



Revista Brasileira de Ciência do Solo

ISSN: 0100-0683

revista@sbcs.org.br

Sociedade Brasileira de Ciência do Solo  
Brasil

Previatello da Silva, Livia; de Jong van Lier, Quirijn; Metri Correa, Marcus; de Miranda,  
Jarbas Honorio; Alves de Oliveira, Luciano  
Retention and Solute Transport Properties in Disturbed and Undisturbed Soil Samples  
Revista Brasileira de Ciência do Solo, vol. 40, 2016, pp. 1-10  
Sociedade Brasileira de Ciência do Solo  
Viçosa, Brasil

Available in: <http://www.redalyc.org/articulo.oa?id=180249980027>

- How to cite
- Complete issue
- More information about this article
- Journal's homepage in redalyc.org

redalyc.org

Scientific Information System

Network of Scientific Journals from Latin America, the Caribbean, Spain and Portugal

Non-profit academic project, developed under the open access initiative

# Retention and Solute Transport Properties in Disturbed and Undisturbed Soil Samples

Lívia Previatello da Silva<sup>(1)</sup>, Quirijn de Jong van Lier<sup>(2)\*</sup>, Marcus Metri Correa<sup>(3)</sup>, Jarbas Honorio de Miranda<sup>(4)</sup> and Luciano Alves de Oliveira<sup>(5)</sup>

<sup>(1)</sup> Universidade de São Paulo, Centro de Energia Nuclear na Agricultura, Programa de Pós-graduação em Ciências, Piracicaba, São Paulo, Brasil.

<sup>(2)</sup> Universidade de São Paulo, Centro de Energia Nuclear na Agricultura, Divisão de Funcionamento de Ecossistemas Tropicais, Piracicaba, São Paulo, Brasil.

<sup>(3)</sup> Universidade Federal Rural de Pernambuco, Departamento de Engenharia Ambiental, Recife, Pernambuco, Brasil.

<sup>(4)</sup> Universidade de São Paulo, Escola Superior de Agricultura "Luiz de Queiroz", Departamento de Engenharia de Biosistemas, Piracicaba, São Paulo, Brasil.

<sup>(5)</sup> Universidade de São Paulo, Escola Superior de Agricultura "Luiz de Queiroz", Programa de Pós-graduação em Engenharia de Sistemas Agrícolas, Piracicaba, São Paulo, Brasil.

\* **Corresponding author:**  
E-mail: qdjvlier@usp.br

**Received:** January 27, 2015

**Approved:** February 12, 2016

**How to cite:** Silva LP, De Jong van Lier Q, Correa MM, Miranda JH, Oliveira LA. Retention and Solute Transport Properties in Disturbed and Undisturbed Soil Samples. Rev Bras Cienc Solo. 2016;40:e0151045.

**Copyright:** This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided that the original author and source are credited.

**ABSTRACT:** Solute transport parameters can be determined in miscible displacement experiments, usually performed in columns with disturbed (sieved) soil samples. Experiments with undisturbed samples are uncommon, due to the difficulty of taking undisturbed samples at the size required for these experiments. Structural alteration of the disturbed material implies modifications in the pore geometry that determines hydraulic properties, including hydraulic conductivity and retention and properties related to miscible displacement. An existing model for prediction of breakthrough curves based on retention properties was tested using material from a medium-textured Ferralsol, and alterations caused by sample disturbance were investigated. Soil water retention curves and miscible displacement parameters were determined in breakthrough experiments with nitrate salts in columns filled with undisturbed and disturbed soil samples. Data obtained from the undisturbed samples showed a higher dispersion, suggesting homogenization of pore geometry and a reduction in the representative elementary volume by the disaggregation and sieving of the soil material. The transport parameters for nitrate determined in disturbed and undisturbed samples were significantly different and the model was able to simulate the observed breakthrough curves after fitting the pore connectivity parameter.

**Keywords:** sampling, retention, miscible displacement, solute transport, leaching.



## INTRODUCTION

Quantifying the components of the solute transport process is important for understanding management practices to control ion movement in soil (Bresler, 1981). Studies on soil solute dynamics not only provide a means to determine solute flow in soils but can also give a physical explanation of phenomena that occur during the movement of mineral fertilizers and other salts, such as percolation, exchange, and adsorption of ions (Nielsen and Biggar, 1961).

The miscible displacement process affecting solutes in porous media can be physically described by the solute transport equation, relating displacement to the movement of the interface between transported and transporting fluids. The solution of this equation includes three components describing solute transport: the dispersion-diffusion coefficient ( $D$ ), the retardation factor ( $R$ ), and the Péclet number ( $P$ ) (Ruiz et al., 2010). These transport parameters can be determined in the laboratory by performing a breakthrough experiment, to be analyzed by analytical or numerical physical-mathematical models (Anami et al., 2008; Fonseca et al., 2009; Rose et al., 2009; Doltra and Muñoz, 2010; Silva et al., 2012). In contrast with analytical solutions, the numerical models do not require boundary conditions that usually are not satisfied during experiments.

