

Application of an Automated Time Domain Reflectometry to Solute Transport Study at Field Scale: Experimental Methodology and Calibration of TDR

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ABSTRACT : Field scale experiments using an automated 144-channel TDR system were conducted which monitored the movement of solute through unsaturated loamy soils. The experiments were carried out on two different field plots of 0.54 ha to study the vertical movement of solute plume created by applying a square pulse of CaCl_2 as a tracer. The residence concentration was monitored at 24 locations on a transect and 5 depths per location by horizontally-positioning 50 cm long triple wire TDR probes to study the heterogeneity of solute travel times and the governing transport concept at field scale. This paper describes details of experimental methodology and calibration aspects of the TDR system. Three different calibration methods for estimation of solute concentration from TDR-measured bulk soil electrical conductivity were used for each field site. Data analysis of mean breakthrough curves (BTCs) and parameters estimated using the convection-dispersion model (CDE) and the convective-lognormal transfer function model (CLT) reveals that the automated TDR system is a viable technique to study the field scale solute transport providing a normal distribution of resident concentration in a high resolution of time series, and that calibration method does not significantly affect both the shape of BTC and the parameters related to the peak travel time. Among the calibration methods, the simple linear model (SLM), a modified version of Rhoades' model, appears to be promising in the calibration of horizontally-positioned TDR probes at field condition.

INTRODUCTION

Numerous studies on solute transport have been conducted at either laboratory or field scale to identify the processes which dominate the transport of chemicals through unsaturated soils. Awaiting that results of laboratory determination on solute transport are not representative of the field scale, there have been growing interest in solute transport at field scale. Research efforts were then oriented to field investigations either using solution samplers (Miller *et al.*, 1965; Biggar, Nielsen, 1976; Starr *et al.*, 1978; Van de Pol *et al.*, 1977; Jury *et al.*, 1982) or taking soil cores (Wild, Babiker, 1976). Application of these measurement techniques was not found suitable for study on the solute transport at field scale due to problems associated with representative nature of water samples from solution samplers (Hansen, Harris, 1975; Grover, Lamborn, 1970; Adams, 1974) and time-series measurement of solute displacement for soil coring and the physical disturbance for both method (Kachanoski *et al.*, 1992).

Nondestructive measurement of field scale solute travel time using vertically-positioned TDR probes was reported by Kachanoski *et al.* (1992) and parameter estimation of field solute transport models using the same technique by Elrick *et al.* (1992). They found that the TDR method was simple, quick and inexpensive for solute transport study. These studies were based on the manual measurement of mass flux densities using TDR probes. For depth-dependent and time-series measurement, TDR probes are often positioned horizontally (Mallants *et al.*, 1994; Vanclooster *et al.*, 1995; Ward *et al.*, 1994). Field study of solute transport especially aiming at investigating the heterogeneity of transport parameters and the governing transport concept requires a large number of TDR probes at multiple locations and depths. Recently, a computer controlled TDR system for measuring soil water content and bulk soil electrical conductivity was developed by Heimoaara and Water (1993a). This system enables one to handle a large number of probes with automated 144-channels suitable for monitoring a high resolution of time-series solute concentrations at multiple locations.

The objective of this study is to develop a new

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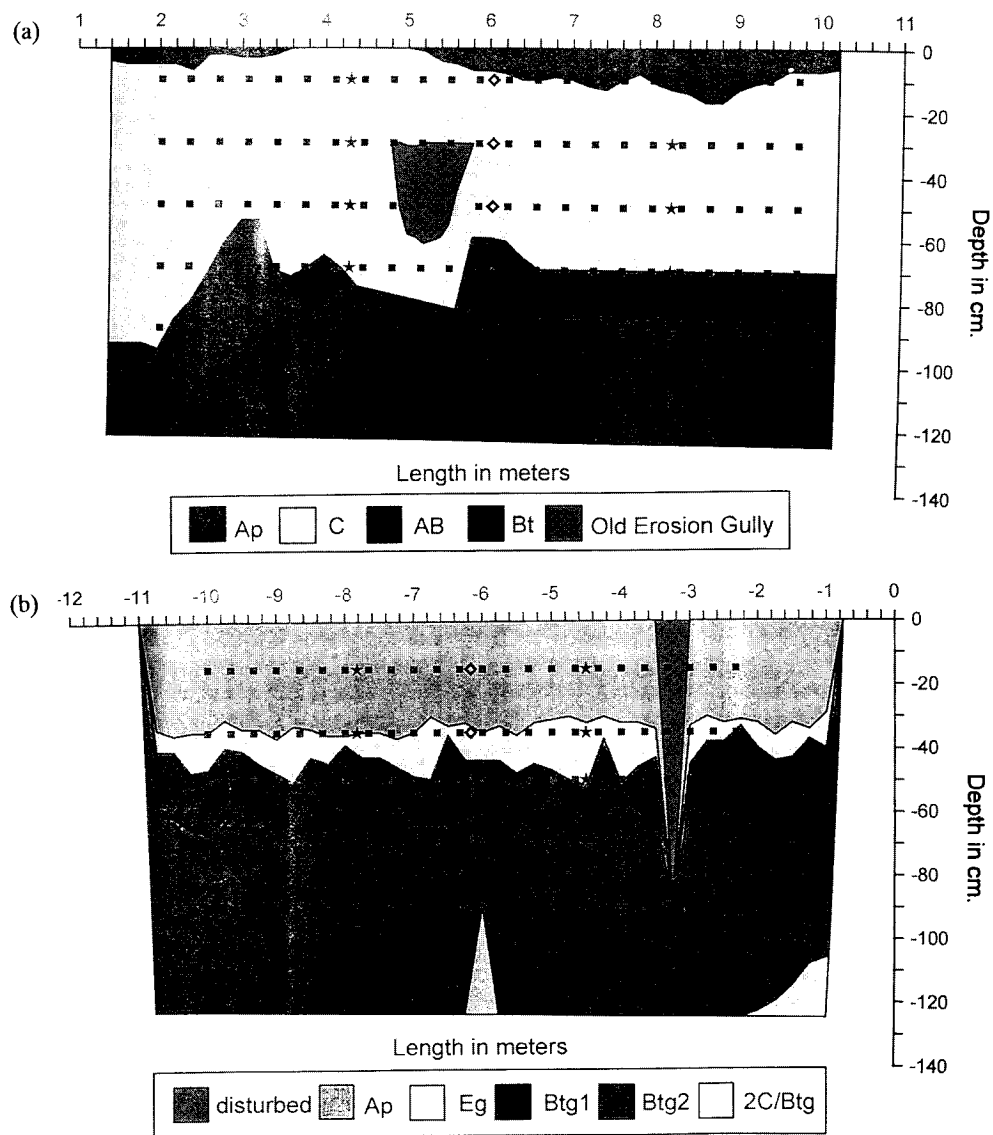


Fig. 1. Schematic depiction of the boundaries of the soil horizons and the position of the TDR probes, the tensiometer cups and thermal sensors in the trench of the study area at the Bekkevoort (a) and the Jülich site (b).

method for monitoring of solute displacement at field using the automated TDR system equipped with horizontally-positioned TDR probes. This paper describes a detailed experimental procedure and calibration of TDR probes. In a companion paper (this issue), a study on the parameter estimation of time-series resident solute travel time density function and the governing transport concept is reported, based on the spatially-averaged mean breakthrough curves.

