Spatial and Temporal Tracer Test Data Analysis

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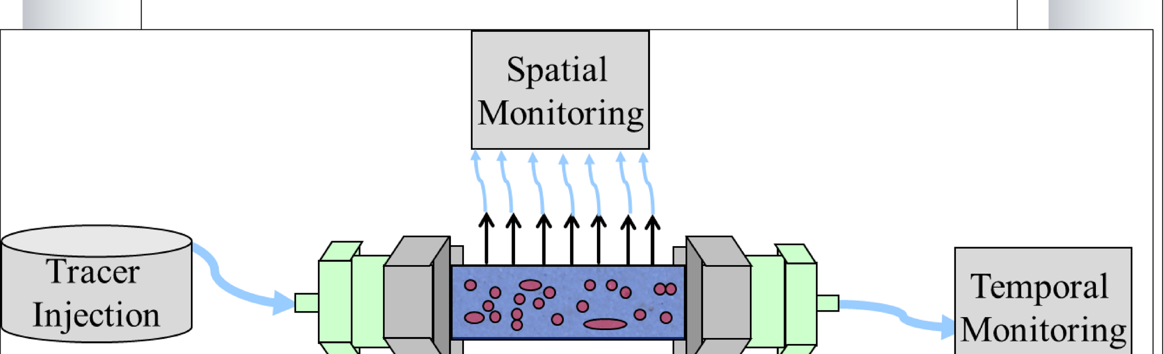
Introduction

Description:
Students are provided data sets that could be obtained by monitoring flow and transport of a tracer or contaminant in the field or in a soil column experiment in the laboratory.

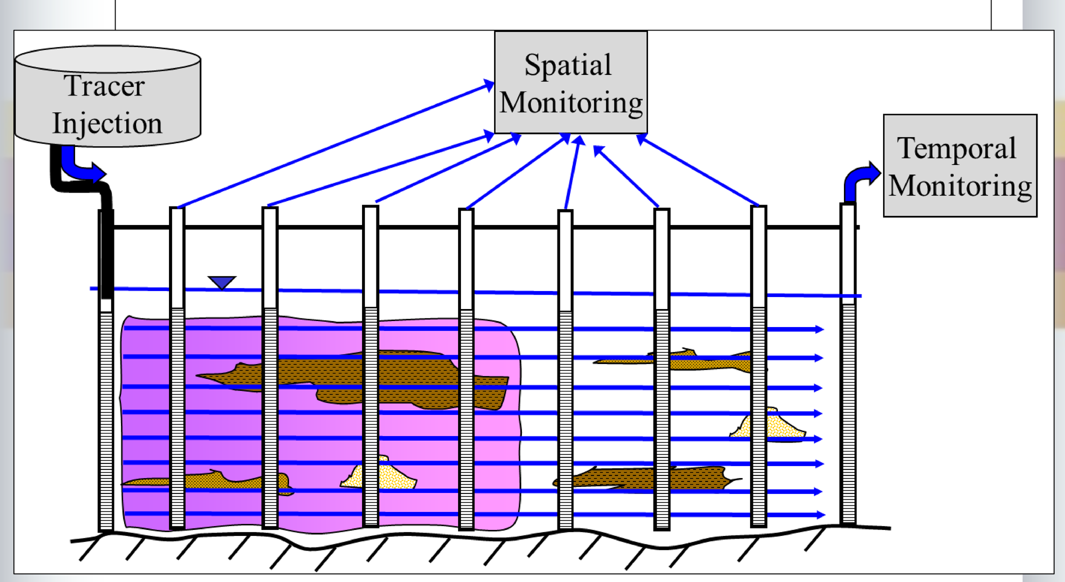
The analysis is designed to illustrate the similarities and differences in spatial and transient data, which supports measurement and monitoring strategies in hydrogeology, soils, and geochemistry. The assignments were also designed to illustrate the link between groundwater flow and solute transport. The goal is the develop problem solving skills by guiding students through calculations with targeted questions. Student engagement is developed through active learning and real-world practical application. The exercises reinforce theory with practical applications of data analysis used to determine solute transport properties and assess the subsurface conceptual model.

