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Comparison of Numerical and Analytical Solutions for Breakthrough Curve Modeling

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ORIGINAL ARTICLE

ABSTRACT: Study of contaminant transport in soil is of primary importance from a various environmental points of view. A modeling study is reported here for simulation of bromide transport. Four soil samples including disturbed and un-disturbed clay-loam and sandy-loam soil were analyzed through bromide injection and modeling contaminant breakthrough curve. Analytical and numerical solutions were applied through using CXTFIT and HYDRUS models, respectively, and compared to simulate the mechanism of bromide transport. The obtained results reveal that the analytical solutions offer more accuracy than the numerical solutions for modeling contaminant transport. This may be attributed to the simplifications of the numerical solutions.

Keywords: breakthrough curve, HYDRUS, CXTFIT, modeling

INTRODUCTION

Contaminant transport in the soil and its modeling is an issue that has been widely considered in recent years and many studies have been performed on it. In fact, contaminant transport, pesticides, chemical fertilizers and, generally, studying the process of transportation of all pollutants to either surface water or groundwater through agricultural, industrial, residential and other types of land, is an very important issue for studying and adjustments of the agricultural management approaches and groundwater pollution control (Lee et al., 2001). Therefore, sediment transportation models have many applications in studying the mechanism of nutrients and pollutants transport and leaching in soils. Practical application of these models can simplify and decrease volume of computations, laboratory costs and increase work speed. Knowing the characteristics of flow in soil pores is necessary for proper management and use of fertilizers, and prevents rapid transport of nutrients which cause loss of fertilizer and groundwater pollution (Constantinos et al., 1990).

Soil structure directly affects many of physical characteristics of soil including specific retention, hydraulic conductivity and nutrients transport. Weak soil structure causes a decrease in plant's available water since lack of aviation in humid condition and increased resistance against infiltration in dry condition, put a limit on plant growth (Campbell, 1988). Most of Sand, loam, and sand-loam soils which are in coarse soils category have no structure or a fragile structure (Nadler et al., 1996).Mentioned specifications and characteristics, require special fertilizing management to lessen nutrients loss. To the best of the authors' knowledge, there are no corresponding studies regarding the comparison of HYDRUS with CXTFIT for modeling bromide in the soils.

MATERIALS AND METHODS

HYDRUS-1D model

HYDRUS-1D model is a developed numerical model of 1D transport of water, nutrients and heat in the soils. This model can simulate saturated and unsaturated conditions and estimate soil characteristics by reverse method (Vrugt et al., 2001). Most of groundwater pollution problems are due to synchronous process of water and nutrients flow, heat transfer and bio-geo-processes.

Based on this process, models can act as valuable tools for studying transportation of a wide ranged organics and minerals in different hydrologic and geochemical conditions (Jaqcues et al., 2008).

CXTFIT model

CXTFIT model can estimate parameters of different pollution transport in 1D uniform flow prediction models using observed data of lab or field experiments through analytical solution. This model can solve various transport-dispersion relations in different initial and boundary conditions using analytical solutions (Simunek et al., 2003).

Application

We took poly-ethylene (PVC) pipes with diameter and height of 10 and 40cm, respectively. To facilitate penetration of pipe in soil, the soil around the pipe was removed frequently while the pipe was penetrating and its entrance was covered with a lace to prevent soil breakage to the pipe. Then PVC pipes together with undisturbed soil were pulled from bottom and taken. The same way was followed to prepare the disturbed column and after

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gathering the soil from the field, he sample was aviated and condensed normally.

Prepared soil columns (disturbed or undisturbed) were connected to Marriott tank for leaching with 0.01 molar CaCl2 solution. The bottom of the soil column was fixed with scotch and screen and their function is holding soil column and preventing soil particles wash out. The Screen pores were big enough to avoid limiting flow. A constant head of 10 cm was considered above each column to fulfill the saturation condition. Exit location is adjustable and its height is adjusted based on required flow. First, columns were gradually saturated form below with 0.01 molar CaCl2 material solutions.

