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1994

Proceedings WWRC-94-11

In

Proceedings of Fourteenth Annual American Geophysical Union: Hydrology Days

Submitted by

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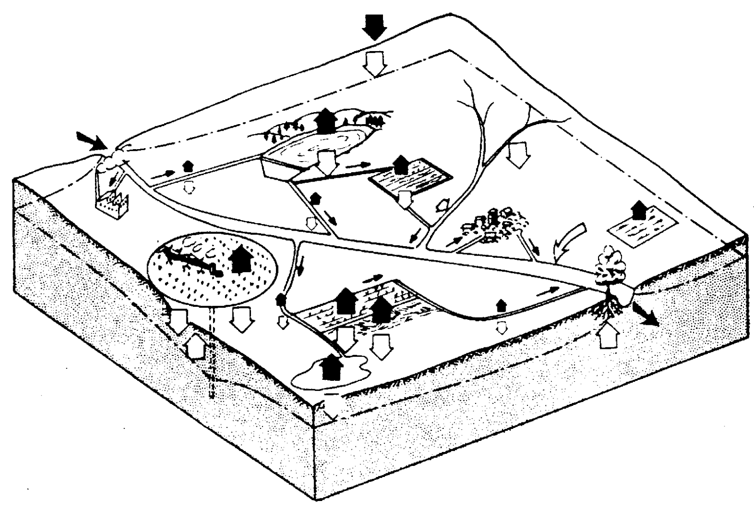
Proceedings
of Fourteenth Annual
American Geophysical Union

HYDROLOGY DAYS



April 5 - 8, 1994
Colorado State University
Fort Collins, Colorado

HYDROLOGY DAYS PUBLICATION

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The Transfer Function for Solute Transport

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ABSTRACT

The transfer function is used to study solute transport in complex soil systems in a simple way by characterizing the output flux as a function of the input flux. The stochastic convective model of the transfer function assumes that solute travel time spreads out at a rate proportional to the square of the distance from the inlet end. Data from a laboratory experiment conducted through long soil columns are used to validate the intrinsic assumptions of the stochastic convective model. Analyses of the experimental data in the homogeneous and heterogeneous soil columns support the assumptions of the transfer function. It is shown that the mean of the probability density function of the travel time is a linear function of log of the travel distance, while the standard deviation is a constant. The stochastic convective model predicts reasonably accurate results of solute transport in the homogeneous and heterogeneous media. Because of the spatial variability of soils, using information obtained at a location closer to the predicting place provides better predictions than using information at farther locations.

INTRODUCTION

More recently the transfer function is applied to simulate the average solute concentration in soils (*Jury*, 1982; *Jury et al.*, 1982; *Sposito et al.*, 1986; *White et al.*, 1986). The transfer function models complex soil systems in a simple way by characterizing the output flux as a function of the input flux. The transformation of an arbitrary input signal into an output signal for a linear system is achieved by means of the impulse response function, which defines the response of the system to a narrow pulse input at the inlet end (*Himmelblau*, 1970, *Jury and Roth*, 1990). The use of the transfer function to represent process models of solute transport is based on a probability density function (pdf) of the travel time of solute molecules. The probability density function characterizes the distribution of possible travel time that a solute molecule might experience in moving from the inlet end to the outlet end. *Jury et al.*, (1982) used the transfer function successfully to describe subsequent movement of a solute pulse down to depth exceeding 360 cm. The model required only a single calibration observing the movement of the solute pulse past 30 cm. The transfer function has the advantage not only of giving mean values but of giving the relative probability of occurrence of extreme movement through soils.

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To test the validity of the transfer function, experiments in soil columns should monitor the outflow concentration as a function of time at various distances from the inlet end, or as a function of distance at various time. However, except for a very recent study (*Khan and Jury*, 1990), this test of the models has not been performed in the laboratory. In particular, the test has not been initiated using large scale experiments.

In this paper data from a laboratory tracer experiment, conducted through 1250-cm soil columns (*Huang et al.*, 1993), are use to validate the intrinsic assumptions of the transfer function. Predictions of solute transport based on the model will be compared with the experimental data.

