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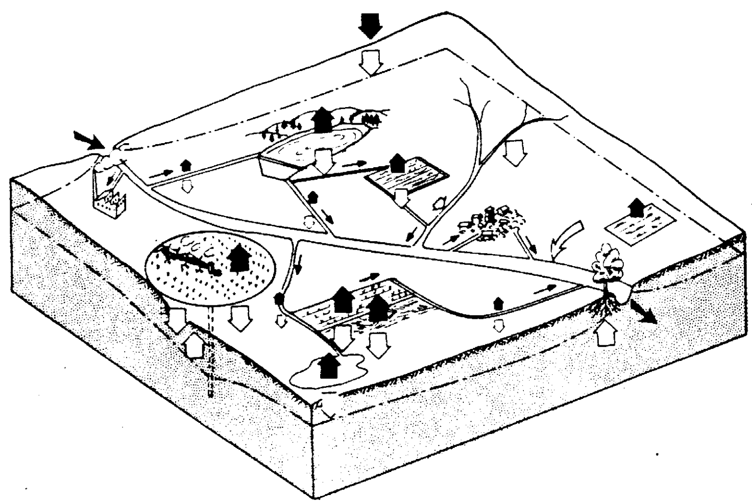

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Field Experiment and Stochastic Analysis of Solute Transport in an Unsaturated Soil

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ABSTRACT

Solute concentration and water content were measured at a depth to 170 cm in an unsaturated field soil. Soil water movement and solute transport in the local scale were studied and the spatial variability of the soil water content and concentration were discussed. As compared with the water content, the concentration distribution shows a large variation. The immobile water content is about 24 to 39 percent of the total water content in the experiment. The flux velocity is described with a log normal distribution function. The mean and variance of the concentration are calculated using the convection equation, the convection-dispersion equation with the stochastic velocity, and the classical convection-dispersion equation. It is shown that the concentration variance is proportional to the concentration gradient and inversely proportional to the local dispersivity. The maximum concentration variance is near the concentration front.

INTRODUCTION

Solute transport in unsaturated soils plays an important role in many contamination problems because contaminant sources are often located near the soil surface, and contaminants may move through the unsaturated zone to the groundwater. The most commonly used model to express the transport precess in the unsaturated zone is a direct extension of the convection dispersion equation of solute transport in saturated soils, which mainly combined two terms: (1) solute displacement by convection with the mean pore water velocity, and (2) hydrodynamic dispersion induced by the fluctuation of pore water velocity from the mean velocity. With the help of numerical models, the convection dispersion equation is successfully used in simulating solute transport through soil columns and soil tanks in the laboratory (*Yang*, 1986, 1988). Because of the inherent spatial variability of soil properties, the traditional deterministic model is suffered from the limitation of its applicability to the field. A number of stochastic models have been proposed to simulate solute transport in soils, which ignore the lateral mixing and treat solute movement as some isolated vertical homogeneous soil columns with different random transport parameters (*Dagan and Bresler*, 1979; *Bresler and Dagan*, 1983; *Jury*, 1982; *Jury et al.*, 1986).

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Field experiments indicate that the small scale variation of soil water velocity is the key factor leading to the field scale dispersivity. In order to study the spacial variability of soil water and solute movement, a field experiment of unsaturated solute transport was conducted under steady-state infiltration. This paper is to analyze the variability of soil water velocity and its effect on the solute transport process.

EXPERIMENT

A solute leaching experiment was performed over 35 days from August 23 to September 25, 1990 on a cultivated field in the northern China. Surface water is the main irrigation resource in this region. In the period of water shortage the groundwater is used as a supplementary resource. Groundwater depth is about 1.2 - 2.0 m. The soil is the loam sand to a depth of 2.0 m. The saturated conductivity measured by the double-ring method is 1.1 - 1.4 cm/day.

The experiment was conducted on a 6.0 x 3.0 m^2 plot. The plot was separated from the nearby soil with polyethylene plastic extending to a depth of 1.2 m below the soil surface. Surrounding the plot there was a protection area with the width of 1.5 m. The plot was divided into 8 1.5 x 1.5 m^2 subplots. The sampling sites were evenly distributed in each subplot. During the whole experiment period the groundwater depth maintained at 2.2 m. Shown in Fig. 1 are the initial water content and soil solute concentration after the pretreatment.