Due to the difficulty of collecting undisturbed samples at the required size, in the order of 1000 cm<sup>3</sup>, breakthrough experiments are normally performed in columns filled with disturbed and sieved soil material. The water retention curve, however, is normally performed in smaller samples (in the order of 100 cm<sup>3</sup>), allowing the use of samples with undisturbed structure.

Any deformation implies modification in the pore space geometry that determines hydraulic properties, including retention and hydraulic conductivity, as well as properties related to miscible displacement. Therefore, the use of samples with a natural structure is preferable for evaluation of the behavior of naturally occurring soils.

Water retention and ion displacement is governed, among other factors, by the geometry of pore space, and it is our hypothesis that a functional relation between both processes is to be expected. Therefore, a model that predicts the breakthrough curve based on water retention properties would be sensitive to modifications in soil structure. Such a model was proposed by Wang et al. (2002), who employed a water retention parameter related to pore size distribution, and another parameter related to pore size connectivity to be estimated independently.

The objective of this paper was to analyze the modifications in breakthrough properties caused by disturbance of soil structure by sieving and repacking, and the correlation of these modifications to changes in the corresponding water retention curves using the model of Wang et al. (2002). To do so, modifications in the water retention parameters were determined from experimental retention desorption curves, whereas changes in miscible displacement parameters were measured by breakthrough experiments using nitrate salts in soil material samples from a medium-textured Ferralsol from Brazil.

## MATERIALS AND METHODS

### Soil

The soil material used in this study was sampled at depths from 0.20 to 0.50 m in a *Latossolo Vermelho-Amarelo* (Santos et al., 2013), a Ferralsol (IUSS Working Group WRB, 2015) from the municipality of Piracicaba, São Paulo, Brazil (22° 44' S and 47° 38' W, altitude 500 m) under conventional tillage management.

Particle size analysis was performed using the densimeter method (Donagema et al., 2011) and yielded  $0.198 \text{ kg kg}^{-1}$  clay,  $0.032 \text{ kg kg}^{-1}$  silt, and  $0.770 \text{ kg kg}^{-1}$  sand, consisting of  $0.320 \text{ kg kg}^{-1}$  coarse sand ( $2.00 - 0.210 \text{ mm}$ ) and  $0.450 \text{ kg kg}^{-1}$  fine sand ( $0.210 - 0.053 \text{ mm}$ ). Bulk density, determined in a soil sample ring, was  $1,230 \text{ kg m}^{-3}$ , and particle density, determined with a pycnometer, was  $2,600 \text{ kg m}^{-3}$ , resulting in a total porosity of  $0.527 \text{ m}^3 \text{ m}^{-3}$ . Soil chemical properties were determined by standard methods according to Donagema et al. (2011), which showed  $\text{pH}(\text{CaCl}_2)$  of 6.2, S of  $14 \text{ g m}^{-3}$ , organic matter of  $13 \text{ kg m}^{-3}$ , P of  $3 \text{ g m}^{-3}$ ,  $\text{K}^+$  of  $2.0 \text{ mol}_c \text{ m}^{-3}$ ,  $\text{Ca}^{2+}$  of  $22 \text{ mol}_c \text{ m}^{-3}$ ,  $\text{Mg}^{2+}$  10 of  $\text{mol}_c \text{ m}^{-3}$ , and H of  $15 \text{ mol}_c \text{ m}^{-3}$ , while Al exhibited a total base sum of  $34 \text{ mol}_c \text{ m}^{-3}$ , CEC of  $49 \text{ mol}_c \text{ m}^{-3}$ , and base saturation of 69 %.

### Breakthrough experiments

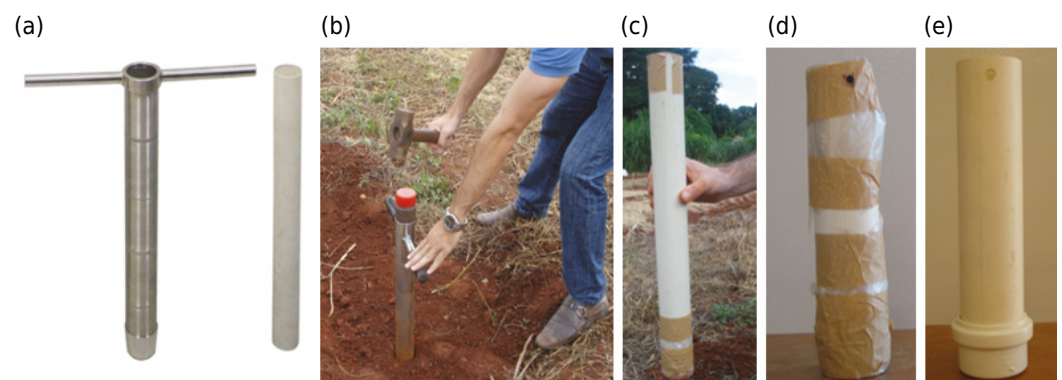
Six breakthrough experiments were performed in PVC tubes with an external diameter of 0.05 m, consisting of three tubes filled with undisturbed and three with disturbed soil samples. To allow maintenance of a constant hydraulic head, an outlet was placed at the top of the tube, 0.1 m above the soil sample surface, to drain excess water.

