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SENSITIVITY ANALYSIS OF HYDRUS-1D MODEL IN THE SIMULATION OF POTASSIUM TRANSPORT IN TWO BRAZILIAN SOILS

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ABSTRACT: In this work we verified the performance of HYDRUS-1D model in the simulation of potassium displacement in segmented columns filled with Haplustox (S1) and Hapludox (S2) soils under unsaturated conditions. For this, the ion transport parameters were obtained by Breakthrough Curves (BTC) applying 1800 mg L^{-1} potassium solution in segmented columns for posterior simulation concentration profile by the model. The sensitivity analysis of the model was done using the Nash-Sutcliffe Efficiency Index (NSI) by doing positive and negative variations of the model input transport parameters. At the end, by the result of the BTC's, was observed that the soil S2 presented greater interaction with the potassium ion. The sensitivity analysis showed that the parameters saturated hydraulic conductivity, saturated water content and retardation factor presented the farthest NSI values from the unit, that is, they promote greater variations for the two studied soils, especially for S2.

KEYWORDS: fertirrigation, miscible displacement, solute dynamics

ANÁLISE DE SENSIBILIDADE DO MODELO HYDRUS-1D NA SIMULAÇÃO DO TRANSPORTE DE POTÁSSIO EM DOIS SOLOS DE TEXTURAS DISTINTAS

RESUMO: O presente trabalho teve por objetivo verificar o desempenho do modelo HYDRUS-1D na simulação do deslocamento do potássio em colunas de solo segmentadas, preenchidas com Latossolo Vermelho Amarelo (S1) e Nitossolo Vermelho (S2), em condições não saturadas. Para tal, os parâmetros de transporte do íon potássio foram obtidos por meio de Breakthrough Curves (BTC), com a aplicação de solução de 1800 mg L^{-1} de concentração de potássio. A solução foi aplicada nas colunas segmentadas para posterior simulação do perfil da

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concentração de potássio pelo modelo. A análise de sensibilidade do modelo foi feita por meio do Índice de Eficiência de Nash-Sutcliffe (NSI), impondo-se variações positivas e negativas aos parâmetros de transporte de entrada do modelo. Ao final, pelo resultado das BCT's, observou-se que o solo S2 apresentou maior interação com o íon potássio. A análise de sensibilidade mostrou que os parâmetros condutividade hidráulica saturada, umidade volumétrica na saturação e fator de retardamento apresentaram os valores mais distantes da unidade de NSI, ou seja, foram os que causaram maiores variações para os dois solos estudados, especialmente para S1.

PALAVRAS-CHAVE: fertirrigação, deslocamento miscível, dinâmica dos solutos

INTRODUCTION

Potassium has high soil mobility and its absorption is highly selective, which is an advantage, since nutrients with high mobility are absorbed more efficiently, although they are much more easily leached (Ernani et al., 2012). Potassium's main roles in a plant are directly linked to vital processes, such as photosynthesis, translocation and ionic balance. Its prime mode of transportation to root is by diffusion, characterized by random thermal movement of ions towards the root, due to the gradient of concentration generated on the root surface.

According to reports by Zanini (1991) and Ruiz et al. (1999), the mass flow can significantly contribute in the process when potassium concentration in the soil solution is high, coinciding with points where the soil moisture values are higher, being related to the water distribution in the soil, which allows the control of this ion in the soil due to the fertirrigation and irrigation practices.

In order to obtain a satisfying efficiency when using water and fertilizers, herbicides and pesticides in the soil, it is of greater importance, regarding both environmental and economic questions, a better understanding of these dynamics on an unsaturated environment (Ladu & Zhang, 2011). However, on these processes involves a large number of variables, and it is necessary to use simulation models for agility, precision and to allow a large number of factors and effects to be considered. Also, there is still some difficulty in involving all these variables so that a model can actually predict the process of displacement and retention of solutes in agricultural environments.

