CONTAMINANT TRANSPORT

MECHANICAL ASPECTS

ADVECTION

\[ v = \frac{Kdh}{\phi e dl} = \text{average linear velocity} \]

DISPERSION/DIFFUSION
due to variable advection
that occurs in the transition zone between
two domains of the fluid with different compositions
(diffusion is caused by chemical gradients)

Later we will look at some fundamental
Some NONMECHANICAL ASPECTS: Decay & Sorption

In the direction of flow we consider

LONGITUDINAL DISPERSION:

Velocity variation within pores:
Velocity variation between pores:
Variation of flow path lengths

TRANSVERSE DISPERSION (normal to the flow path):

Splitting of flow paths
These physical mixing processes are combined and referred to as "Mechanical Dispersion"

Mechanical dispersion is related to average pore velocity by dispersivity ($\alpha$)

$$Mechanical\ Dispersion = D = \alpha \bar{v}$$

- dispersivity ($\alpha$)
- units of length
- increases with increased heterogeneity and thus with travel distance

**Diffusion:**
Movement of dissolved species from areas of high concentration to low concentration

**Fick's Law:**

$$Flux = F = -D \frac{\partial C}{\partial l}$$

- $D$ in open water for common groundwater ions
  - $\sim 1 \times 10^{-9}$ to $2 \times 10^{-9}$ m$^2$/sec
- $D^*$ represents $D$ in porous media, and is reduced due to tortuosity and effective porosity
  - $D^* \sim 2 \times 10^{-11}$ to $5 \times 10^{-10}$ m$^2$/sec

Some suggest $D^* = D \frac{\phi_e}{\tau}$

$$\tau = \frac{\text{actual path}}{\text{direct path}}$$
Transport Equations
The combined mechanical and chemical diffusion process is treated with a Fick's Law approach

\[ F = -D \frac{\partial C}{\partial l} \]

But here D is Hydrodynamic Dispersion expressed as

\[ D = \alpha v + D^* \]

Studies indicate scale dependence of dispersivity, \( \alpha \).

Dispersivities at various scales & measured by various methods as compiled by Stan Davis et al. Table B1 in the book, "Ground Water Tracers"

<table>
<thead>
<tr>
<th>Single-Well Injection Withdrawal Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of Aquifer</td>
</tr>
<tr>
<td>Alluvial</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Multiple-Well Tracer Test (including two-well tracer tests)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of Aquifer</td>
</tr>
<tr>
<td>Chalk</td>
</tr>
<tr>
<td>Alluvial</td>
</tr>
<tr>
<td>Alluvial</td>
</tr>
<tr>
<td>Fractured dolomite</td>
</tr>
<tr>
<td>Fractured carbonate</td>
</tr>
<tr>
<td>Fractured crystalline</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Single-Well Tracer Test with Surface Geophysics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of Aquifer</td>
</tr>
<tr>
<td>Alluvial</td>
</tr>
</tbody>
</table>
### Table B1 CONTINUED Dispersivities at various scales & measured by various methods from "Ground Water Tracers"

<table>
<thead>
<tr>
<th>Type of Aquifer</th>
<th>Location</th>
<th>Approximate Distance Traveled by Solute (meters)</th>
<th>( \alpha_L ) (meters)</th>
<th>( \alpha_T ) (meters)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alluvial</td>
<td>Lyons, France</td>
<td>1,000</td>
<td>12</td>
<td>4</td>
<td>Fried, 1975</td>
</tr>
<tr>
<td>Limestone</td>
<td>Brunswick, GA</td>
<td>1,500</td>
<td>61</td>
<td>18</td>
<td>Brediehoef &amp; Pinder, 1973</td>
</tr>
<tr>
<td>Alluvial</td>
<td>Rocky Mtn. Arsenal, CO</td>
<td>4,000</td>
<td>30</td>
<td>30</td>
<td>Konikow, 1977</td>
</tr>
<tr>
<td>Alluvial</td>
<td>Arkansas River Valley, CO</td>
<td>5,000</td>
<td>30</td>
<td>9</td>
<td>Konikow &amp; Brediehoef, 1974</td>
</tr>
<tr>
<td>Glacial deposit</td>
<td>Long Island, NY</td>
<td>1,000</td>
<td>21.3</td>
<td>4.3</td>
<td>Pinder, 1973</td>
</tr>
<tr>
<td>Basalt</td>
<td>Snake River</td>
<td>4,000</td>
<td>91</td>
<td>137</td>
<td>Robertson, 1974</td>
</tr>
</tbody>
</table>

