

A REVIEW OF SOLUTE TRANSPORT MODELING IN SOILS AND HYDRODYNAMIC DISPERSIVITY

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Abstract. The knowledge of solute transport process in the porous media has an important role for addressing chemical pollution, loss of nutrients, groundwater contaminating rate and drainage water quality. The aim of this paper was to review the hydrodynamic dispersivity parameter and the models of dispersion - mass and stochastic to evaluate the solute transport process in soils. Solute transport models, convective - dispersive Equation (CDE) and convective lognormal transfer (CLT) are fitted to experimental breakthrough curves (BTC's) and solute transport parameters are estimated. It should be investigated which of the CDE or CLT model explain the BTCs more reliably. The review indicates that the soil physical properties and experiment conditions can determine the appropriate model that characterizes the BTCs. The travel time distribution and the variance of solute molecule velocities vary with flow rate. Mohammadi and Vanclooster (2012) indicated that the mean solute travel time, μ_t , increases partially with the travel distance and decreases with the flow rate. The review shows that the mean travel time distribution depends on the flow rate. Generally, well - controlled solute transport experiments on soils are essential to the knowledge of the solute transport processes and parameters for different flow rates and soil types.

Keywords: Solute transport, breakthrough curve (BTC), convection dispersion model (CDE), convective lognormal transfer (CLT)

Abbreviations			
<i>CDE</i>	convection dispersive equation	<i>BTC</i>	break thorough curve
<i>C</i>	solute concentration (ML^{-3})	<i>D₀</i>	molecular diffusion coefficients
<i>V_m</i>	pore water velocity (LT^{-1})	<i>pdf</i>	probability density function
<i>t</i>	time (T)	<i>D</i>	hydrodynamic dispersion coefficient (L^2T^{-1})
<i>z</i>	distance from the top boundary in the direction of flow (L)	<i>V</i>	is average pore water velocity (LT^{-1})
<i>E_x</i>	mean of the travel time distribution at any distance of x	μ	geometric mean of the solute travel time
<i>Var_x</i>	variance of the travel time distribution at any distance of x	<i>CD</i>	convective - dispersive
<i>SC</i>	stochastic - convective	<i>CLT</i>	convective lognormal transfer
μ_{sa}^2	Mean of solute particle immigration distance	λ	hydrodynamic dispersivity coefficient (L)
σ_{sa}^2	standard deviation of solute particle immigration distance	σ^2	geometric variance of solute travel time

INTRODUCTION

Arid and semi-arid regions are facing soil salinization and the lack of water resources. Information is scarce about the soil solute transport for efficient soil and water management. The behavior of solutes and cations under various climate and soil conditions can be assessed using models that simulate solute transport (Haghighi-Fashi and Ejlali, 2015). Solute transport in soil is affected by a large number of physical, chemical, and microbial soil properties. The solute transport in the porous media is a key factor in soil

physics for understanding root zone leaching rate and addressing chemical pollution, loss of nutrients, groundwater contaminating rate, the salt distribution profiles and drainage water quality (Nimbi et al., 2003). Concern about soil and water pollution has led to several studies focused on water and solute transport processes in soil.

Solute transport models

There are several mathematical models applied to predict solute transport in soil. Among these models, convection dispersive equation (CDE) has been widely used to estimate solute transport. For one-dimensional steady-state flow and for a neutral tracer, CDE is given by (Fried and Combarnous, 1971):

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial z^2} - V \frac{\partial c}{\partial z} \quad (1)$$

where c is the solute concentration (ML^{-3}), t is time (T), z is distance from the top boundary in the direction of flow (L), D is hydrodynamic dispersion coefficient (L^2T^{-1}), and V is average pore water velocity (LT^{-1}).