MATERIALS AND METHODS

Experimental Site

Field tracer experiments were conducted at two different sites. Each experimental site was located at Bekkevoort, Belgium and Jülich, Germany respectively. Trenches were made up to a depth of 1.2 m in order to get information on soil profile development and to install the TDR probes. Configuration of the soil horizons and the probe positions is schematically depicted in Fig. 1. The soil in the Bekkevoort site is an Eutric Regosol (FAO classification), being a young soil with high base saturation and few traces of

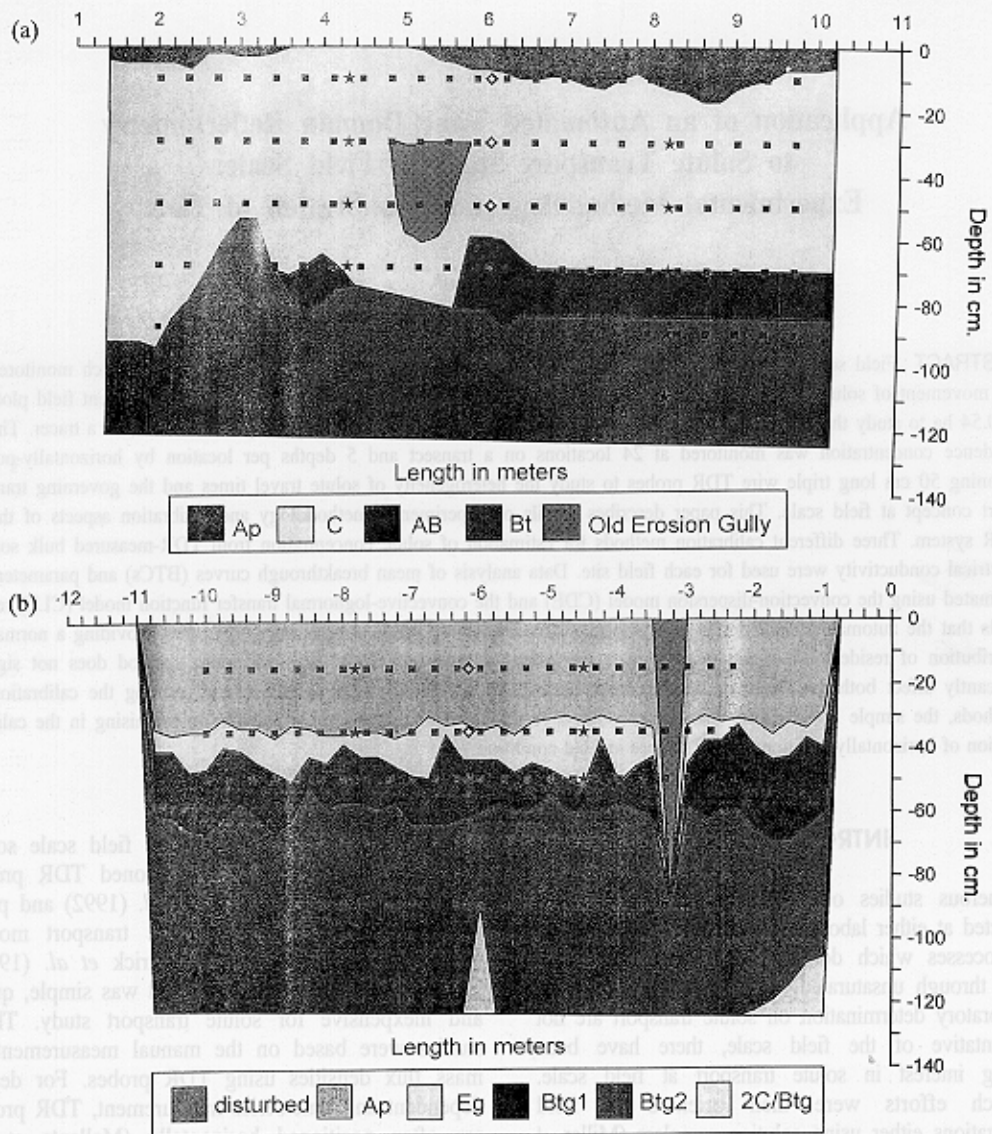


Fig. 1. Schematic depiction of the boundaries of the soil horizons and the position of the TDR probes, the tensiometer cups and thermal sensors in the trench of the study area at the Bekkevoort (a) and the Jülich site (b).

profile development. The soil profile exhibits 4 different horizons with varying thickness: Ap (0~20), C (20~70), AB (70~90), Bt (>90 cm). At the Jülich site, the soil is characterized as a Stagnic Podzolvisol. The soil profile exhibits 5 distinct horizons: Ap (0~30 cm), Eg (30~40), Btg1 (40~60), Btg2 (60~100), C (>100) showing strong profile development. The E horizon shows the lowest clay percent due to the transport of clay to a deeper horizon while the Btg1 horizon contains a high clay content as a result of accumulation of clay and minerals transported from the E horizon. At the boundary between the E and B horizons, tongues in a size of a few centimetres are present as a result of shrinkage and swelling of Btg1 horizon influenced by shallow perched ground water table. Table 1 shows basic soil properties measured at different depths for both experimental sites. The soil types are classified as loamy with clay percent ranging 14.1 to 15.5% at Bekkevoort and silt loamy with 13.8 to 23.6% at Jülich over 1 m depth from the soil surface.

Experimental Design

After investigation of the soil profile development, one side of the trench was covered by a plastic sheet as a barrier in order to prevent possible interference of the disturbed soil region. Then 50 cm long triple-wire TDR probes (0.4 cm diameter, 4.6 cm spacing) were positioned horizontally at 24 different locations (35 cm spacing) and 5 different depths, 10, 30, 50, 70, 90 cm for Bekkevoort and 15, 35, 50, 70, 90 cm for Jülich (Fig. 1). In addition, thermal sensors were installed in the middle of the trench wall at 4 depths

Table 1. A summary of basic soil properties of two the experimental sites, Bekkevoort and Jülich respectively.

Depth (cm)	Textural fractions (%)			Organic Carbon (%)	CEC (meq/100)
	Sand	Silt	Clay		
Bekkevoort					
10	53.30	32.64	14.06	2.2	0.14
30	48.68	36.54	14.78	0.8	1.15
50	38.09	46.45	15.46	0.4	6.85
70	34.54	50.07	15.39	0.3	6.82
90	45.49	39.94	14.57	0.6	7.10
Jülich					
15	14.72	66.41	18.87	1.7	10.06
35	15.12	66.56	18.32	0.9	8.03
50	15.45	61.27	23.28	0.4	14.51
70	20.33	56.06	23.59	0.5	9.28
90	19.68	56.18	24.14	0.1	10.17

to monitor the variations of soil temperature, and tensiometer cups at 5 depths at two locations. A plastic greenhouse was built over the plot covering an area of 4.5 m × 12 m. The greenhouse provided an experimental condition independent of natural rainfall during the solute displacement experiment. Water was applied on the plot using an irrigation system before and after application of the solute to maintain a steady downward flux. Static sprinklers were arranged at 28 grid points (4 transversal and 7 longitudinal) with spacing of 1.25 m in transversal and 2 m in longitudinal direction (Fig. 2). Preliminary test on the performance of static sprinklers for the given arrangement revealed that uniformity coefficient was found the highest in the middle area (1.25 m × 8 m) of the plot under an operating pressure of 1.5 KPa. Therefore the study area to investigate the field solute transport was selected in the middle of the plot where 120 TDR probes were positioned.

Prior to the application of a solute, a steady state condition was imposed by the application of a constant flux of 2.84 cm day⁻¹ at Bekkevoort and 1.50 cm day⁻¹ at Jülich for a period of 3 weeks. An on-off system was introduced to apply irrigation water frequently to minimise a possible the risk of nonsteady state condition of the water flux. The observed coefficient of variation (CV) of the irrigation rate ranged between 6 and 8% in the study area. The steady state condition was assured by the analysis of the pressure heads and water contents as measured by tensiometers and TDR probes respectively.