Undisturbed soil samples were taken with a specially designed auger (Figure 1). Excess soil on the top and bottom of the samples was removed, resulting in a final sample height of 0.23 m. Figure 1 shows some details of the undisturbed sampling process.

For experiments with disturbed samples, the soil material was air dried and sieved through a 0.002 m mesh. Columns were filled with the material in order to obtain uniformity and homogeneity, subdividing the total mass in portions. The portions were subsequently added to the tube and compacted, applying light pressure with a wooden disc.

The breakthrough experiments were performed at the Soil Physics Lab of the Biosystems Engineering Department of the University of São Paulo in Piracicaba, São Paulo, Brazil. Breakthrough curves (BTC) were determined by adding a solution with  $50 \text{ g m}^{-3}$  of nitrate to the soil surface contained in the columns. For each of the three columns with disturbed and undisturbed samples, a distinct inorganic nitrate salt was used:  $\text{Ca}(\text{NO}_3)_2$ ,  $\text{NH}_4\text{NO}_3$ , and  $\text{KNO}_3$ . Nitrate was used due to its high solubility and for its agronomic and environmental importance. In addition, from an electrochemical standpoint, there is a difference between nitrate and other oxyanions regarding adsorption by soil particles. Nitrate is adsorbed exclusively by electrostaticity, thus depending solely on soil particle charges (Alcântara and Camargo, 2005).

Saturation and leaching were performed according to Rossi et al. (2007) and Silva et al. (2012). After verification of a permanent flow regime, a solution containing the respective



**Figure 1.** Details of the undisturbed sampling process. (a) Auger used to take the undisturbed samples; (b) Sampling; (c) PVC tube with undisturbed sample; (d) Sample after removing excess and drilling the outlet; (e) PVC tube with drain and cap at the bottom.

50 g m<sup>-3</sup> nitrate source was applied to the columns, one component per column. Mariotte flasks were used to ensure a constant nitrate application rate to the column.

The column outflow was sampled in 15 mL acrylic flasks. The accumulated outflow was expressed relative to the column pore volume  $V_p$  (m<sup>3</sup>), calculated as the product of column volume  $V$  (m<sup>3</sup>) and soil porosity  $\alpha$  (m<sup>3</sup> m<sup>-3</sup>). The NO<sub>3</sub><sup>-</sup> concentration in each sample was determined by spectrophotometry (Yang et al., 1998).

Values of nitrate concentration ( $C$ ) as a function of applied volume ( $V_a$ ) for each soil column were transformed into their relative equivalents. The concentration was divided by the concentration of the applied solution ( $C_0$ ), and the applied volume was expressed relative to the column pore volume ( $V_p$ ). Using the obtained relative solute concentration ( $C/C_0$ ) and relative volume ( $V_a/V_p$ ), transport parameters (retardation factor -  $R$ , Péclet number -  $P$ , slope -  $S$ , dispersion-diffusion coefficient -  $D$ , and dispersivity -  $\lambda$ ) were calculated by inverse modeling using the CFITIM module from Stanmod 2.0 (STudio of ANalytical MODels) (Šimůnek et al., 2008). The water flux density in the soil was determined by dividing the outflow volume by the column cross-section and by the time.

### Water retention experiments

Water retention (desorption) curves were determined for the disturbed and undisturbed soil samples in metal rings of 0.03 m height and 0.05 m diameter, with three replicates. The sample water content was determined after equilibrium at nine tensions: 0.10, 0.20, 0.40, and 1.0 m on a tension table, and 3.0, 5.0, 10, 50, and 1.5 10<sup>2</sup> m in a pressure chamber. The Brooks and Corey (1964) equation was fitted to the data using the RETC software (van Genuchten et al., 1991):

$$S = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left( \frac{h_b}{h} \right)^n \quad \text{Eq. 1}$$

in which  $S$  is the effective saturation,  $\theta$  is the water content (m<sup>3</sup> m<sup>-3</sup>),  $\theta_s$  is the saturated water content (m<sup>3</sup> m<sup>-3</sup>),  $\theta_r$  is the residual water content (m<sup>3</sup> m<sup>-3</sup>),  $h_b$  is the air entry matric potential (m), and  $n$  is a fitting parameter related to pore size distribution.

### Relation between retention and breakthrough properties

To correlate retention and breakthrough properties, the Wang et al. (2002) model was applied. According to this model, relative solute concentration  $c(t)/c_0$  is described by:

$$\frac{c(t)}{c_0} = 1 - \left[ \frac{nR}{(n(m+1) + 2)V_a/V_p} \right]^{\frac{2+(m+1)n}{2+mn}} \quad \text{Eq. 2}$$

in which  $n$  is the retention curve fitting parameter (Equation 1),  $m$  is a parameter related to pore connectivity, normally considered equal to -2, and  $R$  is the retardation factor given by:

$$R = 1 + \frac{\rho k}{\theta} \quad \text{Eq. 3}$$

in which  $k$  (m<sup>3</sup> kg<sup>-1</sup>) is the distribution coefficient,  $\rho$  (kg m<sup>-3</sup>) is the soil bulk density, and  $\theta$  (m<sup>3</sup> m<sup>-3</sup>) is the soil water content.