According to CDE, the probability density function (pdf) of travel time of solute particles is defined as follows (Jury and Roth, 1990):

$$f(z,t) = \frac{z}{2\sqrt{\pi Dt^3}} \exp\left[-\frac{(z-Vt)^2}{4Dt}\right] \quad (2)$$

In this function, the mean (E_x) and variance (Var_x) of the travel time distribution at any distance of x from the desired depth is given by:

$$E_x(t) = \frac{x}{z} E_z(t) \quad \text{or} \quad E_x(t) = \frac{x}{V} \quad (3)$$

$$\text{Var}_x(t) = \frac{x}{z} \text{Var} E_z(t) \quad \text{or} \quad \text{Var}_x(t) = \frac{2Dz}{V^3} \quad (4)$$

Eq.(4) shows that the expected mean time is independent of D and the variance of travel time scales linearly with depth. The basic assumption of this model is homogeneous and steady-state conditions with complete solute mixing regime. In the past decades, a number of experiments have examined the validity of the CDE model to quantify solute transport in soil media in the laboratory and the field (Rao et al., 1980; Li et al., 1994). Despite many studies on solute transport field, there are limitations such as narrow range of velocity and experimental conditions (Shukla et al., 2002). Some researchers have tried to change the model adapted for transient conditions (Vanderborght et al., 1997) or non-homogeneous soils (Steenhuis et al., 2001) and eventually using the model to predict the natural soil behavior. Due to the spatio-temporal variability of soils and faults of the above models for estimating solute transport in soil, as an alternative, the researchers have tried to use the transfer functions. Transfer functions are used to model the output flow characteristics as a function of input flow properties (Himmelblue, 1970). One of the most important transfer functions is statistical or stochastic - convective (SC) method.

Mohammadi and Vanclooster (2011) investigated the flow rate dependency to the solute transport within an undisturbed Inceptisol core. They found that the flow regime was

partially as stochastic - convective (SC) at high flow rates and convective - dispersive (CD) at low flow rates. Results of their study demonstrated that the mixing of solutes decreases with an increase in flow rate, due to the reduced tortuosity of solute flow paths.

In SC process, the transport distances of a solute particle at a constant time, t , is described as follows:

$$z = vt \quad (5)$$

Since the velocity (v) is variable, the distance distribution at any time is given by:

$$f(Z) = f(vt) = \frac{1}{t} f_v\left(\frac{z}{t}\right) \quad (6)$$

Where is the spatial distribution of the velocity. Eq. (6) describes the distribution of solute transport distance. The mean, μ_{sa}^2 , and standard deviation, σ_{sa}^2 of solute particle immigration distance at any time are defined as function of time (Jury & Roth, 1990):

$$\mu_{sa} = \int z f(z) dz = \int z \frac{1}{t} f_v\left(\frac{z}{t}\right) dz \quad (7)$$

$$= t \int v f_v(v) dv$$

$$= t \mu_v \quad (8)$$

$$Q_{sa}^2 = \int z^2 f(z) dz - \mu_{sa}^2 = \int z^2 \frac{1}{t} f_v\left(\frac{z}{t}\right) dz - \mu_{sa}^2$$

$$= t^2 \int v^2 f_v(v) dv - (t \mu_v)^2 = t^2 \left(\int v^2 f_v(v) dv - \mu_v^2 \right)$$

$$= t^2 \sigma_v^2$$

where the μ^2 and σ^2 are the mean and standard deviation of solute particle immigration distance at reference time. Jury (1982) has defined the pdf of convective lognormal transfer (CLT) model as:

$$f_f(z,t) = \frac{1}{\sqrt{2\pi\sigma_1 t}} \exp \left[-\frac{(\ln(t/z) - \mu_1)^2}{2\sigma_1^2} \right] \quad (9)$$

where μ is geometric mean of the solute travel time, σ^2 is the geometric variance of solute travel time, and t is time of solute transport.

