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Full Length Research Paper

A simple method for estimating the convection-dispersion equation parameters of solute transport in agricultural ecosystem

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The convection-dispersion equation (CDE) is the classical approach for modeling solute transport in porous media. So, estimating parameters became a key problem in CDE. For statistical method, some problems such as parameter uniqueness are still unsolved because of more factors. Due to the advantage of clear physical concept and unique parameter values, the simple deterministic method became very useful alternatives. In this paper, a simple method was proposed to estimate both D and R, and the validity was verified by experiment, which can be applied in agriculture and environmental fields for predicting soil quality property.

Key words: Convection-dispersion equation (CDE), parameters estimation, agricultural system.

INTRODUCTION

Transport of agri-chemicals through soils affects both crop production and groundwater quality. The classical approach of modeling solute transport in porous media uses the deterministic convection-dispersion equation (CDE). For this reason, estimating parameters is a key problem for applying CDE (Buchter et al., 1995; Kool et al., 1987).

Methods of estimating CDE transport parameters can be divided into statistical and deterministic approaches. Statistical parameter estimation techniques consist of the least sum of square, maximum likelihood and moment analysis methods (Bresler and Naor, 1987; Jury and Sposito, 1985; Parker and van Genuchten, 1984; Toride et. al., 1995).These methods are complicated and require a special program. Meanwhile, for different initial values, there are different fitting parameters. Some problems such as parameter uniqueness are still unsolved because of more factors. Controvertibly, the deterministic method has the advantage of clear physical base and unique parameter values and simple deterministic method are very useful alternatives. Rifai et al. (1956) presented a method to estimate the dispersion coefficient (D) from the slope of the breakthrough curve (BTC) at a time corresponding to the displacement of one pore volume. The disadvantage is that only one data point of BTC is used. Elprince et al. (1977) modified this method by using two parameters, dispersion coefficient and retardation factor (D, R), but there is still a shortage of few data used. When the Pacelet number is larger than 5, the BTC can be approximated by a normal distribution (Levenspiell and Smith, 1957; Fried and Combarnous, 1971) or a lognormal distribution (Rose and Passioura, 1971), and the parameters can be estimated by the method of probability property. Yamaguchi (1989) had

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modified Rifai's method (1956) using four points different to the estimated parameters. But the change of slope of BTC is more intensive; the estimation parameters are more different with other method (Li, 1999). BTC is a time-consuming method. Shao et al. (1998) presented an approximate method to estimate parameters by boundary-layer theory not needed to make BTC, but it is difficult to detect the boundary layer in practice. The objective of this study was to propose simple method to estimate both D and R of CDE simultaneously under the condition which the BTC were made or not. The results could be useful for applying CDE to predict the agri-chemicals transport in soils.

THEORY AND ERROR ANALYSIS

One-dimensional transient solute transport through a homogeneous medium during steady-state water flow is traditionally described by CDE:

$$R\frac{\partial c_r}{\partial t} = D_0\frac{\partial^2 c_r}{\partial x^2} + u_0\frac{\partial c_r}{\partial x} \quad (1)$$

Where, Cr(x,t) is the volume-averaged resident concentration of the solution in the liquid phase, u_0 is the mean velocity and assumed constant, D_0 is the dispertion coefficient and supposed constant, R is retardation factor, t is time and x is the distance.

The boundary and initial conditions for a semi-infinite column experiment are:

$$c(x,0) = 0 \quad (2a)$$

$$-D\frac{\partial c_r}{\partial x} + uc_r\Big|_{x=0} = uc_0 \quad (2b)$$

Where, the initial solute concentration in the soil column is 0, and the concentration of solute supplied at the soil column inlet is c_0. The solution of Equation (1) under the condition of Equation (2) is (van Genuchten and Parker,1984):

$$\frac{c_r}{c_0} = \frac{1}{2}erfc[\frac{x-ut}{2\sqrt{Dt}}] + \frac{1}{2}\exp[\frac{ux}{D}]erfcc[\frac{x+ut}{2\sqrt{Dt}}] \quad (3)$$