Application of Solute

As soon as the steady state condition was achieved,

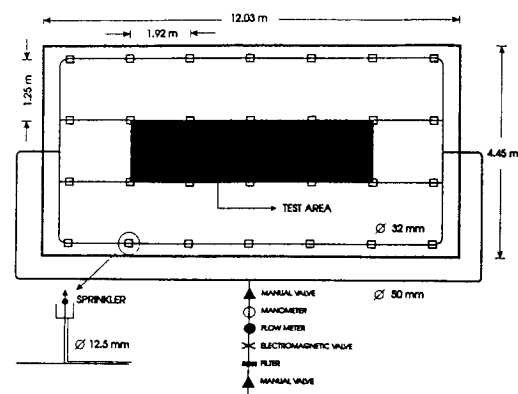


Fig. 2. Layout of the irrigation system in the greenhouse used for the field tracer experiments. The study area is indicated with marked shadow.

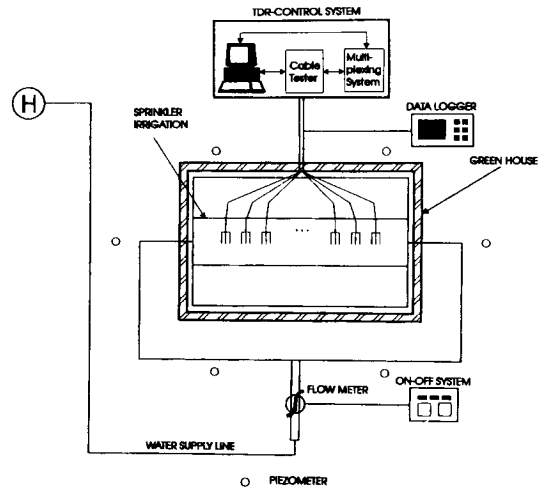
Table 2. Experimental conditions at two field sites for monitoring solute transport.

	Bekkevoort	Jülich
Soil:		
Classification	Eutric Regosol	Stagnic Podzoluvisol
Type (Clay %)	Loam (14.1-15.5)	Silt Loam (13.8-23.6)
Irrigation:		
Intensity (cm day ⁻¹)	114	144
Cycle (min min ⁻¹)	0.3/20	0.5/48
Flux (cm day ⁻¹)	2.8	1.5
CV (%)	6	8
Solute Application:		
Type	Pulse	Pulse
Tracer	CaCl ₂ ·2H ₂ O	CaCl ₂ ·2H ₂ O
Input Conc. (g l ⁻¹)	87.5	80.0
Duration (day)	0.23	0.33
Mass (g m ⁻²)	567	400
CV (%)	19	13
Monitoring:		
Frequency (hrs)	2	4
Duration (day)	42	65

a square pulse of solute (CaCl₂ · 2H₂O) with a concentration of 87.5 g l⁻¹ (Bekkevoort) and 80.0 g l⁻¹ (Jülich) was applied uniformly over an area of 1.75 times the study area using a hand sprayer. The CV of solute application was 19% and 13%, and the pulse duration was 5.7 hrs and 8 hrs with 0.65 cm and 0.5 cm of application depth for each site respectively, resulting in the solute flux density identical to the water flux density applied during the steady-state condition. All of this resulted in an application of the solute with 567 and 400 gm⁻². Table 2 shows a summary of the experimental conditions applied at both sites.

Monitoring of the BTC

Immediately after the application of the solute, irrigation water was introduced again for leaching the solute plume downward with the same flux density as applied during the steady state condition. A schematic representation of the field experimental design is given in Fig. 3. Measurement of the waveforms guided by the triple TDR probes was done by the 144-channel automatic TDR monitoring system consisting of a control box, multiplexer and cable tester (Tektronix 1502B). Sequential retrieval of the waveform was done using a multiplexing system (4 main switch boxes) connected to 24 coaxial switch boxes, one of which again connects 6 TDR probes.

**Fig. 3.** Scheme of the experimental set-up consisting of different units used for monitoring of solute transport at field scale.

One cycle of the sequential measurement lasted 35 minutes. The measurement frequency was 2 hrs for Bekkevoort and 4 hrs for Jülich and was controlled by the control box containing a 52 Mb hard disk. The waveform data were stored on the hard disk and retrieved every 3 days using a portable PC. Parallel to the measurement of the waveforms, soil temperature was monitored at hourly intervals using a data logger system. This information was required since the bulk soil electrical conductivity, as measured by the TDR, was found to be sensitive to soil temperature (Heimovaara *et al.*, 1995). The solute movement was monitored for 42 days for Bekkevoort and 65 days for Jülich after which breakthrough of all applied solutes was nearly achieved at the bottom of the soil profile.

CALIBRATION OF TDR

Different steps are required for the calibration of the TDR probes in order to properly measure the soil water content and solute concentration. The first step is related to the probe geometry such as the travel time in the Epoxy resin of the TDR probe and the probe length. Following the approach used by Heimovaara *et al.* (1993b), an accurate determination of soil water content using the unbalanced triple wire TDR probes was done by measurement of the probe geometry. Determination of the solute concentration in the soil water requires a sequence of calibration steps. The first step is the determination of the cell constant (K_p) and cable resistance (R_{cable}) which are required to convert the TDR-measured resistance (R)

to the bulk soil electrical conductivity (EC_a). The second step is to relate the bulk soil electrical conductivity to the electrical conductivity (EC_w) of soil water. This step is the most important part of the calibration procedure since difficulties arise for horizontally-positioned TDR probes as compared to the vertically-positioned TDR probes. For the latter probes, calibration constants involved in the relation of EC_a and relative concentration of soil water are removed (Kachanoski *et al.*, 1992). The last step is to obtain the relationship between the solute concentration (C) and the electrical conductivity of soil water.

Probe Geometry

The probe geometry can be determined by measurement of the total travel time of an electromagnetic wave along the probe in both air and water (Heimovaara, 1993b). The total travel time (Fig. 4) can be given as a function of the refraction index as follows:

$$\Delta t_p = \Delta t_o + \Delta t_s = \Delta t_o + L n_{aa}/c \quad (1a)$$

$$\Delta t_p = \Delta t_o + \Delta t_s = \Delta t_o + L n_{aw}/c \quad (1b)$$

where Δt_p , Δt_o , Δt_s are the total travel time, the travel time in Epoxy resin, the travel time in the probe embedded in the soil, and n_{aa} , n_{aw} are the refraction indices of the dielectric medium of air and water, and L , c are the probe length, the velocity of light in free space (3×10^8 m s⁻¹) respectively. The refraction index can be related to the dielectric permittivity as:

$$n_a = (K_a)^{1/2} \quad (2)$$

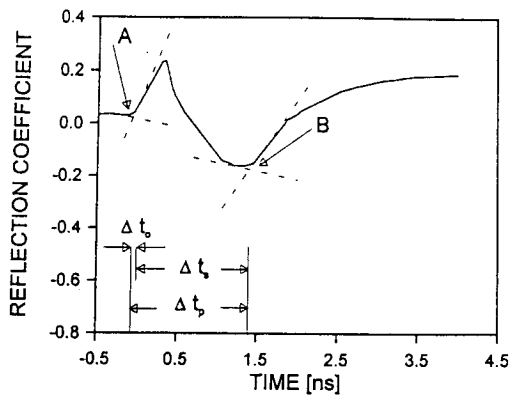


Fig. 4. Total travel time, Δt_p , consisting of the travel time in the Epoxy resin, Δt_o , and the travel time in the soil, Δt_s , in the TDR waveform. Points A and B indicate the first and second reflection points obtained with the double reflection analysis procedure.

where n_a and K_a are the refraction index and the apparent dielectric permittivity of the material between the probes. The dielectric permittivity of air, K_{aa} , is equal to 1. The dielectric permittivity of water, K_{aw} , is dependent on the temperature of water, and given by (Hasted, 1973):

$$K_{aw} = 87.740 - 0.40008T + .398 \times 10^{-4} T^2 - 1.410 \times 10^{-6} T^3 \quad (3)$$

The probe geometry parameters can then be solved by substituting the values of n_a for air and water obtained through (2) and (3). The moisture content was determined using the relationship given by Topp *et al.* (1980):

$$\theta = (-530 + 292 K_a - 5.5 K_a^2 + 0.043 K_a^3) / 10^4 \quad (4a)$$

$$\text{with } K_a = \left[\frac{c \Delta t_s}{2L} \right]^2 \quad (4b)$$

This calibration was done for all TDR probes prior to the experiment. Information on these calibration parameters was stored in a sensor file required for the execution of the waveform analysis program.

