Solute transport characteristics of a deep soil profile in the Loess Plateau, China postprint

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Abstract

Understanding solute transport behaviors of deep soil profile in the Loess Plateau is helpful for ecological construction and agricultural production improvement. In this study, solute transport processes of a deep soil profile were measured by a conservative tracer experiment using 25 undisturbed soil cores (20 cm long and 7 cm diameter for each) continuously sampled from the surface downward to the depth of 500 cm in the Loess Plateau of China. The solute transport breakthrough curves (BTCs) were analyzed in terms of the convection-dispersion equation (CDE) and the mobile-immobile model (MIM). Average pore-water velocity and dispersion coefficient (or effective dispersion coefficient) were calculated using the CDE and MIM. Basic soil properties and water infiltration parameters were also determined to explore their influence on the solute transport parameters. Both pore-water velocity and dispersion coefficient (or effective dispersion coefficient) generally decreased with increasing depth, and the dispersivity fluctuated along the soil profile. There was a good linear correlation between log-transformed pore-water velocity and dispersion coefficient, with a slope of about 1.0 and an average dispersivity of 0.25 for the entire soil profile. Generally speaking, the soil was more homogeneous along the soil profile. Our results also show that hydrodynamic dispersion is the dominant mechanism of solute transport of loess soils in the study area.

Full Text

Preamble

Solute transport characteristics of a deep soil profile in the Loess Plateau, China

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Abstract

Understanding solute transport behaviors in deep soil profiles of the Loess Plateau is essential for ecological restoration and agricultural production improvement. This study investigated solute transport processes in a deep soil profile using a conservative tracer experiment with 25 undisturbed soil cores (each 20 cm long and 7 cm in diameter) continuously sampled from the surface to a depth of 500 cm in the Loess Plateau of China. The solute transport breakthrough curves (BTCs) were analyzed using both the convection-dispersion equation (CDE) and the mobile-immobile model (MIM). Average pore-water velocity and dispersion coefficient (or effective dispersion coefficient) were calculated using the CDE and MIM. Basic soil properties and water infiltration parameters were also determined to explore their influence on solute transport parameters. Both pore-water velocity and dispersion coefficient (or effective dispersion coefficient) generally decreased with increasing depth, while dispersivity fluctuated along the soil profile. There was a strong linear correlation between log-transformed pore-water velocity and dispersion coefficient, with a slope of approximately 1.0 and an average dispersivity of 0.25 for the entire soil profile, indicating that the soil became more homogeneous along the profile. Our results also demonstrate that hydrodynamic dispersion is the dominant mechanism of solute transport in loess soils of the study area.

Keywords: solute transport; loess soil; pore-water velocity; dispersion coefficient; hydraulic conductivity; Loess Plateau

1 Introduction

Solute transport represents a critical pathway for nutrient flow to plant roots and agrochemicals to groundwater (Shao et al., 1998; van der Zee and Leijnse, 2013). Understanding soil water and soluble substance behavior is vital for enhancing nutrient use efficiency and protecting shallow groundwater systems. However, field-scale soil solute transport is complex and influenced by hydraulic properties and soil heterogeneity (Huang et al., 1995; Seuntjens et al., 2002; Mallants, 2014). Consequently, both theoretical and experimental models have been developed to investigate solute transport behavior in soils (e.g., Tsuboyama et al., 1994; Seuntjens et al., 2002; Gao et al., 2010; Koestel et al., 2013; Venkatraman et al., 2014). Theoretically-driven mathematical models such as the convection-dispersion equation (CDE) can simulate non-reactive solute transport through saturated porous media under laboratory and field conditions (Lapidus and Amundson, 1952; Nielsen and Biggar, 1962). Additionally, the mobile-immobile model (MIM) can describe anomalous transport in heterogeneous porous media (van Genuchten and Wierenga, 1976).

