Phosphorus Transport Through a Saturated Soil Column: Comparison Between Physical Modeling and HYDRUS-3D Outputs

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Abstract: The objective of the present study was to understand Phosphorus transport from soil columns at different water flux densities and to compare computer simulation results using HYDRUS-3D and the physical model against column-experiment data. Towards that end, two water flux densities (0.0075, 0.0065 m sec^{-1}) and P concentration rates (33 mol cm^{-3}) were used. The soil used has a silty clay- loam texture. The numerical model (HYDRUS-3D) successfully predicted P transport in the present experiment. Overall, the HYDRUS-3D model successfully simulated the water flow in the columns; however, it overestimated the final adsorbed PO$_4$ concentrations in the soil. The present column experiment is useful for assessing relative behavior of P in increasing the movement of phosphorus ions out of the soil profile and into ground waters.

Key words: Phosphorus transport, HYDRUS-3D model, groundwater pollution, soil column, adsorption, steady flow

INTRODUCTION

Phosphoros is a critical element in both natural and agricultural ecosystems throughout the world (Onweremadu, 2007) as its limited availability is often the main constraint for plant growth in highly weathered soils of the tropics (Bunemann *et al.*, 2004). Phosphorus deficiency problems are common in well-weathered Oxisols and Ultisols because of strong acidic reactions and an abundance of Al and Fe ions (Saleque *et al.*, 2004). A substantial problem to human health is contamination of ground waters through leaching of phosphorus. Usage of fertilizers and leakage of phosphorus through the soil has been a concern throughout the world. A considerable number of laboratory experiments have been conducted to enable modeling of contaminant transport to improve the simulation capability of models. HYDRUS-3D is a software package for simulating water, heat and solute transport in three-dimensional, variably saturated media (Simunek *et al.*, 2005). Many researchers have used Hydrus to predict solute transport in the soil column (Pang *et al.*, 2000; Ventrella *et al.*, 2000). Phosphorus (P) in solutions is attached to positively charged sites on the surface of soil particles and is strongly adsorbed to the soil, forming stable bonds with the soil's functional group. The soil adsorbs P molecules found in the soil solution; phosphorus then interacts with soil particles in its exchangeable form. Although phosphate is strongly adsorbed to soil particles, many recent studies have shown that phosphate can easily be found in subsurface fresh water (Enright and Madramootoo, 2003; Simard, 2005). The reason behind such results is the under-sorption and desorption process that is controlled by the equilibrium constant. As the concentration of phosphate increases in the soil solution, the phosphate is adsorbed to soil while, when the concentration of phosphate in the solution is depleted, the phosphate that has been adsorbed in the soil dissolves back into solution. Also, the macropore flow path is important to load phosphate through the soil (Stamm *et al.*, 1998; Hooda *et al.*, 1999). In order to improve predictions of phosphate transport in soil, computer modeling can be useful for simulating P distribution under laboratory and field conditions. Phillips (2006) investigated the accuracy of the HYDRUS-2D model in simulating the transport of reactive chemicals like potassium in undistubed soil columns. The results showed that the HYDRUS model was successful in simulating water flow but it was not very conclusive with regard to reactive solute transport. Ben-Gal and Dudley (2003) simulated P movement and P distribution patterns under continuous application of P fertilizer from a subsurface, point-source emitter applied HYDRUS-2D. Both simulated and experimental results showed that an increase in P uptake by plants and greater P mobility, was observed under continuous applications of water and fertilizer as opposed to intermittent applications. However,

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Ben-Gal and Dudley (2003) concluded that the Langmuir isotherm, provided within the HYDRUS-2D model, is inadequate for describing P sorption. It assumes instantaneous equilibrium between the solid and solution interfaces. Rassam and Cook (2002) modeled water flow and solute transport in soil with a high concentration of acid sulfatteof tile drained fields using the HYDRUS-2D model. They concluded that numerical modeling as employed by the HYDRUS-2D model provided an effective tool in understanding the mechanisms involved in such a complex system, hence is a valuable management tool.