A steady state infiltration rate, 4 mm/day, was applied with chloride as a tracer. Water was never ponded on the soil surface and evaporation was minimized by covering the plot with polyethylene plastic. Soil samples were taken every 5 days at the depths of 15, 30, 45, 60, 75, 90, 105, 120, 135, 150 and 170 cm in each subplot. The soil samples were used to determine water content and solute concentration.

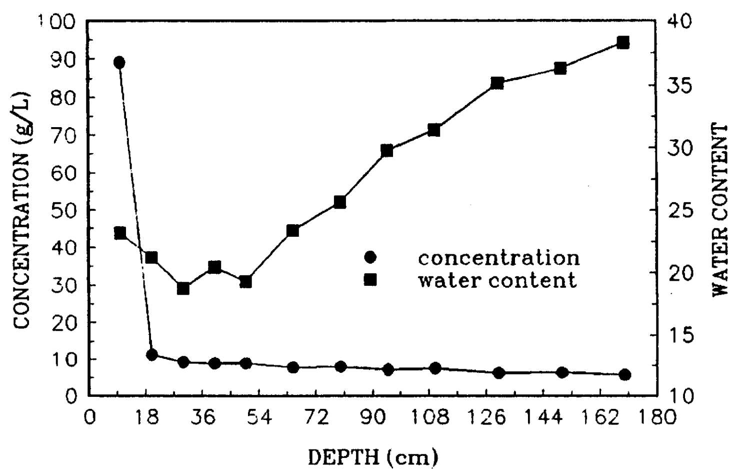

Fig. 1. The initial profiles of water content and concentration.

DISTRIBUTION OF SOLUTE TRANSPORT VELOCITY

The distribution of solute concentration profile measured at the time of 21 days (September 13, 1990) is presented in Fig. 2. The concentration profiles at the subplots display a considerable disparity. The solute transport velocity can be determined by

$$V = z/t \tag{1}$$

where V is the solute transport velocity, z the depth of the concentration front which may be represented by the median or mode of the concentration profile at the corresponding sampling time t.

Solute transport velocity determined in the 8 subplots at time 8, 14, 21, 27, and 33 days are listed in Table 1. In the experiment process the infiltration rate was accurately controlled and its relative error was less than 5%. It can be seen from Table 1 that the coefficient of variation (*CV*) of the solute transport velocity is between 14% and 39%. *CV* is larger at the shallow soil than at the deep soil because of the heterogeneity resulted from cultivation and root activities near the soil surface. The results in Table 1 also indicates that a concentration profile measured at one subplot can not be used to represent the average concentration distribution in the experimental field.

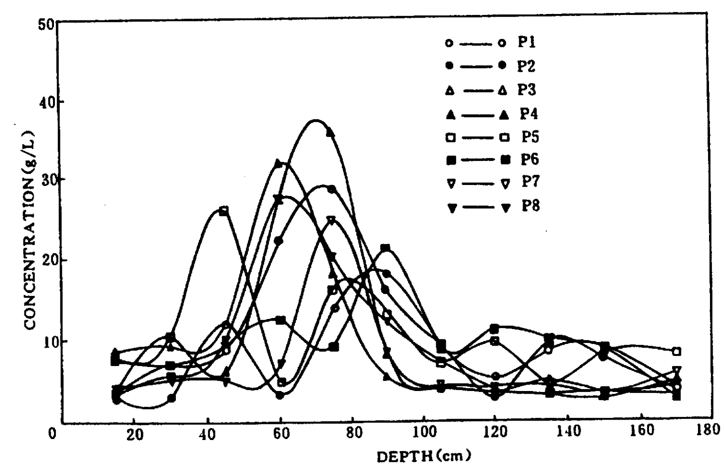

Fig. 2. Concentration profiles at different sampling locations on September 13,1990.

Table 1. Solute transport velocity (mm/day) calculated using Eq. 1 and the experimental data.

time (day)	SUBPLOTS								CV (%)
	1	2	3	4	5	6	7	8	
8	3.28	4.15	2.47	4.25	2.47	2.47	2.47	0.69	39
14	2.48	2.20	2.57	2.57	2.48	3.63	4.45	2.48	18
21	2.42	1.68	3.29	2.48	3.10	2.42	3.10	2.85	18
27	2.32	2.83	1.96	2.27	2.60	2.96	2.92	1.96	15
33	1.82	2.88	2.09	2.03	2.50	2.13	2.50	2.33	14