Theoretical models are widely employed to conduct experiments on various aspects of solute transport in soils (Lennartz, 1999; Zhou et al., 2011; Chotpantarat et al., 2012). However, the well-controlled boundary conditions required for theoretical models are difficult to establish at the field scale. Undisturbed soil columns with well-preserved natural layers can provide valuable information on solute transport behavior at local scales (Seyfried and Rao, 1987; Mallants, 2014). While most undisturbed soil columns range from a few to several tens of centimeters in depth, some large columns can reach depths of 100 cm (Vanclooster et al., 1995; Garré et al., 2010).

The Loess Plateau of China contains the largest deposit of loess soil in terms of both area and depth and experiences the most severe soil and water loss, resulting in ecosystem degradation (Shi and Shao, 2000). Consequently, efforts have been made to investigate the spatial distribution of soil water and nutrients at various scales to restore and reconstruct degraded ecosystems (Fu et al., 2000; Gao et al., 2015; Li et al., 2015). Research on solute transport processes in Loess Plateau soils has focused primarily on repacked (Zhou et al., 2011) and undisturbed (Jiang et al., 2012; Yang et al., 2013) soil columns sampled from the surface to depths of less than 100 cm. Little research has examined solute transport behavior in deep soil profiles. Some studies focusing on hydrological properties of deep soil layers indicated that soil hydrological properties varied little at depths >500 cm (Wang et al., 2013; Li et al., 2016). Since solute transport depends largely on water movement, evaluating solute transport processes in soil profiles from 0–500 cm depth could have significant implications for soil nutrient management and groundwater quality protection.

In this study, we conducted a solute transport experiment using undisturbed soil cores collected in vertical succession from a deep soil profile in the Loess Plateau, and characterized the effects of soil properties and water infiltration parameters on solute transport processes. Parameters for water infiltration and solute transport breakthrough curves (BTCs) were determined under steady-state flow conditions. The BTCs were fitted using both the CDE and MIM. Basic soil properties were used to explain variations in solute transport processes along the soil profile.

2.1 Undisturbed soil core sampling

Undisturbed soil cores were collected from a corn field at Yangling (34°30 N, 108°07 E) situated in the Loess Plateau of China. The site has an annual mean temperature of 12.8°C and mean annual precipitation of 530 mm. The soil is classified as Lou soil (Eum-orthic Anthrosol according to Chinese Soil Taxonomy;

Wang et al., 2006). The undisturbed soil cores were collected from September 28 to October 2, 2017, when the corn was ripe and ready for harvest.

A soil pit (150 cm long, 100 cm wide, and 500 cm deep) was excavated, and one vertical face was smoothed with a shovel. Soil cores were sampled using a transparent acrylic cylinder (7 cm internal diameter, 24 cm height) with a 5 mm wall thickness and a sharp bottom edge for cutting through the soil profile. The cylinder was gently driven into the soil in 3-cm increments using a rubber hammer and then removed, with soil outside the cylinder scraped off. This process was repeated until the soil core reached approximately 20 cm depth, as measured by a tape attached to the cylinder wall. The soil core was then cut off and sealed at the bottom with filter paper, a perforated plate, and a lid with a drainage hole. The top end was plugged with soil in a plastic bag to prevent sample loss. A total of 25 undisturbed soil cores (20 cm long, 7 cm diameter) were collected from the surface to the smoothened face depth (0–500 cm) and transported to the laboratory.

2.2 Water infiltration and solute transport experiment

In the laboratory, soil cores were placed on custom-made shelves, with each core surface covered by filter paper to prevent crust formation during watering. Small sampling bottles were placed beneath the cores to collect drainage water. Deionized water was applied to the core tops using Mariotte bottles to maintain a constant water head, which was recorded for each core for subsequent calculations. The water table in the Mariotte bottle was measured to calculate infiltration rate at short intervals during the early period and longer intervals during the later period. The infiltration experiment was terminated when the wetting front reached the core bottom. The ponded water at the soil surface was then removed, and 0.2 mol/L NaCl solution was used as a tracer to seamlessly replace the deionized water. Subsequently, effluent was continuously collected in a 25 mL graduated cylinder at fixed intervals and titrated with 0.1 mol/L AgNO solution to determine Cl concentration until it approached 0.2 mol/L.