THEORY

For the convection-dispersion equation, its travel time pdf (Fickian pdf) can be written as follows (*Jury and Roth*, 1990)

$$f(l, t) = \frac{l}{2\sqrt{\pi D t^3}} \exp[-\frac{(l - Vt)^2}{4Dt}] \tag{1}$$

and the cumulative travel time distribution function (cdf) is

$$P(l, t) = \int_0^t f(l, t')dt' = \frac{1}{2}[\mathrm{erfc}(\frac{l - Vt}{2\sqrt{Dt}}) + \exp(\frac{Vl}{D})\mathrm{erfc}(\frac{l + Vt}{2\sqrt{Dt}})] \tag{2}$$

The mean and variance of the travel time distribution Fickian pdf at any distance from the inlet end of x are

$$\mathrm{E}_x(t) = \frac{x}{l}\mathrm{E}_l(t)$$
$$\mathrm{Var}_x(t) = \frac{x}{l}\mathrm{Var}_l(t) \tag{3}$$

where E_l and Var_l are the mean and variance of the travel time distribution at a specified distance of l. The relationship of the variance indicates that the spreading rate of the solute travel time is proportional to the travel distance.

Proposed by *Jury* (1982), the travel time pdf of the convective lognormal transfer function model (CLT) has the form of

$$f(t) = \frac{1}{\sqrt{2\pi}\,\sigma t} \exp[-\frac{(\ln t - \mu)^2}{2\sigma^2}] \tag{4}$$

and the cumulative travel time distribution function is

$$P(t) = \frac{1}{2}\{1 + \mathrm{erf}[\frac{(\ln t - \mu)}{\sqrt{2}\sigma}]\} \tag{5}$$

where μ and σ are the mean and standard deviation of the CLT. When the convective lognormal transfer function is applied at different locations, the pdf and cdf can be written as follows

$$f(x, t) = \frac{1}{\sqrt{2\pi}\,\sigma_l t} \exp\{-\frac{[\ln(tl/x) - \mu_l]^2}{2\sigma_l^2}\} \tag{6}$$

and

$$P(x, t) = \frac{1}{2}(1 + \mathrm{erf}\{\frac{[\ln(tl/x) - \mu_l]}{\sqrt{2}\sigma_l}\}) \tag{7}$$

where μ_l and σ_l are the mean and standard deviation of the lognormal transfer function at distance l. The mean and standard deviation at distance x are related to those at l by

$$\sigma_x = \sigma_l$$
$$\mu_x = \mu_l + \ln(x/l) \tag{8}$$

Equations (8) involves the assumptions (*Jury and Roth*, 1990)

$$f(x, t) = \frac{l}{x} f(l, \frac{tl}{x})$$
$$P(x, t) = P(l, \frac{tl}{x}) \tag{9}$$

The Fickian travel time pdf can be modified so that it obeys (9) at different distances of a column in a steady state flow experiment, by defining distance-dependent parameters through the following relations (*Jury and Roth*, 1990)

$$V_x = V_l$$
$$D_x = \frac{x}{l}D_l \tag{10}$$

The processes, which obey (9), are called stochastic convective models. The mean and variance of the stochastic convective models at any distance, x, are calculated by

$$E_x(t) = \left(\frac{x}{l}\right) E_l(t)$$

$$Var_x(t) = \left(\frac{x}{l}\right)^2 Var_l(t) \qquad (11)$$

These models predict that solute travel time will spread out (as defined by the variance) at a rate proportional to the square of the distance from the inlet end. Since the stochastic convective models are similar, I only use the convective lognormal transfer (CLT) function in the following discussion.

RESULTS

A laboratory experimental data (*Huang et al.*, 1993) were used to validate the intrinsic assumptions of the stochastic convective model (CLT). The laboratory tracer experiments were conducted through 1250-cm long, horizontally placed soil columns during steady saturated water flow. Two columns, each of which had a cross-sectional areas of 10 × 10 cm^2, were used: a uniformly packed homogeneous sandy soil column and a heterogeneous column containing layered and mixed formations of various shapes and sizes of soils. The tracer experiments were carried out after establishing steady-state flow, by replacing tap water with a 6 g/L NaCl solution. The concentration of NaCl in the columns at various time was measured at 50- or 100-cm intervals. Observed breakthrough curves in the homogeneous sandy column were relatively smooth, while those in the heterogeneous column were somewhat irregular and exhibited extensive tailing. More detail about the experiments was given by *Huang et al.* (1993). Based on the experimental data, a nonlinear optimization procedure (*Marquardt*, 1963; *Parker and van Genuchten*, 1984) was applied to compute the parameters of the transfer function, i.e., μ and σ of the CLT. The parameters were determined by minimizing the sum squared errors between the measurements and estimates by the model.

