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Application of an Automated Time Domain Reflectometry to Solute Transport Study at Field Scale: Transport Concept

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ABSTRACT : The time-series resident solute concentrations, monitored at two field plots using the automated 144-channel TDR system by Kim (this issue), are used to investigate the dominant transport mechanism at field scale. Two models, based on contradictory assumptions for describing the solute transport in the vadose zone, are fitted to the measured mean breakthrough curves (BTCs): the deterministic one-dimensional convection-dispersion model (CDE) and the stochastic-convective lognormal transfer function model (CLT). In addition, moment analysis has been performed using the probability density functions (*pdfs*) of the travel time of resident concentration. Results of moment analysis have shown that the first and second time moments of resident *pdf* are larger than those of flux *pdf*. Based on the time moments, expressed in function of model parameters, variance and dispersion of resident solute travel times are derived. The relationship between variance or dispersion of solute travel time and depth has been found to be identical for both the time-series flux and resident concentrations. Based on these relationships, the two models have been tested. However, due to the significant variations of transport properties across depth, the test has led to unreliable results. Consequently, the model performance has been evaluated based on predictability of the time-series resident BTCs at other depths after calibration at the first depth. The evaluation of model predictability has resulted in a clear conclusion that for both experimental sites the CLT model gives more accurate prediction than the CDE model. This suggests that solute transport at natural field soils is more likely governed by a stream tube model concept with correlated flow than a complete mixing model. Poor prediction of CDE model is attributed to the underestimation of solute spreading and thus resulting in an overprediction of peak concentration.

INTRODUCTION

Understanding the mechanism of conservative solute transport at field scale is essential for predicting the fate of contaminants and agrochemicals in the unsaturated zone. Various transport models in either a deterministic or a stochastic form, have been proposed to describe the movement of solute at local or field scale. Until now, the most widely used are the convection-dispersion equation (CDE) and the convective lognormal transfer function (CLT) model (Jury *et al.*, 1982). The CDE model is based on the assumption of constant pore water velocity, hydrodynamic mixing and instant equilibrium between the liquid and soil phase. On the other hand, the CLT model assumes that solute particles transport through independent stream tubes. Accordingly, these two models conceptualize the solute transport processes as two extremes: one with complete lateral mixing and the other independent movement with no mixing between different sizes of pores.

A number of field experiments demonstrated that the solute transport mechanism is dependent on the soil type and features such as tonguing, macropores and structural voids (Van Wesenbeeck *et al.*, 1991; Flury *et al.*, 1994; Bronswijk *et al.*, 1995). Many questions, therefore, were raised with respect to the use of the CDE model when the solute transport studies shifted from laboratory to field condition. Nevertheless, some studies reported the successful description of solute transport behaviour with the CDE model in either laboratory (Biggar, Nielsen, 1967) or field (Schulin *et al.*, 1987) condition. Application of the CLT model to field solute transport study (Butters, Jury, 1989) revealed that the model could predict well the spreading of solute pulse to a depth of 3 m after calibration at 0.3 m. However, the CDE model underpredicted the solute spreading beyond 0.3 m after calibration. Tseng, Jury (1994) compared the two different model hypotheses by performing numerical experiments with hypothetical random fields and they found that the observed dispersion in the mean field data was

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intermediate between the two extreme process hypotheses and none of them was accurate over the entire range of testing. Comparison of these models was also reported by Costa *et al.* (1994) who found that the LEACHM (Wagenet, Hutson, 1989), a numerical version of the CDE model, gave the better prediction of solute movement under unsaturated steady-state condition than the CDE and CLT model.

To compensate for the problems associated with the assumptions of CDE model, such as validity of the transport process in the the vertical direction and spatial heterogeneity of soil hydraulic and solute transport properties, a few attempts were made to modify the classical CDE model proposing the mobile and immobile concept (Van Genuchten, Wierenga, 1976) and the regional stochastic model (Parker, Van Genuchten, 1984) by assuming a lognormal distribution of the pore water velocity across the field. As argued by Bronswijk (1995), modifying the CDE model by adding new concepts or more parameters becomes often meaningless since different sets of parameters might give equally best fits to observed data. Rather, more in-depth analysis of the model would be a prerequisite for better understanding and thus improving the knowledge of transport in field soils. To do so, high quality data sets of solute transport in real conditions are required.

So far, most studies on solute movement conducted at field scale are based on either solution samplers or soil coring. Problems associated with the solution samplers are disruption of flow paths, representativeness of solute concentration and difficulties involved in the extration of solution in dry soils. With respect to the solute transport mechanism, the representativeness of solute concentration, whether it is flux or resident type of concentration, is an important issue because the physics behind the mechanism dominating the flow processes is contingent to this. Furthermore, since the analytical solutions of both the CDE and CLT equations are different for the flux and resident concentration, an unclear picture of solute concentration would give a misleading interpretation of the results. The main disadvantages related to soil coring are that sampling disturbs the soil profile and that the frequency of sampling is low. Furthermore, an instantaneous observation of the solute concentration profile may not provide convincing or conclusive information unless the results are reproducible.