The probability of the log-transformed solute transport velocity, *Ln*(V), is plotted in Fig. 3 based on the 40 values in Table 1. The resulting relationship appears to be a straight line. Therefore, the observed values of V are better described by a lognormal distribution. The mean value and standard deviation of *Ln*(V) can be determined as 0.94 and 0.16, respectively. The coefficient of variation is 0.17. *Biggar and Nielsen* (1976) monitored solute movement with solute samplers under ponding in twenty 6.5 x 6.5 m^2 plots randomly located in a 150-ha agricultural field. They found that the apparent velocity of the solute peak was distributed lognormally, and the mean value, standard variation (σ_{lnV}), and coefficient of variation (*CV*) of *Ln*(V) were equal to 3.01, 1.25 and 0.475, respectively. *Van de Pol et al.* (1977) conducted a field experiment on water and solute transport under unsaturated steady-state condition on an 8 x 8 m^2 plot. It was found that the pore scale velocity and the apparent dispersion coefficient were lognormally attributed and the mean value, standard variation, and coefficient of variation of *Ln*(V) were 1.203, 0.504, and 0.427, respectively. The velocity variability in the present experiment is relatively small compared with the above two experiments.

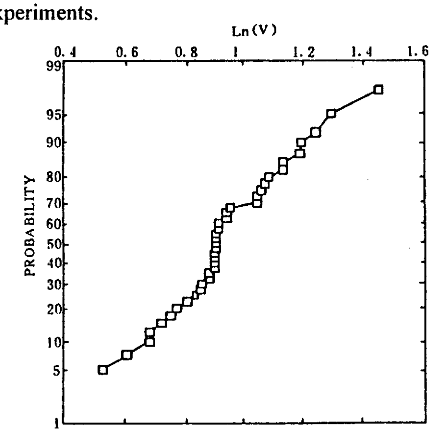

Fig. 3. Probability distribution of the solute transport velocity.

The field local scale dispersivity can be determined from the variability of solute transport velocity. As shown by *Russo and Dagan* (1991), the effective longitudinal dispersion coefficient for unsaturated soil can be expressed in the same form as that for saturated soil, which depend on the velocity variance, correlation scale and travel time (*Dagan*, 1984, 1986). In this paper we assume that water flow is vertical and steady. The solute transport velocity does not change along the vertical profile and is randomly distributed in the horizontal plane. The depth of solute movement at any point (x, y) on the plane at time t can be represented as $V = z/t$. The variance of solute transport depth is

$$\sigma_z^2 = \langle z'^2 \rangle = \sigma_V^2 t^2 \tag{2}$$

When the pore scale dispersion is neglected, the effective dispersion coefficient can be determined by (*Dagan*, 1986)

$$D_z = \frac{1}{2}\frac{d\sigma_z^2}{dt} = \sigma_V^2 t \tag{3}$$

Thus D_z is not a constant, but grows linearly with the travel time and travel distance of the solute body. In Eq. 3 the effective dispersion coefficient is proportional to the variance of the velocity. Expressing the effective dispersion coefficient D_z as a product of the effective dispersivity α and the average solute transport velocity V, that is, $D_z = \alpha V$, we obtain $\alpha = 0.068t$ (cm) from the experiment. For t = 14, 21, and 27 days, the effective dispersivities are 0.94, 1.4, and 1.8 cm, respectively. The dispersivity determined in a laboratory in a repacked soil column for the same soil is about 0.1 to 0.2 cm. The effective dispersivity determined from the variance of solute transport velocity in the field scale is a order large as the pore scale dispersivity.

STOCHASTIC ANALYSIS OF THE EXPERIMENTAL DATA

Average Concentration and Variance Based on the Convection Model (Model A)

Neglecting the pore scale dispersion, solute transport in a homogeneous profile can be expressed as follows

$$\frac{\partial C}{\partial t} = -V\frac{\partial C}{\partial z} \tag{4}$$

and the boundary and initial conditions for the experiment are

$$C(z,0) = \begin{cases} C_1, & 0 \le z \le L \\ C_2, & L < z \end{cases} \tag{5}$$

$$C(0,t) = C_0, \qquad t > 0 \tag{6}$$

where C is the concentration, t the time, C_1 and C_2 are the initial concentration at the depth $z = -L$ and $z > L$, respectively, C_2 is also the concentration of infiltration water, and V the constant velocity along the soil profile. The probability of the velocity is a lognormal distribution in a mathematical form of

$$P(V) = \frac{1}{\sqrt{2\pi}\,\sigma_{LnV}}\exp\left[\frac{-(LnV-\overline{LnV})}{2\sigma_{LnV}}\right] \tag{7}$$