Where,

$$D = \frac{D_0}{R} \quad u = \frac{u_0}{R} \quad (4)$$

For Equation (3), the second term can be negligible at the high Brenner number (B=uL/D). So, we can neglete the second term:

$$\frac{c_r}{c_0} = \frac{1}{2}erfc[\frac{x-ut}{2\sqrt{Dt}}] \quad (5)$$

Equation (5) can be transferred:

$$1 - 2\frac{c_r}{c_0} = erf[\frac{x-ut}{2\sqrt{Dt}}] \quad (6)$$

Equation (6) was inverse operated:

$$arcerf(1 - 2\frac{c_r}{c_0}) = \frac{x-ut}{2\sqrt{Dt}} \quad (7a)$$

$$\sqrt{t}arcerf(1 - 2\frac{c_r}{c_0}) = \frac{x-ut}{2\sqrt{D}} \quad (7b)$$

Where, $arcerf$ is the inverse operation of the error function, the values can be obtained from tables (Tables of the Error Function and Its Derivative, 1954) through inverse checking. If x equal fixed L, setting ξ equal to:

$$\xi = \sqrt{t}arcerf(1 - 2\frac{c_r}{c_0}) \quad (8)$$

Equation 7b can change the relationship between BTC and time t:

$$\xi = \frac{L}{2\sqrt{D}} - \frac{u}{2\sqrt{D}}t \quad (9)$$

Similarly, there is similar solution for effluent curve:

$$\frac{c_f}{c_0} = \frac{1}{2}erfc[\frac{x-ut}{2\sqrt{Dt}}] + \frac{1}{2}\exp[\frac{ux}{D}]erfcc[\frac{x+ut}{2\sqrt{Dt}}] \quad (10)$$

Where, the C_f is the effluent concentration. Using same method, the Equation (10) can be transfered to the style of Equation (9). But the ξ equal $\sqrt{t}arcerf(1 - 2\frac{c_f}{c_0})$

not $\sqrt{t}arcerf\ (1 - 2\frac{c_r}{c_0})$.

Thus, Equation (9) shows there exist a linear relationship between ξ and t. The intercept and slope are functions of D and u, and can be used to fit these