Goals:
- Recognize and describe differences in spatial and temporal data
- Understand physical representation of statistical moments of concentration data
- Be able to plot data sets, determine slopes, and input equations into spreadsheets
- Identify processes impacting fluid flow and solute transport behavior through observation and analysis of concentration monitoring data
- Understand the importance and practical applicability of mass balance calculations and dimensional analysis

Conceptualization:
These two data sets could be collected using a soil column (below) with tracer or contaminant injection at one end and extraction at the other.



Similarly, these two data sets could be collected in the field (below) with an injection/extraction system or simply a set of wells that allows monitoring along the direction of flow and transport.



Moment Analysis Background

<u>Purpose</u>: to evaluate spatial or temporal properties (statistics) of a tracer or contaminant plume.

<u>1-D Spatial Moments (absolute) M_n</u>
(general) n^{th}: $M_n = \int cx^n dx = \Sigma cx^n \Delta x$
0^{th}: $M_0 = \int cdx = \Sigma c\Delta x$ (total mass in plume)
1^{st}: $M_1 = \int cxdx = \Sigma cx\Delta x$ (mean location of plume)
2^{nd}: $M_2 = \int cx^2dx = \Sigma cx^2\Delta x$ (spread of plume)

<u>1-D Temporal Moments (absolute) M_n</u>
(general) n^{th}: $M_n = \int ct^n dt = \Sigma ct^n \Delta t$
0^{th}: $M_0 = \int cdt = \Sigma c\Delta t$ (total mass)
1^{st}: $M_1 = \int ctdt = \Sigma ct\Delta t$ (mean arrival time)
2^{nd}: $M_2 = \int ct^2dt = \Sigma ct^2\Delta t$ (degree of spreading)

<u>Normalized</u> (μ_n'): (always divide by the 0^{th} moment M_0); dx = spatial; dt=temporal
(general) $\mu_n' = M_n/M_0 = \int cx^n dx/\int cdx = \Sigma cx^n\Delta x/\Sigma c\Delta x$

<u>Central</u> (μ_n^c): (general); dx=spatial; dt=temporal
$\mu_n^c = \int(x-\mu_1')^n cdx/\int cdx = \Sigma(x-\mu_1')^n cdx/\Sigma c\Delta x$
μ_2^c = variance = $\sigma^2 = M_2/M_0 - \mu_1'^2$
$= \int(x-\mu_1')^2 cdx/\int cdx = \Sigma(x-\mu_1')^2 cd\Delta x/\Sigma c\Delta x$
$\mu_2^c = D2t$ or $d\mu_2/dt = 2D$; D is Dispersion Coeff.

<u>Spatial Moment</u>
M_0 = total mass (over distance)
Normalized M_1 = average location of plume center
M_2 = spread in distribution about that center
d(normM_1)/dt = dx/dt = velocity of plume

<u>Temporal Moment</u>
M_0 = total mass (through time)
Normalized M_1 = average time of arrival of plume (get velocity if you know the center of distribution)
M_2 = spread in time about that arrival time

<u>Spreadsheet Calculations</u>
The formulas for the zeroeth and first normalized temporal moments are below. For spatial moments and moments of higher order, students solve from these formulas and the notes above. Given a data set with *n* concentration-time data points, beginning with point- '1':

$$\mu_0 = \sum_{i=2}^{n}\left(\frac{C_i + C_{i-1}}{2}\right)(t_i - t_{i-1})$$

$$\mu_1' = \frac{\sum_{i=2}^{n}\left(\frac{t_iC_i + t_{i-1}C_{i-1}}{2}\right)(t_i - t_{i-1})}{\mu_0}$$