Many numerical models have been tested, such as NCSWAP, LEACHM (Hutson and Wagenet, 1992; RZWQM Team, 1995), CHAIN-2D (Simunek and Van Genuchten, 1994), CHAIN _IR (Zhang, 1997) and HYDRUS-2D (Simcnek *et al.*, 1999b). As a result of increasing concerns over groundwater pollution with phosphorus, the objectives of the present study were defined as follows:

- Study P transport from soil columns with water flux at different P concentrations
- Compare computer simulation results using numerical and physical models with column-experiment data

MATERIALS AND METHODS

The research was conducted during the cropping season between 2009 and 2010 at Omidie, southeastern Iran. The study site is located at latitude 31°-53'-14" N and 48°-40'-34" E, with an elevation of 55 meters (handheld Global Positioning System – GPS) (Garmin Ltd, Kansas, USA). The predominant parent material underlying the area from which most soil was formed is coastal plain sand (Benin formation) of the Miocene-Oligocene geological era. These soils are referred to as silty clay loam and are characteristically acidic, have low cation exchange capacity, low base saturation and low fertility and are challenged by multiple nutrient deficiencies (Oti, 2002). The area has a semi-arid tropical climate (Igwe and Stahr, 2004) with two distinct seasons, namely the wet and dry seasons. Rainfall distribution is bimodal with peaks during the months of July and September. Temperatures are high and change only slightly during the year.

Some physical and chemical properties are illustrated in Table 1.

Soil columns: The columns had an ID of 10 and 100 cm long. They were made of transparent polyvinyl chloride (PVC). The physical model used in the experiments (designed and built in the Water Science Faculty of Shahid Chamran University, Ahvaz) consists of a PVC pipe 100 cm tall. The model had three parts - input, output

and porous media- which were placed on a foot stool; water and contaminants were flowed from the bottom of the column. To prevent soil particles from falling off the top of the column, a Plexiglas plate was placed on the soil column. Water, along with contaminants, was flowed from the source through a pipe into the porous media. To prevent air from entering the system, a control valve was placed along this path. Sampling tubes were placed on the body model in flowing lengths 5, 12, 25, 50 and 75 cm from the bottom of the model. Drainage pipes were placed 32, 55 and 82 cm from the bottom of the model. The schema used in the physical model is shown in Fig. 1.

Water and phosphate application: The soil columns were saturated by adding water from the bottom of the column to reach saturated conditions and phosphate solution was applied at steady rate. The soil columns at different depths were monitored to collect the leachate. The water was applied at two different constant rates: 0.0075, 0.006 m sec^{-1} with a P concentration of 33 mol cm^{-3}. The P concentration was calculated with a scanning spectrophotometer. BTC curves were extracted at different depths and are shown in Fig. 4 to 15. At the end of experiment at each depth, the soil was changed to execute experiments at another depth.

Soil hydraulic properties: The van Genuchten-Mualem model (Van Genuchten, 1980) was used to describe the water retention and conductivity (K(h)) functions for both matrix and macropore domains (Mualem, 1976):

$$\theta(h) = \theta_r + \frac{\theta(h) \quad \theta_r}{\theta_s \quad \theta_r} \qquad h < h_e \qquad (1)$$
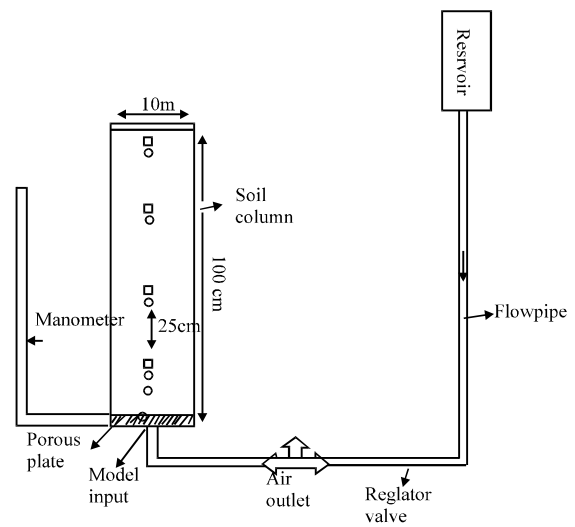$$= \theta_s \qquad\qquad h > h_e$$

Fig. 1: Schema of physical model

Table 1: The number of physical and chemical properties of soil used in the present study

