Hydrodynamic dispersion

Dispersive transport of contaminants results from the heterogeneous distribution of water flow velocities within and between different soil pores (Figure 1, left). Dispersion can be derived from Newton’s law of viscosity which states that velocities within a single capillary tube follow a parabolic distribution, with the largest velocity in the middle of the pore and zero velocities at the walls (Figure 1, left). For this reason contaminants in the middle of a pore will travel faster than contaminants that are farther from the center. Since the distribution of contaminant ions within a pore depends on their charge, as well as on the charge of pore walls, some contaminants may move considerably faster than others. In some circumstances (e.g., in fine-textured soils), anion exclusion may occur. Since the anions in such soils are located predominantly in the faster moving liquid in the center of a pore away from the negatively charge solid surface, anionic contaminants may travel faster than the average velocity of water (e.g., Nielsen et al. 1986). Based on Poiseuille’s law, one can further show that velocities in a capillary tube depend strongly on the radius of the tube, and that the average velocity increases with the radius to the second power. Since soils consist of pores of many different diameters, contaminant fluxes in pores of different diameters will be significantly different, with some contaminants again traveling faster than others (Figure 1, right). Furthermore, contaminants may travel according to pathways of different length. All these factors result in a bell-shaped distribution of velocities and thus of arrival times, typical of a breakthrough curve.

Figure 1: Distribution of velocities in a single pore (left) and distribution of velocities in a pore system (right) resulting in different arrival times of contaminants (modified from Šimůnek and van Genuchten, 2006).

The above pore-scale dispersion processes lead to an overall (macroscopic) hydrodynamic dispersion process that can be described mathematically in approximately the same way as molecular diffusion using Fick’s first law. Addition of the dispersion and diffusion processes leads to the following expression for the contaminant mass flux in the liquid phase \( J_h \):

\[
J_h = -\theta D_h \frac{\partial c}{\partial z} = -\theta (D_m + D) \frac{\partial c}{\partial z}
\]

(Eq. 1)
where $D_h$ is the hydrodynamic dispersion coefficient $[L^2T^{-1}]$ that accounts for both molecular diffusion and mechanical dispersion (Fetter, 1999), $D_m$ is the mechanical dispersion coefficient $[L^2T^{-1}]$, and $D$ is the liquid phase diffusion coefficient $[L^2T^{-1}]$. The mechanical dispersion coefficient in one-dimensional systems has been found to be approximately proportional to the average pore-water velocity $v = q/\theta$ $[LT^{-1}]$, with the proportionality constant generally referred to as the (longitudinal) dispersivity $\lambda$ (Biggar and Nielsen 1967). The discussion above holds for one-dimensional transport; multi-dimensional applications require the use of a more complicated dispersion tensor involving longitudinal and transverse dispersivities (e.g., Bear 1972).

Dispersivity is a transport parameter that is often obtained experimentally by fitting measured breakthrough curves with analytical solutions of the advection-dispersion equation. The dispersivity often changes with the distance over which contaminants travel, the so-called dispersion-scale effect. Values of the longitudinal dispersivity usually range from about 1 cm for relatively short, packed laboratory columns, to about 5 or 10 cm for field soils. Longitudinal dispersivities can be significantly larger (up to hundreds of meters) for regional groundwater transport problems (Gelhar et al. 1985). If no other information is available, a good first approximation is to use a value of one-tenth of the transport distance for the longitudinal dispersivity (e.g. Anderson 1984), and a value of one-hundred of the transport distance for the transverse dispersivity when multi-dimensional applications are considered.

In many cases, especially in groundwater sediments, flow is three-dimensional. In such case, a three-dimensional flow and transport equation should be used. Often, such flow systems can be simplified to a two-dimensional system. For a two-dimensional flow system, the advection-dispersion equation for a sorbing chemical element undergoing radioactive decay is written as (Bear, 1972):

$$ R \frac{\partial C}{\partial t} = D_{ij} \frac{\partial}{\partial x_j} \left( \frac{\partial C}{\partial x_i} \right) - q_i / n_e \left( \frac{\partial C}{\partial x_i} \right) - R \mu C $$  \hspace{1cm} (Eq. 3)

where $D_{ij}$ is the hydrodynamic dispersion tensor, $q_i$ is the $i$-th component of the Darcy flux, and $x_i$ ($i = 1,2$) is spatial coordinate. The hydrodynamic dispersion $D_{ij}$ now accounts for dispersion in the direction of the main flow component, characterized by the longitudinal ($\alpha_L$) dispersivity, and in the direction orthogonal to the main flow direction, characterized by the transversal ($\alpha_T$) dispersivity, and is given by (Frind and Hokkanen, 1985):

$$ D_{11} = \alpha_L v_1^2 / <v> + \alpha_T v_2^2 / <v> + D_p $$  \hspace{1cm} (Eq. 4)

$$ D_{22} = \alpha_T v_1^2 / <v> + \alpha_L v_2^2 / <v> + D_p $$  \hspace{1cm} (Eq. 5)

$$ D_{12} = D_{21} = (\alpha_L - \alpha_T) v_1 v_2 / <v> $$  \hspace{1cm} (Eq. 6)

where $<v> = (v_{12} + v_{22})^{0.5}$.

