HYDRUS-2D simulations of water and potassium movement in drip irrigated tropical soil container cultivated with sugarcane

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ABSTRACT

Subsurface drip irrigation is increasingly being used for sugarcane production in Southeast Brazil in attempts to conserve water, especially after extreme droughts in 2014 and 2015. Correct design of a subsurface drip system is essential to provide information about water and solutes dynamics in the subsurface, leading to possible water savings. While field investigations demand much time and financial resources, numerical models can also provide much information about expected water and solute distributions in the soil profile. The objective of this study was to use HYDRUS-2D for simulations of water and potassium movement in containers packed with a subsurface drip-irrigated tropical soil cultivated with sugarcane and comparing simulated and observed data through statistical parameters. Investigations were carried out in a greenhouse during 240 days after the tillering stage. Spatial and temporal distributions of water content and potassium concentrations were collected using Time Domain Reflectometry (TDR) to calibrate and validate HYDRUS-2D. Simulations were carried out using hydraulic properties fitted directly to measured retention date, as well as estimated using pedotransfer functions (Rosetta Lite and the class pedotransfer of Carsel and Parrish). RMSE and MAE indicated a favorable capacity of the model to simulate soil water content using with measured properties and a better performance than estimated properties by pedotransfer functions. For the potassium concentrations, a less than optimal performance was obtained with HYDRUS-2D using both the measured hydraulic properties and the pedotransfer functions. A better understanding and accurate determination of solute concentrations in soil, uptake parameters, the crop root growth and distribution should be necessary for improve the simulations and observed data. The inability of HYDRUS-2D to accurately estimate potassium concentrations was not necessarily a limitation of model, but rather a limitation of knowledge about the soil and plant parameters involved.

1. Introduction

First introduced in 1532, sugarcane has always been important for Brazil's economy. Brazil at present is not only the largest sugarcane producer in the world, followed by India and China, but also the largest producer of sugar and ethanol derived from sugarcane. Responsible for more than 50% of the world's sugar market, sugarcane is cultivated in nearly all parts of the country. Severe droughts during 2014 and 2015 had a direct impact on sugarcane productivity. Productivity decreased especially dramatically in the Brazilian Southeast where rainfall remained far below the long-term average, along with high temperatures (CONAB, 2015).

Subsurface drip has become a viable alternative to traditional irrigation methods in terms of optimizing water and nutrient applications (e.g., Keller and Bliesner, 1990; Ramos et al., 2012). Investigations conducted in São Paulo State, Brazil, about the viability of subsurface drip in sugarcane cultivation demonstrated an increase of 24% in stem yield and 23% in sugar yield relative to no irrigation (Gava et al., 2011). Dalri and Cruz (2002) studied the effect of subsurface drip frequency on the initial development of sugarcane and found an average increase of 45% in fresh stem and leaf mass in relation to the control without irrigation. Júnior et al. (2012) further showed a significant increase in sugar (25.3 Mg ha⁻¹) and ethanol (20 m³ ha⁻¹) productivity with fertigation of 90 kg N ha⁻¹ and 60 kg K ha⁻¹ by subsurface drip. Dalri and Cruz (2008) observed increases in sugarcane production of 43 and 62% for the second and third harvests, respectively, thus demonstrating good adaptation with this type of irrigation.

Because of the high potassium demand of crops cultivated in tropical soils, many studies have focused on the potassium dynamics in
such soils (Miranda et al., 2005; Melo et al., 2006; Rivera et al., 2006; Pinho and Miranda, 2014). Kolachi and Jalali (2007) found that potassium concentrations can increase substantially in groundwater by leaching. Groundwater near agricultural areas often show potassium concentrations above the limit for potable water (12 mg L\(^{-1}\)) according to World Health Organization (2011) and Griffioen (2001).

The rational use of natural resources, and avoiding or limiting environmental impacts because of poor management, requires a thorough understanding of water and solute transport processes in irrigated soil environments. Time Domain Reflectometry (TDR) has many advantages for monitoring water and solute transport processes such as its precision, the use of multiple readings, repetition without destruction of the soil, and security (Bizari et al., 2014; Coelho and Or, 1996; Elaiuy et al., 2015; Souza and Folegatti, 2010). However, field investigations with TDR are often time-consuming and costly, plus may have some environmental impact because of the use of trenches during their installation.

