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Estimating transverse dispersivity based on hydraulic conductivity

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HIGHLIGHTS

- Transverse vertical dispersivity (TVD) is inversely proportional to hydraulic conductivity.
- TVD is also shown to be inversely proportional to effective grain size.
- A novel regression equation for estimating transverse vertical dispersivity is presented.
- New transverse vertical dispersivity values are calculated for previous studies.
- A previously published equation for estimating TVD when $v >$ critical velocity is validated.

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ABSTRACT

The modeling of depletion timeframe for a non-aqueous phase liquid (NAPL) layer is partially dependent on transverse vertical dispersivity. This paper provides guidance for estimating this parameter over the wide range of soil textures in which NAPL resides at contaminated sites. Transverse dispersivity is re-calculated for several previous NAPL dissolution studies based on a consistent methodology for estimating model input parameters. Through the compilation of a number of case studies from the literature including multiple NAPL dissolution experiments, the trend of transverse vertical dispersivity appears to be inversely proportional to the effective grain diameter when groundwater velocity (v) is below a critical threshold (v_c). A novel regression equation is derived for estimating transverse dispersivity based on hydraulic conductivity when $v < v_c$ and the NAPL length is on the order of meters. The critical velocity for NAPL pool dissolution appears to range from 3 to 5 m/d based on a limited number of studies with NAPL pool lengths of 1 m or more. The method derived by Klenk and Grathwohl (2002) is validated for estimating a correction factor for dispersivity when $v > v_c$.

1. Introduction

Sites with NAPL contamination may require expensive, long-term remediation, particularly when NAPL layers are present in the subsurface (Parker et al., 2003; Kavanaugh et al., 2013). The rate of dissolution from the surface of horizontal NAPL layers is proportional to transverse vertical dispersivity (Hunt et al., 1988; Johnson and Pankow, 1992), and this dispersivity

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may be dependent on groundwater velocity at some sites (Klenk and Grathwohl, 2002; Olsson and Grathwohl, 2007; Chiogna et al., 2010).

A wide range of transverse dispersivity (α_{TV}) has been cited in the literature. For example, Klenk and Grathwohl (2002) cite laboratory studies where with a range in α_{TV} from 0.05 to 1 mm. Schafer and Therrien (1995) calibrated a field-scale model simulating dissolution from NAPL using $\alpha_{TV} = 10$ mm. The wide range of α_{TV} in these studies indicates that there is relatively high uncertainty in this parameter, which contributes to substantial uncertainty in estimates of timeframes for NAPL depletion.

NAPL layers are formed at contaminated sites in a wide range of soil textures including silt, sand, or gravel; however, most of the work on estimating dispersivity in laboratory experiments has been conducted using medium to coarse sand or relatively large diameter spherical glass beads. There is a need to better understand how to estimate dispersivity for a wide range of soil textures and groundwater velocity at contaminated sites because these experimentally-derived dispersivity values are unlikely to be broadly applicable to field sites. It is typically assumed that transverse vertical dispersivity is directly proportional to the mean grain size, d_{50} [L] (de Josselin de Jong, 1958; Perkins and Johnston, 1963; Klenk and Grathwohl, 2002; Olsson and Grathwohl, 2007; Chiogna et al., 2010). As shown below, the proportionality of mean grain size is not representative of α_{TV} trends observed during experiments in sand with a broad range in grain and pore size.

A companion paper demonstrated that soil tortuosity correlates with hydraulic conductivity (Carey et al., 2016), and in some cases α_{TV} has been shown to be related to tortuosity (e.g. Klenk and Grathwohl, 2002). The objective of this study was to evaluate if α_{TV} may be correlated to hydraulic conductivity, given that K is commonly measured at contaminated sites. In response, a detailed literature review was conducted to tabulate results of previous laboratory experiments where estimates of vertical dispersion were available. In a number of cases, α_{TV} is re-analyzed in this present study using a consistent methodology for estimating the tortuosity coefficient (from Carey et al., 2016) and free-water diffusion coefficient (Hayduk and Laudie, 1974). A regression equation is derived based on the compiled dispersivity estimates from other studies, and compared to an earlier regression equation (Chiogna et al., 2010). Results of various NAPL pool dissolution studies are used to indicate a new lower limit for critical velocity (v_c) when NAPL pools are relatively long (e.g. greater than 1 m), and the sensitivity of pool depletion timeframe to critical velocity is discussed.

2. Background

Hydrodynamic dispersion represents the overall spreading of a contaminant plume along the direction of bulk groundwater flow and is comprised of two components: molecular diffusion and mechanical dispersion. Vertical dispersion transverse to the direction of flow is the driving process for mass dissolution from the surface of a NAPL pool. Transverse vertical dispersion is generally caused by deviations from the bulk groundwater flow direction due to tortuous flow paths, vertical heterogeneity, and diffusion between active flow channels.

Transverse vertical dispersion, or D_z [L^2/T] may be calculated using

$$D_z = \alpha_{TV} v + \tau D_o \tag{1}$$

where τ is the tortuosity coefficient [dimensionless], and D_o is the free-water diffusion coefficient [L^2/T]. The first term on the right side of Eq. (1) represents mechanical dispersion, and the second term represents the effective diffusion coefficient. Mechanical dispersion processes contributing to transverse vertical dispersivity include the effect of tortuous, or sinuous flow paths as well as molecular diffusion between streamlines. The latter component of mechanical dispersion is a physical mixing process. When groundwater velocity is below a critical threshold (v_c), this mixing process is complete and transverse dispersivity is mainly influenced by flow path sinuosity.

Transverse dispersivity tends to increase as the scale of contaminant migration increases, due to a corresponding increase in the vertical heterogeneity. Transverse dispersivity measured based on a large-scale field test (e.g. hundreds of meters) represents macro-scale field conditions; the transverse dispersivity which drives NAPL layer dissolution typically occurring over a scale of only meters will be smaller than the macro-scale dispersivity.

2.1. Factors influencing pore-scale transverse dispersion

For this study, pore-scale refers to a scale on the order of meters. Naturally-occurring in situ conditions which may influence local-scale α_{TV} include:

- When velocity is sufficiently high, there is insufficient time for diffusion to equalize concentrations within water flowing through a pore space, resulting in a reduction in the apparent dispersivity (after Perkins and Johnston, 1963; Klenk and Grathwohl, 2002). See below for a more detailed discussion regarding the influence of velocity on α_{TV};
- Well-graded soil with a broad distribution (i.e. large variance) in particle and pore size distribution will have higher dispersivity relative to poorly-graded (i.e. well sorted) soil (Perkins and Johnston, 1963; Nimmo, 2004);
- The dispersivity of a porous medium will increase as the tortuosity of the porous medium increases, which corresponds to a decrease in the tortuosity coefficient (τ). For example, Klenk and Grathwohl (2002) demonstrated that the transverse dispersivity in the capillary fringe is relatively high due to increased tortuosity resulting from the presence of entrapped air.