Because only convection is considered, the concentration front should move downward as a piston flow. For an inert solute and a realization of velocity V in the region, the concentration at the depth z and time t is

$$C'(z,t,V) = C_0[H(z,Vt) - H(z-Vt-L)] \tag{8}$$

where

$$H(z) = \begin{cases} 0, & z \leq 0 \\ 1, & z > 0 \end{cases} \tag{9}$$

$$C_0 = C_1 - C_2; \qquad C' = C - C_2$$

In the homogeneous soil, V is a random variable, the average concentration in the region can be calculated by

$$\overline{C'} = \int_0^\infty C'(z,t,V)P(V)dV \tag{10}$$

Substituting Eqs. (8) and (9) into Eq. (10), we have

$$\overline{C'} = C_0(\phi_1 - \phi_2) \tag{11}$$

where

$$\phi_1 = \phi\left(\frac{Ln(z/t)-\overline{LnV}}{\sigma_{LnV}}\right) \qquad \phi_2 = \phi\left(\frac{Ln\frac{z-L}{t}-\overline{LnV}}{\sigma_{LnV}}\right) \qquad \phi = \int_z^\infty \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{\eta^2}{2}\right)d\eta \tag{12}$$

The variance of concentration can be expressed as

$$\sigma_C^2 = \int_0^\infty [C'(z,t,V) - \overline{C}(z,t)]^2 P(V)dV \tag{13}$$

where σ_C^2 is the variance of concentration. By substituting Eqs. (8) and (10) into (13), we obtain the following result

$$\sigma_C^2 = C_0^2(\phi_1 - \phi_2)(1 - \phi_1 + \phi_2) \tag{14}$$

The average concentration and variance at September 6, 13, and 19 (that is, t = 8, 14, and 21 days) can be calculated from Eqs. (11) and (13). It can be seen from Fig. 4 that under the effect of spatial variability, the average concentration profile does not move in a piston shape. The concentration profile is flattened eventually and its peak decreases with time. Compared with the experimental data, the model reproduces the concentration profile very well (Fig. 5), but the variance calculated from the model is somewhat larger than the experiment result. One of the reasons may be that in the model the pore scale dispersion is neglected. Figure 4 also shows that the maximum value of variance is located near the concentration front.

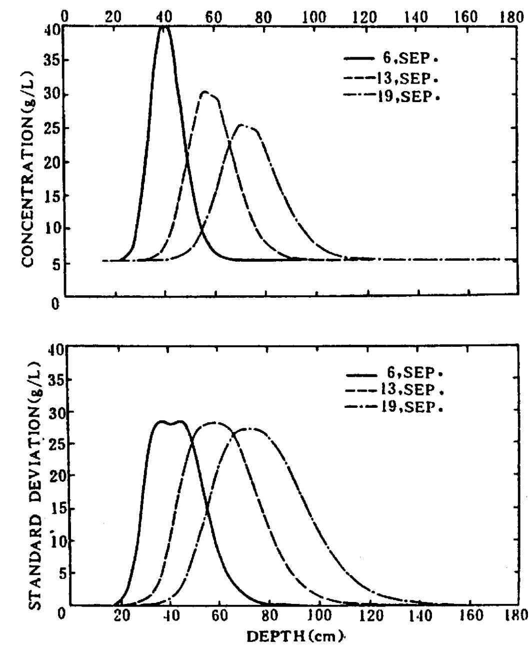

Fig. 4. Profiles of the average concentration and standard deviation.