#### Break through Curves

- **Cо** continuous source starting at \( t=0 \)
- Initially fresh water
- **C outflow**
- **Contour C/Cо, versus x location at one time**
- **C=0**
- **Graph C/Cо versus x for 3 different times**
- **Graph C/Cо at one x location as a function of time**

Note: \( t' \) would be average travel time to this point. Why?
Mechanical Transport Equations can be derived by considering an elemental volume as we did for the flow equations. We leave the derivation to a later course & consider the practical analytical forms:

\[
\frac{\partial C}{\partial t} = D_l \frac{\partial^2 C}{\partial l^2_l} + D_t \frac{\partial^2 C}{\partial l^2_t} + D_v \frac{\partial^2 C}{\partial l^2_v} - v_l \frac{\partial C}{\partial l}
\]

- \(C\) concentration in fluid
- \(t\) time
- \(l\) spatial coordinate
- \(D\) dispersion tensor
- \(v\) interstitial velocity
- \(l_l\) reflects the flow direction
- \(l_t\) reflects the direction transverse laterally to flow
- \(l_v\) reflects the direction transverse vertically to flow

Note differing form of flow equations:

\[
\frac{\partial h}{\partial t} = S \left[ \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \right]
\]

Equation for mechanical transport in 1-D:

\[
\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x}
\]

- \(C\) concentration in fluid
- \(t\) time
- \(x\) spatial coordinate
- \(D\) dispersion tensor
- \(v\) interstitial velocity
Analytical Solution for transport in 1-D flow field

continuous source

1D spreading

without chemical reaction

This is an appropriate model for transport along a sand column
It will over estimate C at x if applied to a case with spreading in the transverse lateral or vertical directions

It will predict the break through curves we looked at earlier

\[ C = \frac{C_0}{2} \left( \text{erfc} \left( \frac{x - \bar{v}_x t}{2\sqrt{D_x t}} \right) + \exp \left( \frac{v_x x}{D_x} \right) \text{erfc} \left( \frac{x + \bar{v}_x t}{2\sqrt{D_x t}} \right) \right) \]

erfc is the complimentary error function

---

**Complementary Error Function (erfc)**

<table>
<thead>
<tr>
<th>( \beta )</th>
<th>( \text{erf} (\beta) )</th>
<th>( \text{erfc} (\beta) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1.0</td>
</tr>
<tr>
<td>0.05</td>
<td>0.056372</td>
<td>0.943628</td>
</tr>
<tr>
<td>0.1</td>
<td>0.112463</td>
<td>0.887537</td>
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<tr>
<td>0.15</td>
<td>0.167964</td>
<td>0.832036</td>
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<tr>
<td>0.2</td>
<td>0.222933</td>
<td>0.777067</td>
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<tr>
<td>0.25</td>
<td>0.277875</td>
<td>0.722125</td>
</tr>
<tr>
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<td>0.332827</td>
<td>0.667173</td>
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<tr>
<td>0.35</td>
<td>0.387932</td>
<td>0.612068</td>
</tr>
<tr>
<td>0.4</td>
<td>0.442932</td>
<td>0.557068</td>
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<tr>
<td>0.45</td>
<td>0.497858</td>
<td>0.502142</td>
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<tr>
<td>0.5</td>
<td>0.552550</td>
<td>0.447450</td>
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<tr>
<td>0.55</td>
<td>0.607233</td>
<td>0.392767</td>
</tr>
<tr>
<td>0.6</td>
<td>0.661816</td>
<td>0.338284</td>
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<tr>
<td>0.65</td>
<td>0.716309</td>
<td>0.283791</td>
</tr>
<tr>
<td>0.7</td>
<td>0.770701</td>
<td>0.229309</td>
</tr>
<tr>
<td>0.75</td>
<td>0.825094</td>
<td>0.174906</td>
</tr>
<tr>
<td>0.8</td>
<td>0.879487</td>
<td>0.119513</td>
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<tr>
<td>0.85</td>
<td>0.933881</td>
<td>0.064119</td>
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<tr>
<td>0.9</td>
<td>0.988275</td>
<td>0.005725</td>
</tr>
<tr>
<td>0.95</td>
<td>0.999999</td>
<td>0.000001</td>
</tr>
<tr>
<td>1.0</td>
<td>1.000000</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Error Function