The CLT model (Jury and Scotter, 1994) can be employed for different solute concentrations and boundary and initial conditions. Later, the transformed depth coordinates in the CLT model was introduced by Ellsworth and Jury (1991). Then, Vanderborght et al. (2001) estimated the apparent dispersivity and variance of the pore water velocity in undisturbed condition of lysimeters. Estimating the apparent dispersivity was done successfully for a wide range of soil types, but their approach was not able to explain the

dependency of apparent dispersivity to the flow conditions (i.e. the flow rate). Subsequently, Mohammadi and Vancllooster (2012) presented a conceptual approach to model the geometric mean travel time of solute transport using the CLT model resulted from the soil moisture characteristic (SMC) knowledge, parameterized using the Kosugi model (1996). The above mentioned approach is further validated on a set of solute transport experiments (Mohammadi and Vancllooster, 2011). Mohammadi and Vancllooster (2012) showed that the mean solute travel time, μ_t , increases partially with the travel distance and decreases with the flow rate. They found that the variance of solute travel time σ^2_t is decreased with the flow rate up to 0.4 - 0.6 Ks and subsequently increased.

In CLT model, it is assumed that the travel time variance of solute transport increases as quadratic with distance, whereas in CDE models, this increase is linearly. Therefore, the change rates of travel time variance of solute transport with distance determines that if the flow type is CDE or SC (Jury and Roth, 1990). The solute transport studies have shown that CDE model is well adapted for the solute transport in small scale laboratory columns and in contrast, the transport in lysimeter scale (Vanderborgh et al., 1997) and the field scale (Jury and Flühler, 1992) is better modeled with the CLT model, specially where the distances from the soil surface becomes larger (Jury et al., 1982).

Hydrodynamic dispersivity

According to CDE, hydrodynamic dispersivity coefficient, $\lambda(L)$ is defined as:

$$\lambda = \frac{D}{V} \quad (10)$$

The $\lambda(L)$ describes the mixing regime in soils (Vanderborgh et al., 2001). The $\lambda(L)$ is an important parameter to describe the solute transport in porous media (Javaux and Vancllooster, 2003). However, the relations between this parameter, experimental conditions, and soil characteristics for different flow regime are not still well known. Hydrodynamic dispersivity depends on the flow conditions and is not constant in the porous medium (Javaux and Vancllooster, 2003).

Vanderborgh and Vereeken (2007) found that the soil texture has no significant effect on hydrodynamic dispersivity coefficient (λ) obtained from soil leaching experiments, whereas, interactions of soil texture, soil experiment scale, and flow rate on λ is significant. For unsaturated regime, λ distribution is not dependent on flow rate in coarse-textured soils, but is increased with flow rate in fine-textured soils. The soil matrix pores are small in fine-textured soils and therefore, the soil matrix has a low hydraulic conductivity. With increasing flow rate, conductivity of inter - aggregates pores and thus, λ increases.

Solute transport may be simulated by knowledge of the saturated hydraulic properties. This agrees with previous studies representing that solute transport properties are related to soil saturation degree or water content (Bejat et al., 2000; van Genuchten et al., 1977), pore size distribution (Li and Ghodrati, 1997), and particle size distribution (Nielsen and Bigger, 1961). Mohammadi et al. (2009) indicated that the knowledge of soil hydraulic properties in small scale homogeneous soil cores under saturated conditions can help to predict the solute BTC.

Shukla et al. (2003) investigated the effects of soil texture and flow rate on solute transport in undisturbed and saturated soil columns with sandy loam and loam textures. They concluded that the two-parameter global dispersion relationship ($D = \lambda V_m + D_0$) well expresses the dispersion process for loam soil, while the single global parameter ($D = \lambda V_m$) is more appropriate for sandy soil. Parameters D , D_0 , and V_m are the apparent diffusion coefficients, the molecular diffusion coefficients and the pore water velocity, respectively.

They observed that the fitted λ is independent of V_m and mixing length and also D is independent of V_m in the low velocity rate, although it was obtained a linear relationship between fitted D and V_m for velocity rates less than 0.1 cm h^{-1} .