Homogeneous medium

Table 1 shows the best-fitting results of μ and σ of the CLT, using the data collected from the homogeneous soil column. At each of the measured locations, the CLT fitted the data very well, as indicated by the high coefficient of multiple determination (r^2) between the observed data and the calculated concentration. Figure 1 presents one example of the measured data and the fitting breakthrough curve at x = 1200 cm.

To examine the assumptions of the model, we assumed that σ of the CLT was a constant along the soil column and used the fitted σ of the model at 50 cm (i.e. σ = 0.0646) as the constant. Then μ's were calculated at other locations using the optimization procedure and the measured data. As shown in Table 1, the CLT fitted the data quite well for a fixed σ and the values of μ are almost the same as those obtained by a simultaneously fitting procedure (μ and σ) in Table 1. Figure 2 compares the fitted μ of the CLT in Table 1 with the theoretical values calculated using (8) at each distance with l = 50 cm and μ_l = 4.368. The fitted and theoretical mean values are well represented by the 1:1 relation, which shows that the assumptions of the transfer function are valid for the example.

Using the parameters of the CLT at one location, we predicted breakthrough curves at other locations. Figures 3 show the data at 50 cm and the predicted concentration using the CLT, based on parameters obtained at locations of 1200 cm and 600 cm. Using the information at 600 cm (closer to 50 cm) gives a more accurate prediction.

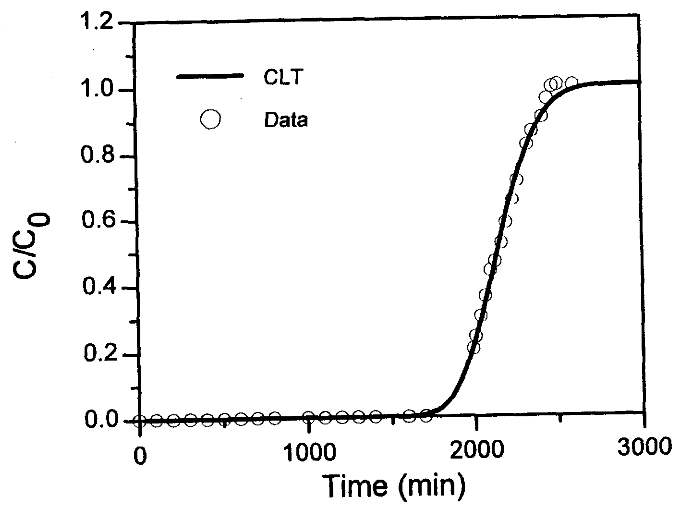

Fig. 1 The fitting and measured breakthrough curves at x = 1200 cm.

Table 1. Estimation of the parameters of the CLT in the homogeneous soil column.

	CLT (Fitting σ and μ)			CLT (σ = 0.0646)	
Distance (cm)	σ	μ	r^2	μ	r^2
50	0.0646	4.368	0.990	4.368	0.990
100	0.0429	5.123	0.992	5.124	0.976
150	0.0450	5.507	0.991	5.508	0.977
200	0.0467	5.796	0.995	5.798	0.984
250	0.0560	6.035	0.997	6.034	0.994
300	0.0582	6.212	0.996	6.213	0.995
350	0.0568	6.373	0.998	6.373	0.995
400	0.0615	6.509	0.998	6.509	0.997
450	0.0628	6.636	0.998	6.636	0.998
500	0.0666	6.746	0.998	6.745	0.998
550	0.0702	6.833	0.998	6.833	0.998
600	0.0614	6.908	0.998	6.908	0.998
650	0.0812	7.038	0.994	7.036	0.993
700	0.0803	7.119	0.997	7.119	0.994
750	0.0902	7.184	0.997	7.180	0.992
800	0.0947	7.257	0.998	7.261	0.985
850	0.0954	7.340	0.999	7.341	0.989
900	0.0837	7.365	0.999	7.364	0.994
950	0.0871	7.433	0.999	7.431	0.989
1000	0.0910	7.493	0.996	7.471	0.988
1050	0.0889	7.539	0.999	7.541	0.991
1100	0.0811	7.600	0.999	7.602	0.994
1150	0.0918	7.639	0.999	7.639	0.987
1200	0.0903	7.669	0.998	7.671	0.987