Numerical models can provide additional insight into prevailing water and solute transport processes in the subsurface. The HYDRUS-2D software (Šimůnek et al., 1999a, 1999b; Šimůnek et al., 2016), in particular, has been used in a large number of drip irrigation and/or fertigation studies (Cote et al., 2003; Doltra and Muñoz, 2010; Kandelous and Šimůnek, 2010; Li et al., 2015; Mguidiche et al., 2015; Provenzano, 2007; Ramos et al., 2012; Rodríguez-Sinobas et al., 2012; Skaggs et al., 2004).

Of these, Mguidiche et al. (2015) simulated volumetric soil water content in the potato crop under subsurface drip irrigation, with the results showing relatively close agreement between simulated and measured data in the root zone. Provenzano (2007) showed the suitability of HYDRUS-2D to simulate water contents around a buried emitter during irrigation. For Roberts et al. (2009) and Mguidiche et al. (2015), a better understanding of the processes that occur in a subsurface drip-irrigated soil profile, such as root growth and distribution, as well as plant water uptake, are essential for reliable modeling of the water and solute transport processes involved.

Other studies used HYDRUS-2D to obtain also general information about solute transport processes in soils. For example, Ajday et al. (2007) reported that nitrogen leaching in fields with shallow root systems can be minimized by appropriate selection of the flow rate, and the time duration and intermittency of irrigation intervals. Doltra and Muñoz (2010) obtained acceptable accuracy of the estimated soil N-NO\(_3\)\(^-\) contents of the upper 90 cm surface soil at four levels of fertigation during crop rotation, while Phogat et al. (2014) used HYDRUS-2D to optimize the drip timescale for perennial horticultural crops to improve fertigation efficiency and limit groundwater contamination. Karandish and Šimůnek (2017) concluded that HYDRUS-2D could be used to determine optimal strategies for deficit irrigation and partial root-zone drying, as a complement or even substitute of time-consuming and expensive field studies.

Most or all of the above studies concerned non-tropical soils. By comparison, few if any HYDRUS-2D investigations have focused on subsurface drip/fertigation applications of tropical soils. The objective of this study was to use HYDRUS-2D for simulations of water and potassium dynamics in greenhouse containers packed with a subsurface drip-irrigated tropical soil cultivated with sugarcane and comparing simulated and observed data using statistical parameters.

2. Materials and methods

2.1. Experimental setup

The experiments were conducted during the tillering stage (2\(^{nd}\) phenological stage) between June/2015 to January/2016 in a greenhouse at the experimental area of the Department of Biosystems Engineering, University of São Paulo (LEB/ESALQ-USP) in Piracicaba, São Paulo, Brazil (22° 43' 33"S, 47° 38' 00"W, elevation of 547 m).

According to the meteorological station installed inside the greenhouse, average temperature, global radiation and relative humidity were 24.8°C; 19.2 MJ m\(^{-2}\) day\(^{-1}\) and 78.7% during the experimental period.

Three 500-L polyethylene containers (120 cm diameter and 60 cm high) were uniformly packed with a sandy loam soil (Oxisol - Ustox) collected in 0–30 cm depth with the initial soil water content of 0.15 cm\(^{-3}\). Packing was done from the bottom of containers using five layers of 10 cm, which the first (bottom) layer consisting of gravel covered by a geotextile blanket to avoid soil losses to the drain outlet. Subsequently four layers were packed in each container. One emitter was installed per container at a depth of 25 cm; button dripers had a flow rate equal to 4.0 L h\(^{-1}\) at a nominal pressure of 100 kPa.

The RB92579 sugarcane variety Saccharum officinarum L. was planted using 30-day old seedlings. Soil samples were collected to determine initial soil conditions such as selected physical and chemical properties (Table 1). A total of sixteen TDR probes (5 cm width and 10 cm length) with three stainless steel rods (3 mm thickness) were installed in four 10-cm layers and in one side of the containers (Fig.1), because of symmetry of the wetted soil volume measures, according to Kandelous et al. (2011). Soil water contents were monitored using a TDR calibration curve developed by Ponciano et al. (2015):
water stress, corresponding to 0.17 cm$^3$ cm$^{-3}$. When reaching this value, irrigation started until the water content in the field capacity (0.24 cm$^3$ cm$^{-3}$), considering the soil area of 11,309 cm$^2$ per container. Drainage during and after the irrigations was estimated from the volume collected through the drains. Fertigation was accomplished using a schedule as documented by Malavolta (1994). Agricultural activities during the experiments are summarized in Table 2.