The applied volume of solution in relation to pore volume is calculated as

$$\frac{V_a}{V_p} = \frac{tv_0}{L} \quad \text{Eq. 4}$$

where  $t$  (d) is time,  $L$  (m) is the length of the soil column, and  $v_0$  (m d<sup>-1</sup>) is the average velocity of the solution, given by

$$v_0 = \frac{K_s}{\theta_s - \theta_r} \quad \text{Eq. 5}$$

where  $K_s$  ( $\text{m d}^{-1}$ ) is the saturated hydraulic conductivity, estimated in each experiment as a function of the observed solute flux.

## RESULTS AND DISCUSSION

### Breakthrough experiment

The disturbed soil material in the columns had a bulk density of  $1230 \text{ kg m}^{-3}$ , corresponding to a total porosity of  $0.527 \text{ m}^3 \text{ m}^{-3}$ . The bulk density of the soil in the undisturbed columns was higher,  $1355 \text{ kg m}^{-3}$  (corresponding to a total porosity of  $0.482 \text{ m}^3 \text{ m}^{-3}$ ), with a standard deviation of  $11 \text{ kg m}^{-3}$  (coefficient of variation of 0.8 %). The difference in density and porosity observed between the disturbed and undisturbed columns results in different hydraulic properties and solute flux properties.

Saturated hydraulic conductivity in the disturbed soil columns was  $0.535 \text{ m d}^{-1}$ , on average, and  $0.134 \text{ m d}^{-1}$  in the column with undisturbed structure. The difference between both values is in agreement with the retention curves, which show an increase in macroporosity for the disturbed soil.

A summary of the analysis of variance for the solutes  $\text{Ca}(\text{NO}_3)_2$ ,  $\text{KNO}_3$ , and  $\text{NH}_4\text{NO}_3$  is shown in table 1, showing no significant difference between the transport parameters evaluated, either for the disturbed or the undisturbed samples. From these results, the experiments performed with any of the cations can be considered replicates.

The multiple means comparison test (Tukey at 5 % probability) for the main nitrate transport parameters obtained from disturbed and undisturbed soil showed differences for all parameters (Table 1). It is clear that these differences are related to structural modifications in the disturbed samples caused by the process of disaggregation and sieving. A similar

**Table 1.** Summary of the analysis of variance (squared means) for solute transport parameters obtained from the solutes  $\text{Ca}(\text{NO}_3)_2$ ,  $\text{KNO}_3$ , and  $\text{NH}_4\text{NO}_3$  in experiments with disturbed and undisturbed soil samples

Source of variation	Degree of freedom	$v$	$P$	$R$	$S$	$\lambda$	$D$
Disturbed soil							
Treatment	2	0.00268 <sup>ns</sup>	21.99 <sup>ns</sup>	0.00014 <sup>ns</sup>	0.025 <sup>ns</sup>	0.038 <sup>ns</sup>	0.031 <sup>ns</sup>
Residue	6	0.01103	29.39	0.00083	0.032	0.079	0.042
Overall mean	-	9.81 <sup>(1)</sup> A	22.75 A	0.94 A	1.42 A	0.0095 <sup>(2)</sup> B	0.092 <sup>(3)</sup> A
CV (%)	-	15.73	23.83	3.07	12.56	28.44	32.07
Undisturbed soil							
Treatment	2	0.00541 <sup>ns</sup>	3.51 <sup>ns</sup>	0.042 <sup>ns</sup>	0.099 <sup>ns</sup>	0.075 <sup>ns</sup>	0.045 <sup>ns</sup>
Residue	6	0.01334	7.08	0.019	0.032	0.381	0.071
Overall mean	-	2.0 <sup>(1)</sup> B	8.69 B	0.82 B	1.03 B	0.0241 <sup>(2)</sup> A	0.048 <sup>(3)</sup> B
CV (%)	-	81.86	30.62	16.61	17.46	25.65	80.94