Mean Arrival Time (MAT): = First normalized temporal moment & Mean Travel Time (MTT):

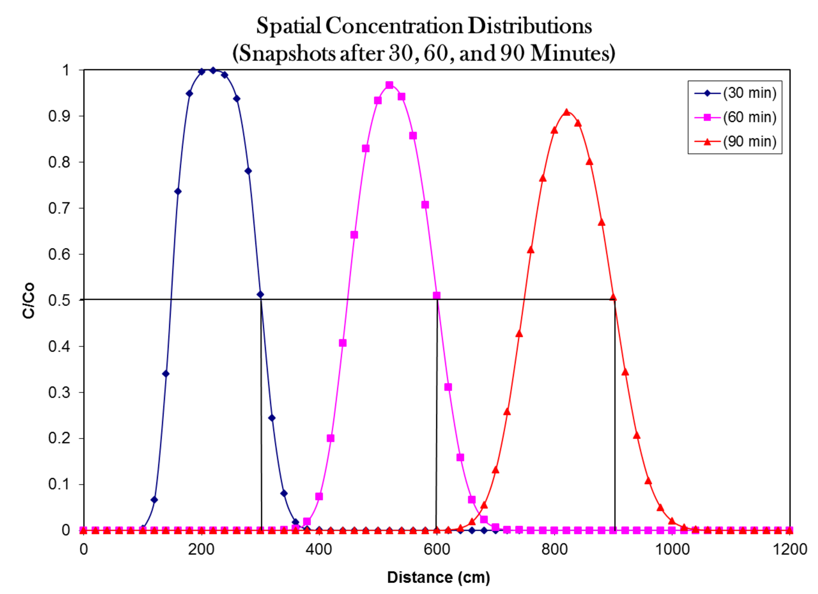
MTT=MAT – Avg. Injection Time of Tracer Pulse

$$MTT = \mu_1' - 0.5t_o$$

where t_o is the total injection time of tracer pulse. When solute mass balance is good (close to 100%) the zeroeth moment can be used as t_o.

Activity Assignment & Solution

Problem #1 Spatial Moment Analysis
Given: Distance (cm) and relative concentration (C/Co) data for a tracer plume at 30, 60, and 90 minutes. The time required to inject the tracer was 15 minutes.
A. Plot snap-shots of the contaminant plume as relative concentration vs. distance for each time (one graph with concentrations from all three locations). What can you observe about the graph? Explain apparent differences in the three curves. What factors may contribute to spreading at this scale?
ANSWER:



B. Calculate the spatial moments for each curve: 0^{th}, 1^{st} normalized and 2^{nd} central, giving appropriate units for each. What is the physical meaning of each of the three moments that you calculated? What are some limitations of the moment analysis?
ANSWER:

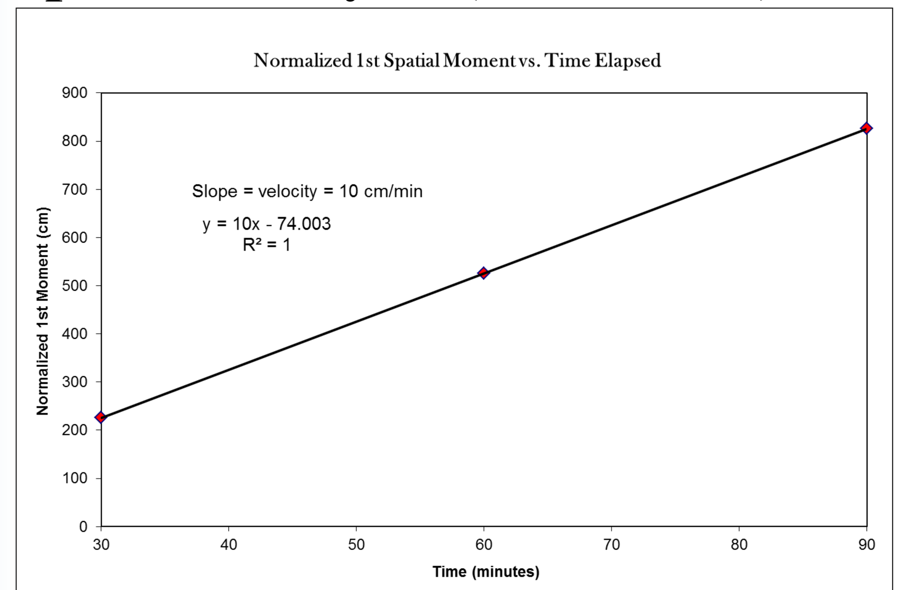
	M0	M1 norm	M2 cent
time (min)	(cm)	(cm)	(cm^2)
30	153	226	2508
60	153	526	3258
90	153	826	4008