Recently, time domain reflectometry (TDR) has been applied to solute transport study as an alternative and interesting device for monitoring conservative solutes in porous media (Dalton *et al.*, 1984; Nadler *et al.*, 1991). Monitoring of solute movement using vertical TDR probes have been demonstrated for laboratory and field scale (Kachanoski *et al.*, 1992; Ward *et al.*, 1995). In these studies, flux type concentrations were measured by taking into account the solute mass leaving the bottom end of the soil volume monitored by the TDR probes. Application of vertical TDR probes to field scale studies, might not be appropriate due to the turtuosive nature of flow in field soils and it is very likely that the percolating solute might leave the TDR detecting volume before the applied solute mass reaches the bottom end of the TDR probes. To overcome this problem, TDR probes are often horizontally positioned (Mallant *et al.*, 1994; Vanclooster *et al.*, 1995; Ward *et al.*, 1995) whereby the probes monitor the resident concentration of the bulk soil volume. The data monitored by horizontally-positioned TDR probes give a clear picture of time-series resident solute spreading at a specific depth. In this study, based on the vertical movement of high frequency time-series resident solute plume monitored from the automated TDR system, the governing transport process at field scale is investigated. Time moments analysis was done to define the variance and dispersion of solute travel time for the resident type concentrations based on the CDE and CLT model parameters. The results of the moments analysis and the model preditability formed the basis for the evaluation of the transport concept at the experimental sites.

THEORY

Model Probability Density Function

For a narrow pulse of a mobile, nonvolatile and nonreactive solute applied uniformly on the soil surface under steady state water flow, the time-normalized travel time *pdf* of flux concentration f^f (l,t) of a solute is given by:

$$f^f(l,t)=\frac{C^f(l,t)}{\int_0^{\infty} C^f(l,t')dt'} \quad (1)$$

where C^f (l,t) is the flux concentration at depth l at time t. When no solute is present in the soil initially, and that the integral of the concentration-time curve at any depth is unity, the travel time flux *pdf* of CDE can be described20s Fickian type distribution (Jury, Sposito, 1985; Jury, Roth, 1990):

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

where V and D are the parameters relating to the pore water velocity and the dispersion coefficient of the CDE model. Assuming that there exists a perfect correlation between solute travel times through successive soil layers, Jury, Roth (1990) generalized the travel time flux *pdf* of CLT model for an arbitrary depth z:

$$f^f(z,t) = \frac{1}{\sqrt{2\pi}\sigma_1 t}\text{Exp}\left[-\frac{(\ln(tl/z)-\mu_1)^2}{2\sigma_1^2}\right] \quad (3)$$

where σ and μ are the parameters of the CLT model at the depth of *l*.

For time-series resident concentration, the travel time *pdf* of CDE model was obtained by Jury, Roth (1990) using the Laplace transform of the Fickian *pdf* of flux concentration:

$$f^r(z,t) = \frac{V}{\sqrt{\pi Dt}}\text{Exp}\left[-\frac{(z-Vt)^2}{4Dt}\right] - \frac{V^2}{2D}\text{Exp}\left(\frac{Vz}{D}\right)\text{Erfc}\left[\frac{z+Vt}{\sqrt{4Dt}}\right] \quad (4)$$

Based on the relationship between resident and flux pdfs (Jury, Roth, 1990), which is given as:

$$f^r(z,t) = \frac{t}{z}f^f(z,t) \quad (5)$$

the travel depth resident pdf (depth-normalized) of the CLT model could be obtained (Jury, Roth, 1990) by simply substituting the travel time flux *pdf* (3) into (5):

$$f_z^r(z,t) = \frac{1}{\sigma_l z\sqrt{2\pi}}\text{Exp}\left[-\frac{\left(\text{in}\left(\frac{tl}{z}\right)-\mu_l\right)^2}{2}\sigma_l^2\right] \quad (6)$$

The travel time resident *pdf* (time-normalized) of the CLT model was proposed by Vanderborght *et al.* (1994) assuming that the time-series resident *pdf* at a particular depth can be expressed as a ratio of the concentration to its time integral and that the time integral of resident *pdf* is constant:

$$f_t^r(z,t) = \frac{l}{z}\frac{1}{\sqrt{2\pi}\sigma_l}\text{Exp}\left[-\frac{\ln(tl/z)-\mu_l)^2}{2\sigma_l^2}-\mu_l-\frac{\sigma_l^2}{2}\right] \quad (7)$$

Moment Analysis of Resident pdf

The general form of time moments for resident concentration *pdf* is given by:

$$T_N^r = \int_0^\infty t^N f^r(z,t)dt \quad (8)$$

and based on the approach by Vanderborght *et al.* (1994), the *pdf* of time normalized resident concentration, $f_t^r(z,t)$, can be written as:

$$f_t^r(z,t)\frac{f_t^r(z,t)}{\int_0^\infty f_t^r(z,t)dt} \quad (9)$$

Substituting (9) into (8) gives the following expression:

$$T_N^r = \int_0^\infty \frac{t^N f_t^r(z,t)}{\int_0^\infty f_t^r(z,t)}dt \quad (10)$$

Since the denominator in (10) is constant with time, the equation becomes:

$$T_N^r = \frac{\int_0^\infty t^N f_t^r(z,t)dt}{\int_0^\infty f_t^r(z,t)dt} \quad (11)$$

Introducing the relationship between resident (time-normalized) and flux *pdfs* given in (5) into (11) on the condition that (5) is valid for both depth and time-series resident *pdfs*, the Nth moment of time-normalized resident *pdf* in the CLT model is reduced to the following form:

$$T_N^r = \frac{\int_0^\infty t^{N+1} f^f(z,t)dt}{\int_0^\infty t f^f(z,t)dt} = \frac{T_{N+1}^f}{T_1^f} \quad (12)$$

Since the Nth time moment of flux pdf is known (Jury, Sposito, 1985), and expressed as:

$$T_N^f = \int_0^\infty t^N f^f(z,t)dt = \left(\frac{z}{l}\right)^N \text{Exp}\left(N\mu_l + \frac{N^2\sigma_l^2}{2}\right) \quad (13)$$

the Nth time moment of time-normalized resident *pdf* is given as:

$$T_N^r = \left(\frac{z}{l}\right)^N \mathrm{Exp}\left(N\mu_l + \frac{N(N+2)}{2}\sigma_l^2\right) \quad (13)$$