### Table 2

<table>
<thead>
<tr>
<th>Date</th>
<th>Agricultural activities</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>June 9 in 2015 (day 1)</td>
<td>Planting and irrigation</td>
<td>19.48 mm (23.70 L)</td>
</tr>
<tr>
<td>August 31 in 2015 (day 84)</td>
<td>Fertigation</td>
<td>15.71 mm (17.75 L) + 0.998 mg cm$^{-3}$ K$^+$</td>
</tr>
<tr>
<td>September 25 in 2015 (day 109)</td>
<td>Fertigation</td>
<td>15.41 mm (17.42 L) + 0.414 mg cm$^{-3}$ K$^+$</td>
</tr>
<tr>
<td>October 13 in 2015 (day 127)</td>
<td>Fertigation</td>
<td>15.64 mm (17.68 L) + 0.437 mg cm$^{-3}$ K$^+$</td>
</tr>
<tr>
<td>November 11 in 2015 (day 156)</td>
<td>Fertigation</td>
<td>14.07 mm (16.84 L) + 0.362 mg cm$^{-3}$ K$^+$</td>
</tr>
<tr>
<td>November 30 in 2015 (day 175)</td>
<td>Fertigation</td>
<td>16.42 mm (18.55 L) + 0.427 mg cm$^{-3}$ K$^+$</td>
</tr>
<tr>
<td>December 14 in 2015 (day 189)</td>
<td>Fertigation</td>
<td>15.78 mm (17.83 L) + 0.466 mg cm$^{-3}$ K$^+$</td>
</tr>
<tr>
<td>December 28 in 2015 (day 203)</td>
<td>Irrigation</td>
<td>16.73 mm (18.90 L)</td>
</tr>
<tr>
<td>January 11 in 2016 (day 217)</td>
<td>Irrigation</td>
<td>16.81 mm (19.00 L)</td>
</tr>
<tr>
<td>January 25 in 2016 (day 231)</td>
<td>Irrigation</td>
<td>16.74 mm (19.1 L)</td>
</tr>
</tbody>
</table>

2.2. HYDRUS-2D simulations

The radially symmetric subsurface drip irrigation process was modeled using HYDRUS-2D (Šimůnek et al., 1999a) based on the following form of the Richards equation for an isotropic soil profile (Cote et al., 2003; Ramos et al., 2012):

$$ \frac{\partial \theta(h)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} [r K(h) \frac{\partial \theta(h)}{\partial r}] + \frac{\partial}{\partial z} [K(h) \frac{\partial \theta(h)}{\partial z} + \frac{\partial K(h)}{\partial z}] - S(h) $$

(2)

where $h$ is pressure head (L), $t$ is time (T), $r$ is the radial coordinate (L), $z$ is the vertical coordinate (L), $K$ is the hydraulic conductivity (LT$^{-1}$), and $S$ denotes root water uptake (LT$^{-1}$) as described with the uptake model by Feddes et al. (1978):

$$ S(h) = \gamma(h) \beta(r, z) W T_p $$

(3)

where $\gamma(h)$ is the soil water stress response function (-), $\beta$ is the normalized root water uptake distribution (LT$^{-1}$), $T_p$ is the potential transpiration rate (LT$^{-1}$), and $W$ is the area of the soil surface (L$^2$) associated with the transpiration process.

2.2.1. Soil hydraulic properties

The soil hydraulic properties were described using the standard equations of van Genuchten (1980) given by:

$$ \theta(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + (k_h h)^n)^m} $$

(4)

$$ K(h) = K_s S^[[1 - (1 - S^{1/m})^{2}]] $$

(5)

where $\theta_r$ and $\theta_s$ are the residual and saturated soil water contents (L$^3$L$^{-3}$), respectively, $a$ (L$^{-1}$), $n$ and $m$ (-) are dimensionless shape parameters of the soil water retention curve, with $m = 1-1/n$, and $S$ is effective saturation given by:

$$ S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} $$

(6)

In this study we used soil hydraulic parameters that were either fitted directly to observed retention curve (Fig. 2) using Eq. (4), or obtained using pedotransfer functions. For the measured hydraulic data, we used undisturbed samples taken from the containers. A total of 9 points were obtained: gravimetric water contents at pressure heads of -10, -20, -40 and -100 cm using a tension table system, and at -300, -500, -1000, -5000 and -15000 cm using the Richards pressure plate approach (Klute, 1986).