Usually the transverse dispersivity is 10 to 20 times smaller than the longitudinal dispersivity. The effect of different ratios for $\alpha_L / \alpha_T$ is seen in Figure 2. As the ratio becomes smaller, the plume will develop a less elongated shape, indicating that more chemicals will move in the direction orthogonal to the main water flow direction. This phenomenon is typical for layered sediments.
In case of a uniform two-dimensional velocity field with the direction of flow parallel to the $x$-axis, Eq. (3) is simplified to (with $v_2 = v_x = 0$):

$$\frac{\alpha_L}{\alpha_T} = \frac{20}{5} = 4$$

$$\frac{\alpha_L}{\alpha_T} = \frac{2}{1} = 2$$
\[ R \frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2} - q_s / n_e \left( \frac{\partial C}{\partial x} \right) - R \mu C \]  

(Eq. 7)

where \( D_L \) and \( D_T \) are the longitudinal and transversal dispersion coefficient, respectively, equal to:

\[ D_L = D_p + \alpha_L \nu \]
\[ D_T = D_p + \alpha_T \nu \]  

(Eq. 8)

For the determination of appropriate dispersivities an extensive literature review was carried out. Details of the review and the data analysis are given by Mallants et al. (1998). Only the main results will be presented here.

![Graph showing longitudinal dispersivity versus scale](image)

Figure 3 Longitudinal dispersivity versus scale: only data with high and intermediate reliability are shown. Dashed line indicates best estimate, i.e. \( \alpha_L = 0.0267 \times \). Horizontal arrows indicate maximum (\( =90m \)), best estimate (\( x > 1000 \text{ m} \)) = 26.7 m, and minimum (\( = 5.5 \text{ m} \)) dispersivity in the range of travel distances between 1000 and 10000 m (from Mallants et al., 1998).

A summary of the longitudinal dispersivities, \( \alpha_L \), whose reliability was estimated to be intermediate or high, is plotted in Figure 3. Also indicated on the graph are the best estimate
relationship $\alpha_L = 0.00267 \times$, where $x$ is travel distance, together with the 25% and 75% values for $\alpha_L/x$. The best estimate represents the 50% value of the $\alpha_L/x$ probability distribution. Note that these relationships are only valid for travel distances smaller than 1000 m. For $x > 1000$ m, a constant value of 26.7 m is proposed.

Figure 3 clearly shows the increasing trend for $\alpha_L$ with increasing travel distance. However, for travel distances larger than or equal to 1000 m, too few reliable data were available to derive a relationship between $\alpha_L$ and $x$. We therefore assumed that $\alpha_L$ remained constant with scale for distances larger than 1000 m. The best estimate value was equal to 26.7 m, which is based on the best estimate relationship $\alpha_L/x = 0.0267$, with $x = 1000$ m. This approach may underestimate $\alpha_L$ at very large distances, but this is conservative. At distances of 1000 m or more, the minimum and maximum value for $\alpha_L$ were equal to the minimum and maximum observed values, respectively.

In addition to the longitudinal dispersivity, also estimates for the horizontal transverse, $\alpha_H$, and the vertical transverse, $\alpha_V$, dispersivity were derived (in case transport is three dimensional, three dispersivities apply, $\alpha_L$, $\alpha_H$, and $\alpha_V$, where $\alpha_H$ accounts for dispersion in the $y$-direction and $\alpha_V$ in the $z$-direction). For these two parameters, $\alpha_H$ and $\alpha_V$, best estimates were calculated directly from the relationship between $\alpha_L$ and $\alpha_H$ and from the relationship between $\alpha_H$ and $\alpha_V$, respectively. In other words, each sampled value for $\alpha_L$ will lead to a value for $\alpha_H$ by using $\alpha_H = \alpha_L/5.08$ (Mallants et al., 1998). The value for $\alpha_H$ thus obtained should be within the minimum (= 0.001 m) and maximum (=12.5m) observed values for $\alpha_H$. The calculated value for $\alpha_H$ will then be used to calculate a value for $\alpha_V$, according to $\alpha_V = \alpha_H/22.7$. This value should be within the following limits: $0.0004 \leq \alpha_V \leq 0.345$ m. A summary of the statistical parameters for each of the dispersivity coefficients is given in Table 1.

<table>
<thead>
<tr>
<th></th>
<th>$\alpha_L$ [m]</th>
<th>$\alpha_L/x$ [-]</th>
<th>$\alpha_H$ [m]</th>
<th>$\alpha_V$ [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>50th percentile (median)</td>
<td>26.7</td>
<td>0.0267</td>
<td>0.1000</td>
<td>0.0022</td>
</tr>
<tr>
<td>minimum</td>
<td>5.5</td>
<td>0.0089$^S$</td>
<td>0.0010$^3$</td>
<td>0.0004$^#$</td>
</tr>
<tr>
<td>maximum</td>
<td>90</td>
<td>0.0870$^+$</td>
<td>12.500$^+$</td>
<td>0.3450$^+$</td>
</tr>
</tbody>
</table>

$^&$ log-uniform distribution ($x \geq 1000$ m); $^S$ log-triangular distribution ($x < 1000$ m)

$^{**}$ values calculated from $\alpha_H = \alpha_L/5.08$; $^{***}$ values calculated from $\alpha_V = \alpha_H/22.7$

$^{#}$ based on observed values; $^S$ 25th percentile; $^*$ 75th percentile
References


