CONTAMINANT TRANSPORT

MECHANICAL ASPECTS

ADVECTION

\[ \bar{v} = \frac{Kdh}{\phi_e dl} = \text{average linear velocity} \]

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

If we only consider advection and start with a "point" of material with \(C_0=1000\, \text{mg/l}\)

A point has no volume so can it have a concentration? So why do we say a "point"?

\[ K = 0.1 \, \text{cm/sec} \]
\[ dh = 10 \, \text{cm} \]
\[ dl = 100 \, \text{cm} \]
\[ \phi = 0.2 \]

How long will it take for the material to move 50cm?

What will the concentration be at that location at that time?
However concentration will decrease due to DIFFUSION and DISPERSION

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 ($\alpha$)

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

- 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:**
\[ \text{Flux} = F = -D \frac{\partial C}{\partial l} \]

- \( D \) in open water for common groundwater ions ~1x10\(^{-9}\) to 2x10\(^{-9}\) m\(^2\)/sec
- \( D^* \) represents \( D \) in porous media, and is reduced due to tortuosity and effective porosity
  - \( D^* \sim 2x10^{-11} \) to 5x10\(^{-10}\) 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

\[ D_1 = \alpha_1 v_1 + D^* \]

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>Type of Aquifer</th>
<th>Location</th>
<th>Distance Between Injection and Observation Wells (meters)</th>
<th>DL (meters)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alluvial</td>
<td>Lyons, France</td>
<td>6 &amp; 12</td>
<td>4.3</td>
<td>Fried, 1975</td>
</tr>
<tr>
<td>Fractured dolomite</td>
<td>Carlsbad, NM</td>
<td>55</td>
<td>38.0</td>
<td>Groves and Bester, 1971</td>
</tr>
<tr>
<td>Fractured carbonate</td>
<td>So. Nevada</td>
<td>121</td>
<td>15.0</td>
<td>Classen and Cordes, 1975</td>
</tr>
<tr>
<td>Fractured crystalline</td>
<td>Savannah River Plant, B.C.</td>
<td>530</td>
<td>134.0</td>
<td>Webster et al., 1970</td>
</tr>
</tbody>
</table>

Single-Well Tracer Test with Surface Geophysics

<table>
<thead>
<tr>
<th>Type of Aquifer</th>
<th>Location</th>
<th>Distance Traveled by Tracer (meters)</th>
<th>DL (meters)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alluvial</td>
<td>Lyons, France</td>
<td>80 m</td>
<td>5-12</td>
<td>0.009-14.5 Fried, 1975</td>
</tr>
</tbody>
</table>

Table B1 CONTINUED Dispersivities at various scales & measured by various methods from "Ground Water Tracers"

Dispersivities Measured on a Regional Scale by Model Calibration

<table>
<thead>
<tr>
<th>Type of Aquifer</th>
<th>Location</th>
<th>Approximate Distance Traveled by Solute (meters)</th>
<th>DL (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 Fried, 1975</td>
</tr>
<tr>
<td>Limestone</td>
<td>Brunswick, GA</td>
<td>1,500</td>
<td>61</td>
<td>18 Bredhoeft &amp; Pinder, 1973</td>
</tr>
<tr>
<td>Alluvial</td>
<td>Rocky Mt. Arsenal, CO</td>
<td>4,000</td>
<td>30</td>
<td>30 Konikov, 1977</td>
</tr>
<tr>
<td>Alluvial</td>
<td>Arkansas River Valley, CO</td>
<td>5,000</td>
<td>30</td>
<td>9 Konikov &amp; Bredhoeft, 1974</td>
</tr>
<tr>
<td>Glacial deposit</td>
<td>Long Island, NY</td>
<td>1,000</td>
<td>21.3</td>
<td>4.3 Pinder, 1973</td>
</tr>
<tr>
<td>Basalt</td>
<td>Snake River</td>
<td>4,000</td>
<td>91</td>
<td>137 Robertson, 1974</td>
</tr>
</tbody>
</table>
Break through Curves

initially fresh water

C₀ continuous source starting at t=0

C outflow

schematic C/C₀ for t=t’
Contour C/C₀ versus x location at one time

Note t’ would be average travel time to this point. Why?

C₀

t₁ t₂ t₃

along the column at various times
Graph C/C₀ versus x for 3 different times

C₀

0.5

0

x

0

first arrival t₁ average arrival time t₂ t₃ constant C=C₀
Graph C/C₀ at one x location as a function of time

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

\[
\frac{\partial C}{\partial t} = D_l \frac{\partial^2 C}{\partial l^2} + D_t \frac{\partial^2 C}{\partial t^2} + D_v \frac{\partial^2 C}{\partial l^2} - \nu_l \frac{\partial C}{\partial l}
\]

C concentration in fluid

Note differing form of flow equations

t time

I spatial coordinate

D dispersion tensor

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

V interstitial velocity

I_l reflects the flow direction

I_t reflects the direction transverse laterally to flow

I_v reflects the direction transverse vertically to flow
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 breakthrough curves we looked at earlier.