Cell Constant and Cable Resistance

The relationship between the resistance of a soil and the bulk soil electrical conductivity is defined using the cell constant, K_p (m⁻¹), as follows:

$$EC_a = K_p T_c / R_s \quad (5)$$

where T_c and R_s are the temperature correction factor and the resistance of the soil (Ω). Since the EC_a in (5) is the conductivity of the soil at 25°C, the T_c gives a correction with reference to the measurement at 25°C:

$$T_c = 1 + \alpha (25 - T) \quad (6)$$

in which α is the temperature coefficient of the sample (°C⁻¹) and T the temperature at which the conductivity was measured. Heimovaara *et al.* (1995) found that α varied linearly with temperature:

$$\alpha = -5.5 \times 10^{-4} T + 0.0342 \quad r^2 = 0.59 \quad (7)$$

The total resistance of the transmission line, R_{tot} , detected by TDR consists of the resistance of the soil, R_s , and the resistance of the cable, connectors and cable tester, R_{cable} . The R_s can then be calculated with:

$$R_s = R_{tot} - R_{cable} \quad (8)$$

The total resistance is obtained from the measured amplitude of the electromagnetic wave at long travel

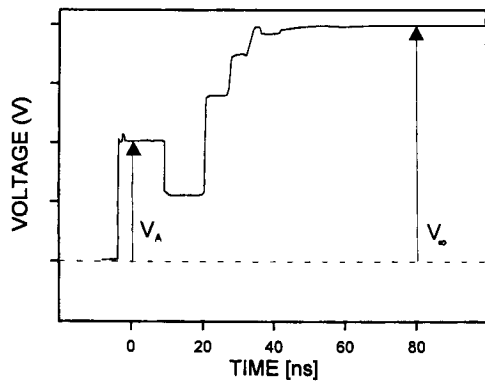


Fig. 5. Complete TDR waveform of a probe in demineralized water showing the voltage steps. The voltage levels used for the conductivity analysis are indicated with V_A and V_∞ .

times along the transmission line since the amplitude is a direct measure of the impedance of the transmission line and that the impedance at low frequencies is equal to the resistance after multiple reflections:

$$R_{\text{tot}} = Z_c \frac{(1 + \rho_\infty)}{(1 - \rho_\infty)} \quad (9)$$

where Z_c is the characteristic impedance (50Ω) of the cable tester (Tektronix 1502B) and ρ_∞ is the reflection coefficient at infinite times in the waveform. The reflection coefficient is calculated from the voltage wave with:

$$\rho_\infty = (V_\infty - V_A) / V_A \quad (10)$$

where V_∞ and V_A are the voltage levels as shown in Fig. 5. Heimovaara *et al.* (1995) found that the resistance of cable for 0.1 m long triple wire probes increases linearly with the cable length and that the contribution of cable resistance was significant at high conductivity ($>2.5 \text{ dS m}^{-1}$). In this study, 4 different solutions with known conductivities ($0.38, 0.75, 1.57, 12.42 \text{ dS m}^{-1}$) were used to determine both the cell constant and the cable resistance. The cell constant, K_p , was obtained by taking the slope of the linear regression function between $1/R_{\text{tot}}$ and the temperature corrected EC_a (EC_a/T_c) as there was no effect of cable resistance on the total resistance at the low conductivity levels. At the highest conductivity level (12.42 dS m^{-1}), significant effect of cable resistance on the total resistance was found such that the value of $1/R_{\text{tot}}$ deviates from the linear regression line as shown in Fig. 6. The cable resistance was then obtained by taking the magni-

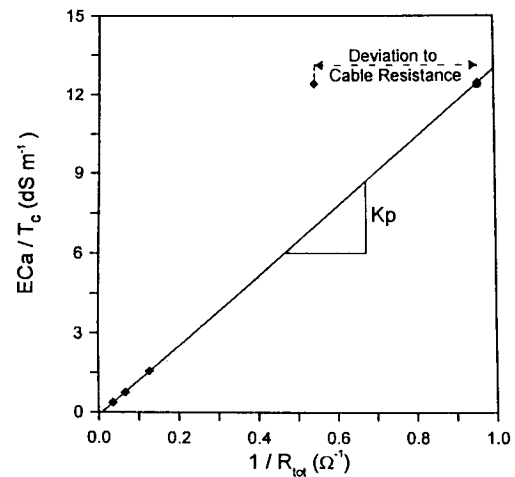


Fig. 6. Relation between $1/R_{\text{tot}}$ and temperature corrected EC_a obtained from measurements of TDR resistance in 4 different solutions of known conductivities. The difference between a deviated point and the linear regression line on the axis of resistance is related to the cable resistance.

tude of the deviation from the linear line since the deviation was clearly induced by the cable resistance at high conductivity. This calibration procedure was done for all TDR probes used in this study. Then the bulk electrical conductivity, EC_a , was calculated using (5) with T_c and R_s obtained through (6) to (10).

Relationship between EC_a and EC_w

Several methods are available in the literature for the relationship in either a direct or indirect way. The direct method is applicable for a repacked soil by relating the TDR-measured EC_a to the known concentration of soil water. For the indirect method, again a few methods are available which are based on the calibration coefficients and conceptual models. Two different approaches using the calibration coefficients have been used. by Ward *et al.* (1994), Mallants *et al.* (1994) and Vanclooster *et al.* (1995). The first approach is to define the calibration coefficient for the pulse application of solute. The coefficient can be obtained by relating a numerical convolution of time series breakthrough curves (BTCs) to the input concentration times the pulse duration, assuming that there is a complete mass recovery and that the time integral of resident concentration is equivalent to that of flux concentration (in case of using CLT model concept) (Vancllooster *et al.*, 1993; Ward *et al.*, 1994) as follows:

$$\beta_{z,x} = \frac{C_o t_o}{\int_0^t \left[\frac{1}{R(z,x,\tau-t_o)} - \frac{1}{R(z,x,t_i)} \right] d\tau} \quad (11)$$

where $\beta_{z,x}$ is the calibration coefficient at depth z and location x , and C_o , t_o are the concentration and duration of solute pulse, and $R(z,x,t_i)$ is the resistance before application of solute pulse. The other approach is to define the calibration coefficient from a step input of solute. A step increase of solute concentration would result in a zero gradient of TDR-measured resistance at a large time for a given depth. At this time, one may assume that the TDR-measured EC_a is equal to the input concentration, C_o , so that:

$$C_o = \beta_{z,x} \left[\frac{1}{R(z,x,t_F)} - \frac{1}{R(z,x,t_i)} \right] \quad (12)$$

where $\beta_{z,x}$ is the calibration coefficient at depth z and location x , $R(z,x,t_F)$ is the TDR-measured resistance at depth z and location x at a large time and $R(z,x,t_i)$ is the initial resistance at depth z and location x before application of step input.

