

COMPARISON OF FLUX AND RESIDENT CONCENTRATION BREAKTHROUGH CURVES (BTCs) IN STRUCTURED SOIL COLUMNS

Dong- Ju Kim

Dept. of Earth and Environmental Sciences, Korea University

ABSTRACT

In many solute transport studies, either flux or resident concentration has been used. Choice of the concentration mode was dependent on the monitoring device in solute displacement experiments. It would be questionable, however, to accept the equivalency in the solute transport parameters between flux and resident concentrations in structured soils exhibiting preferential movement of solute. In this study, we investigate how they differ in the monitored breakthrough curves (BTCs) and transport parameters for a given boundary and flow condition by performing solute displacement experiments on a number of undisturbed soil columns. Both flux and resident concentrations have been simultaneously obtained by monitoring the effluent and resistance of the horizontally-positioned TDR probes. The study reveals that soil columns having relatively high flux densities exhibited great differences in the degree of peak concentration and travel time of peak between flux and resident concentrations. The peak concentration in flux mode was several times higher than that in resident one. This was mainly due to the bypassing of solute through soil macropores.

1. INTRODUCTION

In recent years studies on solute transport behaviour in soils have drawn increasing attention because of ever-growing concerns about environmental hazard of applied agrochemicals and nuclear waste disposals on land and water quality. Among them most important issues have been on how the applied solutes move along the vadose zone and permeate to the ground water. Several attempts were made on the use of existing model or development of new model to describe the solute transport mechanism. A common approach used for model validation among many soil scientists was to conduct a breakthrough experiment at either laboratory or field scale in order to obtain necessary information on the movement of chemicals.

Two different expressions of solute concentration, i.e., flux and resident concentrations, were possible for both theoretical equations and monitoring techniques. A limiting case in the solute transport study was monitoring data rather than model developing. Depending on the mode of concentration detected by measuring device, each model type for transport mechanism was chosen. No priority exists on the choice of the

type of model or equation and reports results of studies. This means that there exists a complete equivalency in the solute transport parameters between two concentration modes.

A number of laboratory-scale solute displacement experiments have been conducted on disturbed or undisturbed soil columns by detecting either flux concentration (Khan and Jury, 1990; Li and Ghodrati, 1994; Ma and Selim, 1994) or resident concentration (Vanclooster et al., 1993; Mallants et al., 1994; Ward et al., 1994) using time domain reflectometry (TDR). So far, no detailed solute transport study has been conducted based on simultaneous measurements of both type concentrations except for theoretical consideration (Parker and van Genuchten, 1984). In this study, we investigate how they differ and affect the transport parameters by monitoring flux and resident concentrations using the electrical conductivity of effluent and resistance of TDR probes horizontally positioned at middle of soil columns and performing parameter estimation of the observed BTCs based on two solute transport models, CDE and CLT.

2. MATERIALS AND METHODS

Solute Displacement Experiment

The site where the structured soil columns were taken was being used as grass land. Soil is classified as Stagnic Podzoluvizol (FAO classification) with indication of eluviation of clay and minerals and influence of seasonally perched groundwater table. Soil type was silt loam with varying clay percent over different horizon. Undisturbed soil columns with a diameter and height of each 20 cm were collected at 12 discrete locations in a 40 m long transect and at 4 different depths per location.

Prior to the breakthrough experiment, the saturated hydraulic conductivity (K_s) and the near saturated hydraulic conductivity were measured using a constant head and crust method (Bouma et al., 1972). From the results of hydraulic conductivity, significant variability of K_s were found among soils at the same horizon with difference in several orders of magnitude. It was believed that this was due to the existence of macropores in the soil. Step application of solute in a soil having macropores has been confronted with difficulties in obtaining a stable resistance of TDR at equilibrium due to bypassing the soil matrix domain and thus requiring an enormous amount of solute. Therefore we decided to use a pulse input of solute.

Both flux and resident concentrations were simultaneously monitored using measurement window of effluent at exit boundary and soil resistance by positioning 15 cm long and 2.5 cm wide parallel TDR probes in the middle of the soil column. A steady state condition was imposed on each column in a period of 15 days before application of solute. During the steady state condition, soil moisture content and resistance were measured by TDR. Solute was applied with ponding condition on top of the soil column in a 1 cm depth of CaCl_2 solution (10 g l^{-1}) as a tracer. After application of solute, ponding condition was again imposed on top boundary to leach the solute plume downward while a free drainage condition was imposed on bottom boundary by installation of a perforated PVC disk to collect the effluent. The effluent concentration was determined by an EC-meter.