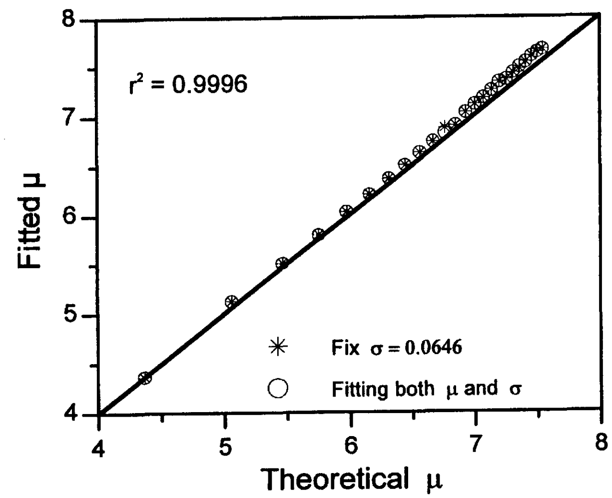

Fig. 2. The comparison between the fitted μ values and the theoretical results of the CLT in the homogeneous column.

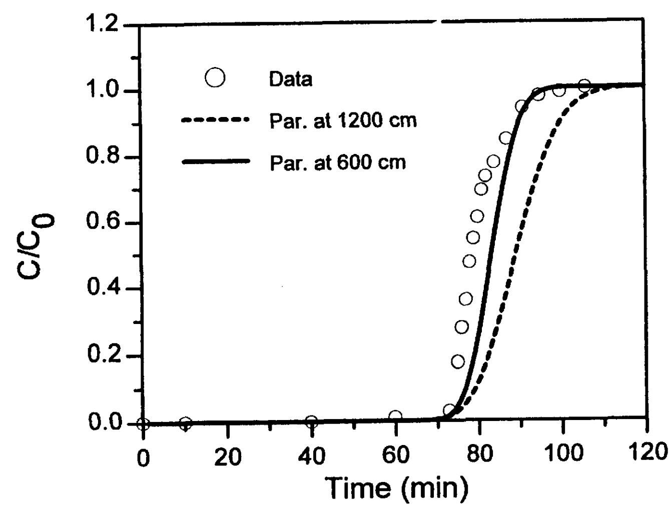

Fig. 3. The comparison between the measured data at 50 cm and the predicted concentration using the CLT, based on parameters obtained at locations of 600 and 1200 cm in the homogeneous column.

Heterogeneous medium

To test validity of the transfer function in the heterogeneous soil, we used available information at the measured location x = 100 and x = 1200 cm, respectively, to predict breakthrough curves at other locations with the CLT, and compared the estimates with the measurements of the solute concentration. Table 2 lists the estimated values of μ for the CLT with different constants of σ in the soil column. The assumed constants of σ were taken from the best-fitting parameters at 100 and 1200 cm, or σ = 0.232 and σ = 0.410, respectively. For the CLT the fitted μ values at the same location are very close assuming the constant of σ as either 0.232 or 0.410 in the whole soil column. Figure 4 indicates that the linear assumption of μ vs. log(x) for the CLT is reasonable for the heterogeneous medium. Figure 5 compares the measured breakthrough curve at x = 1200 cm with predicted results by the CLT. The predictions were based on information (σ and μ) obtained at 100, 600 and 900 cm, respectively. The CLT predicts reasonably good results, especially for predictions based on parameters obtained at the location closer to the predicting points.