In addition, two theoretical models are available. One is Mualem's model (Mualem, Friedman, 1991) which utilizes information on the parameters of the moisture retention characteristic. The other is Rhoades' model (Rhoades *et al.*, 1989) derived from the two-pathway conductance model. Rhoades *et al.* (1989) proposed a quadratic equation, hereafter referred to original Rhoades' model (ORM), relating the bulk soil electrical conductivity to the conductivity of soil water based on the assumption that the conductivity of soil water in the continuous liquid pathway, EC_{wc} , is equal to the conductivity of soil water in series-coupled pathway, EC_{ws} . The functional relationship between EC_a and EC_w is given by:

$$EC_{wc} = \frac{-B + \sqrt{B^2 - 4AC}}{2A} \quad (13)$$

with

$$A = [\theta_s(\theta_w - \theta_{wc})]$$

$$B = -[\theta_s EC_a - (\theta_s + \theta_{ws})^2 EC_s - (\theta_w - \theta_{ws})(\theta_{ws} EC_s)]$$

$$C = -[\theta_{ws} EC_s EC_a]$$

where θ_s , θ_{ws} and θ_{wc} are the volumetric contents of solid particles, soil water in series-coupled and in the separate continuous liquid pathway, respectively, and EC_s , EC_{ws} and EC_{wc} are the specific electrical conductivities of these three elements. Following em-

pirical equations were proposed to determine the parameters such as θ_s , θ_{ws} , θ_{wc} and EC_s involved in the model, derived from basic soil properties.

$$\theta_s = \rho_b / \rho_s \quad (14)$$

$$\theta_{ws} = 0.468 \theta_w + 0.064 \quad (15)$$

$$EC_s = 0.023 * \%Clay - 0.021 \quad (16)$$

where ρ_b , ρ_s are the densities of bulk soil and solid particles.

All of these methods, however, are not suitable for estimating the electrical conductivity of soil water from the TDR-measured EC_a for horizontally-positioned TDR probes under the field condition. In case of the calibration coefficient obtained from the pulse input, there will be difficulties when preferential movement of solute occurs bypassing the TDR-detecting volume that contradicts the assumption of complete mass recovery. The step input of a solute at field condition is not realistic since continuous application of solute would require an enormous amount of solute and even more if there is a preferential movement through soil macropores. With respect to the conceptual models, Vanclouster *et al.* (1994) showed that the Rhoades' model (under condition of equilibrium between mobile and immobile phases) gives a better description of the relationship between EC_a and EC_w than the Mualem model. This was due to the large uncertainties in the parameters of the moisture retention function. However, the Rhoades' model given in the form of (13) can not be applied to the breakthrough condition where a non-equilibrium between mobile and immobile soil water concentrations prevails mostly during migration of the applied solute. Hence, a new approach was proposed by Kim *et al.*, (1994) adapting the ORM applicable only to the equilibrium condition to a transient non-equilibrium condition such as a breakthrough condition. The new approach is based on the assumption that the solute exchange between the continuous liquid pathway (mobile phase) and the series-coupled pathway (immobile phase), caused mainly by molecular diffusion, is negligible compared to the hydrodynamic dispersion, during a relatively short time period of breakthrough condition. A distinct feature of the new approach is the introduction of a fractional factor to distinguish the soil water concentration (EC_{ws}) in the immobile phase from the one (EC_{wc}) in the mobile phase. Application of the new approach revealed that the typical non-linear behaviour, initially present in the ORM, vanishes resulting into a simple linear model (SLM). In SLM, the bulk soil electrical conductivity, EC_a , is

associated with two components and given by:

$$EC_a = [EC_a]_{im} + \theta_{wc} EC_{wc} \quad (17)$$

The first one, $(EC_a)_{im}$, represents the contribution of the bulk soil conductivity in the immobile phase and the other the contribution of the conductivity in the mobile phase. In fact, this component was found to be constant and could be determined by the initial conditions of EC_a and EC_{wc} . The latter component can be expressed using the soil water content in mobile phase, θ_{wc} , that is the slope of SLM and the conductivity of soil water in the mobile phase, EC_{wc} . Validity of the new approach was verified by comparing results of the SLM with those obtained from the method of using the calibration coefficient obtained from the step input of solute when applied to the TDR-measured BTC data on a number of short soil columns sampled in the vicinity of the field plot at the Jülich site (Kim *et al.*, 1995). In this study, three calibration methods, i.e., ORM, SLM and the calibration coefficient (CC) from the pulse input, were used to compare the effect of the different methods on the mass recovery and parameter estimation.

Relationship between EC_w and C

The relationship between EC_w ($dS\ m^{-1}$) and C ($g\ l^{-1}$) was established by measurement of the conductivities of solutions with different levels of known concentrations. The solutions were prepared by adding a certain amount of $CaCl_2 \cdot 2H_2O$ to the irrigation water used in the field experiment. Then a linear equation was obtained by relating EC_w to C. Results for both experimental sites are shown in Fig. 7.

DATA ANALYSIS

Mean BTCs and Calibration Methods

For each calibration method, the mean BTC data were obtained by averaging the 24 individual BTCs over each depth. The individual BTCs were obtained using the calibration parameters in the models. Table 3 shows the mean and standard deviations of the parameters for each depth. For the Bekkevoort soil, the initial EC_a measured during the steady state condition is nearly constant at the different depths but for the Jülich soil it shows variations. The EC_a in the tailing part of the BTC is slightly higher than zero in the Bekkevoort soil, but in the Jülich soil it increases slightly with depth indicating a possible solute exchange between mobile and immobile region at larger depths. The soil water contents in both the ORM and SLM were obtained by averaging

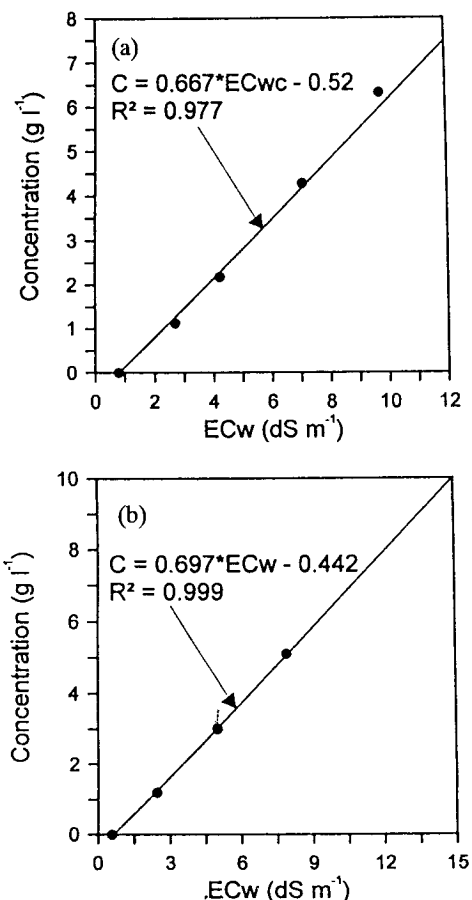


Fig. 7. Relation between EC_w and C obtained for irrigation water used at the Bekkevoort (a) and Jülich (b) site. Regression equations were derived for the ranges of EC_w of the BTC data.

the measured values during steady state condition. The different values of parameters for each experimental site are attributed to the differences in textural compositions (Table 1).

Mass Recovery and Parameter Estimation

In order to identify the effect of the different calibration methods on the mass recovery and solute transport parameters, the mean BTC data were used. Mass recovery was determined by taking the ratio between the input concentration times pulse duration, $C_0 t_0$ and the time convolution of the mean BTC. Since a complete mass recovery was assumed for the calibration method of CC, mass recovery was calculated for the calibration methods of ORM and SLM. For the parameter estimation, the mean BTCs

Table 3. Results of the calibration coefficients and model parameters used in the different calibration methods (mean values with standard deviation between parantheses).