For the pedotransfer functions we used both the Rosetta Lite function of Schaap et al. (2001) and the class pedotransfer function of Carsel and Parrish (1988) as implemented in HYDRUS-2D. For the Rosetta estimates we used the measured granulometric data as well as the measured values of bulk density and water contents at -330 and 15000 cm. Table 3 lists the estimated hydraulic parameters.

![Fig. 1. Distribution of TDR probes in the container: (a) front vision, and (b) top vision.](image_url)

Table 3 lists the estimated hydraulic parameters.

![Fig. 2. Observed data fitted soil water retention curve of the sandy loam soil.](image_url)


2.2.2. Root water uptake

The spatial root distribution was described using the model of Vrugt et al. (2001):

\[ \beta(r, z) = \left(1 - \frac{r}{r_m}\right)^2 \exp\left(-\frac{r^2}{r_m^2} - \frac{z^2}{z_m^2}\right) \]  

(7)

where \( \beta(r, z) \) denotes the dimensionless two-dimensional spatial distribution of root water uptake, \( r_m \) is the maximum rooting length in the radial direction (L), \( r \) is the radial distance from the origin of the plant (L), \( p_1(\cdot) \) and \( r^* \) (L) are empirical parameters (\( p_1 \) equals unity for \( r > r^* \)), and some constant for \( r \leq r^* \) to be fitted to the root data), \( z_m \) is the maximum rooting depth (L), \( z \) (L) is the depth in the soil profile (\( z \geq 0 \)), \( p_k(\cdot) \) and \( z^* \) (L) are empirical parameters (similarly as for \( p_1 \) and \( r^* \), \( p_k \) equals unity for \( z > z^* \)).

Only a single sugarcane plant and a simple root distribution model were considered, in which the roots expanded vertically into all available space in the containers (\( z_m = 50 \) cm), but concentrated mainly above the dripper (\( r^* = 2 \) cm, \( z^* = 25 \) cm) where water and potassium were applied, and then extended horizontally to 30 cm (\( r_m = 30 \) cm).

Reductions of root water uptake due to the water stress, \( \alpha_i(h) \), were described using the formulation of Feddes et al. (1978):

\[
\alpha_i(h) = \begin{cases} 
0, & h > h_1 \text{ or } h \leq h_4 \\
\frac{h - h_1}{h_2 - h_1}, & h_1 < h \leq h_2 \\
1, & h_2 < h \leq h_3 \\
\frac{h - h_4}{h_4 - h_1}, & h_4 < h \leq h_5 
\end{cases}
\]  

(8)

where \( h_1, h_2, h_3, \text{ and } h_4 \) are the threshold parameters. Eq. (8) assumes that water uptake is at its potential rate when the pressure head is between \( h_2 \) and \( h_3 \), decreases linearly when \( h > h_2 \) or \( h < h_3 \), and becomes zero when \( h < h_4 \) or \( h > h_5 \). The following parameters of the Feddes et al. (1978) model were used: \( h_1 = -10, h_2 = -25, h_3 = -150 \) to -500, \( h_4 = -16000 \) cm, which were taken from Taylor and Ashcroft (1972) for sugarcane.

Potassium in a soil can generally be subdivided into four different fractions: structural, non-exchangeable, exchangeable and in soil solution, whereby the latter can be taken up directly by plants with mass flow of water uptake (Barber, 1995; Sparks, 1987). Consequently, we assumed that potassium was passively taken up by the root system of sugarcane (Šimůnek and Hopmans, 2009) by moving with the soil solution.