Vanderborght et al. (2001) investigated the relationship between soil properties, experimental conditions, and solute transport and found that the dispersivity was increased in all the soils with an increase in leaching rate. Ingrid et al. (1999) found a power law relationship between dispersion and water content velocity. They reported that the dispersivity is a function of the both soil media properties and water content. Javaux et al. (2006) found that the identification of micro heterogeneity is required to predict the flow rate dependency of the solute transport processes. Soil texture affects the soil break through curve (BTC) shape. Sandy soils have a more symmetrical BTC, whereas BTC is asymmetric for clay and loam soils (Gonzalez and Ukrainczyk, 1999). BTC symmetry increases in coarse-textured soils with an increase in flow rate. In clay soils having a loose structure, the flow velocity is low (mixing time is large) and then, the solute mixing will be increased. In fine-textured soils, stagnant water leads to a high mixing, low slope BTC and a poor leaching. Krupp and Elrick (1986) found that the λ parameter depends highly on soil moisture content.

Wilson and Gelhar (1974) have demonstrated a 10-fold increase in longitudinal λ with the reduction of soil moisture from saturation. With increasing flow rate, the pore domain contributing into solute transport increases and thus, the variance of solute mixing time will be increased and λ diminished (Vanderborght et al., 1997). An increase in soil moisture content associated with a higher flow rate can cause the reduced tortuosity or shorten flow paths and thus, the reduced arrival time distribution domain of solutes and diminished λ (Maciejewski, 1993). Khan and Jury (1990) reported an increased D with the depth when high flow rates were imposed. In contrast, they observed a constant D for lower flow rates. In unsaturated soils, hydrodynamic dispersivity variation is more complicated than that in saturated soils (Javaux and Vanclooster, 2003; Javaux et al., 2006).

Soil saturation degree has a high effect on dispersivity. The greater λ in leaching experiments (for saturated soil surface conditions) reflects the significant effect of flow and transfer through macro - pores, which are active under saturated conditions (Vanderborght and Vereecken, 2007). Brunsriet al. (2008) showed that the λ increases pronouncedly with soil moisture content of unsaturated soils. However, they found that the maximum λ is obtained in unsaturated soils, 1.13 cm for sandy soil and 1.35 cm for loam in water contents of 0.13 and 0.20, respectively. Maximum λ in sandy soil was less than that in loam. This indicates that the loam soil has more dispersivity than sandy soil and thus, λ is higher due to the finer texture. The effect of flow rate and heterogeneity of the porous medium on governing transport and mixing regime is sophisticated to estimate (Ursino and Gimmi, 2004; Mohammadi and Vanclooster, 2011). Thus, there is a need to knowledge of governing transport concept and evaluate the solute transport parameters for different flow rates and soil types. Performing well-controlled transport experiments on undisturbed soils (e. g. at the core or lysimeter scale) is essential to control the boundary conditions. In recent years, many attempts have been made to understand the mechanism of water and solute transport in the agricultural fields. To prevent the pollution and estimate the risk caused by contaminants, it is essential the knowledge of the governing processes of solute transport from the soil surface into the soil root zone and eventually into the groundwater. Therefore, the solute dispersion into the soil should be concerned. The present paper reviews solute dispersion and the CDE and SC models to apply for solute transport processes.

SOLUTE TRANSPORT

Soil BTCs are obtained at different flow rates and the models are fitted to the experimental BTCs to investigate which of the models is suitable to describe the solute diffusion process. It should be assessed which of the CDE model and CLT model assumptions have a more accuracy in soil condition, considering the assumption of complete mixing regime of the solutes in CDE model. Shukla et al. (2003) found that the CDE model is better modeled in homogeneous soils. This finding is partially consistent with observation of Mohammadi and Vanclouster (2011) who demonstrated that the CDE provides an appropriate fitting to the experimental BTCs at low flow rates. In addition, Bejat et al. (2000) reported a well fit of the CDE model with a mean R^2 between 0.72 and 0.99 in undisturbed soils. Zhang (1994) demonstrated that the flow regime is CDE in disturbed and saturated homogenous soils. It seems that the validity of the CDE dispersion model for saturated and homogeneous soils, across a wide range of pore water velocity that is found by Shukla et al. (2003). Shukla et al.(2003) reported that the variability between BTCs may be resulted from the measured water content and average pore water velocity. It seems that for choosing the suitable model describing solute transport, soil physical condition is more effective factor than the experimental conditions in consistent with earlier finding of Bejat et al. (2000) and Krupp and Elrick (1968) who observed that solute transport properties are affected by soil hydraulic and physical properties.