Calibration of TDR Measurements

For determination of TDR-measured resident concentration, soil columns at the end of BTC experiment were saturated with the same CaCl_2 concentration as input solution to obtain the calibration coefficient (Mallants et al., 1994; Ward et al., 1994) from the TDR resistance at the equilibrium between the input concentration and soil solution in the TDR-detecting region. The step increase of solute concentration results in a zero gradient of TDR impedance at a large time for a given depth. At this time, one may assume that the impedance corresponds to the input concentration, C_o , so that

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

where β_z is the calibration coefficient at depth z , $R(z, t_F)$ is the TDR measured impedance of depth z at a large time and $R(z, t_i)$ is the initial impedance of depth z before application of step input. Once the calibration coefficient is obtained, the solute concentration at depth z and time t , $C(z, t)$, in response to addition of solute with the concentration, C_o , can be determined by:

$$C(z, t) = \beta_z \left[\frac{1}{R(z, t)} - \frac{1}{R(z, t_i)} \right] \quad (2)$$

The electrical conductivity of flux concentration as measured by the EC -meter was calibrated using the following relationship between EC (dS/m) and C (g/l) obtained from measurements of EC in solutions of known concentrations:

$$\text{EC} = 1.341 C + 0.76 \quad (r = 0.98) \quad (3)$$

3. RESULTS AND DISCUSSIONS

Most of the monitored BTCs in both the flux and resident concentration showed distinct features in peak concentration and travel time of peak concentration for different flux densities of effluent, and presence of bimodal shape. The BTCs are grouped into 4 different types. Type 1 represents the BTCs having much higher and earlier peak in flux than resident concentration. In type 2, the flux concentration shows still much higher peak but the peak almost equals to that of resident concentration. Type 3 shows the BTCs having the same magnitude of both the peak concentration and travel time in the flux and resident concentrations. Type 4 corresponds to the BTC showing earlier and higher peak of resident than flux concentration. In fact, this type was the one of our expectation to obtain from the column displacement experiment since the resident concentration was monitored at 10 cm from the inlet boundary and the flux at 20 cm. However, most of the BTCs have been found to be type 1, 2, 3.

A few important features can be noted from the comparison of different types. For type 1, most of solutes moves preferentially along the macropores and only a small part of the applied solutes enters into the

soil matrix region. Occurrence of peak travel time in both the flux and resident appears to greatly differ. This can be explained such that either the preferential movement through the macro region, consisting of the main component of flux concentration, is unlikely detected by the probe bypassing the TDR-detecting volume or that the contribution of solutes in the macro region is so small in areal ratio compared to the matrix region. Comparison of the flux densities between type 1 (0.13 cm hr^{-1}) and type 2 (0.68 cm hr^{-1}) implies that soils having higher flux densities are more likely to yield the same peak travel time in both the flux and resident modes. This would be due to the increased chances of detecting the solutes by the probe on one hand and the increased area of macropores on the other hand since the number and area of macropores are proportional to the flux density in the macro region. Another feature is related to the occurrence of bimodal peak in the flux concentration of the BTC. Note that the BTC of type 2 having the highest flux density is in unimodal shape but the other types show bimodal BTCs. This is due to the fact that the solute interchange between the macro and matrix region is almost negligible during the storm flow through the macropores. However, chemical diffusion between the two regions are quite significant for soils having a rather moderate flux density because the solute interchange may occur during the relatively increased solute travel time. It is interesting to see that the type 3, having the intermediate flux density (0.36 cm hr^{-1}) between those of type 1 and 2, exhibits both the simultaneous travel time of peak concentration in flux and resident and a distinct bimodal shape in flux concentration. In type 3, the flux concentration predicted from parameters of resident BTC well coincides with the second peak of the measured flux concentration. The first peak is attributed to the preferential movement of solutes through the macro region which was not detected by the probe. This result clearly indicates that the TDR-measured concentration most likely represents solutes present in the soil matrix region.

Type 4 shows the BTC obtained from a soil column without dominant macropores since the flux density was very small with 0.02 cm hr^{-1} and the peak of resident concentration appears before that of flux concentration although the flux concentration shows a bimodal shape with the relatively low first peak. The predicted flux concentration gives a good agreement with the measured in the peak travel time but the peak concentration is underestimated. This suggests that even in a homogeneous structured soil, care should be taken in the use of the solute transport parameters obtained from the TDR-measured resident BTC to predict the flux concentration.

4. REFERENCES

1. Bouma, J., and J. L. Denning, Field measurements of unsaturated hydraulic conductivity by infiltration through gypsum crusts, *Soil Sci. Soc. Am. Proc.*, 36, pp.846-848 (1972).
2. Khan, A. U., and W. Jury, A laboratory study of the dispersion scale effect in column outflow experiments, *J. Hydrol.*, 5, pp.119-131 (1990).
3. Li, Yimin, and M. Ghodrati, Preferential transport of Nitrate through soil columns containing root channels, *Soil Sci. Soc. Am. J.*, 58, pp. 653-659 (1994).

4. Ma, L., and H. M. Selim, Tortuosity, mean resident time, and deformation of breakthroughs from soil columns, *Soil Sci. Soc. Am. J.*, 58, pp.1076-1085 (1994).
5. Mallants, D., M. Vanclooster, M. Meddahi, J. Feyen, Estimating solute transport in undisturbed soil columns using time domain reflectometry, *J. Contam. Hydrol.*, 17, pp.91-109 (1994).
6. Parker, J. C., and M. Th. van Genuchten, Flux-averaged and volume-averaged concentrations in continuum approaches to solute transport, *Water Resour. Res.*, 20, pp.866-872 (1984).
7. Vanclooster, M., D. Mallants, J. Diels, and J. Feyen, Determining local scale solute transport parameters using time domain reflectometry, *J. Hydrol.*, 148, pp.93-107 (1993).
8. Ward, A. L., R. G. Kachanoski, and D. E. Elrick, Laboratory measurements of solute transport using time domain reflectometry, *Soil Sci. Soc. Am. J.*, 58, pp.1031-1039 (1994).