After cutting material solution flow, 1 liter CaBr2 0.01 molar (C0) solutions were injected immediately as pulse to columns. Then CaCl2 0.01 molar flows injected to the columns again, and Bromide concentration (C) of drained water was measured after injection in 5-15 min periods and.

This process was continued until reaching constant Bromide concentration in the drained water. Measured concentrations converted to relative concentration (C/C0) and infiltration curves were achieved by plotting (C/C_0) against (t) or pore volume (Pv). Each pore volume (Py) is total occupied pores bye fluid in soil column and is calculated by the following relation:

$$P_v = \theta_s \times V_t \qquad (1)$$

Where P_v in cm^3, θ_s is volume of saturated moisture in cm^3/ cm^3 and V_t is soil column bulk density cm^3. Number of pore volume is derived by dividing drained solution by P_v.

Measuring Bromide concentration (Br) in exit solution was done using a PH meter gauge equipped with Bromide selector electrode made by Crison co,Spain. Bromide concentration measuring domain of this gauge is from 1 micromole per liter to 1 mol per liter, and temperature of 0 to 500°C and measurement balance time of one minute. The gauge calibrated using Bromide standard solutions with concentrations of 10-1, 10-2, 10-3, 10-4, 10-5 mol/liter and prepared for measuring Bromide ion during substitution of bromide solution pulse.

RESULTS AND DISCUSSIONS

Model evaluation

Three statistical parameters were applied here for evaluating the applied models' performances, namely coefficient of determination (R^2), root mean square error (*RMSE*) and scatter index (*SI*), expressions for which are as follows.

$$R = \frac{\sum_{i=1}^{N}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{N}(x_i - \bar{x})^2 \sum_{i=1}^{N}(y_i - \bar{y})^2}} \qquad (2)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_i - x_i)^2}{N}} \qquad (3)$$

$$SI = \frac{RMSE}{\bar{x}} \qquad (4)$$

Where, x_i is the value observed at the *i*th time step, y_i is the corresponding simulated value; N is number of time steps, $\bar{x}$ is mean of observational values and $\bar{y}$ is mean value of the simulations.

Sensitivity analysis of HYDRUS-1D model

In HYDRUS-1D model, soil's hydraulic model can be determined in using eight different models, presented in Table 1.

Table 1. Hydraulic models considered in HYDRUS1D

code	Model
1	Van Genuchten – Mualem
2	Modified Van Genuchten
3	Brooks – Corey
4	Kosugi (log-normal)
5	Dual Porosity (Durner, Dual Van Genuchten – Mualem)
6	Dual Porosity (mobile-immobile, water c. mass transfer)
7	Dual Porosity (mobile-immobile, head mass transfer)
8	Dual-permeability

To study the effect of soil hydraulic model on HYDRUS-1D predicted concentration, all 8 models were defined in the model and amount of outflow concentration from each soil sample was simulated individually. Table 2 sums up statistical parameters related to use of each model. According to the table, the choice of hydraulic models has little effect on hydraulic status of observed soil sample in both coarse textile sandy-loam and fine textile clay-loam samples.

From the values presented in Table 2 it is clear that HYDRUS-1D accuracy in simulation of Bromide concentration in undisturbed sand-loam is less than other samples. Analysis of curves shown in figures 1-4 indicates that mass transport behavior (in the time period) in disturbed clay-loam is much better than other samples and fitting of curves related to observed and simulated values in different time coordinates is better than the other.

In other words, although statistical indicators can indicate general accuracy of each model in each alternative, but detailed investigation (and dynamic) of model behavior and modeling process requires exact information about its performance in each time point, and it's gained by observation of available continuous curves shown in above figures. Study of these curves show that model's relative performance and accuracy in peak values of sand-loam, undisturbed clay-loam is reduced and is underestimated for clay-loam and undisturbed sand-loam and overestimated in disturbed sand-loam.