Table 2. Estimation of the parameters of the CLT in the heterogeneous soil column, assuming σ is a constant. The constants in the table are taken from the best-fitting parameters at x = 100 and 1200 cm, respectively.

	CLT (σ = 0.232)		CLT (σ = 0.410)	
Distance (cm)	μ	r^2	μ	r^2
100	4.465	0.999	4.433	0.983
200	5.132	0.991	5.105	0.998
300	5.617	0.998	5.587	0.992
350	5.741	0.991	5.714	0.998
400	5.906	0.993	5.878	0.996
500	6.041	0.999	6.010	0.989
600	6.199	0.977	6.178	0.999
700	6.575	0.932	6.576	0.979
800	6.497	0.957	6.485	0.993
900	6.743	0.976	6.713	0.999
1000	6.941	0.976	6.919	0.999
1100	7.030	0.970	7.017	0.998
1200	7.156	0.978	7.133	0.999

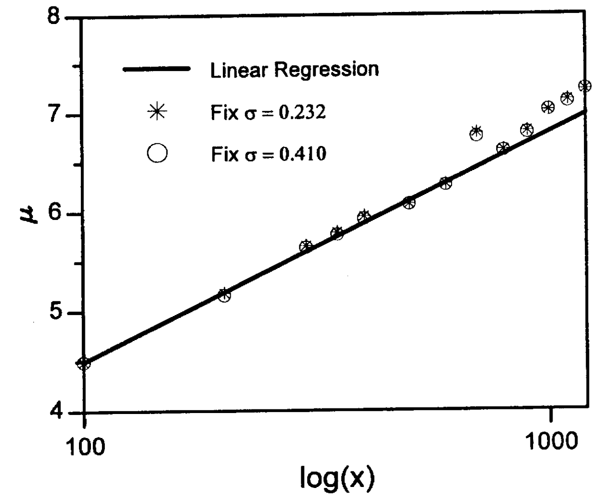

Fig. 4. The linear assumption of μ vs. log(x) for the CLT in the heterogeneous medium.

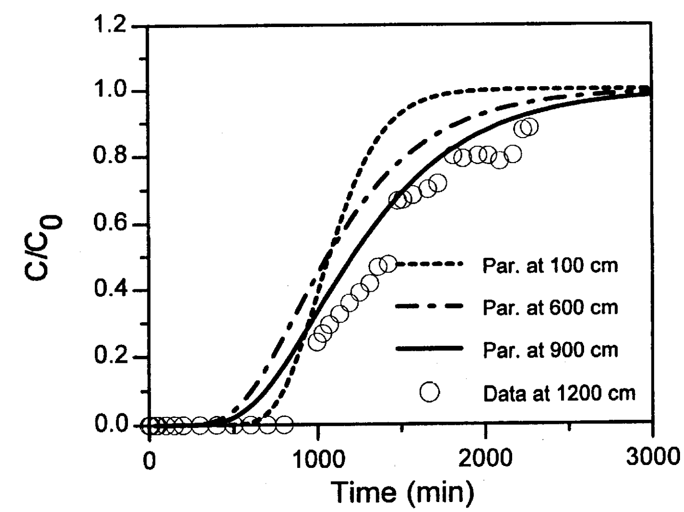

Fig. 5. The predictions of the concentration at x = 1200 cm by the CLT, using the parameters (σ and μ) obtained at 100, 600 and 900 cm in the heterogeneous column.

CONCLUSIONS

Using the laboratory experiments through 1250-cm soil columns, we tested the intrinsic assumptions of the stochastic convective transfer function (CLT). For solute transport both in the homogeneous and heterogeneous media, the assumptions of the CLT are shown to be quite reasonable for the one-dimensional, area-averaged concentration data. It is demonstrated that the mean values of the travel time pdf change linearly with log of the travel distance while the standard deviation is kept as a constant.

Based on available information or measured concentration vs. time somewhere in the soil columns, breakthrough curves were predicted by the CLT. Compared with the measurements, the CLT predicted the solute concentration reasonably well for these examples. Due to the spatial variability of the soil, using information obtained at a location closer to the predicting place provides better predictions than using information collected at farther locations.

ACKNOWLEDGEMENTS

The author is grateful to Mr. K. Huang for providing some data for this analysis.

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