RAW	Clay	Silt	Sand	SOC	Ca	Al	CEC	Alsat	pH (Kcl)
	---------------------------- (g kg^{-1}) ----------------------------				---------------------------- (cmol kg^{-1}) ----------------------------				
1	530	60	610	14	6.6	4.0	19.0	42	6.1
2	300	90	350	25	6.8	3.5	14.0	45	6.0
3	350	420	230	30	7.5	4.4	18.0	56	6.8
4	640	200	160	12	4.3	5.3	20.5	32	6.5
5	300	160	560	23	8.2	3.6	15.5	43	6.0

SOC: Soil organic carbon, Alsat: Aluminium saturation, Ca: Calcium, Al: Aluminium CEC: Cation exchange capacity

$$k(h) = K_s K_r(h) \qquad h < 0$$
$$= K_s \qquad h >= 0 \qquad (2)$$

$$K_r(h) = \frac{\{1(\alpha h)^{n1}[1 + (\alpha h)^n]^m\}^2}{[1 + (\alpha h)^n]^{m/2}} \qquad (3)$$

$$S_e = \frac{\theta(h) \quad \theta_r}{\theta_s \quad \theta_r} \qquad (4)$$

$$M = 1 - 1/n \qquad n > 1 \qquad (5)$$

Where :
$\theta(h)$ = The soil water content at the matrix head, (h)
h = The soil matrix head (L)
θ_S = The saturated water content (L^3 L^{-3})
K_S = The saturated hydraulic conductivity (LT^{-1})
h_e = The air-entry potential (L^{-1})
K_r = The relative hydraulic conductivity (-)
S_e = The relative water saturation (-)
     m, n and α are the fitting parameters of the retention curve
θ = The residual water content (L^3 L^{-3})
$K(h)$ = Unsaturated hydraulic conductivity (LT^{-1})
     The values of α, m and n are obtained by fitting Eq. 2 to the soil water retention data using the RETC model (Van Genuchten *et al.*, 1991)

Theory:
Water flow equation: The Richard equation describes one-dimensional transient water flow in soil (Richards, 1931):

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\frac{\partial \theta}{\partial z} + K(h)\right] \qquad (6)$$

Where :
$\theta(h)$ = The volumetric water content (L^3 L^{-3})
$K(h)$ = The unsaturated hydraulic conductivity (LT^{-1})
z = The vertical coordination (L) taken positively upward
h = The matrix head (L)
t = The time (T)

Solute transport equation: Solute transport in porous media can be described with the one-dimensional convective-dispersive equation (CDE) (Simunek *et al.*, 1999a):
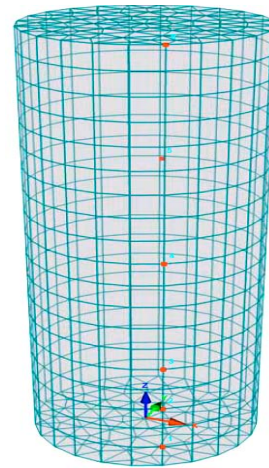

Fig. 2: Defined model in HYDROUS-3D and sampling depths

$$\frac{\partial \theta C}{\partial t} + \frac{\partial p_b S}{\partial t} = \frac{\partial}{\partial z}\left[\theta D \frac{\partial C}{\partial z}\right] - \frac{\partial q_w C}{\partial z} \qquad (7)$$

Where :
S = The sorbed solute concentration (MM^{-1})
ρ_b = The soil bulk density (ML^{-3})
q_w = The volumetric water Flux (LT^{-1})
C = The solute concentration in solution (ML^{-3})
D = The effective dispersion coefficient (L^2 T^{-1})