In this context, many models (analytical and numerical) have been developed to help on this prediction in the soil profiles, among them: MOUSE (Steenhuis et al., 1984), GLEAMS

(Knisel & Devis, 2000), HYDRUS 1-D (Simunek et al., 2005), STANMOD (Simunek et al., 2008), MIDI (Miranda & Duarte, 2002), WANISIM (Lekakis & Antonopoulos, 2015) and CTRW (Shahmohammadi-Kalalagh & Beyrami, 2015). Thus, this work aimed to verified the performance of the HYDRUS-1D model in the simulation of potassium concentration profiles in segmented soil columns filled with two different textured soils under unsaturated conditions.

MATERIAL AND METHODS

The work was carried out at the Soil Physics Laboratory at College of Agriculture "Luiz de Queiroz" (ESALQ), University of São Paulo (USP), Piracicaba, São Paulo, Brazil. Were used for potassium displacement simulations Haplustox (S1) and Hapludox (S2) soils, both dry in the air. The physical-water properties of these soils are showing in Table 1.

Initially, in order to obtain a profile of the potassium concentration along the profile depth, the potassium solution (1800 mg L^{-1}) was applied to a segmented column filled with soils S1 and S2 under an unsaturated conditions with 0.7 m height, that is, 10 rings with 0.07 m high and 0.05 m diameter (Figure 1A). The fact of segmentation into rings are to allow the obtention of potassium concentration in each band and thus make possible the comparison with the simulations performed by the HYDRUS-1D model. In both columns, a pre-calibrated peristaltic pump applied a potassium solution at a constant flow rate of 2.80 cm^3 min^{-1}. Urge to mention that this flow was selected so that there was no depth formation in the column first ring.

The test was carried out until the solution reached the eighth ring of each column. So, then the process of removing the rings was initiated and the solution extraction step was started. The final potassium concentration values of each ring were obtained by correcting according to the water content of the soil of each ring and of the amount of water that was added to extract the solution (Eq.1).

$$[K^+]_{corr} = \frac{U_{paste}.[K^+]}{U_{ring}} \qquad (1)$$

where,

$[K^+]_{corr}$ – potassium ion concentration corrected by water content, mg L^{-1}

U_{paste} – paste water content used to extract the solution, g g^{-1}

$[K^+]$ – potassium ion concentration determined by saturated solution extraction, mg L^{-1}

U_{ring} – ring water content after the solution application, g g^{-1}.

The model input parameters related to the potassium transport in soils were obtained by numeric fitting of breakthrough curves (BTC) (Table 2). For this, PVC columns (0.2 m height and 0.05 m diameter), were filled with soil material, previously mentioned, in constant, equivalent and homogeneous layers. A drain was installed on the top of the column which had the function of maintaining the hydraulic charge of 0.01 m (Figure 1B).

In order to promote water saturation in the columns and to initiate the tests were adopted same procedures as Miranda et al. (2005) and Rossi et al. (2007), replacing only the water distilled by deionized water and using a specific ion meter for potassium. Following, a potassium solution at 1800 mg L^{-1} was applied and batch sequential volumes of 15 cm^3 effluents were collected, representing fractions of 0.079 and 0.069 pore volumes (PV) of S1 and S2, respectively. The PV was calculated as a function of the total soil porosity (α) and the soil volume in the column (392.7 cm^3). A potassium-specific ion meter was used to aid in the effluent collection process, and the BTC test was interrupted only when the relative concentration (C/Co) was equal to the unity, that is, the concentration of potassium apllied being equal to the concentration of potassium in the outlet.

Transport parameters were estimated according to Pinho & Miranda (2014). Thus, to performance analysis sensitivity of the model, the input parameters saturated hydraulic conductivity (Ko), saturation water content (θ_s), pore water velocity (v), dispersion coefficient (D) and retardation factor (R) were varied positively and negatively (±15%, ±30% e ±60%), keeping the others fixed. It is emphasized that dispersivity (λ) varies as a function of v and D parameters, and θ_s was assumed to be α.