Tables are listed in the back of ground water hydrology books
Analytical Solution for transport in 1-D flow field
slug source
3D spreading
without chemical reaction

\[ C(x = vt + X, y = Y, z = Z) = \frac{M}{8(\pi t)^{3/2} \sqrt{D_x D_y D_z}} \exp \left( \frac{X^2}{4D_x t} + \frac{Y^2}{4D_y t} + \frac{Z^2}{4D_z t} \right) \]

**IMPORTANT!** \(X, Y, Z = \) distance from center of mass

Maximum concentration will occur at the center of mass
Where \(X=Y=Z=0\)

\[ C_{\text{max}} = \frac{M}{8(\pi t)^{3/2} \sqrt{D_x D_y D_z}} \]
So we just considered an Analytical Solution for transport in 1-D flow field.

slug source

3D spreading

without chemical reaction

\[
C(x = vt + X, y = Y, z = Z) = \frac{M}{8(\pi t)^{\frac{3}{2}} \sqrt{D_x D_y D_z}} \exp\left(\frac{x^2}{4D_x t} \frac{y^2}{4D_y t} \frac{z^2}{4D_z t}\right)
\]

\(X Y Z\) = distance from center of mass in each direction

NEXT Analytical Solution for transport in 1D flow field.

continuous source

3D spreading

without chemical reaction
Analytical Solution for transport in uniform 1D flow
continuous source

3D spreading
without chemical reaction

Upper case Y and Z
Are the source width and height

If source is on the water table such that spreading is only downward

Omit (/2) on Z terms
Analytical Solution for transport in uniform 1D flow
continuous source
3D spreading
without chemical reaction

\[
C(x, y, z, t) = \frac{C_0}{4} \left( \text{erfc} \left( \frac{x - v_x t}{\sqrt{2D_x t}} \right) \right)
\]

If source is of full vertical extent in a confined aquifer
OR
if you are far from a limited extent source in a confined aquifer

Change Co/8 to Co/4
Omit z terms

Decay

\[
\frac{dN}{dt} = -\lambda N
\]

or \( N = N_0 e^{(-\lambda t)} \)

where \( \lambda = \frac{0.693}{T_1/2} \)

0.693 is the natural log of 0.5
Retardation - Adsorption

\[ R = \frac{V_{\text{water}}}{V_{\text{contaminant}}} = \left(1 + \frac{\rho_b}{\phi_e} K_d\right) \]

Equation for transport in 1-D with Decay, Retardation, Reaction, Source

Divide D's and V's by R

\[
\frac{\partial C}{\partial t} = \frac{D_x}{R} \frac{\partial^2 C}{\partial x^2} - \frac{\bar{V}_x}{R} \frac{\partial C}{\partial x} + \frac{W(C - C')}{R\phi b} + \frac{\text{CHEM}}{\phi} - \lambda C
\]

- C: concentration in fluid
- t: time
- b: aquifer thickness
- x: spatial coordinate
- D: dispersion tensor
- R: retardation coefficient
- v: interstitial velocity
- W: source fluid flux
- \phi: porosity
- C': concentration of source fluid
- CHEM: chemical reaction source/sink per unit volume of aquifer
- \lambda: decay constant
Analytical Solution for transport in uniform 1D flow
continuous source
3D spreading
With Decay

\[ C(x, y, z, t) = \frac{C_o}{8} \exp \left( \frac{x}{2\alpha_x} \left( 1 - \sqrt{1 + \frac{4\lambda\alpha_x}{v}} \right) \right) \]