Depth (cm)	EC _{a,ini} *	EC _{a,tail} **	Calibration	θ _w	θ _{wc}	ORM		SLM	
			Coefficient β _(z,x)			θ _{ws}	θ _s	EC _s	[EC _a]im
Bekkevoort									
10	0.144(0.020)	0.029(0.007)	3.332(0.891)	0.350(0.014)	0.122(0.007)	0.228(0.006)	0.618(0.011)	0.302	0.096(0.020)
30	0.127(0.019)	0.012(0.007)	6.025(1.084)	0.353(0.013)	0.124(0.007)	0.229(0.006)	0.634(0.016)	0.319	0.079(0.020)
50	0.125(0.024)	0.011(0.008)	6.305(1.444)	0.359(0.009)	0.127(0.005)	0.232(0.004)	0.640(0.007)	0.334	0.075(0.025)
70	0.117(0.012)	0.017(0.006)	5.939(0.964)	0.351(0.013)	0.123(0.007)	0.228(0.006)	0.641(0.005)	0.333	0.069(0.013)
90	0.115(0.016)	0.021(0.008)	6.283(0.833)	0.358(0.019)	0.127(0.010)	0.232(0.009)	0.640(0.014)	0.208	0.065(0.017)
Jülich									
15	0.316(0.047)	-3.3E-9(1.4E-8)	4.673(1.550)	0.377(0.011)	0.137(0.006)	0.240(0.005)	0.553	0.45	0.319(0.430)
35	0.463(0.084)	2.5E-9(9.3E-9)	4.544(1.017)	0.409(0.033)	0.154(0.017)	0.256(0.017)	0.612	0.465	0.355(0.079)
50	0.619(0.104)	0.004(0.012)	3.938(1.034)	0.467(0.013)	0.185(0.007)	0.283(0.006)	0.587	0.534	0.484(0.097)
70	0.525(0.057)	0.028(0.020)	3.518(1.068)	0.452(0.021)	0.177(0.011)	0.276(0.010)	0.612	0.645	0.397(0.057)
90	0.417(0.077)	0.045(0.025)	4.253(1.303)	0.430(0.032)	0.165(0.017)	0.265(0.015)	0.602	0.511	0.305(0.065)

*Initial bulk soil electrical conductivity

**Tail bulk soil electrical conductivity

were transformed to probability density functions (*pdfs*) by dividing the concentrations with the area under the curve. Two transport models were used to fit the measured BTCs. One is the convection-dispersion equation (CDE) based on the assumption that complete lateral mixing occurs during the migration of solute through soil pores. The other is the convective-lognormal transfer function (CLT) model (Jury *et al.*, 1982) that assumes independent movement of solute through different sizes of pores. Since the TDR-measured BTC data represent the resident concentration, the probability density function (*pdf*) of travel time for resident concentration type CDE with pulse input of the solute was used, which according to Jury and Roth (1990) can be written as:

$$f'(z,t) = \frac{V}{\sqrt{\pi Dt}} \exp\left[-\frac{(z-Vt)^2}{4Dt}\right] - \frac{V^2}{2D} \exp\left(\frac{Vz}{D}\right) \operatorname{Erfc}\left[\frac{z+Vt}{\sqrt{4Dt}}\right] \quad (18)$$

where z , t are the depth and time, and V , D are the pore water velocity ($L T^{-1}$), the dispersion coefficient ($L^2 T^{-1}$). The *pdf* of the time-normalized resident concentration of CLT obtained from a pulse input of a solute is given by (Vanderborght *et al.*, 1994):

$$f'(z,t) = \frac{l}{z} \frac{1}{\sqrt{2\pi\sigma_t^2}} \exp\left[-\frac{(\ln(l/z))^2}{2\sigma_t^2} - \mu_t - \frac{\sigma_t^2}{2}\right] \quad (19)$$

where μ , σ are the model parameters, and l is the depth of the BTC observation. Parameters of both models were obtained by fitting the mean BTC data using the least square optimization method.

RESULTS AND DISCUSSION

Mean BTCs and Mass Recovery

Fig. 8 shows the results of the mean BTCs in the different calibration steps described above. For the relationship between EC_a and EC_w, the calibration method of SLM was used. The resistance (R) of the tailing part (Fig. 8a) for the Bekkevoort soil does not return to the initial values. This caused values of the EC_a in the tailing part slightly higher than zero as was shown in Table 3. Since the difference between them did not decrease with time, we believe that this was not induced by the physical non-equilibrium effect (van Genuchten, Wierenga, 1976; Kachanoski *et al.*, 1992). Therefore, in this study, the initial EC_a was set equal to the tail value of EC_a since the small concentration but long tailing in time would significantly affect the time moments. The BTCs for the Jülich soil show large differences in the resistance and the initial EC_a across different depths, primarily caused by the difference in clay percent.

After converting from EC_a to either EC_w or C , the BTCs for both soils show transient movement of resident solute concentrations at different depths. The peak concentration decreased with the increase of the spreading around the peak travel time across depth

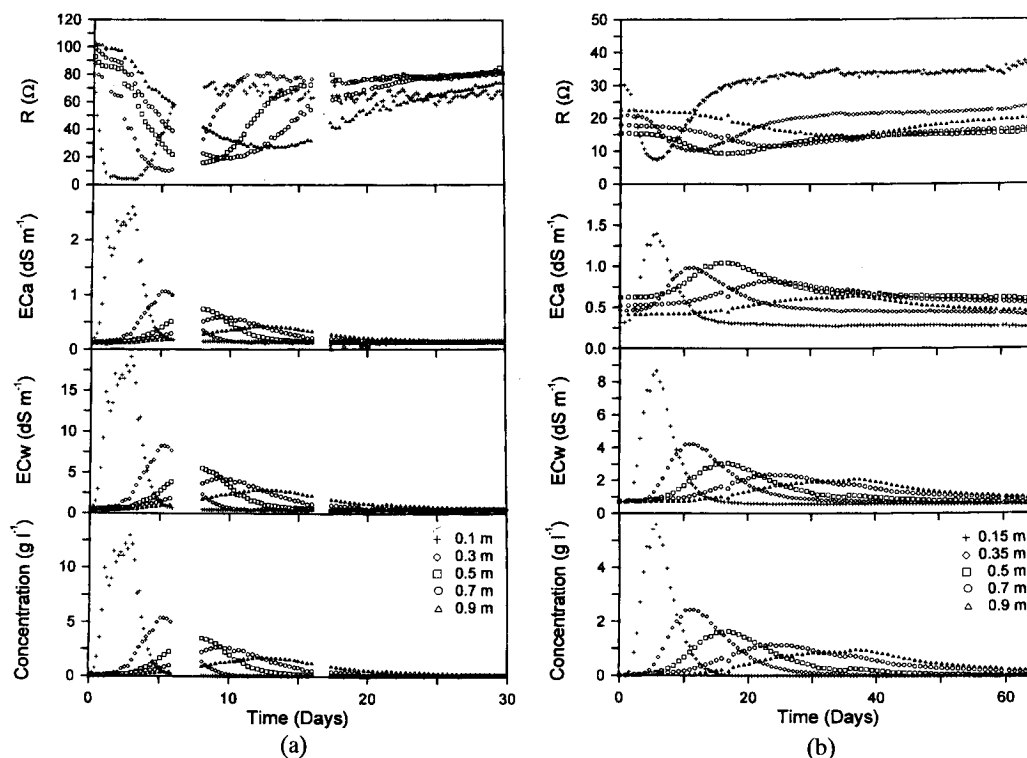


Fig. 8. The mean BTC data obtained through different calibration steps for Bekkevoort (a) and Jich (b). The BTCs for the Bekkevoort soil show two gaps in the data due to PC crash during monitoring.

indicating the solute dispersion process. A normal distribution of BTC was found for both soils showing a nearly symmetrical distribution around the peak. This is in contrast with the results obtained by Jury *et al.* (1982). The reason behind this is explained by that the BTCs observed by them were more likely flux type concentrations since they used suction samplers for monitoring the solute concentrations whereas the BTCs in this study are time-series resident type concentration. As shown by Parker, van Genuchten (1984), the rapid breakthrough and rather long tailing is typical of the time-series flux concentration in CDE for media of high dispersivity. However, in Fig. 8, the measured BTCs in resident concentration exhibit somewhat a delayed peak and more spreading. This behaviour can be clearly identified by comparing the time moments of both the flux and resident concentration *pdfs* for CDE and CLT model. Details of the relationships between time moments and parameters of both models are given in the companion paper (this issue).