Nash-Sutcliffe Efficiency Index (NSI) were calculated by Eq. 2 to verify which parameter had the greatest influence on the simulations of potassium dynamics of the HYDRUS-1D model, as well as which parameter should be determined with greater precision and atention. It is emphasized that this index varies from $-\infty$ to 1, indicating a better accuracy when it approaches 1.

$$\mathrm{NSI} = 1 - \frac{1/n.\sum\left(O_i - S_i\right)^2}{1/n.\sum\left(O_i - \bar{O}\right)^2} \quad (2)$$

where,

NSI – Nash-Sutcliffe Efficiency Index, dimensionless

n – number of observations

O_i – observed data

S_i – estimated data

Ō – average of observed data.

RESULTS AND DISCUSSION

Figure 2 shows the breakthrough curves (BTC) elaborated for the soils under this study, which represent the displacement of the potassium ion in relation to the different soils. To obtain maximum relative concentration (C/Co), Haplustox (S1) and Hapludox (S2) soils required approximately 3.5 pore volume (PV). However, there was a displacement of the S1 curve to the left, which indicates a lower interaction between this type of soil and the potassium ion (Figure 2A).

According to Nielsel and Biggar (1962), when C/Co is equal to 0.5, the corresponding PV is the first indication of the existence or not of interaction between the solute and the soil. Thus, for S1 the PV for C/Co equal to 0.5 was equal to unity, that is, there was no interaction with the colloidal fraction of the soil (Figure 2A). For S2 this value was higher than the unit, evidencing that, when flowing through the soil profile, part of the solute was adsorbed (Figure 2B).

Table 2 shows the potassium ion transport parameters obtained for the soils under study. The retardation factor (R) was higher than the unit for both soils, but higher for S2, confirming a higher adsorption of the potassium ion in relation to S1, corroborating with the results obtained by Pinho & Miranda (2014). Another factor to consider is the pore water velocity of the solution that was smaller for S2. About Peclet number (P), small values indicate that the diffusion transport dominates over the convection transport. At higher values, the convection transport dominates over the diffusion.

For S1, the potassium ion reached greater depths along the column, compared to S2 (Figures 3 and 4). The textural difference between soils influenced notably the displacement of potassium along the column, mainly in the first four rings, modifying its final depth of reach, maintaining certain conformity with the front of wetting. The potassium distribution along the columns showed a typical tendency for each soil type. A concentration of 266.56 mg L^{-1} was observed to the depth of 0.56 m (eighth ring) in S1 column, while for S2, at a depth of 0.28 m (fourth ring), a concentration of 99.15 mg L^{-1} was observed (Figures 3 and 4). Similar results in which the soil textural class influenced the ions displacement were observed by Oliveira et al. (2010), Ribeiro et al. (2011) and Pinho & Miranda (2014).

From the potassium concentration of 1800 mg L^{-1}, the maximum value found for S2 was remained close to 1725 mg L^{-1}. The difference between applied and collected values is due to the effect of adsorption of the potassium ion on the soil, the effect of which is detected by the retardation factor (one of the transport parameters used as input data in the model), as commented previously and observed by Table 2.

Figure 3 and 4, respectively, also shows the simulation of the potassium ion displacement in S1 and S2 by HYDRUS-1D model, as well as the simulation obtained by the sensitivity analysis performed for the model input parameters. It is possible to observe that the model predicted satisfactorily the potassium displacement to the soils S1 and S2, presenting Nash-Sutcliffe Efficiency Index (NSI) values of 0.86 and 0.93, respectively.

Tan et al. (2015) used the HYDRUS-1D model to describe the transport of water and nitrogen in paddy fields in different irrigation managements. The authors commented that the modeling by HYDRUS-1D is a useful system approach that covers all processes related to water and nitrogen management for supporting the strategic and tactical decision process in sustainable rice production. Tafteh & Sepaskhah (2012), also by HYDRUS-1D, simulated water and nitrate leaching under furrow irrigation in rapeseed and maize fields, and concluded that the model was able to simulate deep percolation and nitrate leaching with good accuracy for both crops.