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Table 2. Statistics of applying different hydraulic models of the HYDRUS model

Model code	Disturbed clay-loam			Undisturbed clay- loam		
	R^2	*RMSE*	*SI*	R^2	*RMSE*	*SI*
1	0.940	0.0007	0.228	0.899	0.003	0.9
2	0.940	0.0007	0.228	0.899	0.003	0.9
3	0.940	0.0007	0.228	0.899	0.003	0.9
4	0.940	0.0007	0.228	0.899	0.003	0.9
5	0.940	0.0007	0.228	0.899	0.003	0.9
6	0.940	0.0007	0.228	0.899	0.003	0.9
7	0.940	0.0007	0.228	0.899	0.003	0.9
8	0.944	0.0006	0.217	0.901	0.002	0.7
	Disturbed sandy-loam			Undisturbed sandy- loam		
1	0.902	0.002	0.898	0.781	0.001	0.389
2	0.902	0.002	0.898	0.899	0.003	0.389
3	0.902	0.002	0.898	0.899	0.003	0.389
4	0.902	0.002	0.898	0.899	0.003	0.389
5	0.902	0.002	0.898	0.899	0.003	0.389
6	0.902	0.002	0.898	0.899	0.003	0.389
7	0.902	0.002	0.898	0.899	0.003	0.389
8	0.814	0.002	0.898	0.862	0.0009	0.277

Table 3. Statistics of applying of the CXTFT model

Model code	Disturbed clay-loam			Undisturbed clay- loam		
	R^2	*RMSE*	*SI*	R^2	*RMSE*	*SI*
Isotherm model	0.952	0.002	0.722	0.920	0.0008	0.235
Non –isotherm model	0.963	0.001	0.366	0.921	0.002	0.667
	Disturbed sandy-loam			Undisturbed sandy- loam		
Isotherm model	0.936	0.0007	0.242	0.857	0.001	0.429
Non –isotherm model	0946	0.0005	0.202	0.925	0.002	0.667

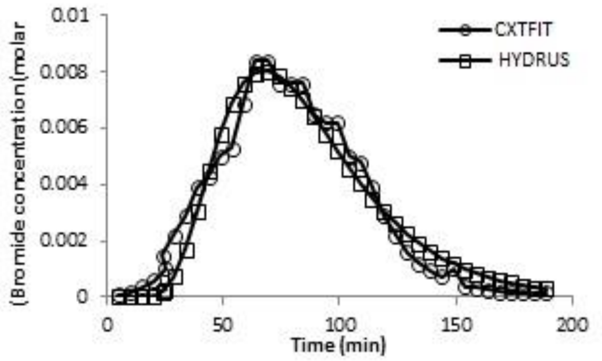

Figure 1. Observed vs. simulated bromide concentration using the Hydrus model in disturbed clay-loam soil

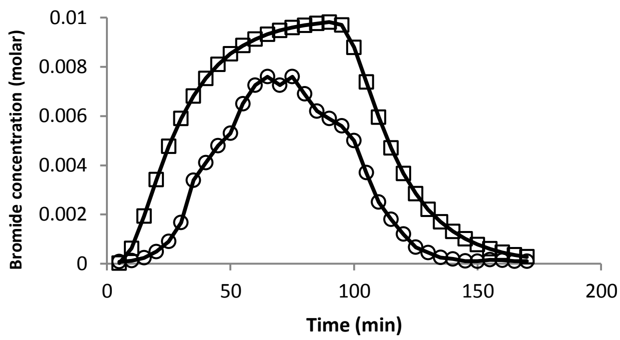

Figure 3. Observed vs. simulated bromide concentration in disturbed sandy-loam soil using Hydrus model