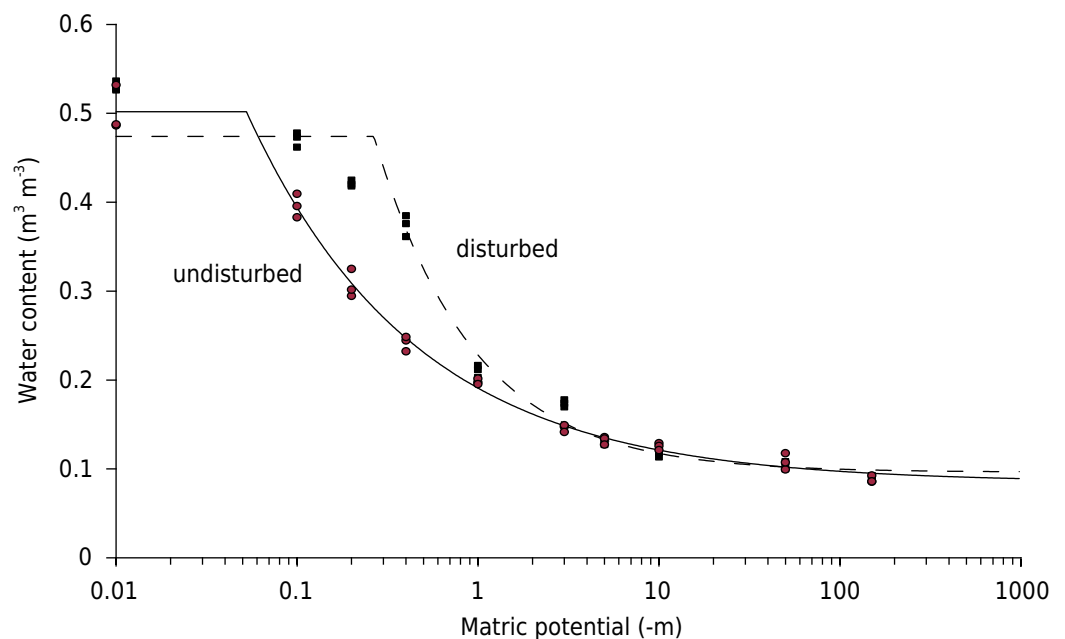
$v$ : average velocity of solution;  $P$ : Péclet number;  $R$ : retardation factor;  $S$ : slope;  $\lambda$ : dispersivity;  $D$ : dispersion-diffusion coefficient; and CV: coefficient of variation. Overall means followed by different letters in the columns are different at a 5 % probability level by the Tukey test. <sup>ns</sup>: non-significant ( $p \geq 0.05$ ) by the F-test. <sup>(1)</sup> In  $\text{m d}^{-1}$ . <sup>(2)</sup> In m. <sup>(3)</sup> In  $\text{m}^2 \text{ d}^{-1}$ .

analysis was performed by Celestino Ladu and Zhang (2011), who found lower values of dispersivity in disturbed and repacked soil, due to a homogenization of structure.

During a flow process through a heterogeneous porous medium, a major part of the solution is transported through some wider channels, making solute molecules move rapidly, a phenomenon called preferential flow (Rosqvist and Destouni, 2000; Gerke, 2006). More preferential flow can be expected in soils with natural structure (Dousset et al., 2007), corroborating the differences observed in transport parameters, especially in reference to dispersivity, as larger values of dispersivity are associated with a predominance of preferential flow (Aggelopoulos and Tsakiroglou, 2008).

### Retention experiment

The results from the retention experiments were in agreement with expected behavior: for matric potentials less negative than 1 m, the disturbed soil showed higher water contents than the undisturbed soil (Figure 2), exhibiting the formation of macropores as a result of the disturbance. Under drier conditions (at more negative potentials), the water contents for disturbed and undisturbed soils were very similar. Fitting parameters of the Brooks and Corey (1964) equation show a higher  $n$  parameter for the disturbed soil (Table 2). A higher  $n$  indicates a more concentrated pore size distribution and directly



**Figure 2.** Water content versus matric potential (“water retention curve”) for disturbed and undisturbed soil samples. Data points correspond to observed values; lines represent the fitted equation 1 (parameters in table 2).

**Table 2.** Fitting parameters for equation 1 (Brooks and Corey, 1964) in disturbed and undisturbed samples

Parameter	Disturbed		Undisturbed	
	Value	Standard Error	Value	Standard Error
$\theta_s$	0.474	0.0095	0.502	0.0065
$\theta_r$	0.096	0.0128	0.085	0.0064
$n$	0.795	0.1424	0.464	0.0303
$h_b^{-1} (m^{-1})$	3.8	0.45	19.1	1.41
$R^2$	0.972		0.994	



affects the predictions of the Wang et al. (2002) model. The  $h_b$  parameter increased and  $q_s$  decreased in the disturbed soil; however, these values do not affect the predictions of the Wang et al. (2002) model.

The three replicates showed similar behavior, with differences in the order of 0.01 to 0.03  $\text{m}^3 \text{m}^{-3}$ . Equation 1 fitted the data points well, with a higher deviation between saturation and matric potential 0.2 m in the disturbed soil, resulting in a slightly lower  $R^2$  in this treatment.

### Relation between retention and breakthrough properties

The retardation factor (Table 1) was smaller than 1, showing that only part of the liquid phase takes part in the transport process. This is the case when the chemical substance (solute) undergoes anionic exclusion or when immobile water regions are present that do not participate in convective movement (Wierenga and van Genuchten, 1989). Consequently, equation 2 from Wang et al. (2002) for reactive solutes was employed.

The diffusion-dispersion equation contains two independent parameters ( $P$  and  $R$ ) fitted to results from a breakthrough experiment by software like Stanmod/CFITIM. The Wang et al. (2002) model, in contrast, is based on information contained in the water retention curve (parameter  $n$ ), adding an independent parameter,  $m$ . Therefore, the statistical performance of CFITIM is expected to be better than that of the Wang et al. (2002) model, as confirmed by the Nash-Sutcliffe efficiency values (Table 3). Using the standard value  $m = -2$ , the performance of the Wang et al. (2002) model was slightly inferior to CFITIM for disturbed soil, and the shape of the predicted curve simulates the experimentally observed behavior well (Figure 3). For the undisturbed soil, a fit with  $m = -2$  resulted in large deviations and a shape that differs from the tendency observed.