The effective dispersion coefficient (D) is given by Bear (1972):

$$D\theta = \lambda_L |q_w| + \theta \tau D_0 \qquad (8)$$

Where :
λ_L = The longitudinal dispersive (L),
D_0 = The aqueous ionic or molecular diffusion coefficient of nitrate in water (L^2 T^{-1}),
τ = The tortuosity factor given by Millington and Quirk (1961):

$$\tau = \frac{\theta^{7/3}}{\theta_s^2} \qquad (9)$$

By manipulating Eq. 7, we obtained the modified Convective-dispersion equation:
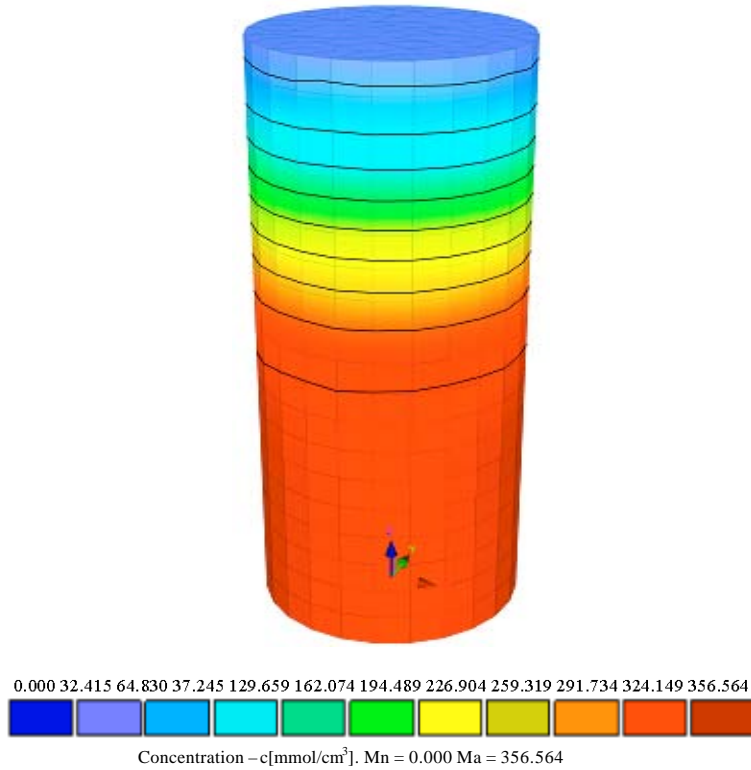
0.000 32.415 64.830 37.245 129.659 162.074 194.489 226.904 259.319 291.734 324.149 356.564

Concentration – c[mmol/cm³]. Mn = 0.000 Ma = 356.564

Fig. 3: P transport and its concentration in soil column

Table 2: T-test analysis tools for equality of data

T-test: Paired two samples for Mean

Test	Values	Test	Values
T-test-100 cm-2		**T-test-75 cm-1**	
t Stat	2.3320535	t Stat	-063949107
t Critical two-tail	1.9766922	t Critical two-tail	1.979599854
T-test-100 cm-1		**T-test-75 cm-1**	
t Stat	1.1575346	t Stat	-1.111394621
t Critical two-tail	1.9799304	t Critical two-tail	1.983971466
T-test-50 cm-2		**T-test-25 cm-2**	
t Stat	0.6973599	t Stat	-0.05949186
t Critical two-tail	1.9855234	t Critical two-tail	2.006646761
T-test-50 cm-1		**T-test-25 cm-1**	
t Stat	-0.814447	t Stat	0.135848981
t Critical two-tail	1.990847	t Critical two-tail	2.012895567
T-test-25 cm-2		**T-test-5 cm-2**	
t Stat	-0.60041	t Stat	-0.38313184
t Critical two-tail	2.0422724 t	Critical two-tail	2.036933334
T-Test-12 cm-1		**T-Test-5 cm-1**	
t Stat	-1.129764	t Stat	0.405223446
t Critical two-tail	2.0369333	t Critical two-tail	2.030107915

$$R\frac{\partial C}{\partial z} = D\frac{\partial^2 C}{\partial z^2} - v\frac{\partial C}{\partial z} \qquad (10)$$

Where:

R = The retardation factor given by the following equation

$$R = 1 + \frac{P_b K_d}{\theta} \qquad (11)$$

Where:

K_d = The partition coefficient of solute $(Cm^3\,g^{-1})$

V = The pore-water velocity (LT^{-1})

Numerical simulation: The water flow and solute transport equations with initial and boundary conditions were solved numerically with the HYDRUS-3D code (Simunek *et al.*, 1999b). The HYDRUS-3D code is based on the Galerkin finite elements method for a space weighting scheme, while the time derivatives for the solute transport equation were approximated by a Crank-Nicholson finite differences scheme. Figure 2 is shown in the definition model in HYDRUS-3d and sampling depths. Figure 3 shows P transport and its concentration in the soil column. The Student's t-test was carried out on the data shown in Table 2.