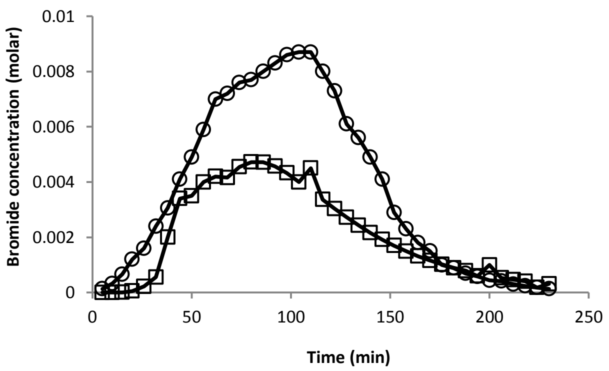

Figure 2. Observed vs. simulated bromide concentration in undisturbed clay-loam soil using Hydrus model

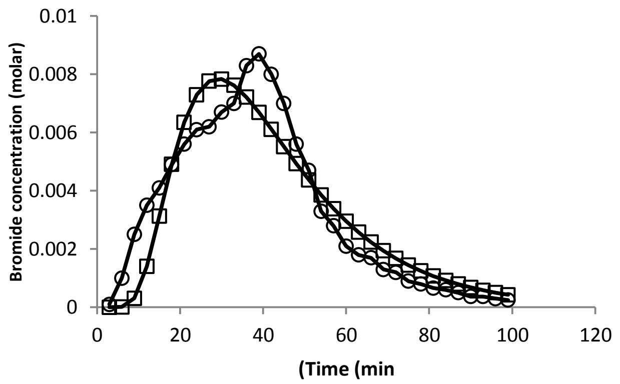

Figure 4. Observed vs. simulated bromide concentration in undisturbed sandy-loam soil using Hydrus model

Also with respect to dispersion (scattering) curves in Figures 5-8 accuracy of HYDRUS-1D model in disturbed clay-loam are more than other 3 samples. If we assume y=ax+b as the equation of straight line fitting these points, a and b values are close to 1 and 0, respectively, which reveals the accuracy of the model in this soil sample.

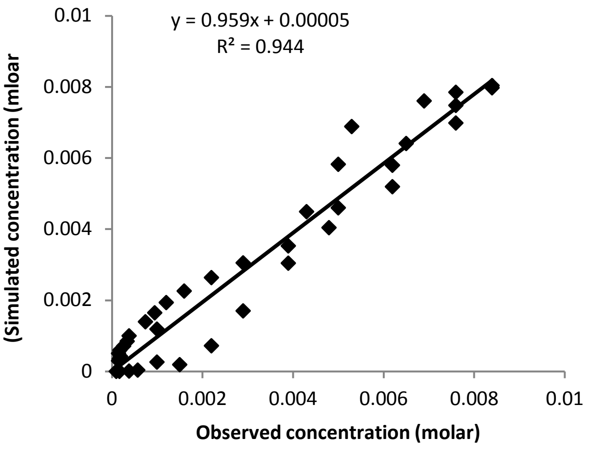

Figure 5. Observed and simulated concentration values with HYDRUS in disturbed clay-loam soil

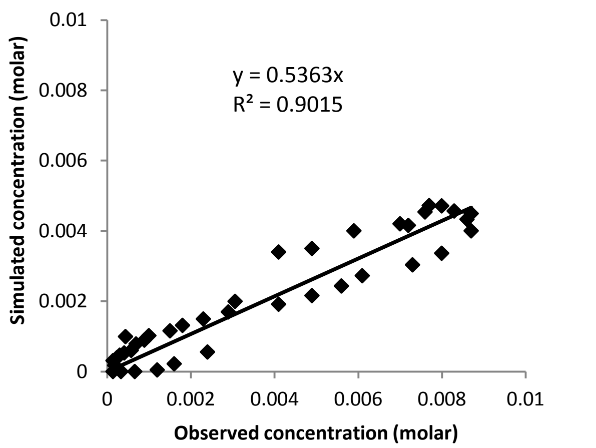

Figure 6. Observed and simulated concentration values with HYDRUS in undisturbed clay-loam soil