The Wang et al. (2002) model predictions were fitted to the experimentally obtained values, resulting in  $m = -2.06$  (disturbed soil) and  $m = -3.55$  (undisturbed soil). These values confirm that  $m = -2$  is an adequate value for the disturbed soil material, but not for the undisturbed soil material, where  $m$  assumes a more negative value. In this respect, it is interesting to note that  $m$  is considered to be related to pore connectivity, with more negative values corresponding to lower connectivity and higher retardation.

Figure 3 also shows that the Wang et al. (2002) model, because of its mathematical structure, does not describe well the beginning of the breakthrough curve, predicting an abrupt increase in relative concentration, which is not observed experimentally.

Observing the experimental data in figure 3, relative maximum concentration ( $C/C_0 = 1$ ) was reached between 1.5 and 2  $V_a/V_p$ . Dispersion between observed values was higher in the experiments with undisturbed soil than in the disturbed soil. The reason for this can be found in the destruction and sieving of soil aggregates, which homogenizes larger structural elements. The small dispersion observed in the experiments with disturbed soil leads to the conclusion that the size of these samples exceeded the representative elementary volume (REV), as described in Bear (1972), Bachmat and Bear (1986), and Kutilek and Nielsen (1994), whereas the REV for the undisturbed soil is larger than the soil column used in our experiments.

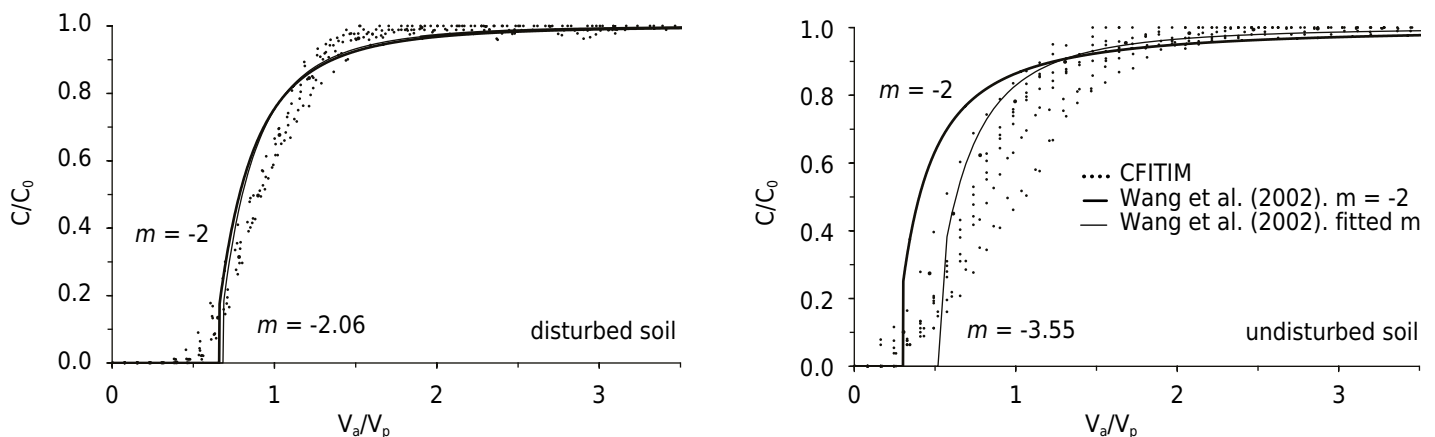
**Table 3.** Nash-Sutcliffe efficiency coefficient for CFITIM and for the Wang et al. (2002) model predictions for  $m = -2$  and for a fitted  $m$

	CFITIM	Wang et al. (2002), $m = -2$	Wang et al. (2002), fitted $m$
Disturbed	0.998	0.978	0.982 ( $m = -2.06$ )
Undisturbed	0.994	0.886	0.957 ( $m = -3.55$ )