The Nth time moments of time-normalized resident *pdf* for the CDE model are evaluated using the Laplace transform:

$$T_N^r = (-1)^N \frac{d^N f^r(S)}{ds^N}\Big|_{s=0} \quad (15)$$

where s is the variable conjugate to t in the Laplace transform operation. The Laplace transform of resident *pdf*, $f^r(s)$, is given by (Jury, Roth, 1990):

$$f^r(s) = \frac{2}{1+\xi}\mathrm{Exp}\left(\frac{Vz}{2D}(1-\xi)\right) \quad (16)$$

with $\xi = \sqrt{1+4sD/V^2}$

Substituting the analytic expression for the resident *pdf* given in (15) into (14), the Nth time moments are obtained (see Appendix). Using the first and second time moments, the variance of the solute travel times is given as:

$$\mathrm{Var}(t) = \int_0^\infty (t-T_1)^2 f(t)dt = T_2 - T_1^2 \quad (16)$$

Table 1 summarizes the results of the time moments analysis of the time-series flux and resident *pdfs* for the CDE and CLT model respectively. Remarkable features are noted from the comparison of time moments and variance. For CDE model the mean travel time of the flux *pdf* is mainly governed by convective flow. However, in case of the resident *pdf* dispersive motion also contributes to the mean displacement. Similar behaviour can be found for the CLT model. The contribution of the dispersive motion causes larger time moments and an increase of the variance of the resident *pdf* as compared to the flux *pdf* for both the CDE and CLT model. The larger values of the first time moment and variance indicate delayed arrival time of the peak concentration and more spreading of solute travel time. All of this gives an impression that the time-series resident *pdf* shows a more likely normal distribution of solute travel times than the time-series flux one. Finally, distinction can be made between the CDE and CLT model on the basis of the behaviour of the variance or spreading of the travel time with distance from the point of injection of the solute pulse. According to the CDE model, spreading of the travel times increases linearly with depth whereas the CLT model reveals that the speading is proportional to the square of the distance from the inlet end. This is clearly identified for both flux and resident *pdfs*.

Dispersion of Travel Time

Based on the time (first and second) moments and variance expressed in the CDE model parameters, Jury, Sposito (1985) developed a fundamental definition for the dispersion of solute travel time of the flux *pdf*, and given as:

$$\text{Dispersion of } f^f(t) = \frac{Z^2}{2}\frac{\mathrm{Var}}{T_1^3} \quad (17)$$

with $Var = T_2 - T_1^2$

In this study, a new definition for the dispersion of the resident *pdf*, derived from the time moments of the CDE model parameters is proposed as follows:

$$\text{Dispersion of } f^r(t) = \frac{Z^2}{(T_1 - \hat{V}ar)^2}\hat{V}ar \quad (18)$$

with $\hat{V}ar = \sqrt{T_2} - T_1$

Additionally, dispersivity length can also be defined using the time moments in a similar manner. Assuming that dispersion coefficient increases linearly with the first power of pore water velocity, and that pore water velocity can be represented as the velocity of a solute moving with ensemble average of travel times over a distance, the following

Table 1. Time moments of solute travel times of time-series flux and resident *pdfs* for the CDE and CLT model.

	CDE		CLT	
	Flux	Resident	Flux	Resident
T_1	$\frac{z}{V}$	$\frac{1}{V}(\frac{D}{V}+z)$	$(\frac{z}{l})\mathrm{Exp}(\mu+\frac{\sigma^2}{2})$	$(\frac{z}{l})\mathrm{Exp}(\mu+\frac{3\sigma^2}{2})$
T_2	$\frac{z^2}{V^2}+\frac{2Dz}{V^3}$	$\frac{1}{V^2}(\frac{4D^2}{V^2}+\frac{4Dz}{V}+z^2)$	$(\frac{z}{l})^2\mathrm{Exp}(2\mu+2\sigma^2)$	$(\frac{z}{l})^2\mathrm{Exp}(2\mu+4\sigma^2)$
Var	$\frac{2Dz}{V^3}$	$\frac{1}{V^2}(\frac{3D^2}{V^2}+\frac{2Dz}{V})$	$(\frac{z}{l})^2\mathrm{Exp}(2\mu+\sigma^2)$ $[\mathrm{Exp}(\sigma^2)-1]$	$(\frac{z}{l})^2\mathrm{Exp}(2\mu+3\sigma^2)$ $[Exp(\sigma^2)-1]$

Table 2. Definition of the dispersion coefficient and dispersivity for time-series flux and resident *pdf* of the CLT model.

	Flux *pdf*	Resident *pdf*
Dispersion (L^2T^{-1})	$\frac{Zl}{2}\frac{[\mathrm{Exp}(\sigma^2)-1]}{\left[\mathrm{Exp}(\mu+\frac{\sigma^2}{2})\right]}$	$\frac{Zl}{\mathrm{Exp}(\mu+\frac{3}{2}\sigma^2)}\frac{\left[\mathrm{Exp}(\frac{\sigma^2}{2})-1\right]}{\left[\mathrm{Exp}(\frac{\sigma^2}{2})-2\right]^2}$
Dispersivity (L)	$\frac{Z}{2}[\mathrm{Exp}(\sigma^2)-1]$	$Z\frac{\left[\mathrm{Exp}(\frac{\sigma^2}{2})-1\right]}{\left[\mathrm{Exp}(\frac{\sigma^2}{2})-2\right]^2}$

expression can be derived for each type of *pdf*:

$$\lambda_{tf} = \frac{Z\mathrm{Var}}{2T_1^2} \quad (19)$$

$$\lambda_{tr} = \frac{ZT_1\hat{\mathrm{V}}\mathrm{ar}}{(T_1-\hat{\mathrm{V}}\mathrm{ar})^2} \quad (20)$$

where λ_{tf} and λ_{tr} are the dispersivities of time-series flux and resident *pdfs*, respectively. The functional expression of dispersion of both flux and resident *pdfs* in terms of time moments and variance allows for calculation of the dispersion coefficient and dispertivity length using the CLT model parameters. Table 2 gives a summary of the definitions of dispersion coefficients and dispertivity lengths obtained for the flux (Jury, Sposito, 1985) and resident *pdfs* (this study) of the CLT model. Irrespective of the type of concentration, the dispersion coefficient of the CLT model increases linearly with depth. However, the dispersion of the CDE model is constant with depth. In fact, the difference of dispersion behaviour between both models provides the second criterion of testing the performance of each model.