0^{th} Moment: Total mass in the system based on the sampled concentrations.
1^{st} Moment, Normalized: The location of the center of mass of the plume.
2^{nd} Central Moment: The spread of the plume about the center of mass.

C. For each data set (30 min, 60 min, 90 min), determine the plume velocity for that specific set using the moments. Assume the times given for each data set are taken from the beginning time of injection. Make sure to adjust for the time of injection by having the time in your calculation begin at the average time of injection, not the beginning. Compare these results to the velocity found by graphing the spatial position of the plume's center of mass versus time, which is the average distance traveled versus time (velocity is the slope, which can be determined using linear regression by adding a trend line in excel). What is the significance of comparing the velocity over all three data sets?

Answer: The velocity for the 30, 60 and 90 min sets is about 10 cm/min. The velocity found by the slope of the normalized first moment vs. time is 10 cm/min (plot at top of column to the left).

Spatial Analysis (Continued)

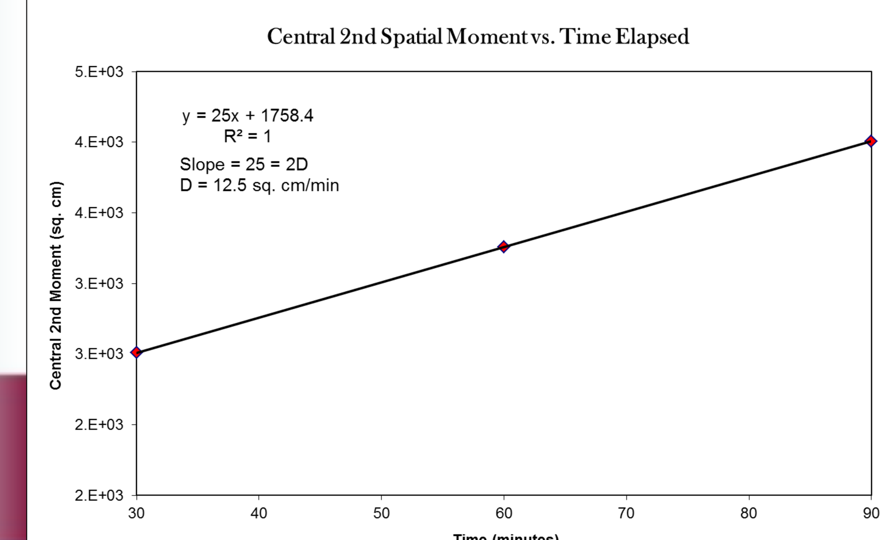


D. Given the injection pulse of 15 min, perform a mass balance. A mass balance calculates the mass recovered during an experiment by dividing the output (mass extracted) by the input (mass injected). However, a mass balance does not necessarily have to be a ratio of quantities of 'mass', which is convenient as the data provided are in relative concentration (C/Co where C is the output monitored concentration and Co is the concentration of the tracer injected).