2.3 Soil property determination

To measure basic physical properties, an additional 50 undisturbed soil samples were collected from the same profile at 10-cm intervals adjacent to the soil cores using a cutting ring (5 cm diameter). Saturated hydraulic conductivity (Ks) was determined using the constant-head method. Soil samples were oven-dried at 105°C for 48 hours after Ks measurement to calculate soil water content and bulk density. Disturbed soil samples were also collected at the same depth intervals (10 cm) for particle size distribution analysis using the laser diffraction method.

2.4 Model description

The CDE and MIM were used to simulate solute transport processes. The one-dimensional equilibrium CDE is given by Equation 1 (Lapidus and Amundson, 1952):

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x}$$

where R is the retardation factor; C is the resident concentration (g/cm³); t is time (min); D is the dispersion coefficient (cm²/min); v is the pore-water velocity (cm/min); and x is distance (cm). For non-reactive tracers, R equals 1.0.

The MIM for non-equilibrium transport, given by van Genuchten and Wagenet (1989), is expressed as follows (Eqs. 2 and 3):

$$\theta_m\frac{\partial C_m}{\partial t} + \theta_{im}\frac{\partial C_{im}}{\partial t} = \theta_m D_m\frac{\partial^2 C_m}{\partial x^2} - \theta_m v_m\frac{\partial C_m}{\partial x}$$

$$\theta_{im}\frac{\partial C_{im}}{\partial t} = \alpha(C_m - C_{im})$$

where is volumetric soil water content (%); is the first-order mass transfer coefficient (min ¹); and subscripts m and im refer to mobile and immobile regions, respectively.

The measured BTCs were fitted to the CDE and MIM to estimate solute transport parameters using the CXTFIT non-linear fitting procedure (Toride et al., 1995). The effective dispersion coefficient (Deff) was derived from Equation 4 and introduced in the MIM to compare solute transport parameters between CDE and MIM (van Genuchten and Dalton, 1986):

$$D_{eff} = D_m + \frac{\alpha\theta_{im}}{\theta^2}v^2$$

where the first term on the right side of Equation 4 denotes hydrodynamic dispersion in the mobile phase, and the second term reflects source-sink effects of solute transfer into and out of immobile regions.

2.5 Data analysis

Solute transport parameters were estimated using the CXTFIT computer program (Toride et al., 1995). Figures were plotted using Sigmaplot 12.5 (Systat Software Inc., UK).

3.1 Soil profile properties

Soil bulk density along the profile ranged from 0.91-1.35 g/cm³, with an average of 1.10 g/cm³ (Fig. 1a [Figure 1: see original paper]). The average bulk density in the 0-20 cm layer was 1.29 g/cm³, similar to values reported for undisturbed Loess Plateau soils by Jiao et al. (2011). Soil compaction initially decreased then increased from the top to the bottom of the profile. Wang et al. (2008) observed bulk density distribution in the 0-100 cm loess soil profile and found that the 10-20 cm layer (the so-called plow pan) exhibited the highest compaction.

The vertical distribution of initial gravimetric water content is shown in Figure 1b. Soil moisture decreased with depth in the surface 0-20 cm layer, then increased with depth in the 20-100 cm layer. Below 100 cm, soil moisture decreased slowly with increasing depth, with no significant differences between individual layers except for the 390-400 cm layer (which may be due to measurement error). Generally, shallow soil layers had low moisture due to evaporation (Heathman et al., 2003; Wang et al., 2008). The relatively high moisture in the surface layer in this study may be attributed to soil sampling following low precipitation events.