RESULTS AND DISCUSSION

Parameter Estimates

Parameters of the CDE and CLT model probability density functions were derived from the mean BTCs measured at different depths using least squares optimization (Jury, Sposito, 1985). In addition, time moments were also calculated. Table 3 shows the results of parameter estimates and time moments in two experimental sites when the simple linear model (Kim *et al.*, 1994; Kim, this issue) was used for calibration of the bulk soil electrical conductivity measured by TDR. The pore water velocities estimated from the CDE model are found rather constant despite the heterogeneity of soil horizons across the depth for both sites. The expected travel times are 14.3 days and 35.6 days for Bekkevoort and Jülich soils respectively, indicating a two or three times higher pore water velocity. Previous findings match reasonably well with the flux densities of downward water movement under steady state conditions which were 2.84 cm day^{-1} for Bekkevoort and 1.50 cm day^{-1} for Jülich. The dispersion coefficients for the Bekkevoort soil are also two or three times higher than for Jülich, implying almost the same dispersivity lengths. Fig. 1 shows the vertical movement of solute plume expressed in the mean resident concentration at field scale. The displacement of center of mass together with the dispersion process are clearly shown in both depth and time scale. From this Figure and Table 3, it seems that the CDE model gives the most realistic estimation of the mean travel time. The travel time of the peak concentration to the depth of 90 cm matches well the first time moments listed in Table 3, resulting in 13 days and 35 days for both the Bekkevoort and Jülich soil respectively. At a given time, more vertical dispersion around the center of mass with faster movement of the solute plume is found for Bekkevoort soil whereas the opposite is true for the Jülich soil. Although the Jülich soil seems to show more spreading of solute travel times for a given depth, this spreading itself is not a direct measure of the dispersion process since soils having lower pore water velocities will always show more spreading of travel times. Table 4 shows the results of the mean travel times and dispersion characteristics estimated using the CDE, CLT model parameters and method of moments (MM). The MM gives higher values of the mean travel time for all depths than the others due to the effect of tailing on the first time moment. Dispertivity lengths are shown to increase with depth, which gives a contradictory result to the assumption of the CDE model. A good agreement is found among the results of dispertivities for the Jülich site. However, the MM for the Bekkevoort site gives much higher values at the first three depths as compared to the other two models. The main cause of the difference is found in the denominator of (18) where the difference between the reduced variance ($\hat{V}ar$) of travel times given as $(T_2)^{0.5}$-T_1 and the first time moment becomes small in that soil (see Table 3). This particular behaviour can also be observed in the dispersivity lengths defined in (19) and (20) as was shown in Fig.

Table 3. Time moments and parameter estimates of time-series resident *pdf* of the CDE and CLT model for the mean BTCs measured at two field sites.

Bekkevoort

Depth (cm)	Time Moments				CDE		CLT	
	T_1	T_2	Var	$\hat{V}ar$	V	D	μ	σ
10	2.46	9.55	3.48	0.63	4.14	5.91	0.65	0.50
30	5.66	39.88	7.87	0.66	5.40	7.00	1.63	0.29
50	8.13	75.32	9.29	0.55	6.34	12.45	1.99	0.28
70	10.25	118.39	13.35	0.63	7.04	26.35	2.20	0.32
90	14.33	238.70	33.23	1.12	6.64	42.41	2.47	0.36

Jülich

Depth (cm)	Time Moments				CDE		CLT	
	T_1	T_2	Var	$\hat{V}ar$	V	D	μ	σ
15	6.43	47.69	6.39	0.48	2.47	3.32	1.64	0.41
35	13.94	226.28	32.06	1.11	2.73	7.68	2.41	0.39
50	20.54	502.59	80.89	1.88	2.68	11.02	2.78	0.39
70	30.61	1098.21	161.53	2.53	2.40	17.49	3.19	0.44
90	35.58	1488.60	222.80	3.00	2.44	16.32	3.47	0.37