Average Concentration and Variance Based on the Convection Dispersion Equation (Model B)

For a inert solute and a realization of random velocity V, the one dimensional convection dispersion equation can be written as

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial z} \tag{15}$$

The boundary and initial conditions for the experiment are

$$C(z,t) = \begin{cases} C_1, & 0 <= z \le L \\ C_2, & L < z \end{cases} \qquad C(0,t) = \begin{cases} C_0, & 0 \le t \le t_0 \\ 0, & t_0 < t \end{cases} \qquad \left.\frac{\partial C}{\partial z}\right|_{z\to\infty} = 0 \tag{16}$$

The solution of Eqs. (15) and (16) is given by *van Genuchten and Alves* (1982):

$$C(z,t,V) = \begin{cases} C_2 + (C_1 - C_2)A(z,t) + (C_0 - C_1)B(z,t), & 0 \le t \le t_0 \\ C_2 + (C_1 - C_2)A(z,t) + (c_0 - C_1)B(z,t) - C_0 B(z,t-t_0), & t_0 < t \end{cases}$$

$$A(z,t) = \frac{1}{2}erfc(\frac{z-L-Vt}{2\sqrt{Dt}}) + \frac{1}{2}\exp(\frac{Vz}{D})erfc(\frac{z+L+Vt}{2\sqrt{Dt}})$$

$$B(z,t) = \frac{1}{2}erfc(\frac{z-Vt}{2\sqrt{Dt}}) + \frac{1}{2}\exp(\frac{Vz}{D})erfc(\frac{z+Vt}{2\sqrt{Dt}}) \tag{17}$$

The average concentration and variance can be evaluated by

$$\overline{C} = \int_0^\infty C(z,t,V)P(V)dV \tag{18}$$

$$\sigma_C^2 = \int_0^\infty [C(z,t,V) - \overline{C}(z,t)]^2 P(V)dV \tag{19}$$

Though $C(z, t, V)$ is expressed analytically, it is not easy to integrate Eqs.(18) and (19) directly. Numerical method may be used for the integration of Eqs. (18) and (19) (*Bresler and Dagan*, 1983), in which the velocity is divided into n-segments (V_{i-1}, V_i) $(i = 1, 2, ..., n)$ based on the following condition

$$\int_{V_{i-1}}^{V_i} P(V)dV = \frac{1}{n}, \qquad i = 1,2,...,n \tag{20}$$

where $V_0 = 0$, $V_n \to \infty$.

The middle point $V_{i-1/2} = (V_{i-1} + V_i)/2$ in each segment (V_{i-1}, V_i) is taken as a representation of the velocity. By substituting $V_{i-1/2}$ into Eqs. (17), (18) and (19), we have

$$\overline{C}(z,t) = \frac{1}{n}\sum_{i=1}^{n} C(z,t,V_{i-1/2})$$
$$\sigma_C^2(z,t) = \frac{1}{n}\sum_{i=1}^{n} [C(z,t,V_{i-1/2}) - \overline{C}(z,t)]^2 \tag{21}$$

This numerical method is quite simple and can be used for more general flow conditions. Numerical results calculated with n = 50, 100, and 200 for the solute velocity probability density $P(V)$ show that the accuracy requirement can be met with n = 50.

Figure 6 represents the observed and predicted results for the pore scale dispersivities α = 0.1, 0.2, 0.4, 0.8, and 1.6 cm at 27 days. As shown in Fig. 6 the average concentration becomes flattened with the increase of the pore scale dispersivity. The calculated results have a good agreement with the experiment data when α was taken between 0.2 and 0.8 cm. As the pore scale dispersivity increases, the variance of the average concentration decreases, that is, the variance is inversely proportional to the pore scale dispersivity, which agrees with the theoretical analytical result of *Vomvaris and Gelhar* (1990).

Average concentration Based on Deterministic Convection Dispersion Equation (Model C)

Average velocity and time varying dispersivity were determined from the experiment data. Substituting those results into the deterministic convection dispersion equation, Eqs. (15) and (16), and taking the effective dispersion coefficient as $D = \alpha V$, we got the average concentration distribution as shown in Fig. 5. However, we can not obtain the variance of concentration from this model.

Figure 5 illustrates the experimental data and the calculated results by Models A, B and C, respectively. Generally speaking, the differences of the calculated results from the three models are not significant. The peak of concentration disparity calculated by the convection model (Model A) and the deterministic convection dispersion equation (Model C) is almost the same. Comparing with the experimental data, the movement of solute front predicted by the three model at 14 days (6, September) is shallower, and movement of solute front predicted at 27 days (19, September) is deeper. The cause of this deviation from the experimental data is that the actual velocity is larger near the soil surface than at the deep soil because of the stronger soil structure and lower water content in the shallow soil. If the effective dispersivity can be determined, it is very simple to use Model C for the determination of average concentration. The stochastic convection model (Model A) is simpler in calculation than the stochastic convection dispersion model (Model B). The average concentration profile calculated by the two models are very close. It is indicated that the spread of solute due to field heterogeneity is much larger than the spread by the pore scale dispersion, so that the later may be neglected. For the concentration analysis in the field, using Model A may be preferable.