In Table 3, we can observe that, for S2, HYDRUS-1D model did not response for all negative variations of saturated hydraulic conductivity (Ko), saturation water content (θ_s) and R. The model did not work for the highest negative variation of Ko and θ_s, in S1 as well. For S1, were found smaller NSI values for all the negative variations and for the greater variation of R (Table 3). On the other hand, for S2, with the exception of the variations that did not let the model work, the NSI values were all higher than 0.86 (Table 3).

From the NSI concept, previously explained, values farther from the unit indicate lower accuracy. Therefore, the input parameters Ko, θ_s and R presented greater sensitivity to variations, evidencing that their determinations for potassium displacement simulations must be performed with more accuracy and precision, taking into account the least possible experimental error, especially for S2.

CONCLUSIONS

Under the conditions studied, the HYDRUS-1D model was able to predict the unidirectional movement of potassium.

The transport parameters saturated hydraulic conductivity, saturation water content and retardation factor presented greater sensitivity to variations for the HYDRUS-1D model, requiring a greater care for determination these parameters, especially for soils with high interaction capacity with the potassium ion.

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Table 1. Physical-water properties texture, bulk density (ρ_b), total porosity (α), saturated hydraulic conductivity (Ko) of the Haplustox (S1) and Hapludox (S2) soils used in simulations.

Soil	Sandy (g kg^{-1})	Silt (g kg^{-1})	Clay (g kg^{-1})	ρ_b (g cm^{-3})	α (cm³ cm^{-3})	Ko (cm h^{-1})
S1	695	120	185	1.37	0.292	18.19
S2	120	250	630	1.18	0.434	8.73

Table 2. Estimated potassium transport parameters for Haplustox (S1) and Hapludox (S2) soils: Peclet number (P), retardation factor (R), dispersion coefficient (D), pore water velocity (v) and dispersivity (λ).

Soil	Potassium transport parameters				
	P	R	D (cm² min^{-1})	v (cm min^{-1})	λ (cm)
S1	4.919	1.750	4.512	1.110	4.066
S2	15.185	2.761	0.411	0.312	1.317

Table 3. Nash-Sutcliffe Efficiency Index for the values of potassium concentration, as a function of the varied input parameter and its variation, for Haplustox (S1) and Hapludox (S2).

Soil	Variation	Input potassium transport parameter				
		Ko	θ_s	λ(v)	λ(D)	R
S1	+60%	0.73	0.92	0.68	0.68	0.69
	+30%	0.79	0.93	0.81	0.73	0.89
	+15%	0.83	0.91	0.80	0.75	0.93
	-15%	0.90	0.77	0.75	0.80	0.56
	-30%	0.79	0.93	0.81	0.73	-0.10
	-60%	-	-	0.56	0.87	-1.07
S2	+60%	0,88	0,98	0,94	0,92	0,86
	+30%	0,90	0,97	0,94	0,92	0,97
	+15%	0,91	0,96	0,94	0,93	0,98
	-15%	-	-	0,93	0,94	-
	-30%	-	-	0,92	0,94	-
	-60%	-	-	0,89	-	-