RESULTS AND DISCUSSION

Phosphate transport in soil columns: The overlay of the BTC curve from experiment and HYDRUS-3D are shown in Fig. 4 to 15. From information on Fig. 4 and 5 it can be seen that in the 5 cm soil column depth the hydrus model accurately predicted the phosphorus movement in the soil. The t-test shows no significant difference between the results of the model and the soil column experiment.
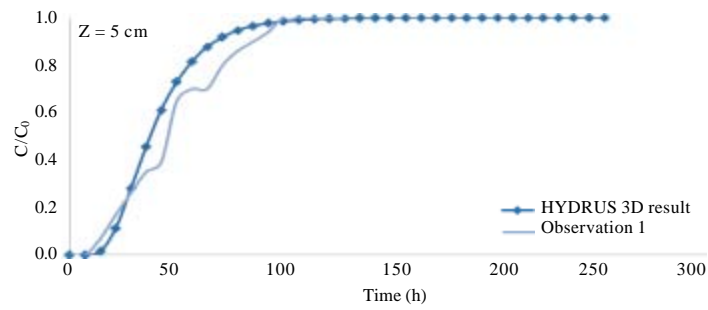
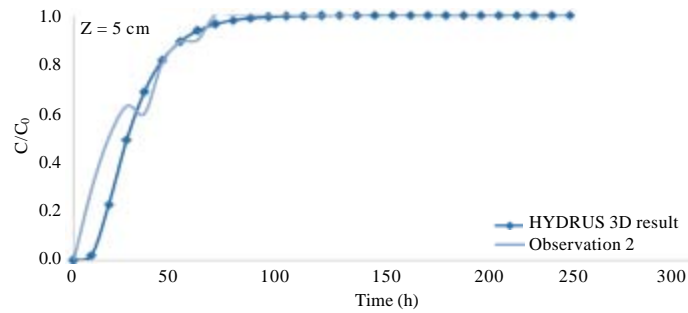Fig. 4: BTC curve from experimental and HYDRUS-3D first test at 5 cm depth

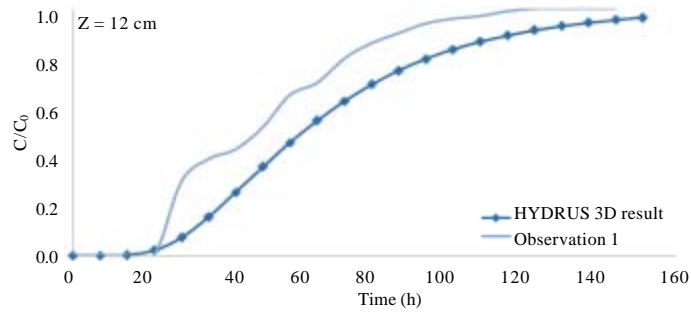Fig. 5: BTC curve from experimental and HYDRUS-3D second test at 5 cm depth

Fig. 6: BTC curve from experimental and HYDRUS-3D first test at 12 cm depth
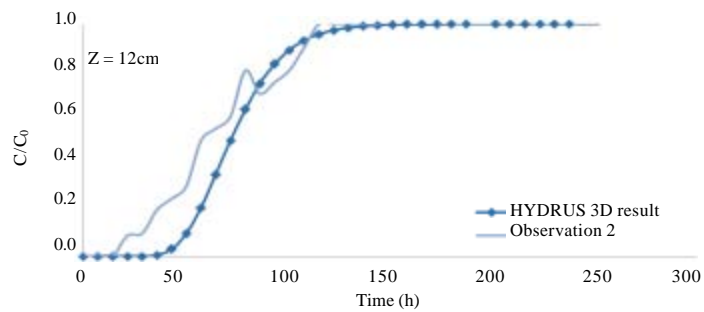