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

erfc is the complementary error function.
Suppose that source enters the up gradient end of a column
At a continuous concentration of \( C_0 = 1000 \text{mg/l} \)

\[ K = 0.1 \text{ cm/sec} \]
\[ dh = 10 \text{ cm} \]
\[ dl = 100 \text{ cm} \]
\[ \phi = 0.2 \]

**Dispersivity** \( \alpha_x = 5 \text{ cm} \)

What will the concentration be at 50 cm after 1000 sec?

average linear velocity

\[ \bar{v} = \frac{Kdh}{\phi dl} = \frac{0.1 \text{ cm}}{\text{sec}} \cdot \frac{10 \text{ cm}}{0.2 \cdot 100 \text{ cm}} = 0.05 \text{ cm/sec} \]

distance traveled in 1000 sec?

\[ d = \bar{v}t = 0.05 \frac{\text{cm}}{\text{sec}} \cdot 1000 \text{ sec} = 50 \text{ cm} \]

By inspection we know that the concentration should be \( 0.5C_0 = 500 \text{mg/l} \)
But let’s carry out the calculation
Experiment with the spreadsheet
http://inside.mines.edu/~epoeter/_GW/22ContamTrans/C1d.xls

Note the values of C using only the first term and then both terms at
times and locations where your intuition allows you to know the
concentration.

When is use of the second term important? When does excel cause it
to be in error?

Analytical Solution for transport in 1-D flow field
slug source
3D spreading
without chemical reaction
Analytical Solution for transport in 1-D flow field
slug source
3D spreading
without chemical reaction

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

IMPORTANT! X Y Z = distance from center of mass

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

\[ C_{\text{max}} = \frac{M}{8(\pi t)^{3/2}} \sqrt{D_x D_y D_z} \]

Suppose a slug source enters a uniform flow field
With an initial mass of \( M_0 = 1000 \text{mg} \)
\[ K = 0.1 \text{ cm/sec} \]
\[ dh = 10 \text{ cm} \]
\[ dl = 100 \text{ cm} \]
\[ \phi = 0.2 \]
dispersivity \( \alpha_x = 5 \text{ cm} \)
dispersivity \( \alpha_y = \frac{1}{5} \alpha_x \)
dispersivity \( \alpha_z = \frac{1}{10} \alpha_x \)

What will the concentration be at 50 cm directly down gradient after 1000 sec?
So we just considered an Analytical Solution for transport in 1-D flow field slug source 3D spreading without chemical reaction

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

\( X, Y, Z = \) 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**

see previous graphic

Upper case $Y$ and $Z$

Are the source width and height

\[
C(x, y, z, t) = \frac{C_0}{8} \left( \text{erfc} \left( \frac{x - v_x t}{2\sqrt{D_x t}} \right) \right)
\]

\[
\left( \text{erf} \left( \frac{y + Y}{2} \sqrt{\frac{x}{D_y}} \right) \right) - \left( \text{erf}\left( \frac{y - Y}{2} \sqrt{\frac{x}{D_y}} \right) \right)
\]

\[
\left( \text{erf} \left( \frac{z + Z}{2} \sqrt{\frac{x}{D_z}} \right) \right) - \left( \text{erf}\left( \frac{z - Z}{2} \sqrt{\frac{x}{D_z}} \right) \right)
\]

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

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

Suppose a source continuously enters that uniform flow field With an initial concentration of \( C_0 = 1,000 \text{mg/l} \)

pause to consider relationship of mass and concentration

\[
\text{Mass} = \text{Conc} \times \text{Volume}
\]

\[
\text{Mass/Time} = \text{Conc} \times \text{Velocity} \times \text{Area} = \text{Conc} \times Q \quad (Q \text{ is discharge})
\]

\[
\text{Mass} = \text{Conc} \times Q \times \text{Time}
\]

Envision the source is submerged and emanates from a 0.5cm high x 1cm wide zone

pause to consider the character of the source geometry

\( v = 0.05 \text{ cm/sec} \)

dispersivity \( \alpha_x = 5 \text{ cm} \)

dispersivity \( \alpha_y = 1/5 \alpha_x \)

dispersivity \( \alpha_z = 1/10 \alpha_x \)

What will the concentration be at 50 cm directly down gradient after 1000sec?

pause to consider the coordinate system
What do you make of the concentration relative to the $C$ we obtained for the slug source?

How much mass enters the system in 1000sec? $M = CQ = CAVD_T$

How would you go about developing a contour map of the plume?

If you did not know the dispersivities, how could you use this equation to estimate them?