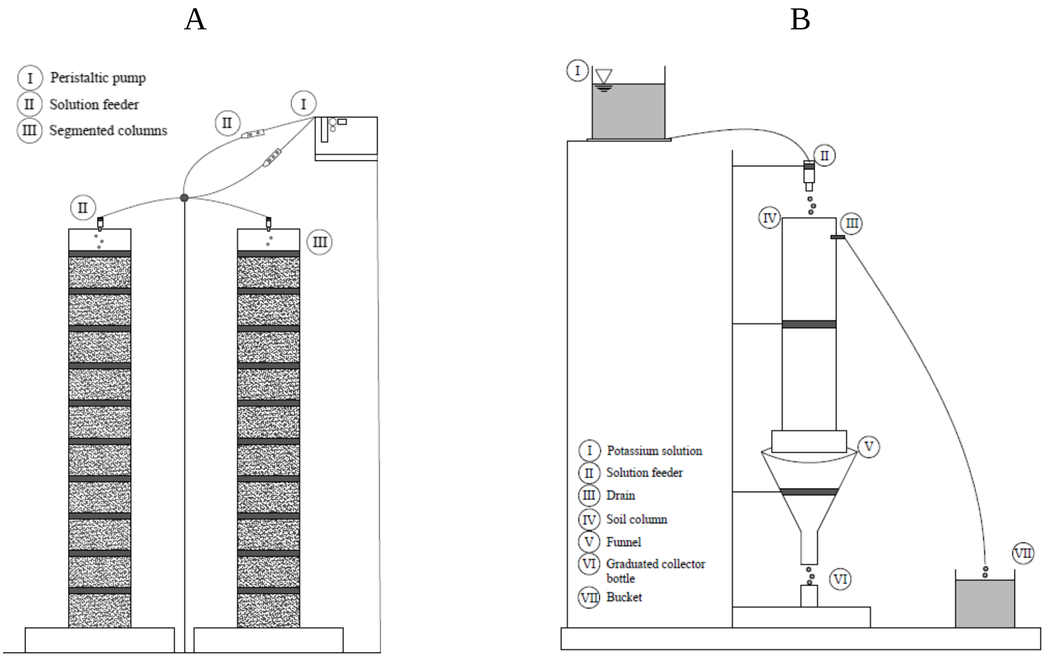

Figure 1. Schemes for (A) potassium solution application in the segmented columns with a peristaltic pump, and (B) the solution collection that crosses the soil column, for the breakthrough curves elaboration.

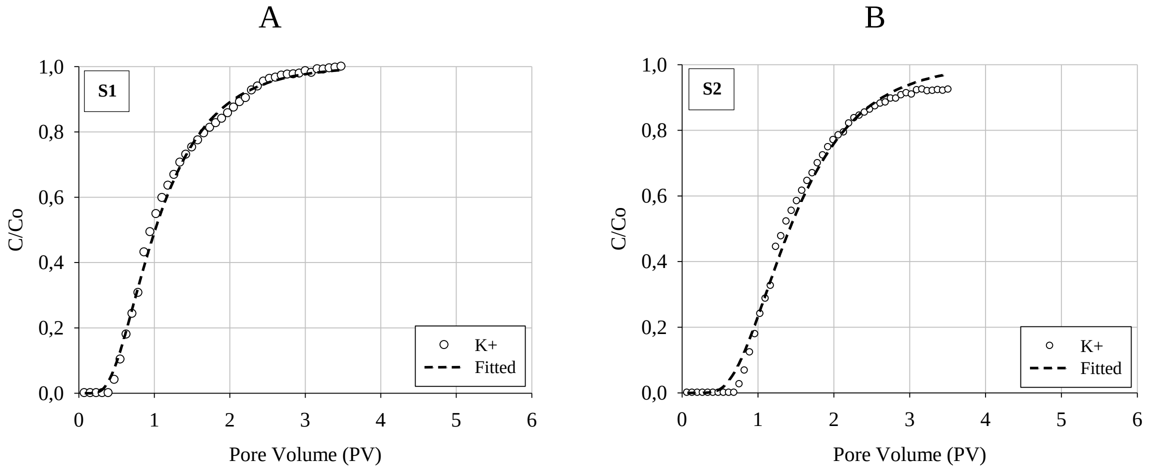

Figure 2. Potassium breakthrough curves for the Haplustox (A) and Hapludox (B) soils used in the experiments.