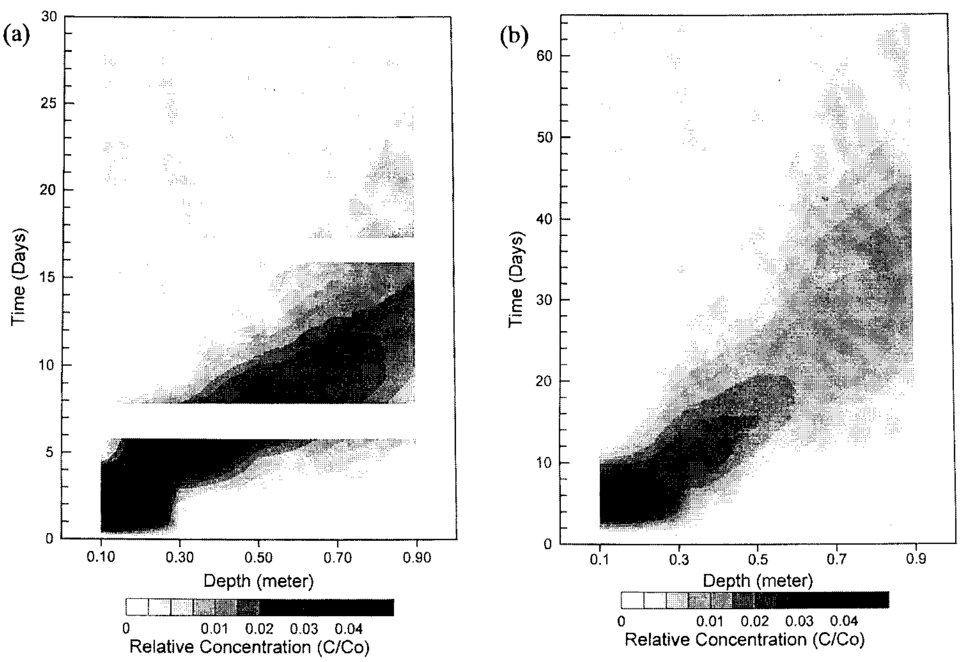

Fig. 1. Vertical distribution of the mean resident solute plume with time monitored using the automated 144-channel TDR system.

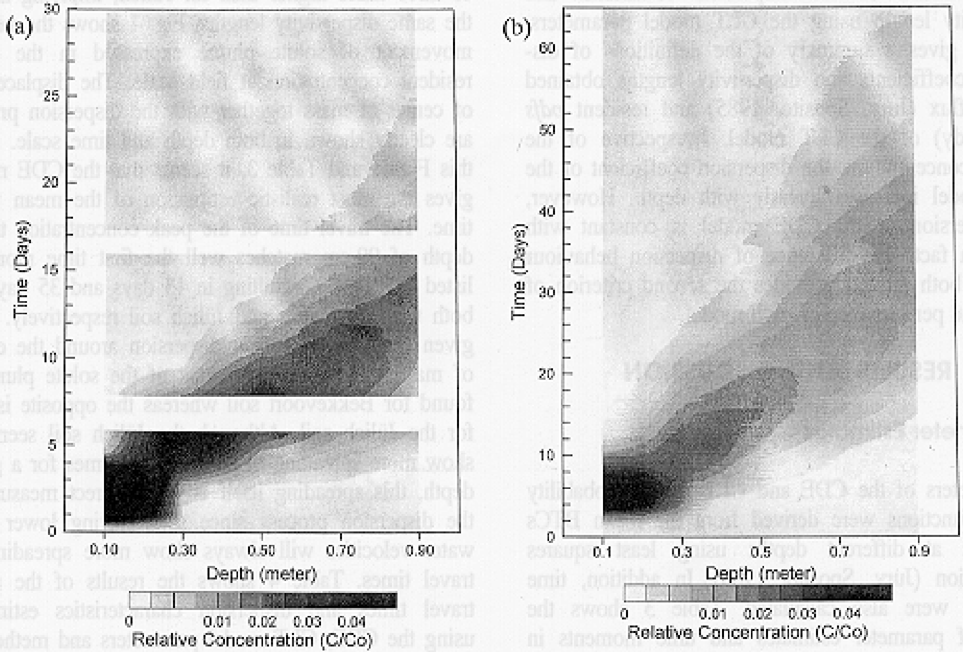

Fig. 1. Vertical distribution of the mean resident solute plume with time monitored using the automated 144-channel TDR system.

Table 4. Mean travel times and dispersion characteristics estimated using the CDE, CLT model parameters and method of moments (MM).

Bekkevoort

Depth (cm)	MM				CDE				CLT			
	T_1	V	D	λ	T_1	V	D	λ	T_1	V	D	λ
10	2.46	4.07	18.83	4.63	2.41	4.14	5.91	1.43	1.91	5.23	6.37	1.77
30	5.66	5.30	23.54	4.44	5.55	5.40	7.00	1.30	5.12	5.86	7.17	1.39
50	8.13	6.15	23.87	3.88	7.89	6.34	12.44	1.96	7.32	6.83	12.71	2.08
70	10.25	6.83	33.40	4.89	9.94	7.04	26.35	3.74	9.02	7.76	26.94	4.04
90	14.33	6.28	51.98	8.28	13.55	6.64	42.41	6.39	11.85	7.60	44.49	7.15

Jülich

Depth (cm)	MM				CDE				CLT			
	T_1	V	D	λ	T_1	V	D	λ	T_1	V	D	λ
15	6.43	2.33	3.05	1.18	6.07	2.47	3.32	1.34	5.18	2.90	3.47	1.53
35	13.94	2.51	8.23	3.28	12.82	2.73	7.68	2.81	11.10	3.15	8.02	3.18
50	20.54	2.43	13.53	5.56	18.68	2.68	11.02	4.12	16.10	3.11	11.51	4.66
70	30.61	2.29	15.76	6.89	29.13	2.40	17.49	7.28	24.26	2.88	18.60	8.56
90	35.58	2.53	22.94	9.07	36.84	2.44	16.32	6.68	32.23	2.79	16.97	7.48

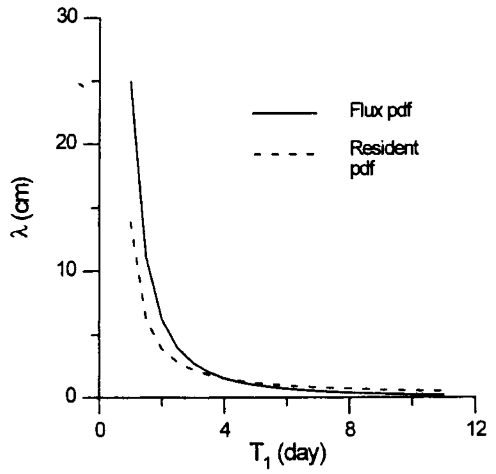

Fig. 2. Dispersivities defined by the time moments analysis of flux and resident *pdfs* and their relationship with the first time moment for a constant variance of 0.5.