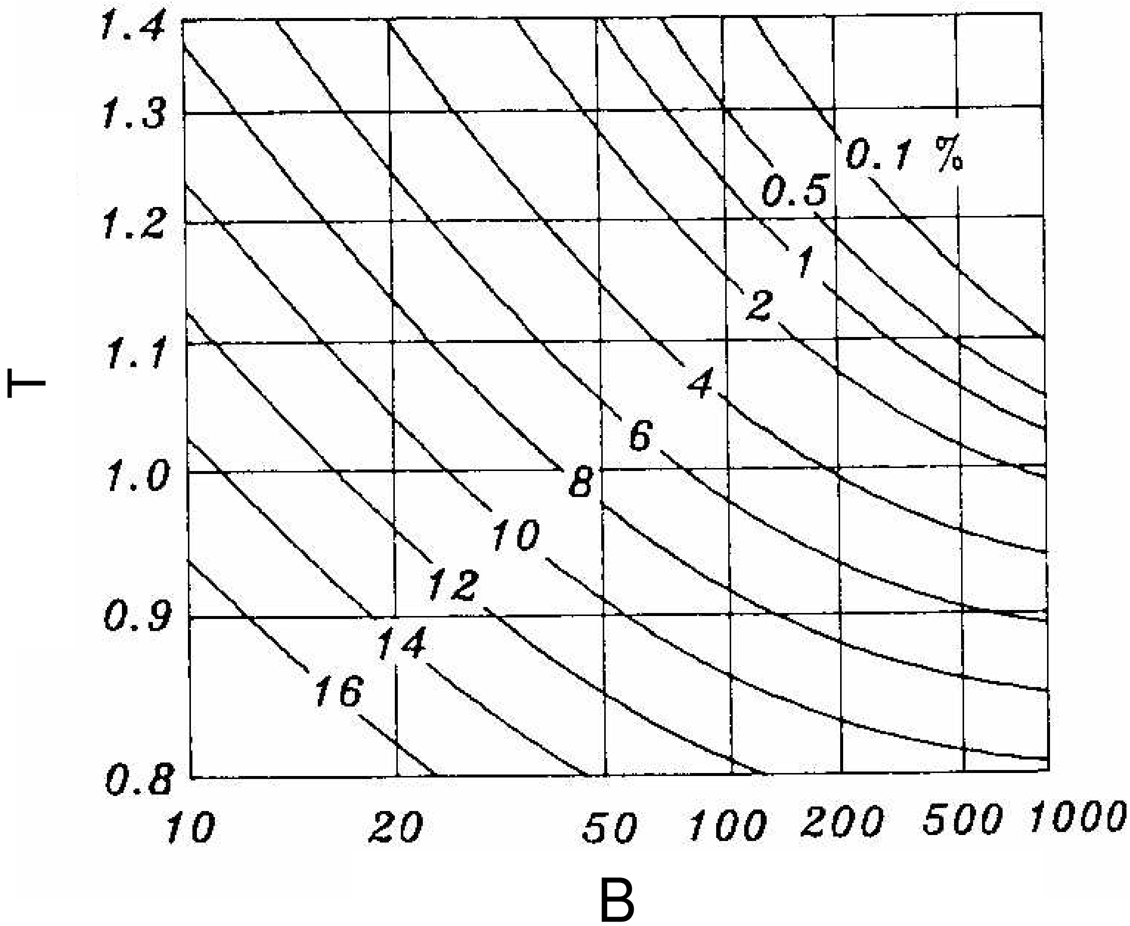


Figure 1. Equal-percentage contibution lines of the second term in the analytical solution [Equation (3), the reduced time is t (log scale) and Brenner number is B (log-log Scale)]. The total percentage was 100, the percentage of second term was gradually decreased with Brenner number increasing. When the Brenner number was more than 100, the percentage of the second term was less than 2. This showed that the second term of the analytical solution can be neglected under Brenner number more than 100 (Yamaguchi, 1989).

parameters, and this was named intercept method. Because BTC is time-consuming, the parmeters were hoped to be estimated not through BTC. Equation (5) can be transferred to be:

$$\frac{arcerf\,(1-2\frac{c}{c_0})}{\sqrt{t}} = \frac{x}{2\sqrt{Dt}} - \frac{u}{2\sqrt{D}} \quad (10)$$

The setting of Y and X equal to:

$$Y = \frac{arcerf\,(1-2\frac{c}{c_0})}{\sqrt{t}}, X = \frac{x}{t} \quad (11)$$

Equation (10) changes a linear relationship between Y and X:

$$Y = \frac{1}{2\sqrt{D}} X - \frac{u}{2\sqrt{D}} \quad (12)$$

If a sieries $\frac{c}{c_0}$ at different point (x_i, t_j) was measured for homogenous column, the parameters can be calculated by Equation (12) not through BTC, and named position-time method.

The main error source is negligibility of the second term of the analytical solution of Equation (3). The percentage contribution of the second term in Equation (3) to the total $\frac{c}{c_0}$ is shown as a function of B and τ in Figure 1, where, B is the Brenner number (B=uL/D) and τ is the number of pore volumes. When Brenner number is larger than 100,

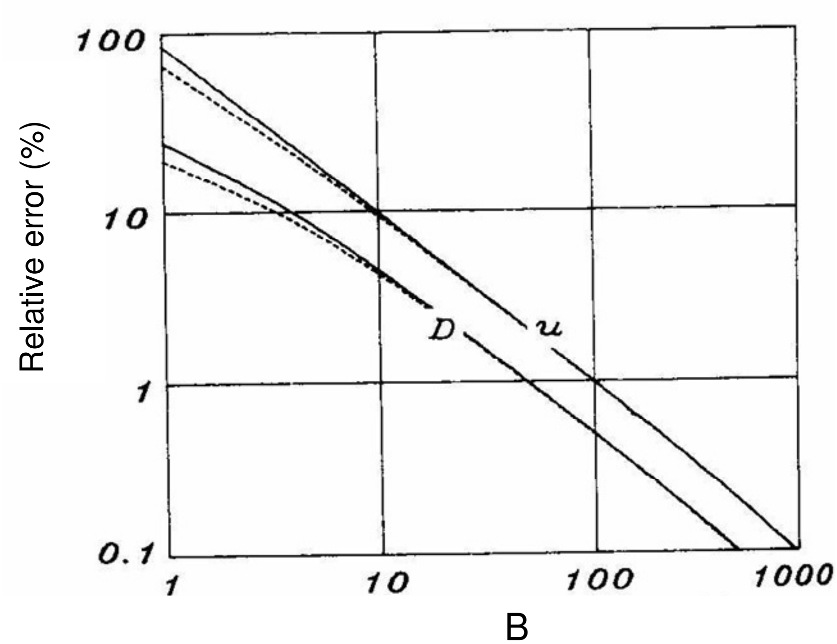


Figure 2. Dependence of relative error (log scale) on Brenner number (log scale) in estimating convective velocity, u and the hydrodynamic dispersion coefficient, D, under e negligibility of the second term of the analytical solution (line is real value, the lash is estimated value). This showed that the estimated parameter values were consistent with the real values under Brenner number more than 100 (Yamaguchi, 1989).