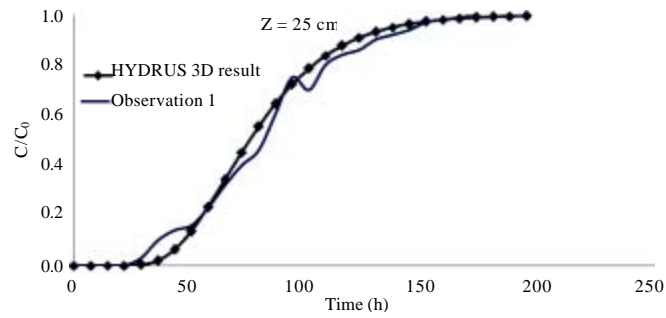Fig. 7: BTC curve from experimental and HYDRUS-3D second test at 12 cm depth

Fig. 8: BTC curve from experimental and HYDRUS-3D first test at 25 cm depth
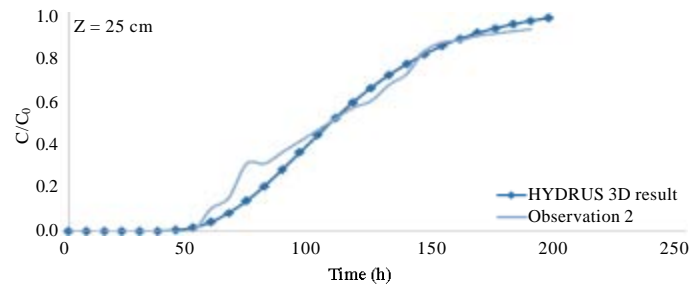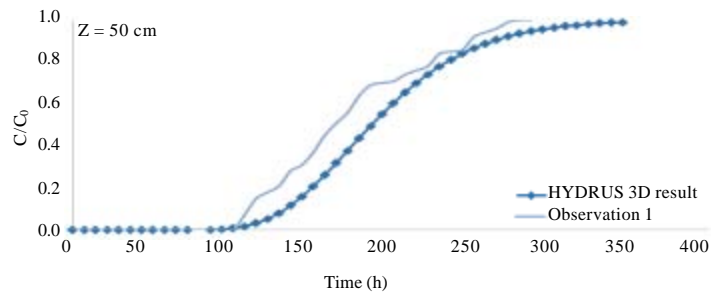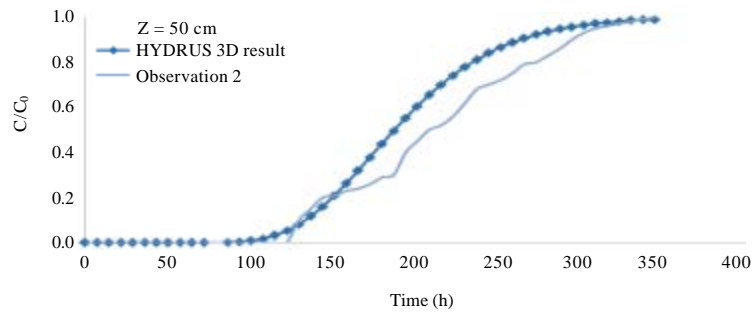

Fig. 9: BTC curve from experimental and HYDRUS-3D second test at 25 cm depth

Fig. 10: BTC curve from experimental and HYDRUS-3D first test at 50 cm depth

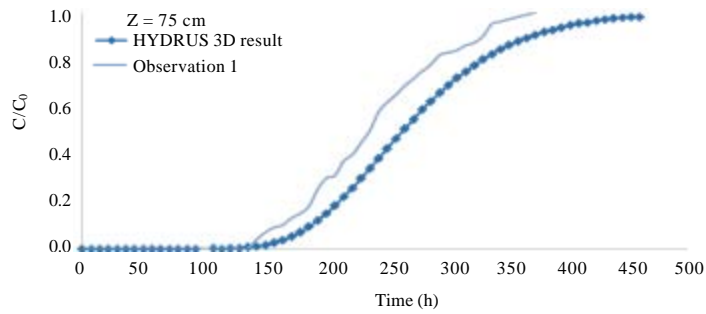Fig. 11: BTC curve from experimental and HYDRUS-3D second test at 50 cm depth