2. For a given variance of travel times at a certain depth, the dispersivity length is inversely related to the first time moment for the flux *pdf* and the difference between the reduced variance and the first time moment for the resident *pdf*. More specifically in case of the resident *pdf*, it is proportional to the pore water velocity when the expected travel time (T_1) is much higher than the reduced variance. Although small differences could be found in the results of dispersivities between different methods, two field soils in this study show comparable results of dispersivity length and its relationship with depth. The values of dispersivity lengths obtained for the two field soils are within a range of 1.3 to 8.6 cm for the depth between 10 cm and 90 cm. These results agree with the result of Ellsworth, Jury (1991) who found 9.1 cm at a depth of 1 m for a loamy sand and Schulin *et al.* (1987) with values ranging between 2.8 and 12.1 cm up to depth of 3.1 m in a stony field soil, but are slightly lower than the result of Butters, Jury (1989) with 5.6 to 23.9 cm field scale disper- sivities for a depth of 30 to 90 cm in a loamy sand soil and Roth *et al.* (1991) with 29 cm for a depth of 40 to 240 cm in a loamy soil.

Transport Concept

The relationship between variance and depth relationship for the two field soils are shown in Fig. 3 and can serve as a first criterion of evaluating each candidate model. Both soils show a strong nonlinear (Bekkevoort) and a weak nonlinear (Jülich) increase of variance with depth. The weak nonlinearity can be viewed as a linear relationship below the second depth, indicating that the transport process obeys the CDE model concept whereas the strong nonlinearity present in the Bekkevoort soil, if a quadratic equation can successfully be fitted, may imply validity of the CLT model concept. The relationships of dispersion with depth are shown in Fig. 4. None of them shows constancy with depth which are far from the CDE model assumption. It becomes obvious that a linear increase can be possibly drawn below the second depth for the Bekkevoort soil while a clear linear relationship is present up to a depth of 70 cm for the Jülich soil. This indicates that both soils obey the CLT model concept to a certain extent of depth. Study on the governing transport concept based on these two criteria appears unreliable due to contradictory results. The unclear results from the variance- or dispersion-depth relationship is attributed to the variations in flow and transport properties across depth since those relationships are based on the assumption of constant pore water velocity and dispertivity.

A more practical evaluation of the model hypotheses would be to compare the observed BTCs with model predictions. Comparisons between the observed and predicted BTC data are shown in Fig. 5. The resident concentration BTCs are predicted at other depths after calibration at the first depth. At the calibration depth an identical BTC is obtained for both models resulting in an almost perfect fitting to the observed BTCs. For the Bekkevoort soil, model predictions using either CDE or CLT concept are poor especially in the peak concentrations and arrival times. Differences between observations and predictions are growing with distance. Since the relation-

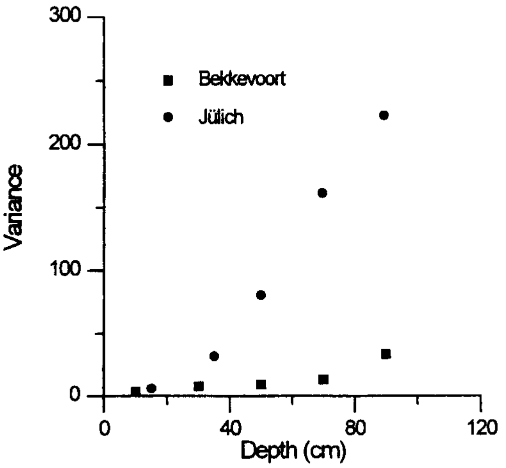

Fig. 3. Relationship between the variance of solute travel times and depth.

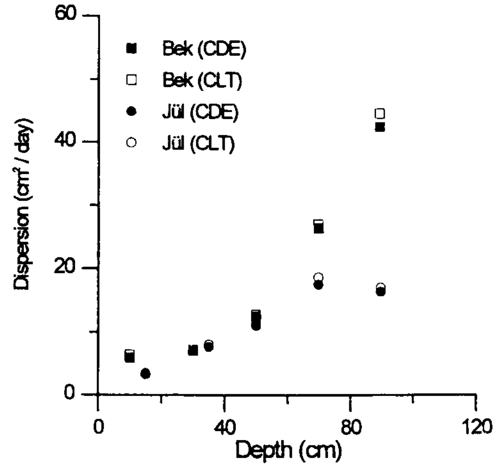

Fig. 4. Relationship between the dispersion of solute travel times and depth.