Clay content initially increased then decreased with depth (Fig. 1c), with maximum values observed in the 30-40 cm layer. Soils with high clay content typically have high water retention capacity, suggesting that water content in the surface layer was strongly influenced by climatic and vegetation conditions in the study area.

3.2 Water flow characteristics

The final infiltration rate for each soil core is shown in Figure 2 [Figure 2: see original paper]. No effluent was collected from soil cores in the 360-380 cm layer after 30 days of water application; therefore, the infiltration rate for this layer was assumed to be zero. Figure 2 demonstrates that soil columns above 200 cm depth had greater infiltration capacity than those below 200 cm. Compared with infiltration rates reported by Wang et al. (2008), this study showed markedly higher rates for the 100-200 cm layer, which may be explained by macro-pores in this layer, particularly with local peak values at 60-80 cm depth. However, Kang et al. (2002) observed a much higher infiltration rate of 0.16 cm/min for the 0-60 cm layer in a winter wheat field in the southern Loess Plateau, and Zhou et al. (2010) reported an infiltration rate of 0.12 cm/min for the 0-10 cm layer in the northern Loess Plateau. These discrepancies may be due to differences in land use and vegetation types.

Vertical variations in Ks along the profile (Fig. 3 [Figure 3: see original paper]) indicated low values in both the 0-200 cm and 350-500 cm layers. Relatively high Ks values in the 200-350 cm layer and at 480 cm depth may be attributed to large soil pores. The differences between final infiltration rate and Ks distributions reflected high spatial variability of soil water infiltration in the study area.

3.3 Solute transport processes

Coefficients of determination (R^2) for BTC curve fitting using both CDE and MIM exceeded 0.9, indicating reliable fitting results. Average pore-water velocity was independently estimated and plotted in Figure 4a [Figure 4: see original paper], showing a general decreasing trend with depth. Average pore-water velocity was higher in soil cores from 0-200 cm depth than from 200-500 cm depth, consistent with the final infiltration rate distribution. Pore-water velocity varied dramatically in the 0-200 cm layer but was distributed uniformly in the 200-500 cm layer, except for the deepest 20 cm. As reported by Mallants et al. (1994), near-surface soils are more heterogeneous.

Mobile-phase velocity (vm) was obtained using the MIM (vm = v/(m/), where vm is mobile-phase velocity (cm/min), v is average pore-water velocity (cm/min), is volumetric soil water content (%), and subscript m refers to the mobile region). The distribution of mobile-phase velocity along the profile is plotted in Figure 4b [Figure 4: see original paper]. High values at 100, 200, 420, and 460 cm depths may be due to very low mobile water fractions, where nearly all water was immobile. Excluding these cases, mobile-phase velocity was less variable than pore-water velocity. Generally, mobile-phase velocity decreased with increasing depth and became nearly constant from 220 cm to 360 cm depth.

Both dispersion coefficient and effective dispersion coefficient were generally larger in shallow than in deep layers (Fig. 5 [Figure 5: see original paper]). The dispersion coefficient varied considerably at 0-200 cm depth but became nearly constant at 200-500 cm depth, except in the deepest layers. Upper profile soils generally had higher porosity and looser structure, facilitating solute transport. Deep soils were more compact, causing high tortuosity in solute transport pathways. Similarly, large dispersion coefficient values for soil cores in the 480-500 cm column were due to macro-pores that could enhance water mobility. Generally, dispersion coefficient is proportional to pore-water velocity, so increases in pore-water velocity result in increased dispersion coefficient. This relationship was observed in this study, where both parameters were high at 0-200 cm depth.

Comparison of dispersion coefficients from CDE and MIM (dispersion coefficient and effective dispersion coefficient, respectively) showed that CDE-derived values were sometimes larger than MIM-derived values, as expected because solute exchange in MIM is equivalent to dispersion in CDE (Wang and Shao, 2007; Zhou et al., 2011). Therefore, the dispersion coefficient fitted by MIM accounted only for hydrodynamic dispersion. However, effective dispersion coefficient values at 160 and 240 cm depths were larger than corresponding dispersion coefficient values due to solute exchange between mobile and immobile regions, which could result in relatively long solute travel distances requiring larger effective dispersion coefficients.