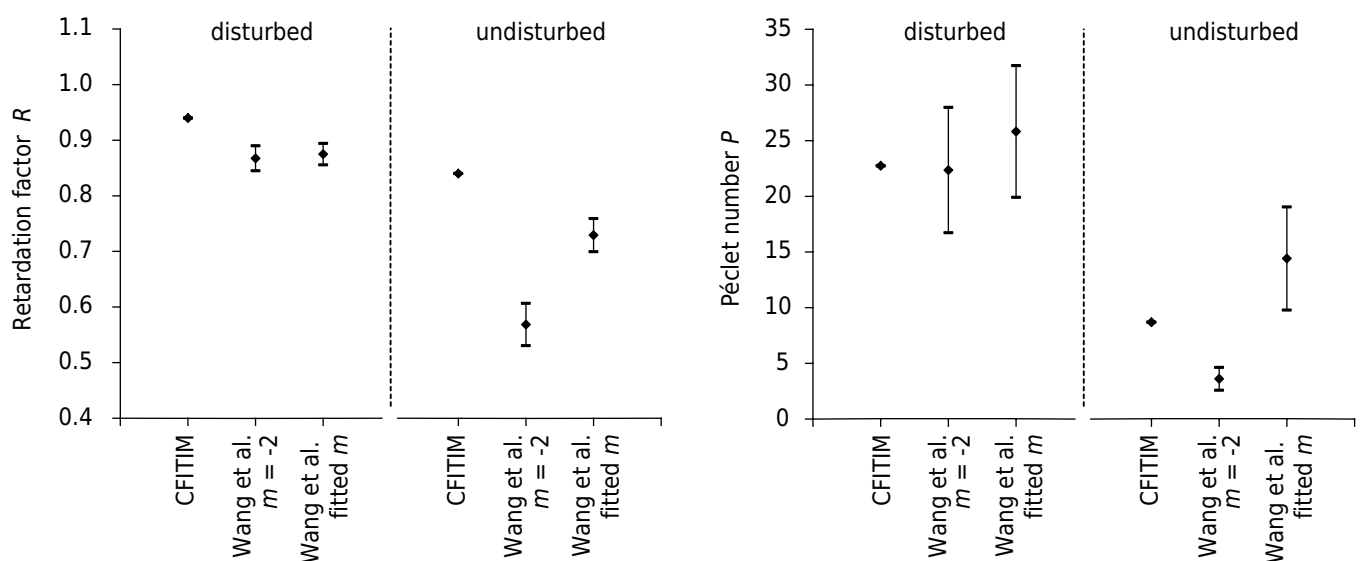


The higher dispersion of values observed in the undisturbed soil leads to a lower Nash-Sutcliffe coefficient and a higher standard deviation (Table 3). Similar observations are reported by several authors. For example, Rossi et al. (2007), in an experiment with two Ferralsols of different texture (a loamy versus a clayey soil), showed that all parameters except dispersivity increased for the disturbed soil. Sampaio et al. (2010) found differences in nitrate transport parameters between disturbed and undisturbed samples of a Ferralsol and made reference to possible compaction and modification of preferential pathways for water flow in their discussion.

An alternative to verify the predictive capacity of the Wang et al. (2002) model is by using the  $C/C_0$  values predicted by the model as a function of  $V_a/V_p$ , fitting the diffusion-dispersion equation to them by Stanmod/CFITIM, thus verifying if the Wang et al. (2002) model is capable of reproducing the experimentally obtained values. Figure 4 shows the results from this exercise. The Wang et al. (2002) model and the diffusion-dispersion equation predict different curve shapes; therefore, the dispersion of fitted values of the Péclet number  $P$  and retardation factor  $R$  by Stanmod/CFITIM is higher in the case of the original experimental breakthrough data. Good fits are observed both for  $P$  and for  $R$  in the



**Figure 3.** Relative solute concentration  $C/C_0$  in the effluent of disturbed and undisturbed soil, as a function of the relative applied volume  $V_a/V_p$ : values observed in three experiments (data points), fitted line by Stanmod/CFITIM, and values predicted by the Wang et al. (2002) model for default parameter value  $m = -2$ , and for fitted  $m$ .



**Figure 4.** Péclet number  $P$  and retardation factor  $R$  obtained from fitting Stanmod/CFITIM to experimental breakthrough data, and to values predicted by the Wang et al. (2002) model for  $m = -2$  and for fitted  $m$ , for disturbed and undisturbed soil material. Error bars represent the confidence interval of 95 %.

disturbed soil. For the undisturbed soil, fitting the  $m$  parameter is an essential step for obtaining better predictions.

## CONCLUSIONS

The Wang et al. (2002) model allows good predictions of breakthrough experiments for the disturbed soil using the standard pore connectivity parameter value of  $m = -2$ . For undisturbed soil samples, a more negative value was fitted to the soil used in this study ( $m \approx -3.5$ ). More research in different soils is needed in order to apply the model.

Experimental breakthrough data dispersion was higher in columns filled with undisturbed material than in those filled with disturbed soil, suggesting that the homogenization of pore structure leads to a reduction in the size of the representative elementary volume (REV) for these properties.

Nitrate transport properties determined in disturbed and undisturbed samples showed significant differences, especially the Péclet number (about 3 times higher in the disturbed soil), mean solution velocity (about 5 times higher in the disturbed soil), dispersivity (about 3 times higher in the undisturbed soil), and the dispersion-diffusion coefficient (about 2 times higher in the disturbed soil).