2.2.3. Simulations of potassium transport

Simulations of potassium transport were carried out using the three-dimensional radially axisymmetric advection-dispersion equation given by:

\[
\frac{\partial \Theta}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \left( \frac{\partial \Theta}{\partial r} + \frac{\partial \Theta}{\partial z} \right) - q_i C \right) 
\]

\[
+ \frac{\partial}{\partial z} \left( \frac{n \Theta}{K_d} \frac{\partial C}{\partial z} + \frac{\partial \Theta}{\partial z} \right) - S(h) C_i
\]  

(9)

where \( C \) is the solution concentration (ML\(^{-3}\)), \( C_i \) is the concentration of the sink term due to root water uptake (ML\(^{-3}\)), \( R \) is the retardation factor (\( \cdot \)), \( q_i \) and \( q_e \) are the radial and vertical volumetric fluid fluxes (L\(^{2}\)T\(^{-1}\)), respectively, and \( D_m, D_a \) and \( D_m \) are components of the dispersion tensor (L\(^2\)T\(^{-1}\)). For solute uptake we assumed a passive potassium uptake process until some maximum value, \( C_{\text{umi}} \) (Šimůnek and Hopmans, 2009).

Assuming linear sorption of potassium by the solid phase, the retardation factor \( R \) is given by:

\[ R = 1 + \frac{2K_d}{\delta} \]  

(10)

where \( \delta \) is the soil bulk density (ML\(^{-3}\)) and \( K_d \) is the potassium distribution coefficient (L\(^{-1}\)M\(^{-1}\) (van Genuchten and Wierenga, 1986). Components of the dispersion tensor are given by the standard equations (Bear, 1988):

\[
\begin{align*}
\frac{\partial D_{r\tau}}{\partial \tau} &= \varepsilon D_{s\tau} + \lambda_i q_{i\tau} + \lambda_r q_{r\tau} \\
\frac{\partial D_{r\tau}}{\partial \tau} &= \varepsilon D_{s\tau} + \lambda_i q_{i\tau} + \lambda_r q_{r\tau} \\
\frac{\partial D_{r\tau}}{\partial \tau} &= \varepsilon D_{s\tau} (\lambda_i - \lambda_r) q_{i\tau} \\
\end{align*}
\]

(11)

where \( D_{r\tau} \) is the potassium ionic diffusion coefficient in free water (L\(^2\)T\(^{-1}\)), \( \varepsilon \) is the tortuosity factor \( (\cdot) \), described here using the Millington and Quirk (1961) formulation, and \( \lambda_i \) and \( \lambda_r \) are the longitudinal and transverse dispersivities (L), respectively, and \( q_{i\tau} \) represents the absolute value of the water flux (L\(^2\)T\(^{-1}\)).

The diffusion coefficient for potassium was set at 1.7 cm\(^2\) day\(^{-1}\) (Miranda et al., 2005). Values of \( \lambda_i \) and \( K_d \) were derived from a simple one-dimensional solute breakthrough experiments, while \( \lambda_r \) was taken to be one-tenth of the value of \( \lambda_i \). The 1-D transport experiments were carried out using 20-cm PVC columns (having inside diameters of 5 cm) filled with the same loamy sand soil as used for the containers. The upper end of the column was fixed at a positive pressure head of 1 cm, while a geotextile membrane and metal grille were used for the bottom boundary. The columns were packed uniformly to the same bulk density as the containers, and then saturated with deionized water for 24 h. After saturation, the columns were washed with deionized water for 24 h to remove most or all ions from the soil exchange complex, after which a solution of 2000 mg L\(^{-1}\) of potassium was applied (Pinho and Miranda, 2014). Breakthrough data were collected and subsequently analyzed using the CFITIM code (van Genuchten, 1981) within the STANMOD software (Šimůnek et al., 1999b).

2.2.4. Initial and boundary conditions

A time-variable flux boundary condition was applied to a semicircle with radius (\( R_0 \)) of 2 cm at 25 cm depth (Fig. 3). The boundary condition with a flux \( q_{d} \) was defined as:

\[ q_{d} = \frac{\text{volume of solution applied/day}}{A_{SW}} \]  

(12)

where the volume of solution applied (L\(^3\)) varied for different events and \( A_{SW} \) is the surface wetted area (L\(^2\)) given by

\[ A_{SW} = 4\pi (R_0)^2 \]  

(13)

where \( R_0 \) is the radius of semicircle (L). During irrigation, the dripper boundary was held at a constant water flux \( (q_d) \). An atmospheric boundary condition was assumed for the entire soil surface. A no-flow boundary condition was established along the left and right edges of the soil profile, and along part of the bottom of the container. A drain was assumed at the bottom of container, with the actual drainage flux being calculated similarly as Eqs. (12) and (13). The initial soil water content was 0.15 cm\(^3\) cm\(^{-3}\), while the initial concentration of potassium was estimated from measured soil chemical properties. For solute (K\(^+\)) transport, a third-type boundary condition was imposed along the
dripper, and zero-flux boundary along all sides except for a zero-concentration gradient along the drain at the bottom of the container.

