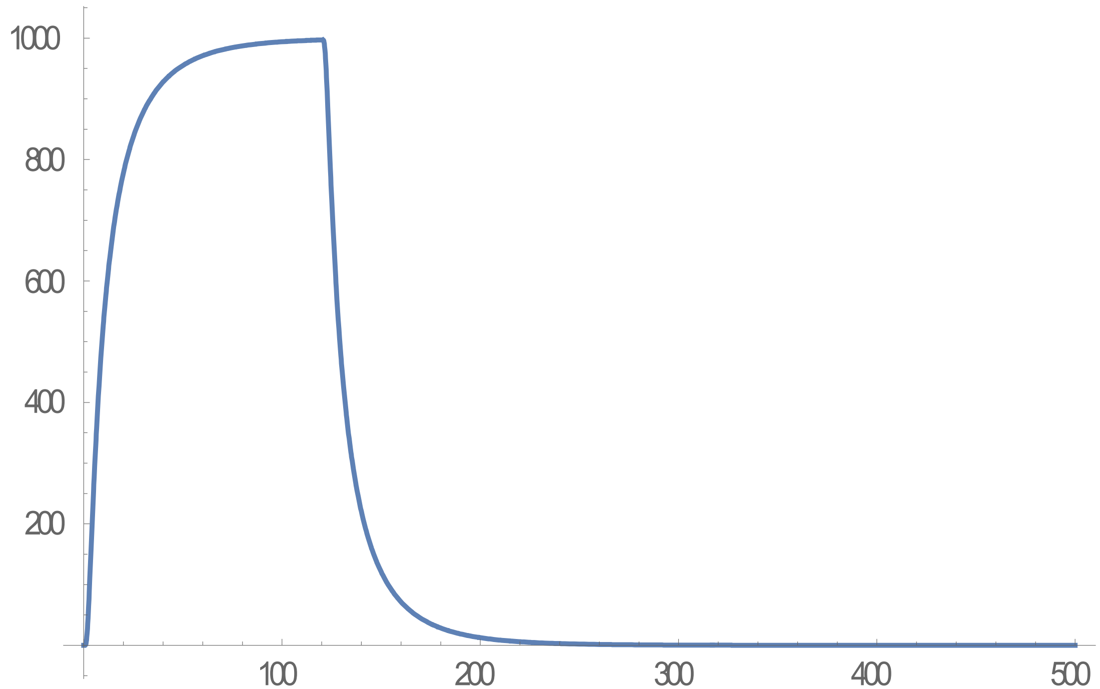
Groundwater Contamination (Contd.)

- If the source is active for time $t = T_0$

$$C(x,t) = \begin{cases} \dfrac{C_0}{2}\left[\operatorname{erfc}\left(\dfrac{x - vt/R}{2\sqrt{Dt/R}}\right) + \exp\left(\dfrac{vx}{D}\right)\operatorname{erfc}\left(\dfrac{x + vt/R}{2\sqrt{Dt/R}}\right)\right] & t \le T_0 \\ \dfrac{C_0}{2}\left[\operatorname{erfc}\left(\dfrac{x - vt/R}{2\sqrt{Dt/R}}\right) + \exp\left(\dfrac{vx}{D}\right)\operatorname{erfc}\left(\dfrac{x + vt/R}{2\sqrt{Dt/R}}\right)\right] - & \\ \dfrac{C_0}{2}\left[\operatorname{erfc}\left(\dfrac{x - v(t-T_0)/R}{2\sqrt{D(t-T_0)/R}}\right) + \exp\left(\dfrac{vx}{D}\right)\operatorname{erfc}\left(\dfrac{x + v(t-T_0)/R}{2\sqrt{D(t-T_0)/R}}\right)\right] & t > T_0 \end{cases}$$