Answer: The mass balance should be a ratio of units of length. The input 'length' is found by the avg. velocity * length of injection and the output 'length' is the zeroeth moment. The mass balance is about 102%.

E. Calculate the dispersion coefficient for the contaminant plume. The dispersion coefficient is equal to ½ the slope of the graph of the second central moment versus time. What are the units of the dispersion coefficient? Does the dispersion coefficient change with time? Do the sizes and shapes of the plume change over time, and why?

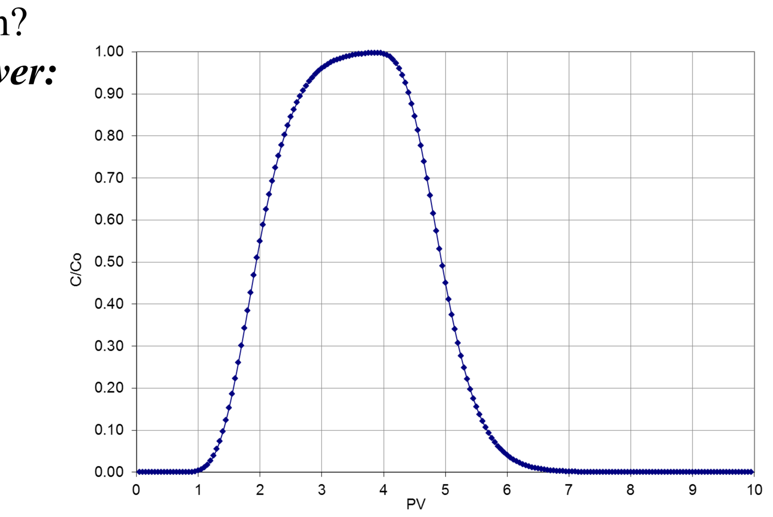
Answer: The slope of the second central moment vs. time is 25 cm2/min (below). The dispersion coefficient is thus 12.5 cm²/min. By looking at the 'snapshot' graph (A) it can be seen that D is constant over time: the plume spreads at a constant rate.



The constant dispersion coefficient means that the rate of plume spreading is constant, or the plume shape is changing (spreading) in a constant manner over time. This type of observation with the constant velocity determined above may be also used with other hydrogeologic data to conceptualize the subsurface hydraulic conductivity heterogeneity or effective homogeneity.

Transient Analysis

Problem #2: Temporal Moment Analysis
Given: Breakthrough curve data (time in min, concentration in mg/L).
F. Plot the breakthrough curve (BTC) as relative concentration (C/Co) versus relative time in pore volumes or PV. What can you observe from the graph?
Answer:



G. Calculate the temporal moments from C/Co and relative time in PV: 0^{th}, 1^{st} normalized, and 2^{nd} central. Describe each conceptually. What is the physical meaning of the moments, and what are the units of these moments?
Answer:

	M0	M1 norm	M2 cent
	(-)	(-)	(-)
Value	3	4	1

0^{th} Moment: Total mass that travels through system over time
1^{st} Moment, Normalized: Average time of the plume arrival
2^{nd} Moment, Central: The spread of the plume over time

H. Determine the contaminant's mean arrival time and hydraulic residence time (travel time, and describe each conceptually and compare with the graph from #F.

Answer: The MAT is equivalent to the first normalized moment. The MTT is MAT minus the average time of injection. Here, the MAT is 390 min (3.5 PV) and the MTT is 223 min (2.0 PV). Compared to the BTC, the MAT appears to be the point where half the mass has reached the sampling port, and the MTT is the point at which C/Co = 0.5. MTT in PV (-) is also the retardation factor (reactive tracer travel time/nonreactive tracer travel time), because the nonreactive tracer travel time is = 1 PV, which adsorption occurred.

I. Perform a mass balance.

Answer: The mass balance is 100.00%. As with the spatial analysis, a mass balance is completed by comparison of the output (zeroth moment) with the amount of tracer injected.

Acknowledgement

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