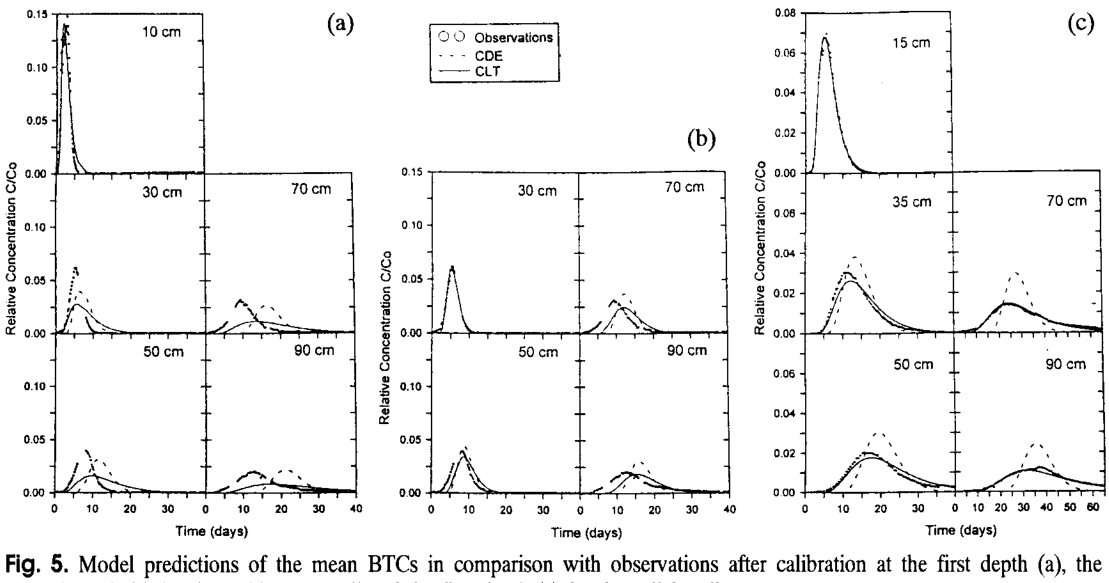

Fig. 5. Model predictions of the mean BTCs in comparison with observations after calibration at the first depth (a), the second depth (b) for the Bekkevoort soil and the first depth (c) for the Jülich soil.

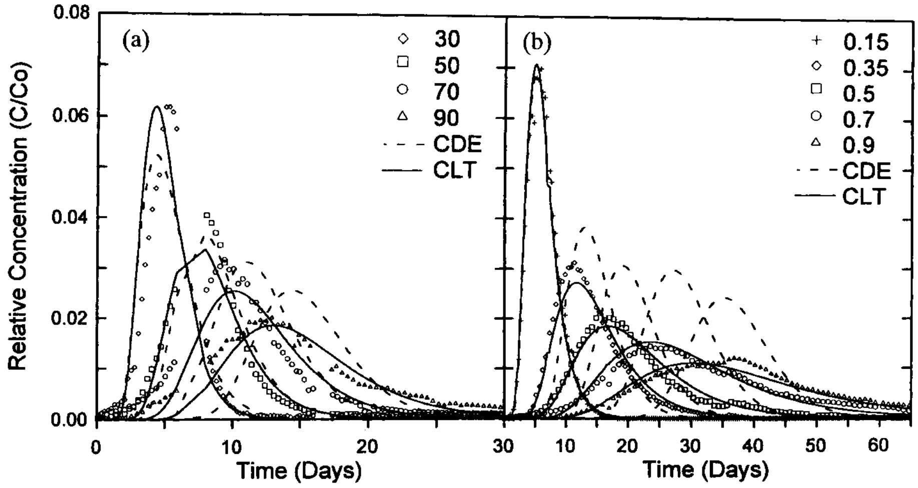

Fig. 6. Model predictions of the mean BTCs in comparison with observations after calibration using the global BTCs at a reference depth of 1 m for the Bekkevoort soil (a) and the Jülich soil (b).

ship of dispersion with depth is shown more likely linear after the second depth, predictions were made again after calibrating at a depth of 30 cm. In this case, the CLT model predictions considerably improved but the CDE model still overestimats the peak concentrations. In contrast, for the Jülich soil, the CLT model gives excellent predictions at all depths with the calibrated parameters obtained from the first depth whereas the CDE model shows similar results to Bekkevoort soil overestimating the peak concentrations. The results of predictability suggest that the CLT model concept is more likely dominating the transport mechanism at both field sites although the CLT model predictions for the Bekkevoort soil are not producing a perfect match with obervations. Poor performance of the CDE model is attributed to the linear increase of variance with depth, which is responsible for the narrower spreading of solute travel times compared to the quadratic increase of variance in the CLT model. As a result, the dispersions of solute are underestimated and the peak concentrations are overestimated. These results are in a good agreement with the findings by Butters, Jury (1989) who found similar differences between the performance of both models.

Another way of testing the model hypothesis with model predictability is to calibrate the model parameters with the global BTC data representing the entire transport regions. The global BTC data can be obtained by transforming the observed BTC data from each depth to a reference depth. The advantage of this approach lies in the fact that heterogeneity of transport properties, possibly present in different soil layers, are lumped and a single property representing longitudinal dispersion is produced encompassing the whole transport volume. In this way more meaningful transport parameters at field scale can be derived and used to evaluate the candidate models. Results of predictions are shown in Fig. 6. For Bekkevoort soil (Fig. 6a), the BTC at the first depth is excluded in the calibration of parameters of the global BTC. The CLT model gives equally good predictions at all depths for both soils. However, the CDE model gives similar results to the previous case, overestimating the peak concentrations especially at larger depths.

SUMMARY AND CONCLUSIONS

The transport mechanism governing the movement of solute at field scale was investigated by applying two candidate models (CDE and CLT), based on the opposite assumptions of solute movement behaviour, to the mean time-series resident type BTC data obtained by an automated TDR system. By implemetation of the time moments analysis on the solute travel time probability density functions of CDE and CLT model, dispersion of travel times for time-series resident concentration was defined in terms of travel time moments. In addtion, the dispersion coefficient of the CLT model was also defined using its model parameters. Estimated dispersivities using those definitions in two field loamy soils, were found in good agreement with those determined using the CDE parameters as well as from other field studies. When the relationship of either variance or dispersion with depth was used, evaluation of the model concept did not result in a clear conclusion due to vertical heterogeneity of the transport properties across different soil horizons. As an alternative, prediction of each model was performed against the observed BTC data after calibrating at the first depth and a reference depth. Results of predictions using two candidate models demonstrated that the CLT model concept was more dominant in the studied soils than the CDE concept. This indicates that solute movement at field scale takes place through different sizes of pores viewed as independent stream tubes with a perfect correlated flow rather than as connected tubes with uncorrelated random lateral mixing.