The results of mean BTCs in C ($g\ l^{-1}$) are shown for three calibration methods in Fig. 9. The methods of SLM and CC give a good agreement in the concentration of BTCs at all depths for both soils.

However, the differences between ORM and SLM or CC are large regardless of depth. The reason for this lies in the fact that in ORM the solute concentrations are equally distributed to mobile and immobile regions and thus the solute concentration (EC_{wc}) in mobile the region are underestimated. Fig. 10 clearly illustrates the difference in the EC_{wc} estimates between ORM and SLM. The difference increases with concentration and at a certain point the non-linearity vanishes showing linearity. The nonlinearity in ORM is due to the assumption of instantaneous equilibrium between mobile and immobile regions from which the quadratic equation (13) has been derived. Results of mass recovery are shown in Fig. 11. SLM gives reasonable estimates in comparison with the reference level (100%). The mass recoveries by ORM are smaller than those by SLM for all depths and soils. Poor estimation by ORM is attributed to the assumption of equilibrium between mobile and immobile regions of the soil which does not hold true for the breakthrough condition. The magnitude of difference between SLM and ORM can be explained by the degree of deviation between the linear parts of each model on which most of peak

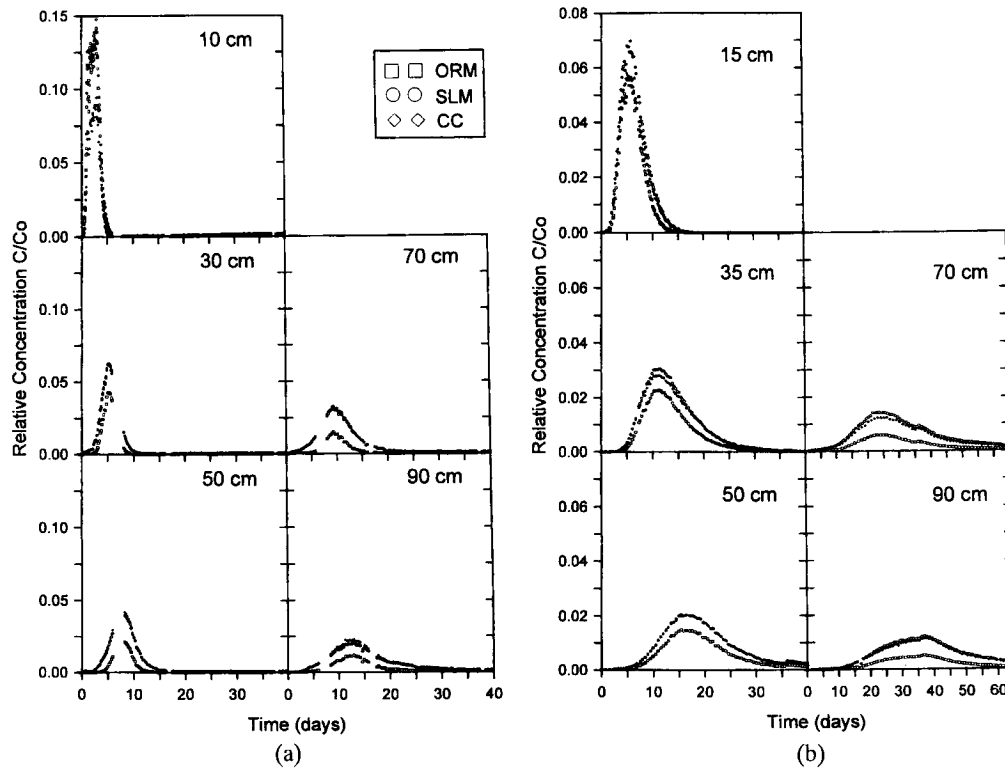


Fig. 9. The mean BTC data obtained using three calibration methods for estimating the concentration of soil water from the bulk electrical conductivity in the Bekkevoort (a) and Jülich (b) soils.

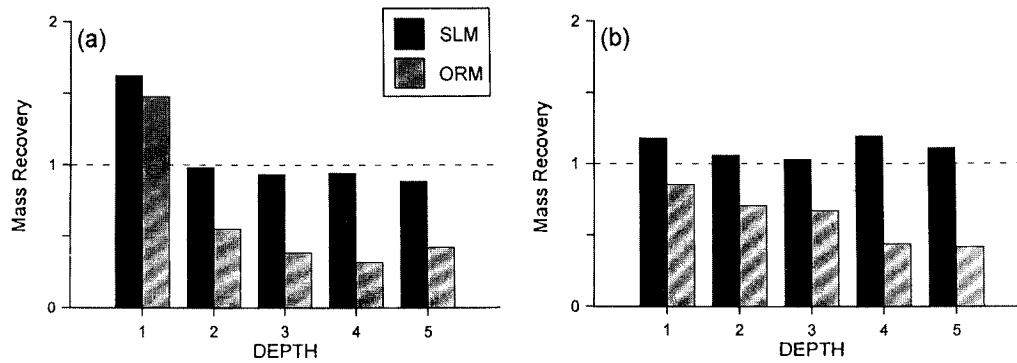


Fig. 10. Mass recovery of the mean BTCs for different calibration methods in the Bekkevoort (a) and Jülich (b) soils.

concentrations falls.

Calibration Method and Model Parameters

Parameters of the mean BTCs obtained through three calibration methods were estimated using the CDE and CLT model *pdfs* and are shown in Table 4. The pore water velocity, *V*, shows more or less constant values for different depths for Jülich soil

indicating relatively small heterogeneity present in the flow properties. Slightly higher differences in the pore water velocities have been found with depth in the Bekkevoort soil. The Bekkevoort soil shows almost two times higher *V* than the Jülich soil. In fact, this high value of *V* is responsible for the nearly two times earlier breakthrough of solute in the Bekkevoort soil as compared to the Jülich soil. The dispersion coefficient, *D*, shows an increase with depth for both soils

regardless the calibration method used. The CLT model parameter, μ , shows an increase with depth, and σ shows relatively constant values for both soils.