THE CLT MODEL PARAMETERS AS A FUNCTION OF FLOW RATE

The mean travel time. Mohammadi and Vanclouster (2012) found that the geometric mean of solute travel time μ_t , increases proportionally with the travel distance and decreases with the flow rates. In addition, they indicated that the σ_t , first, decreases with flow rate and finally, rises to reach the saturated condition.

The variance of travel time. The lower water content may lead to increase the velocity variations and reduce solute mixing. Hence, solutes must travel a longer distance to achieve better mixing (Ingrid et al., 1999). Mohammadi and Vanclouster (2011) found that the mixing of solutes reduced when the flow rate increased, due to the decrease of the tortuosity of the solute flow paths. Since that the water velocity in macro - pores is high, so the variance of solute travel time distribution may be increased. Some researchers believe that the U-shaped change in solute transport variance with the flow rate is due to the heterogeneous nature of soil (Javaux et al., 2006). The effect of tortuosity of the solute flow path, as one of the factors involved in hydrodynamic dispersivity depends on the solute flow rate. Maraqa et al. (1997) reported that the tortuosity of the water flow paths has reduced with an increase in soil water content, reducing mixing of the solute.

Changes of hydrodynamic dispersivity coefficient with the flow rate. The relationship between the water flow rate, q , and hydrodynamic dispersivity coefficient, λ , needs to be assessed. In general, the dispersivity may be flow rate dependent according to Vanderborght et al. (2001) finding who found the dispersivity is not an intrinsic soil property. The dispersivity may be varied with changes in soil texture according to the observations of Vanderborght and Vereecken (2007). In addition, hydrodynamic dispersivity depends on the flow conditions and is not constant in the porous medium (Javaux and Vanclouster, 2003). As the flow rate is increased, the soil pore domain contributing into solute transport increases and therefore, the variance of solute mixing time will be increased and λ diminished (Vanderborght et al., 1997). The higher flow rate can cause the reduced

tortuosity or shorten flow paths and thus, the reduced arrival time distribution domain of the solutes and reduced λ (Maciejewski, 1993).

The dispersion coefficient is influenced by pore water velocity, which is a function of porous media properties and water content (Padilla et al., 1999; Toride et al., 2003; Costa and Prunty, 2006). The dispersivity of the soil under unsaturated conditions may be higher than dispersivity in near saturation (Maraqa et al., 1997). A review of dispersivity provided by Vanderborght and Vereecken (2007) demonstrated that for the short travel distance (0 to 30 cm), the dispersivity was increased clearly with increasing the flow rate. However, this increase was not occurred for long travel distance. They observed that dispersivity was increased with an increase in flow rate in fine - textured soils and decreased in coarse - textured soils. Vanderborght and Vereecken (2007) reported that the dependency of dispersivity on the flow rate is more in fine - textured soils than the activity of large interaggregate pore spaces. Mohammadi and Vanclouster (2011) observed that the activation of macro - pores and large interaggregate pores in fine-textured soils may explain the increased dispersivity with increasing flow rate, but not in soils with a coarser texture.

In general, flow rates and heterogeneity of the porous medium affect the mixing regime, but the effect of heterogeneity and flow rate on governing solute transport regime is complicated (Ursino and Gimmi, 2004).

CONCLUSION

To identify the mixing regime of solute in soils, two solute transport models, CDE and CLT are fitted to experimental BTC's and solute transport parameters are estimated. The review demonstrates that the soil physical properties and experiment conditions are important factors to determine the appropriate model characterizing the BTCs and solute flow regime. The validity of the CDE and CLT model for different conditions (e.g. saturated or unsaturated condition, range of pore water velocities, and soil texture needs to be evaluated. The review indicates that the σ depends on the flow rate and mean travel time distribution varies with the flow rate. In general, the dispersivity is flow rate dependent. Therefore, well-controlled solute transport experiments on soils are essential to the knowledge of the solute transport processes and parameters for different flow rates and soil textures.

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