APPENDIX

Time Moments of Time-Series Resident *pdf* of CDE Model

The Laplace transform of resident *pdf*, $f_t^r(s)$, is given by (Jury, Roth, 1990):

$$f_t^r(s) = \frac{2}{1+\xi}\mathrm{Exp}\left(\frac{Vz}{2D}(1-\xi)\right) = g(\xi)\,h(\xi) \quad \text{(A1)}$$

with $\xi = \sqrt{1+4sD/V^2}$

where $g(\xi)=2/(1+\xi)$ and $h(\xi)=\mathrm{Exp}(Vz(1-\xi)/2D)$. The first time moment is obtained by the first derivative of $f_t^r(s)$:

$$\frac{df_t^r(s)}{ds} = \left(g(\xi)\frac{dh(\xi)}{d\xi} + h(\xi)\frac{dg(\xi)}{d\xi}\right)\frac{d\xi}{ds} \quad \text{(A2)}$$

$$\frac{dg}{d\xi} = -\frac{2}{(1-\xi)^2} \quad \text{(A3)}$$

$$\frac{dh}{d\xi} = -\frac{Vz}{2D}\mathrm{Exp}\left(\frac{Vz}{2D}(1-\xi)\right) \quad \text{(A4)}$$

$$\frac{d\xi}{ds} = \frac{2D}{V^2\xi} \quad \text{(A5)}$$

Substituting (A3-5) into (A2) and rearranging gives:

$$\frac{df_t^r(s)}{ds} = \left(-\frac{Vz}{2D} - \frac{1}{1+\xi}\right)\left(\frac{2D}{V^2\xi}\right)\left[\frac{2}{1+\xi}\mathrm{Exp}\left(\frac{Vz}{2D}(1-\xi)\right)\right] = u(s)\,f_t^r(s) \quad \text{(A6)}$$

$$\text{with } u(s)=\left(-\frac{Vz}{2D} - \frac{1}{1+\xi}\right)\left(\frac{2D}{V^2\xi}\right) \quad \text{(A7)}$$

The second derivative of $f_t^r(s)$ is given:

$$\frac{d^2f_t^r}{ds^2} = f_t^r(s)\left(\frac{du}{d\xi}\frac{d\xi}{ds}\right) + u(s)\frac{df_t^r(s)}{ds} \quad \text{(A8)}$$

$$\frac{du}{ds} = \frac{2D}{V^2\xi}\left[\frac{1}{(1+\xi)^2} + \frac{1}{\xi}\left(\frac{Vz}{2D} + \frac{1}{1+\xi}\right)\right]\frac{2D}{V^2\xi} \quad \text{(A9)}$$

Substituting (A1, 5, 7, 8, 9) into (A6), the second time moment is expressed as:

$$\frac{d^2f_t^r}{ds^2} = \left(\frac{2D}{V^2\xi}\right)^2\frac{2}{1+\xi}\mathrm{Exp}\left(\frac{Vz}{2D}(1-\xi)\right)\left[\frac{1}{(1+\xi)^2} + \frac{1}{\xi}\left(\frac{Vz}{2D} + \frac{1}{1+\xi}\right) + \left(-\frac{Vz}{2D} - \frac{1}{1+\xi}\right)^2\right] \quad \text{(A10)}$$

Noting that at s=0, ξ=1, the first and second time moments are given as function of V and D:

$$T_1^r = (-1)\frac{df_t^r(s)}{ds}\Big|_{s=0} = \frac{1}{V}\left[\frac{D}{V} + z\right] \quad \text{(A11)}$$

$$T_2^r = (-1)^2\frac{d^2f_t^r(s)}{ds^2}\Big|_{s=0} = \frac{1}{V^2}\left[\frac{2D}{V} + z\right]^2 \quad \text{(A12)}$$

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시간영역 광전자파 분석기 (Automatic TDR System)를 이용한 오염물질의 거동에 관한 연구: 오염물질 운송개념

김 동 주

요 약 : 현장에서의 주요 운송 메카니즘을 연구하기 위하여 시간별 잔존수 농도분포곡선 자료를 이용하였다. 운송개념을 대표하는 모델로서 2개의 상반된 가설에 근기한 모델, 즉 CDE와 CLT모델을 사용하였으며 파라미터 추정을 위하여 깊이별 평균농도자료에 최적화기법을 적용하였으며 잔존수 농도의 도달시간을 나타내는 확율밀도함수를 이용하여 모멘트해석도 시행되었다. 모멘트 해석결과 잔존수농도의 1차 및 2차 시간 모멘트는 침출수농도의 것들보다 크게 나타났다. 또한 시간 모멘트를 이용하여 오염물질 운송시간의 변이도와 확산 파라미터도 도출되었다. 변이도 및 확산계수와 운송거리간의 상관관계는 침출수농도 및 잔존수농도에 대해서 동일하게 나타났다. 이러한 관계를 이용하여 2가지 모델을 검정하였으나 운송거리에 따른 운송 파라미터의 불규칙한 변화로 확정적 결론을 얻을 수 없었다. 따라서 첫 번째 깊이에서 얻은 파라미터를 이용하여 다른 깊이에서의 오염물질 운송 방식을 예측하여 실측자료와 비교하여 각 모델을 검정하였다. 그 결과 CLT 모델이 CDE 모델보다 현장실측자료에 근접하였다. 이는 오염물질이 이동함에 따라 완전한 혼합이 발생하는 것이 아니라 상관흐름 즉, "오염물질이 각 층을 통과할 때 빠른 물질은 빠르게 느린 물질은 지속적으로 느리게 움직인다"는 사실을 뒷받침한다고 볼 수 있다. 특히 첨두농도에 대한 CDE 모델의 과대예측은 오염물질 확산의 과소평가에 기인하는 것으로 나타났다.