the percentage contribution of the second term is less than 2% (Figure 1). This showed there was reason to neglect the second term of analytical solution under Brenner number more than 100. The relationship between relative error in estimating u and D using complete and negligibility of the second term analytical solution and Brenner number is shown in Figure 2. When Brenner number is more than 100, there are no difference between the parameters estimation without the second term and real parameter values.

Because in a wide range Peclet number $1 < ud/D_m < 10^6$ (where d is mean diameter of the soil particles, D_m is the molecular diffusion coefficient), $D \cong ud$ (Bear, 1979); the Brenner number was changed:

$$B = \frac{uL}{D} = \frac{ud}{D}\frac{L}{d} \cong \frac{L}{d} \quad (13)$$

So, the condition of the negligibility of the second term of the analytical solution can be satisfied through adjusting the length of soil column L and soil particle diameters. The relative error in estimating u and D is < 1% and < 0.5%, respectively, when the Brenner number is $B \cong \frac{L}{d} > 100$ (Figure 2). In experience, the soil was sieved with 2 mm mesh and if the length of soil column is more than 20 cm, the condition of B > 100 can be satisfied; the above method can be used to estimate the parameters of CDE.

MATERIALS AND METHODS

The experimental soil samples were loam soil. The pH and organic matter of soil were 8.12 and 1.27% respectively. The contents of different particles of > 0.25, 0.25 to 0.05, 0.05 to 0.01, 0.01 to 0.005, 0.0005 to 0.001 mm, < 0.001 were 1.1, 5.6, 47.8, 15.0, 17.9 and 12.8% respectively. The experimental setup is schematically shown in Figures 1 and 2. The soil column was a plexiglass cylinder, 10 cm in diameter and 40 cm long, and perforated at 20 and 30 cm from the top. The air-dried soils sieved with 2 mm mesh were uniformly packed in layers and made the average dry density in the column (1.3 g/cm^3). The holes were used to insert the selective Cl^- iron electrode and to get the Cl^- concentration in different times. A 0.16 N solution of $CaCl_2$ was applied with a positive displacement after the soil column had been saturated with Mariotte bottle under 3 cm high water head. The mean water velocity was $u_0 = 1.03 cm/h$, and the porosity was 0.51. Under the basis, the leaching solution was collected and the Cl^- concentration of the effluent solution was measured by titration with $AgNO_3$ solution.