## REFERENCES

- Aggelopoulos CA, Tsakiroglou CD. Quantifying soil heterogeneity from solute dispersion experiments. *Geoderma*. 2008;146:412-24. doi:10.1016/j.geoderma.2008.06.014
- Alcântara MAK, Camargo OA. Adsorção de nitrato em solos com cargas variáveis. *Pesq Agropec Bras*. 2005;40:369-76. doi:10.1590/S0100-204X2005000400008
- Anami MH, Sampaio SC; Suszek M, Gomes SD, Queiroz MMF. Deslocamento miscível de nitrato e fosfato proveniente de água residuária da suinocultura em colunas de solo. *Rev Bras Eng Agríc Amb*. 2008;12:75-80. doi:10.1590/S1415-43662008000100011
- Bachmat Y, Bear J. Macroscopic modelling of transport phenomena in porous media. 1: The continuum approach. *Transp Porous Media*. 1986;1:213-40. doi:10.1007/BF00238181
- Bear J. Dynamics of fluids in Porous Media. New York: Elsevier; 1972.
- Bresler E. Convective and pore scale dispersive solute transport in unsaturated heterogeneous fields. *Water Resour Res*. 1981;37:1683-93. doi:10.1029/WR017i006p01683
- Brooks RH, Corey AT. Hydraulic properties of porous media. Fort Collins: Colorado State University; 1964. (Hydrology, 3).
- Celestino Ladu JL, Zhang D. Modeling atrazine transport in soil columns with HYDRUS-1D. *Water Sci Eng*. 2011;4:258-69. doi:10.3882/j.issn.1674-2370.2011.03.003
- Doltra J, Muñoz P. Simulation of nitrogen leaching from a fertigated crop rotation in a Mediterranean climate using the EU-Rotate\_N and Hydrus-2D models. *Agric Water Manage*. 2010;97:277-85. doi:10.1016/j.agwat.2009.09.019
- Donagema GK, Campos DVB, Calderano SB, Teixeira WG, Viana JHM, organizadores. Manual de métodos de análise do solo. 2ª ed. rev. Rio de Janeiro: Embrapa Solos; 2011.
- Dousset S, Thevenot M, Pot V, Šimunek J, Andreux F. Evaluating equilibrium and non-equilibrium transport of bromide and isoproturon in disturbed and undisturbed soil columns. *J Contam Hydrol*. 2007;94:261-76. doi:10.1016/j.jconhyd.2007.07.002
- Fonseca B, Teixeira A, Figueiredo H, Tavares T. Modeling of the Cr(VI) transport in typical soils of the North of Portugal. *J Hazard Mater*. 2009;167:756-62. doi:10.1016/j.jhazmat.2009.01.049
- Gerke HH. Preferential flow descriptions for structured soils. *J Plant Nutr Soil Sci*. 2006;169:382-400. doi:10.1002/jpln.200521955

- IUSS Working Group WRB. World Reference Base for Soil Resources 2014, update 2015 International soil classification system for naming soils and creating legends for soil maps. World Soil Resources Reports No. 106. Rome: FAO; 2015.
- Kutilek M, Nielsen DR. Soil hydrology: geo-ecology textbook. Catena: Cremlingen-Destedt; 1994.
- Nielsen DR, Biggar JW. Miscible displacement in soils: I. Experimental Information. Soil Sci Soc Am J. 1961;25:1-5. doi:10.2136/sssaj1961.03615995002500010008x
- Rose DA, Abbas F, Adey MA. The effect of surface solute interactions on the transport of solutes through porous materials. Eur J Soil Sci. 2009;60:398-411. doi:10.1111/j.1365-2389.2009.01122.x
- Rosqvist H, Destouni G. Solute transport through preferential pathways in municipal solid waste. J Contam Hydrol. 2000;46:39-60. doi:10.1016/S0169-7722(00)00127-3
- Rossi P, Miranda AJH, Duarte SN. Curvas de distribuição de efluentes do íon nitrato em amostras de solo deformadas e indeformadas. Eng Agríc. 2007;27:675-82. doi:10.1590/S0100-69162007000400010
- Ruiz HA, Ferreira PA, Rocha GC, Borges Jr JCF. Transporte de solutos no solo. In: De Jong van Lier, Q, editor. Física do solo. Viçosa, MG: Sociedade Brasileira de Ciência do Solo; 2010. p.213-40.
- Sampaio SC, Caovilla FA, Opazo MAU, Nóbrega LHP, Suszek M, Smanhotto A. Lixiviação de íons em colunas de solo deformado e indeformado. Eng Agríc. 2010;30:150-9. doi:10.1590/S0100-69162010000100016
- Santos HG, Jacomine PKT, Anjos LHC, Oliveira VA, Oliveira JB, Coelho MR, Lumbrreras JF, Cunha TJF. Sistema brasileiro de classificação de solos. 3ª ed. Rio de Janeiro: Embrapa Solos; 2013.
- Silva NF, Lelis Neto JA, Texeira MB, Cunha FN, Mir AJH, Coelho RD. Distribuição de solutos em colunas de solo com vinhaça. Irriga. 2012;1:340-50. doi:10.15809/irriga.2012v1n01p340
- Šimůnek J, van Genuchten MTh, Šejna M. Development and applications of the HYDRUS and STANMOD software packages, related codes. Vadose Zone J. 2008;7:587-600. doi:10.2136/vzj2007.0077
- van Genuchten MTh, Leij FJ, Yates SR. The RETC code for quantifying the hydraulic functions of unsaturated soils. Version 1.0. EPA Report 600/2-91/065, U.S. Salinity Laboratory. Washington, DC: USDA; 1991.
- Wang Q, Horton R, Lee J. A simple model relating soil water characteristic curve, soil solute breakthrough curve. Soil Sci. 2002;167:436-43. doi:10.1097/00010694-200207000-00002
- Wierenga PJ, van Genuchten MTh. Solute transport through small, large unsaturated soil columns. Ground Water. 1989;27:35-42. doi:10.1111/j.1745-6584.1989.tb00005.x
- Yang JE, Skogley EO, Schaff BE, Kim JJ. A simple spectrophotometric determination of nitrate in water, resin soil extracts. Soil Sci Soc Am J. 1998;62:1108-15. doi:10.2136/sssaj1998.03615995006200040036x