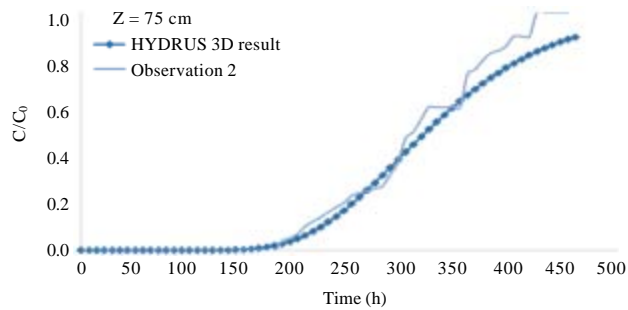Fig. 12: BTC curve from experimental and HYDRUS-3D first test at 75 cm depth

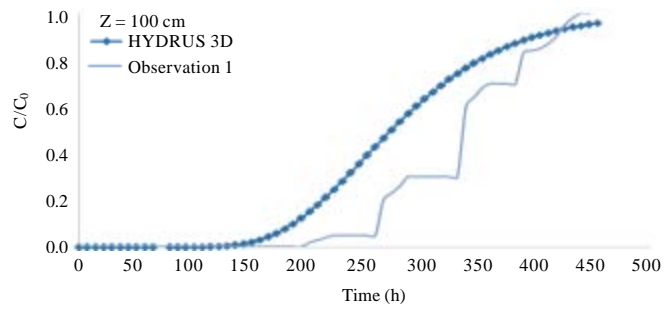Fig. 13: BTC curve from experimental and HYDRUS-3D second test at 75 cm depth

Fig. 14: BTC curve from experimental and HYDRUS-3D first test at 100 cm depth
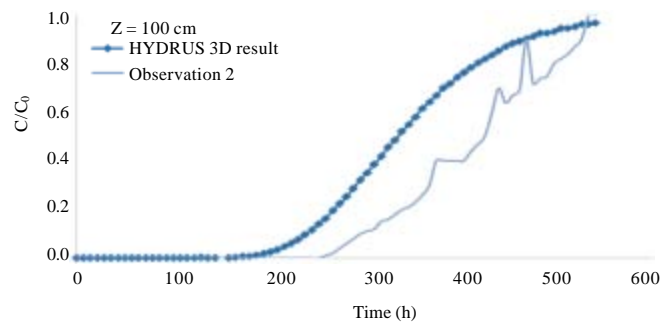

Fig. 15: BTC curve from experimental and HYDRUS-3D second test at 100 cm depth

Fig. 6 and 7, comparing the BTC curve at 12 cm depth, show that the result of the two methods in the second experiment has a higher retardation factor, which indicates that the phosphorus adsorption isotherm is more effective in the hydrus model. This can be been seen in Fig. 8 and 9. The results show that the hydrus results at 25 cm depth most closely match column outputs. As illustrated in Fig. 10 and 11, results of the hydrus model at 50 cm depth show faster phosphorus movement than was actually observed in the first experiment. This phenomenon is demonstrated in Fig. 12 and 13, which show results at 75 cm depth. Figure 14 and 15 show the BTC curve at 100 cm depth. These figures illustrate that the result of the hydrus model at 100 cm depth in the soil column does not show good similarity in both experiments. The predicted solute movement by the model is slower than in reality.

A comparison between the HYDRUS-3D outputs and observed data from the soil column indicate that the model made sufficiently accurate predictions. Break-through curves are shown in Fig. 4 to 14. In all figures it is clear that the outputs of the hydrus model are close to the experiment results. The phosphorus leached through the soil profile and reached different depths in the soil column. Previous studies have indicated that although phosphate is strongly adsorbed to soil particles, its ions can move through soil columns. This phenomenon specifies the effect of macropores on the transport process. For this reason we must use light rates of P fertilizer and minimize irrigation water to reduce the loss of phosphorus. Additionally, it is obvious that the results of the experiment with field conditions may be different than with laboratory conditions and it is therefore necessary for this test to be done under field conditions. The difference between the model and experiments may be as a result of rapid movement of water through the soil without sufficient time for reaction between the soil and the solute (Hillel, 1998). As illustrated in Fig. 4 to 14, as the soil depth in the experiment increases, the difference between the model and soil column outputs also increases. This phenomenon may be related to the increase in error due to preferential flow paths and/or the choice of the incorrect adsorption isotherm.

ACKNOWLEDGMENT

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