How might you set up the problem if 8g/d arrived at the water table over a 1m$^2$ area in an aquifer with the properties and conditions used for the example?

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Analytical Solutions for transport provide smoothed representations of plumes
Be sure to practice using this topic's exercises

View an animation of contaminant transport

Consider how what you see will affect:

1) the predictions you make using the analytical solutions

2) the concentrations you obtain in samples from field sites

View DVD

NOW CONSIDER THE NON-MECHANICAL ASPECTS OF CONTAMINANT TRANSPORT
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

For a material with a half-life of 12 yrs, how much is left after 40 yrs? (Hint figure it as a % of initial mass)

\[ N = N_0 e^{-\lambda t} \]

\[ \lambda = \frac{0.693}{T_{1/2}} \]
It is often said that material is essentially gone after 7 half-lives. How much is left then?

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

\[ \lambda = \frac{0.693}{T_{1/2}} \]
What is the Retardation Coefficient for a site with $K_d = 0.01\text{ml/mg}$

effective porosity of 0.3

particle density of 2.65 g/cc

$$R = \frac{V_{\text{water}}}{V_{\text{contaminant}}} = \left(1 + \frac{\rho_0 K_d}{\phi_e} \right)$$

What is the Retardation Coefficient for a site with

Ground water velocity = 0.05 cm/sec

Contaminant velocity = 0.0009 cm/sec

$$R = \frac{V_{\text{water}}}{V_{\text{contaminant}}} = \left(1 + \frac{\rho_0 K_d}{\phi_e} \right)$$
Equation for transport in 1-D with Decay, Retardation, Reaction, Source
Divide D's and V's by R

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

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
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

Same modifications apply for downward & no vertical spreading

\[
C(x, y, z, t) = \frac{C_o}{8} \exp \left( \frac{x}{2\alpha_x} \left( 1 - \sqrt{1 + \frac{4\lambda\alpha_x}{v}} \right) \right) \left( x - \frac{v}{\sqrt{\alpha_x}} t \right) \left( 1 + \sqrt{1 + \frac{4\lambda\alpha_x}{v}} \right) \frac{41}{2}\text{erf} \left( \frac{y}{2\sqrt{\alpha_y}} \right) \frac{41}{2}\text{erf} \left( \frac{z}{2\sqrt{\alpha_z}} \right)
\]

\[
D_y \frac{x}{v} \text{ if } D^* \text{ is ignored then equivalent to } \alpha_y \frac{x}{v} \text{ which } = \alpha_y X
\]

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

\[
C(x, y, z, t) = \frac{C_o}{2} \exp \left( \frac{x}{2\alpha_x} \left( 1 - \sqrt{1 + \frac{4\lambda\alpha_x}{v}} \right) \right) \left( x - \frac{v}{\sqrt{\alpha_x}} t \right) \left( 1 + \frac{4\lambda\alpha_x}{v} \right) \frac{41}{2}\text{erf} \left( \frac{y}{2\sqrt{\alpha_y}} \right) \frac{41}{2}\text{erf} \left( \frac{z}{2\sqrt{\alpha_z}} \right)
\]

\[
\text{If } R > 1 \text{ Divide } v \text{ by } R
\]

\[
\text{ON THE CENTER LINE}
\]

\[
i.e. \quad y = z = 0
\]

\[
\text{If } R > 1 \text{ Divide } v \text{ by } R
\]
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 \( \bar{v} \) by \( R \)

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Analytical Solution for transport in uniform 1D flow

**STABLE STATE ON THE CENTER LINE**

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

If \( R > 1 \) Divide \( \bar{v} \) 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?)

A transport model for your exploration:
http://inside.mines.edu/~epoeter/_GW/22ContamTrans/TransportModel/tdpf1.0web/pflow/pflow.html

Explore plume spreading as a function of heterogeneity as represented by K variation AND
local heterogeneity as represented by the input dispersivity
Create grid. Make sure you understand the size of the system you are working with.
Properties: Run at least 1 homogeneous and 1 heterogeneous model
Calculate heads
Choose particle movement for flow (this is by random walk ... advecting based on Ks and gradient
then randomly displacing each particle based on dispersivity)
Be aware of the number of particles you use given spacing, grid size and your drawn area
Use the same particles for the above comparison of 1 homogeneous and 1 heterogeneous model
Choose # days per second such that you will get transport across your grid in a matter of a minute
or so (make a rough estimate of travel time given gradient, K, porosity and distance)
Always choose to show center of mass, std deviation bars of particles and plot the variance of
particle locations.
Run both your homogeneous and heterogeneous models with and without local dispersion. When
you use local dispersion make sure it is a reasonable value. Try varying the value.
For all cases note the spatial variance of the particles. Explain the results.
When does it stop plotting spatial variance? Why?