RESULTS AND DISCUSSION

Parameters estimated by intercept method

Based on Equations 8 and 9, ξ of the three different

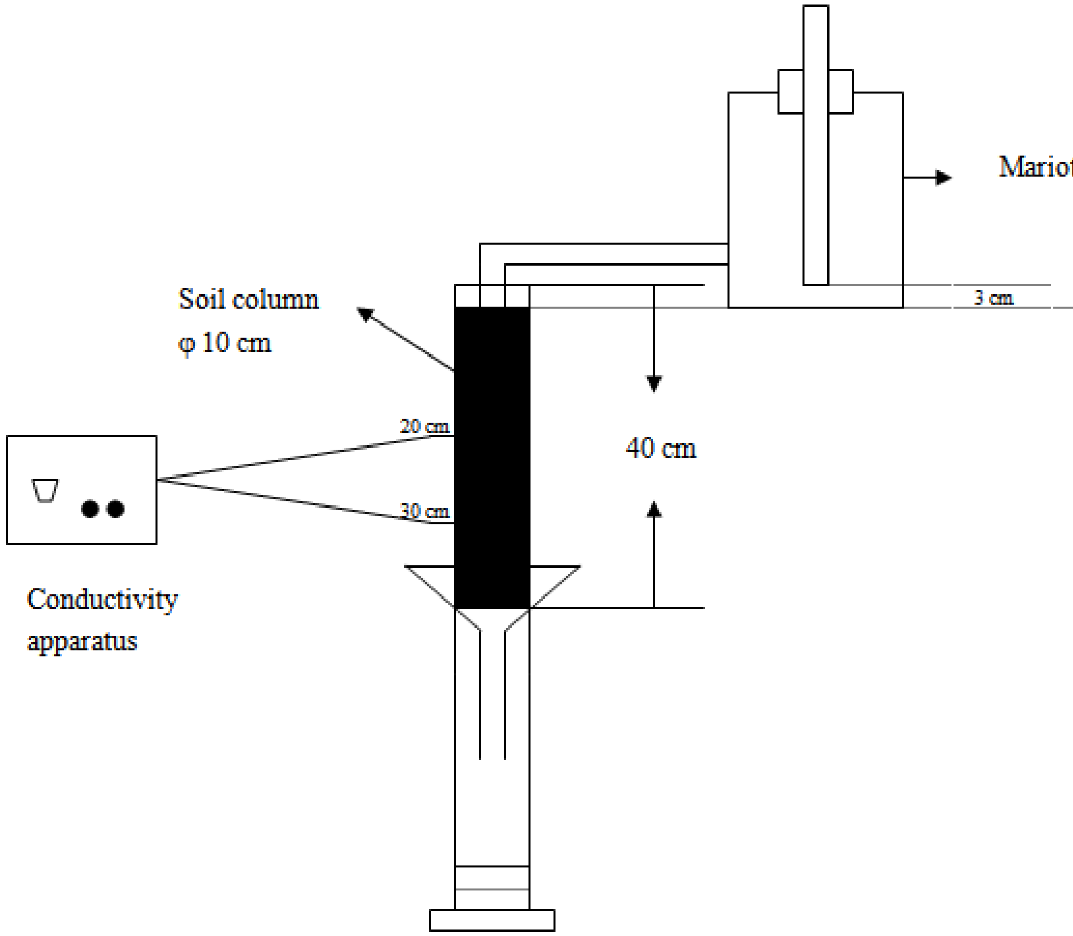
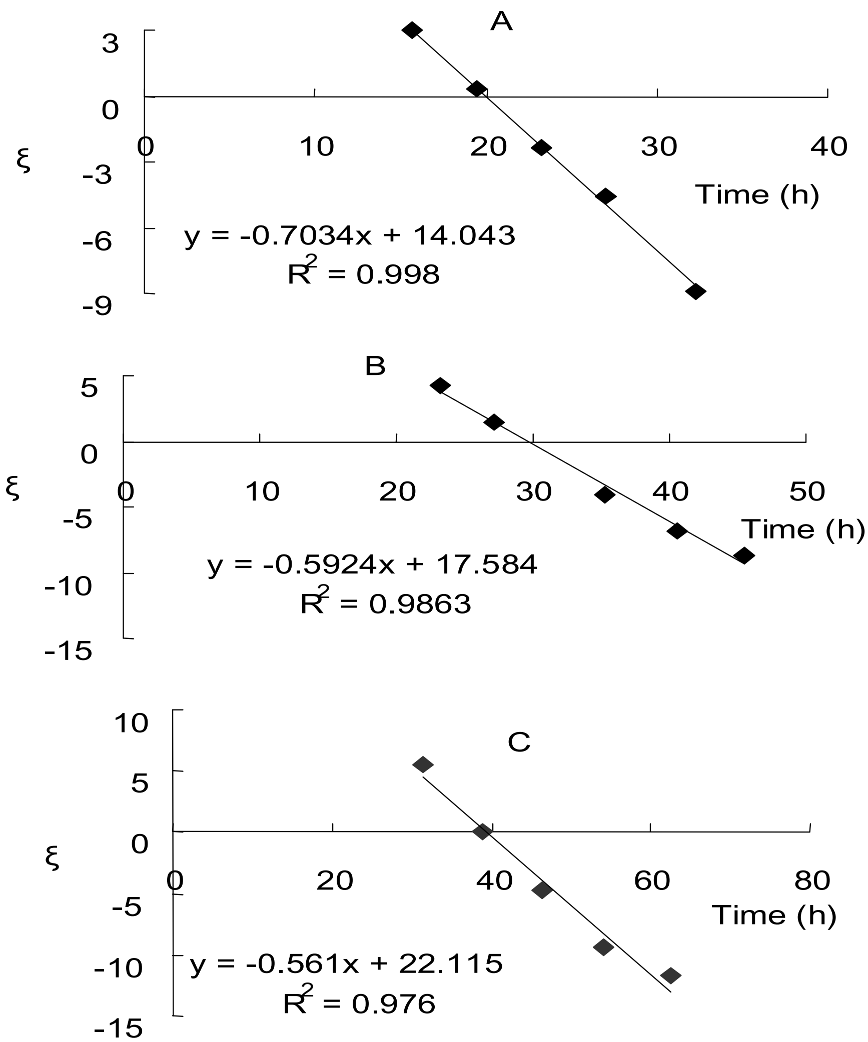