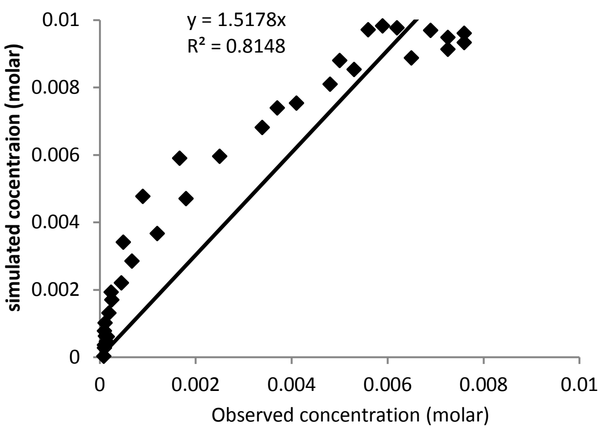

Figure 7. Observed and simulated concentration values with HYDRUS in disturbed sandy-loam soil

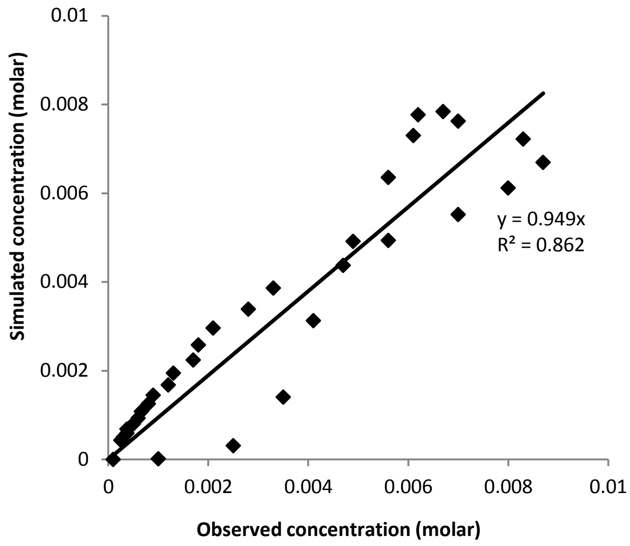

Figure 8. Observed and simulated concentration values with HYDRUS in undisturbed sandy-loam soil

According to the figures and tables above, it is seen that in all 4 soil samples, Bromide transport non-isothermal model has more relative accuracy than non-isothermal transport model. On the other hand, comparing both isothermal and non-isothermal models in all 4 soils suggests that accuracy of these models is the most in clay soil sample. Comparing tables 2 and 3 (related to numerical and analytical method results) shows that accuracy of the numerical solution method is less than the analytical method in studied soils, generally.

In numerical solution (HYDRUS-1D) we used the Galerkin finite element method which is based on network and is presented for solution of partial differential equations. Comparing statistical indicators values in table 2 and 3 and also curves in figs. 1 to 8 we can conclude that accuracy of analytical method in Bromide concentration approximation in all tested soils is more than the numerical method. It is because of assumptions and errors in mesh generation of numerical method which does not exist in the analytical method. Therefore, the CXTFIT model is based on analytical method and presents more accurate results.

The non-isothermal models have higher accuracy due to taking into account more detailed pollution transport (in this paper Bromide), therefore, Bromide transport in clay-loam and sand-loam soils follows non-isothermal model that is obvious in Table 2.

CONCLUSIONS

The following concluding remarks were resulted in the present study:

1. The most accurate results were obtained for the disturbed clay-loam soil sample through application of the both HYDRUS and CXTFT models.
2. In the all experimented soil samples, analytical solution offers more accurate results than the numerical solution alternative.
3. Bromide transport in the both disturbed and un-disturbed soils is governed by non isotherm pollutant transport laws.

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