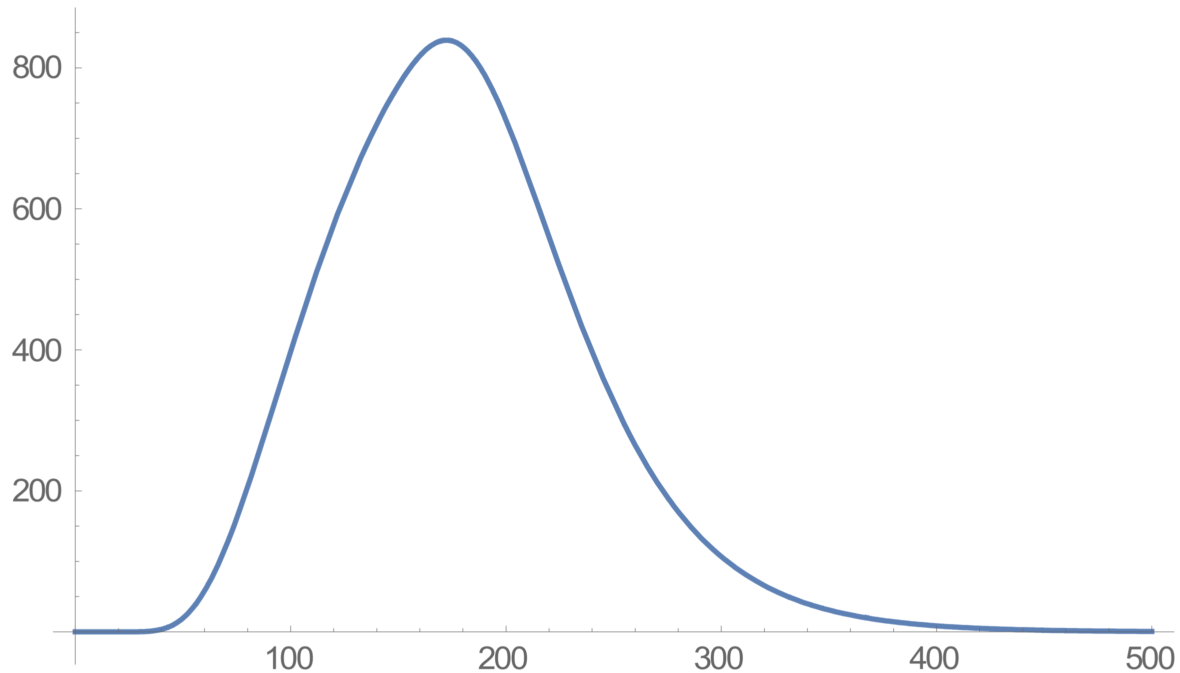
Groundwater Contamination (Contd.)

- **Given v=0.1 m/day, D=0.1 m²/day, C_0 =1000 mg/l, T_0 =120 days**
- For $x = 1.5\ m,\ t = 500\ day$



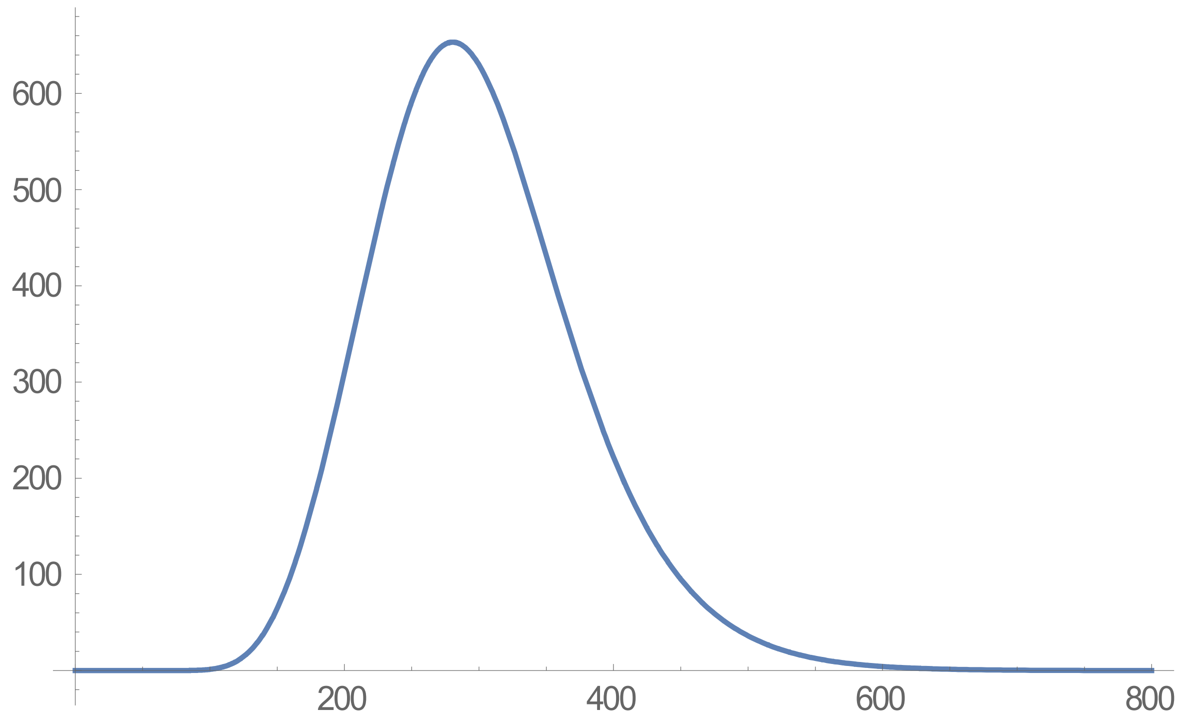
Groundwater Contamination (Contd.)