If R > 1
Divide \( \nabla \) by R

Upper case Y and Z
Are the source width and height
Same modifications apply for downward & no vertical spreading

Note this includes a simplification of \( D = \alpha_x v \)

\[ D_y \frac{x}{v} \] if \( D^* \) is ignored then equivalent to \( \alpha_y \frac{v}{v} \) which = \( \alpha_y x \)
Analytical Solution for transport in uniform 1D flow continuous source 3D spreading with Decay

Upper case Y and Z
Are the source width and height

ON THE CENTER LINE

i.e. $y = z = 0$

If $R > 1$
Divide $\nabla$ by R

---

Analytical Solution for transport in uniform 1D flow continuous source 3D spreading with Decay

Upper case Y and Z
Are the source width and height

AT STEADY STATE

i.e.
Mass is decaying as fast as it is being supplied at the source

If $R > 1$
Divide $\nabla$ by R

---

$C(x, y, z, t) = \frac{C_o}{2}\exp\left(\frac{x}{2\alpha_x}\left(1 - \sqrt{1 + \frac{4\lambda\alpha_x}{\bar{v}}}\right)\right)$

$erfc\left(\frac{x - \bar{v}t}{2\sqrt{\alpha_x\bar{v}}}\left(1 + \sqrt{\frac{4\lambda\alpha_x}{\bar{v}}}\right)\right)$

$erf\left(\frac{Y}{2\sqrt{\alpha_y x}}\right) - erf\left(\frac{Z}{2\sqrt{\alpha_z x}}\right)$

$C(x, y, z, steadystat e) = \frac{C_o}{4}\exp\left(\frac{x}{2\alpha_x}\left(1 - \sqrt{1 + \frac{4\lambda\alpha_x}{\bar{v}}}\right)\right)$

$erf\left(\frac{y + \frac{Y}{2}}{2\sqrt{\alpha_y x}}\right) - erf\left(\frac{y - \frac{Y}{2}}{2\sqrt{\alpha_y x}}\right)$

$erf\left(\frac{z + \frac{Z}{2}}{2\sqrt{\alpha_z x}}\right) - erf\left(\frac{z - \frac{Z}{2}}{2\sqrt{\alpha_z x}}\right)$
Analytical Solution for transport in

uniform 1D flow

\[
C(x, y, z, t) = C_0 \exp \left( \frac{x}{2\alpha_x} \left[ 1 - \sqrt{1 + \frac{4\lambda_x}{\sqrt{v}} \left( \frac{x}{2\sqrt{\alpha_x}} \right)^2} \right] \right)
\]

\[
C(x, y, z, \text{steadystate}) = C_0 \exp \left( \frac{x}{2\alpha_x} \left[ 1 - \sqrt{1 + \frac{4\lambda_x}{\sqrt{v}} \left( \frac{x}{2\sqrt{\alpha_x}} \right)^2} \right] \right)
\]

\[
\begin{cases}
\text{erf} \left( \frac{y}{2\sqrt{\alpha_y x}} \right) - \text{erf} \left( \frac{y}{2\sqrt{\alpha_y x}} \right)
\end{cases}
\]

\[
\begin{cases}
\text{erf} \left( \frac{z}{2\sqrt{\alpha_z x}} \right) - \text{erf} \left( \frac{z}{2\sqrt{\alpha_z x}} \right)
\end{cases}
\]

STEADY STATE ON THE CENTER LINE

i.e. Mass is decaying as fast as it is being supplied at the source

i.e. \( y = z = 0 \)

If \( R > 1 \) Divide \( \nabla \) by \( R \)

THINK IN TERMS OF ORGANIZING THE ANALYTICAL SOLUTIONS IN TERMS OF

THE TYPE OF SOURCE:

SLUG OR CONTINUOUS

TYPE OF SPREADING:

1D, 2D, 3D

TYPE OF CONTAMINANT BEHAVIOR:

DECAYING, ADSORPING

(and if so steady-state? center-line?)