Figure 3. The schematic diagram about Cl^- transport in a soil column experiment.

positions was significantly linearly related with t (Figure 4). The parameters D and R can be calculated by the intercept and slope of ξ and t. The parameters R estimated by intercept method were similar with that by CXTFIT and parameters D was more than 17% by CXTFIT (Table 1). After the second term was neglected, all contribution to the analytical solution was formed by first term; the parameters were amplified to meet these requirements, this maybe a reason for the parameters by the intercept method than the CXTFIT. No matter which method, the parameters D increased along with the length of soil column; this reason maybe that the soil porosity was more complex with the stretching; hydro-dispersion is more intensive. In order to compare the precision of the estimated parameters, the simulated breakthrough curve for three positions by three methods were compared; the simulated results were no obvious different with the measured one although the simulated one was higher than others (Figures 5 and 6). Especially for the first term approximate method (neglect of the second term of the analytical solution) and intercept method, the simulated results were as same as the results by the measured CXTFIT. This showed that intercept method can be used to estimate parameters of CDE equation and had high precision to predict the solute transport in soils.

Parameters estimated by position-time method

Compared with the intercept method, the position-time method needs to measure the BTC. Figure 6 is the linear relationship between Y and X for a series C/C0 at different time at 20 and 30 cm positions. The parameters D and R calculated were 0.645 and 0.97 according to Equation 12, respectively; these approximated the mean values by the intercept method at these 2 points. This showed the parameters by position-time method were an average condition. Figure 7 is the results predicted by the effluent BTC at 40 cm by parameters through 20 and 30 cm positions. The difference between the predicted and measured values was little. The position-time method can be used to estimate the parameters of CDE not through the making of BTC.



4. The linear relationship between ξ and time, $\xi = \sqrt{t}\, arcerf\,(1 - 2\frac{c}{c_0})$.

Figure A, B, C were the measured points at 20cm, 30cm, and effluent, respectively.

Table 1. The parameters by the intercept method compared with CXTFIT method.

Parameter	Intercept method				CXTFIT method			
	20 cm	30 cm	effluent	Average	20 cm	30 cm	effluent	Average
D	0.507	0.728	0.818	0.684	0.554	0.587	0.612	0.584
R	0.97	0.96	0.99	0.97	1.03	1.03	1.01	1.02

Because the intercept method and position-time me-thod are derived from the basic solution of Con-vection-Dispersion Equation, they have clear physical concept, and is fast and easy to calculate. The simulated result by the calculated and measured parameters coin-cided. These can provide a simple method to approxi-mate parameters in CDE.

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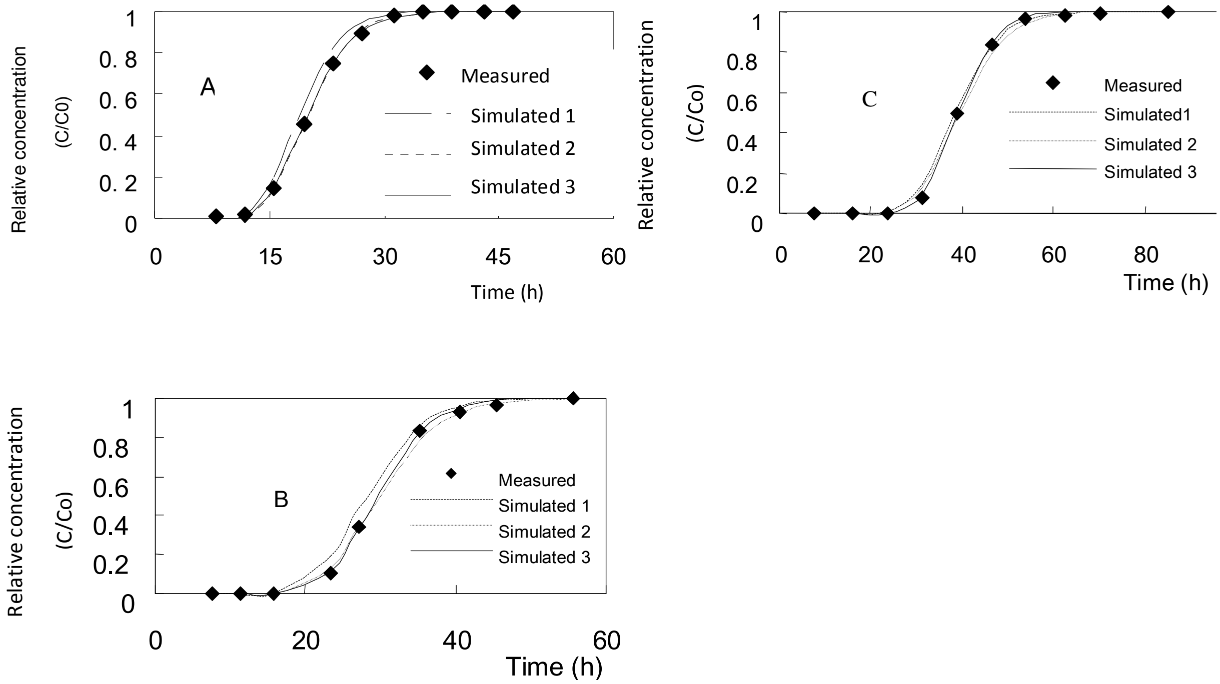