Solute transport in structured soils can approach equilibrium CDE when local equilibrium assumptions are met (Parker and Valocchi, 1986). With low pore-water velocity, mean residence time exceeds the characteristic time for solute exchange between mobile and immobile phases, improving the validity of local equilibrium assumptions for compact soils. In this study, close agreement between dispersion coefficient and effective dispersion coefficient for soil cores from 240–460 cm depths indicated that deep soil layers were largely homogeneous. Soil bulk density increased downward from 200 cm depth (Fig. 1), indicating that deep soils are more compact than shallow soils. For deep soil cores (200–500 cm), solute transport could be described by the CDE model due to soil compaction.

In this study, estimated dispersion coefficient values increased with pore-water velocity ($R^2 = 0.84$, $P < 0.01$). For each soil core, dispersivity (, cm) described the relationship between pore-water velocity and dispersion coefficient (= D/v, where D is dispersion coefficient (cm^2/min) and v is pore-water velocity (cm/min)). Calculated dispersivity fluctuated along the profile, ranging from 0.16–5.31 cm with an average of 1.61 cm. Dispersivity is generally considered characteristic of the entire medium (Bear, 1972), with typical values of 0.1–2.0 cm for repacked homogeneous soil columns, one to several times higher than those for heterogeneous columns (Huang et al., 1995).

Pore-water velocity and dispersion coefficient values for all soil cores were combined to evaluate their relationship across the entire profile using a linear regression equation (Eq. 5):

$$D = \lambda v^n$$

where n is an empirical parameter, typically in the range of 1–2 (Saffman, 1959; Beven et al., 1993).

Log-transformed pore-water velocity and dispersion coefficient showed a strong linear correlation (Fig. 6 [Figure 6: see original paper]). Dispersivity ( ) and exponent (n) values were determined from the regression between log-transformed parameters. Combining all soil cores yielded ensemble mean values of 2.25 cm for dispersivity and 1.1561 for the exponent. Such small dispersivity values for undisturbed soil columns were also compiled by Jury (1985) and observed by Mallants (2014), likely reflecting the relatively homogeneous nature of the loess soil profile, particularly in deeper layers. The exponent value near 1.0 indicates that hydrodynamic dispersion is the primary solute transport process in the study area. A similar exponent value (n = 1.2) was observed by Jaynes et al. (1988) in a bromide leachate experiment under continuous flood conditions. Due to soil heterogeneity, correlations between vertical distributions of solute transport parameters and soil properties were not conclusive. However, the above discussion suggests that spatial fluctuations in solute transport parameters can be qualitatively explained by specific soil physical properties.

4 Conclusions

A conservative tracer experiment was conducted to characterize solute transport processes in a deep loess soil profile (0–500 cm depth) in the Loess Plateau. Average pore-water velocity was determined independently from the experiment, and dispersion coefficients were calculated by fitting the CDE and MIM to solute concentration versus time data. The final infiltration rate initially increased then decreased with depth, showing a negative correlation with soil bulk density. BTC data for all soil cores could be explained by both CDE and MIM.

Measured pore-water velocity had larger values in shallow soil layers, with fluctuations driven by macro-pores. Both dispersion coefficient and effective dispersion coefficient generally decreased with depth, except in a few layers. Close agreement between the two parameters below 200 cm depth indicated that deep soil layers were largely homogeneous. Dispersivity varied considerably across the entire profile and had a smaller magnitude than typical values reported for some soil cores. Log-transformed pore-water velocity and dispersion coefficient exhibited a linear correlation, indicating relatively homogeneous soil. Our results further demonstrate that hydrodynamic dispersion is the main spreading mechanism for solute transport in loess soils of the study area.

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Note: Figure translations are in progress. See original paper for figures.