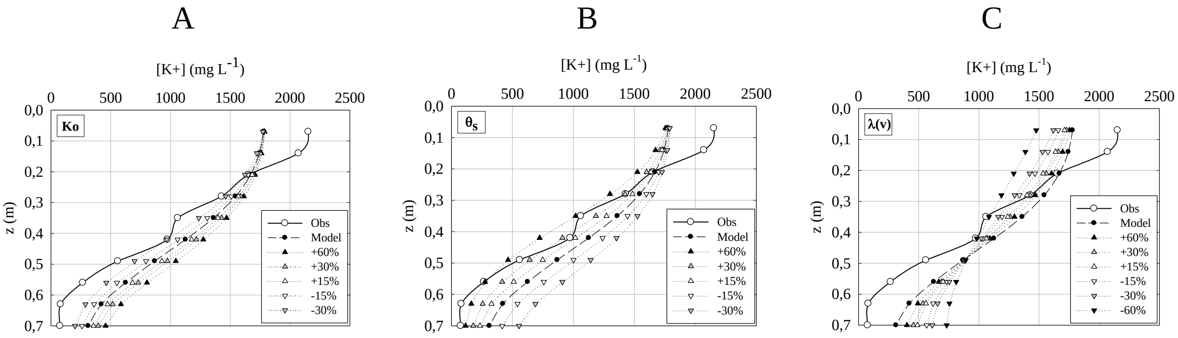

Figure 3. Observed and simulated potassium distributions, when subjected to positive and negative variations of the input parameters (A) saturated hydraulic conductivity (Ko); (B) saturation water content (θ_s); (C) pore water velocity (v); (D) dispersion coefficient (D); and, (E) retardation factor (R), for Haplustox soil.

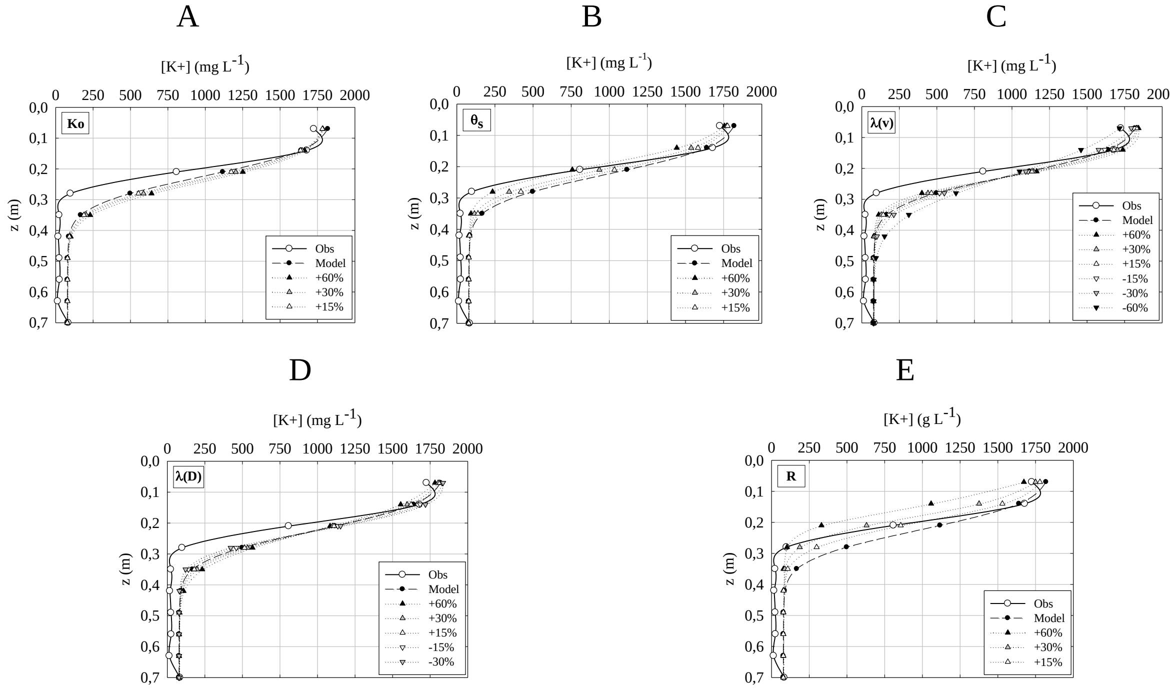

Figure 4. Observed and simulated potassium distributions, when subjected to positive and negative variations of the input parameters (A) saturated hydraulic conductivity (Ko); (B) saturation water content (θ_s); (C) pore water velocity (v); (D) dispersion coefficient (D); and, (E) retardation factor (R), for Hapludox soil.