Figure 5. Comparison of the measured BTC simulated at 3 different positions. The simulated 1 was a result that the parameters estimated by the intercept method and the simulated whole analytical solution. The simulated 2 was a result that the parameters estimated by intercept method and the simulated approximate analytical solution that neglected the second term. The simulated 3 was a result by CXTFIT program. A, B, C were the measured points at 20 cm, 30 cm, and effluent, respectively.

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REFERENCES

Bear J (1979). Hydraulics of groundwater. McGraw Hill, Inc., NewYork.

Bresler E, Naor A (1987). Estimating transport parameters in soils by a maximum likelihood approach. Soil Sci. Soc. Am. J. 51:870-875

Buchter B, Hinze C, Flury M, Fluher H (1995). Heterogeneous flow and solute transport in an unsaturated stony soil monolith. Soil Sci. Soc. Am. J. 59:14-21

Elprince AM, Day PR (1977). Fitting solute breakthrough equation to data using two adjustable parameters. Soil Sci. Soc. Am. J. 41:39-41

Fried JJ, Combarnous MA (1971).Dispersion in porous media. In Advance in Hydrosci. Vol.7. Academic Press Orlando, FL.

Jury WA, Sposito G (1985).Field calibration and validation of solute transport models for the unsaturated zone. Soil Sci. Soc. Am. J. 49:1331-1341

Kool JB, Parker JC, Van Genuchten MTh (1987). Parameter estimation for unsaturated flow and transport models - A Review. J. Hydrol. 91:255-293

Levenspiel O, Smith WK (1957). Notes on the diffusion-type model for longitudinal mixing of fluids in flow. Chem. Eng. Sci. 6:227-233

Parker, Van Genuchten MTh (1984). Determining transport parameters from laboratory and field tracers experients. Virginia Agric. Exp. Stn. Bull. 84-3

Ren Li, Li Baoguo, Zeng Fan, Xing Weiling (1999).Application of two new methods for determining the parameters of solute transport in soils. SHUILI XUEBAO (11):1-6 (In Chinese)

Rifai MNE, Kaufman WJ, Todd DK (1956). Dispersion phenomena in laminar flow through porous media. Inst. Of Eng. Res. Ser. 93(2). Salinity Eng. Res. Lab. Univ. of Cali. Berkeley.

Rose DA, Passioura JB (1971). The analysis of experiments on hydrodynamic dispersion. Soil Sci. 111:252-257

Shao M, Horton R, Miller RK (1998).An approximate solute to the Convection-Dispersion Equation of solute transport in soil. Soil Sci. 163:339-345

Toride NF, Leij, Van Genuchten MTh (1995). The CXTFIT Code for Estimating transport parameters from laboratory and field tracers experiments. U.S. Salinity Laboratory. Res. Report No.137

Yamaguchi T, Moldrup P, Yokosi S (1989). Using breakthrough curves for parameter estimation in the Convection-Dispersion Model of solute transport. Soil Sci. Soc. Am. J. 53:1635-1641