The effect of the calibration method on the parameters was demonstrated using a scatterplot. Results of the scatterplot are shown in Fig. 12 for both solute transport models. For the CDE model, V does not seem to be affected by the calibration method showing a good agreement between SLM or ORM and CC for both soils. However, the dispersion coefficient, D , is underestimated in case of ORM only for the Bekkevoort soil. The CLT model parameters, μ and σ , show similar results to the CDE model

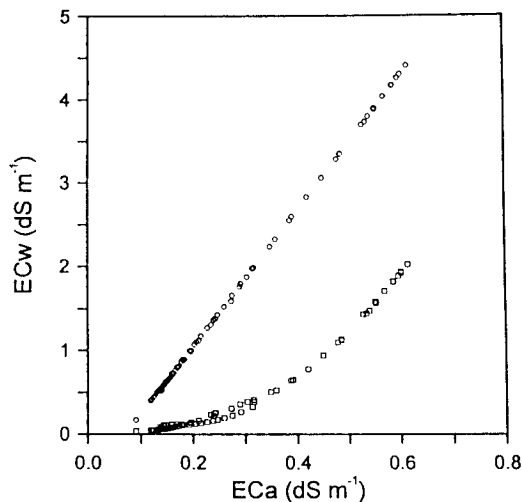


Fig. 11. Relation between EC_a and EC_w for the simple linear model (SLM) and original Rhoades' model (ORM) for the Bekkevoort soil at a depth of 0.7 m.

parameters showing some deviations of σ in case of ORM for the Bekkevoort soil. The relatively large deviation in those parameters between ORM and the other two methods is attributed to the underestimation of the peak concentration by ORM (Fig. 9a). In general, it appears that the parameters related to the travel time of the solute, such as V and μ , are independent on the calibration methods but parameters related to the solute dispersion, such as D and σ , are affected by the calibration method. Although the calibration coefficient from the pulse input may not be appropriate for field soils having preferential flow, a good agreement between CC and SLM for both soils implies the potential use of SLM under field condition. Since so far no standard method in either direct or indirect way has been available for the horizontally-positioned TDR probes under field condition, SLM can be preferably used over ORM.

SUMMARY AND CONCLUSIONS

In this study, a detailed description of experimental procedures has been given for monitoring the vertical movement of a conservative solute at field scale using an automated 144-channel TDR system. The BTC data obtained using the horizontally-positioned triple wire probes were found to give a high resolution of time-series resident concentration for each depth and location and thus providing a high quality of data sufficient to study the spatial variability of solute transport parameters and the governing model concept at field scale. The mean BTC obtained for both experimental sites appeared to be a normal distribution rather than a lognormal one due to the characteristic of the time-series resident concentration. Application of

Table 4. Parameters of the CDE and CLT models fitted to the mean BTCs obtained from the three calibration methods.

Depth (cm)	SLM				Calibration Coefficient				ORM			
	CDE		CLT		CDE		CLT		CDE		CLT	
	V	D	μ	σ	V	D	μ	σ	V	D	μ	σ
Bekkevoort												
10	4.14	5.91	0.65	0.50	4.06	5.29	0.68	0.48	4.18	5.29	0.66	0.47
30	5.40	7.00	1.63	0.29	5.42	7.05	1.63	0.29	5.48	4.52	1.65	0.23
50	6.34	12.45	1.99	0.27	6.38	12.48	1.98	0.27	6.38	6.67	2.02	0.20
70	7.04	26.35	2.20	0.32	7.05	25.85	2.20	0.31	7.16	13.13	2.23	0.22
Jülich												
15	2.47	3.32	1.64	0.40	2.48	3.49	1.63	0.41	2.56	2.74	1.69	0.36
35	2.73	7.68	2.41	0.39	2.75	7.77	2.40	0.39	2.79	6.41	2.41	0.35
50	2.68	11.02	2.78	0.39	2.70	11.14	2.77	0.39	2.75	9.25	2.78	0.36
70	2.40	17.49	3.19	0.43	2.41	16.59	3.19	0.42	2.51	14.46	3.18	0.39
90	2.44	16.32	3.47	0.37	2.44	15.73	3.48	0.37	2.51	13.76	3.47	0.34

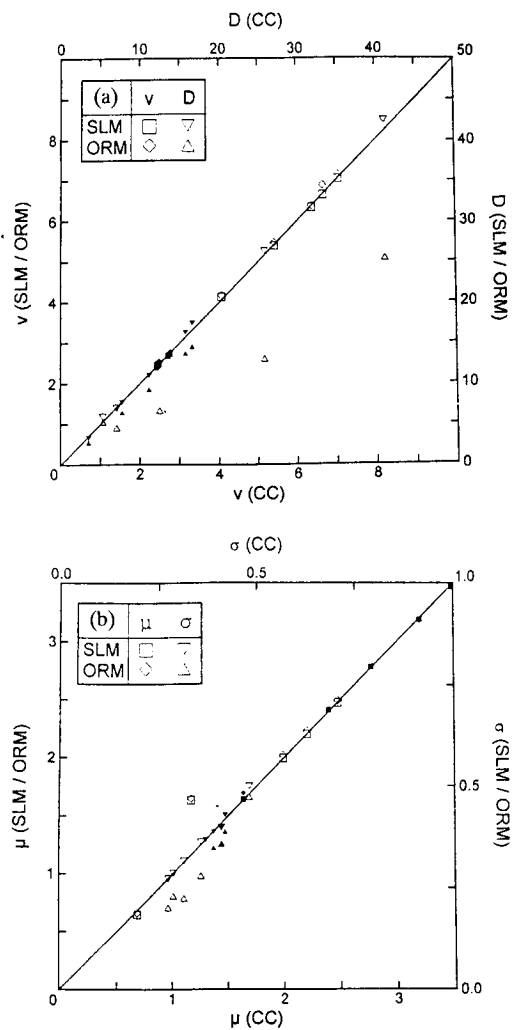


Fig. 12. Scatterplot of the parameters of V and D for the CDE model (a), and μ and σ for the CLT model (b), comparing the calibration coefficient (CC) method with the SLM and ORM method. The symbols for the Bekkevoort soil are empty and those for the Jülich soil are black.

three calibration methods available for the BTCs obtained under field condition reveals that the SLM (simple linear model) was more suitable than the ORM (original Rhoades' model) for defining the relationship between the bulk soil electrical conductivity (EC_a) as measured by TDR and the conductivity of soil water (EC_w). The effect of the calibration method on the solute transport parameters was found such that both parameters, V and μ of the CDE and CLT model, relating to the solute travel time, were not significantly affected, but D and σ relating to the variance of the solute travel time were slightly affected. Good

agreement between the methods of calibration coefficient (CC) from the pulse input and SLM provides a potential use of SLM for calibration of the horizontally-positioned TDR probes under field condition in comparison with ORM. A more detailed analysis of time moments on the transport parameters of the time-series resident type concentrations using the method of moments and consequent study on the governing transport concept is described in a companion paper.

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시간영역 광전자파 분석기(Automatic TDR System)를 이용한 오염물질의 거동에 관한 연구: 실험방법 및 검정

김 동 주

요 약 : 자동 TDR 시스템을 이용하여 약 0.54 헥타 크기의 2개 현장에서 오염물질의 거동을 모니터링하였다. 오염물질의 수직적 플룸을 관측하기 위하여 추적자로서 CaCl_2 를 순간주입(Pulse)방식으로 투입하였으며 오염물질 이동 시간의 공간적 이질성과 현장규모의 운송모델 개념을 파악하기 위하여 횡방향으로 24개 지점과 5개의 다른 깊이, 즉 120개 지점에 50 cm 길이의 TDR 탐사침을 설치하여 잔존수 농도를 측정하였다. TDR에 의해 관측된 전기전도도를 검정하기 위하여 3가지의 다른 방법을 사용하였다. 깊이별 24개 지점에서 얻어진 평균 BTC 자료를 이용하여 CDE 모델과 CLT 모델의 파라미터를 추정한 결과 TDR 방법은 실내실험 뿐만아니라 현장에서의 오염물질 거동 분석에 유용하다는 결론을 얻었다. 또한 3가지 검정방법은 BTC 모양과 특히 오염물질의 침투운송시간과 관련된 파라미터에 큰 영향을 미치지 않으며 사용된 검정방법 중 SLM 방법이 수평적으로 설치된 TDR 탐사침에 대해서 가장 적합한 것으로 나타났다.