- **Given v=0.1 m/day, D=0.1 m²/day, C_0 =1000 mg/l, T_0 =120 days**
- For $x = 12\, m,\ t = 500\, day$



Groundwater Contamination (Contd.)

- **Given v=0.1 m/day, D=0.1 m²/day, C_0 =1000 mg/l, T_0 =120 days**
- For $x = 24\ m,\ t = 800\ day$



Groundwater Contamination (Contd.)

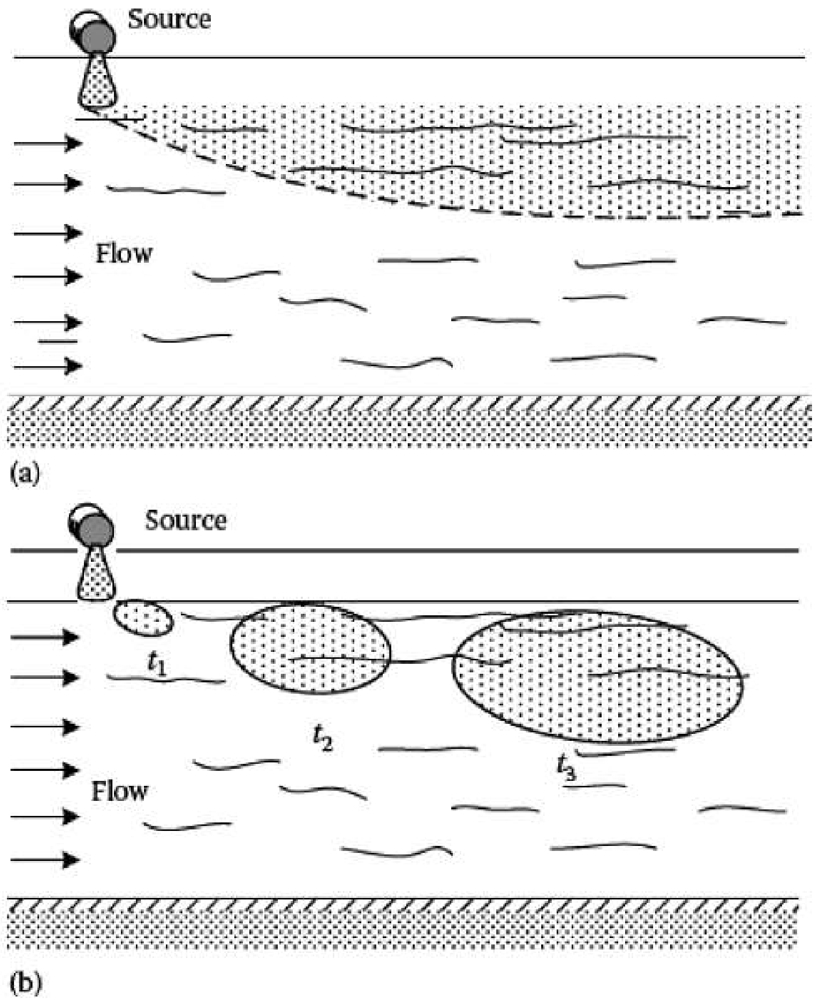
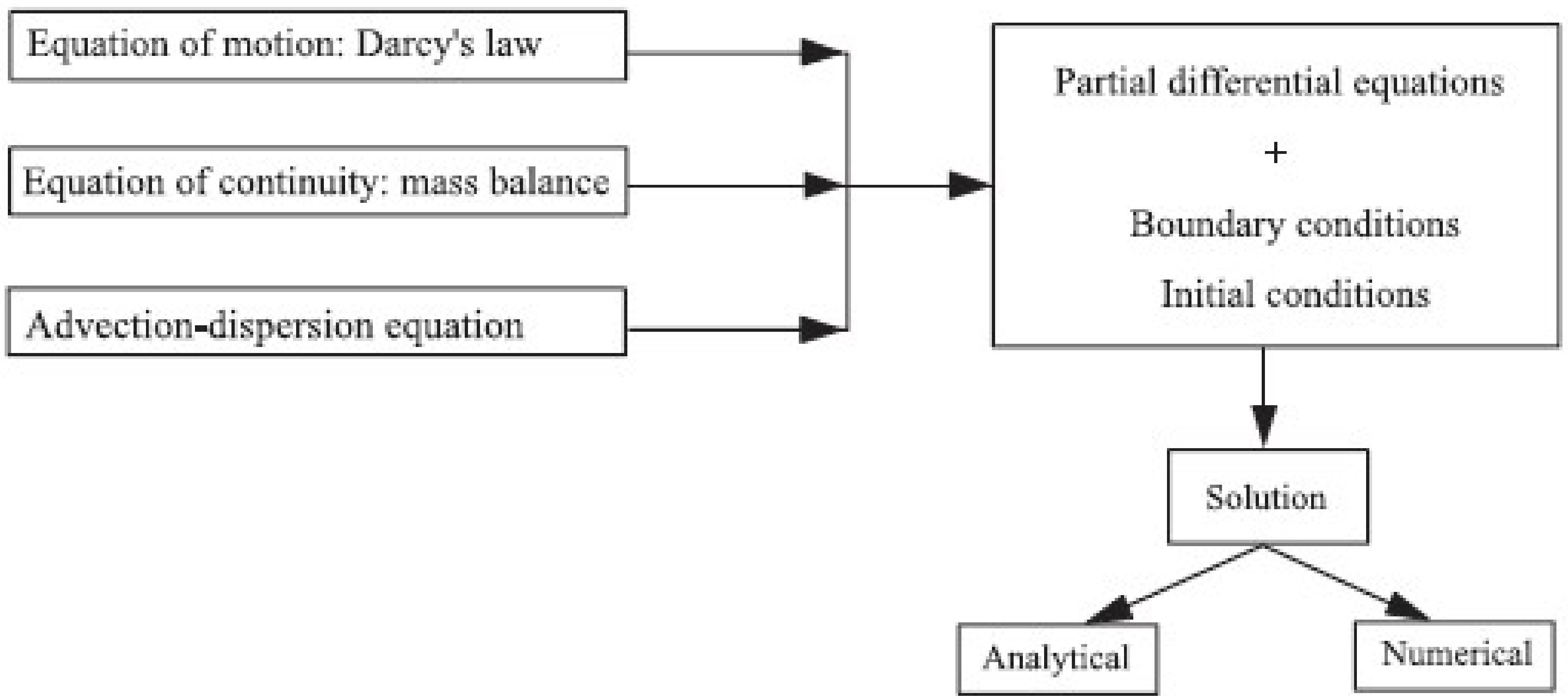


FIGURE 5.10 (a) Continuous release (leaching). (b) Instantaneous injection (spill) of contaminant from a point source into an aquifer with isotropic sand in a 2D uniform field.

Basic Framework



Thank you