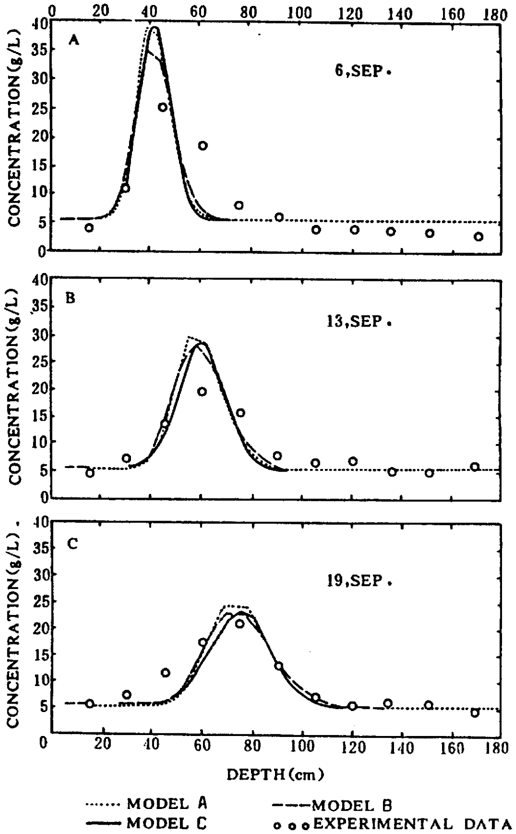

Fig. 5. Average concentration profiles estimated by three models, compared with the data collected on (A) September 6, (B) September 13, and (C) September 19, 1990.

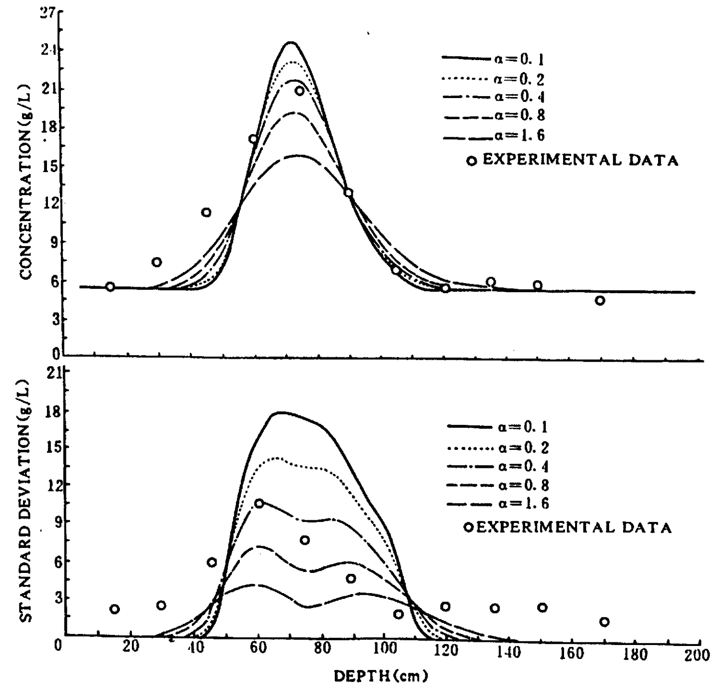

Fig. 6. Profiles of average concentration and standard variance estimated by the convection-dispersion equation.

SUMMARY AND CONCLUSIONS

In the field soil, the solute transport velocity has an intense variability even under a constant infiltration condition. The velocity can be described using a lognormal distribution.

By assuming solute transport velocity to be randomly distributed in the horizontal direction and constant in the vertical direction, the effective dispersivity may be determined from the variance of solute velocity. For the experiment, the effective dispersivity is one order large as the pore scale dispersivity, and the effective dispersivity is proportional to the solute transport time or the travel distance.

The average concentration and variance is determined based on the measured lognormal velocity distribution by the stochastic convection model (Model A), the stochastic convection dispersion model (Model B), and the deterministic convection dispersion equation with a time varying dispersivity (Model C). The average concentrations predicted with these three models are very close, and have a good agreement with the experimental data. The variance calculated using Model A and B is proportional to the concentration gradient and inversely proportional to the pore scale dispersivity. The maximum variance is distributed near the concentration front.

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