2.3. Flow domain and finite element mesh

The dripper can be considered as a semicircle source (Fig. 3), because the radially symmetric of subsurface drip irrigation process (Kandelous et al., 2011; Kandelous and Šimůnek, 2010). The transport domain was set as a rectangle (in a radial direction) with a width of 60 cm (half of the container diameter) and a depth of 50 cm, discretized into 1959 two-dimensional elements involving 1035 nodes (Fig. 3). Several observation nodes were included (Fig. 4) at selected locations in the flow domain to follow simulated soil water contents and potassium concentrations versus time. The observation nodes had very similar coordinates as the TDR probes installed in the containers to allow comparisons of observed and simulated data.

2.4. Estimation of potential evapotranspiration

Potential evapotranspiration was calculated using the Penman-Monteith equation (Allen et al., 1998) as implemented in the HYDRUS-1D software (Šimůnek et al., 1998). The simulations require daily estimates of potential evaporation and transpiration. Fig. 5 shows the partitioning of potential evapotranspiration ($ET_p$) into potential evaporation ($E_s$) and potential transpiration ($T_p$) in correspondence to the leaf area index (LAI) per unit surface of soil below the canopy. At sowing nearly 100% of $ET$ comes from evaporation, while at full crop cover more than 90% of $ET$ comes from transpiration (Allen et al., 1998). Specific crop data we used were as follow: crop height (120 and 230 cm for 2nd and 3rd phenological stages, respectively); albedo (0.23 and 0.31 for 2nd and 3rd phenological stages, respectively) and LAI (2.5 and 7.5 for 2nd and 3rd phenological stages, respectively), the latter calculated using:

$$\text{LAI} = \frac{1}{\alpha_i} \ln(1 - \text{SCF})$$

where $\alpha_i$ is a constant for radiation extinction by the canopy (-) and SCF is the surface cover fraction (-). The values of daily potential transpiration ($T_p$) and soil evaporation ($E_s$) obtained (Fig. 6) were used as time-variable boundary conditions in the model during the experimental period. A maximum $T_p$ of 7.9 mm occurred on day 237 (31st January 2016), when the average temperature, global radiation and relative humidity were the highest during the experiments.

2.5. Statistical analysis

Model performance for predicting soil water contents and potassium concentrations were evaluated in terms of the Root Mean Square Error (RMSE) and the Mean Absolute Error (MAE):

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} (a_i - b_i)^2}{n}}$$

$$\text{MAE} = \frac{\sum_{i=1}^{n} |a_i - b_i|}{n}$$

where $a_i$ and $b_i$ represent the observed and simulated water contents or potassium concentrations. The Surfer software was used for comparisons and mapping of the observed and simulated soil water content and potassium concentrations.
potassium concentrations at selected dates. We used kriging as the gridding method, while the statistical analyses were carried out at preselected dates.

3. Results and discussion

3.1. TDR calibration for potassium concentration

In this study we used an indirect TDR-based method for determining potassium concentrations. The approach requires careful correlation of the indirect electrical conductivity measurements ($E_{C_{TD}}$) with directly observed solution values ($E_{C_S}$) in the soil system being used. Fig. 7 shows a relatively high correlation between $E_{C_{TD}}$ and $E_{C_S}$ as reflected by an $R^2$ value of 0.923, albeit with relatively high RMSE and MAE values (1.447 and 1.063 dS m$^{-1}$, respectively) indicating a less than satisfactory fit. The calibration could be improved by carrying out multiple linear regression between electrical conductivity and TDR measured soil water contents:

$$E_{C_S} = 1.9790E_{C_{TD}} - 0.0630\theta + 0.0391$$

(17)

where $E_{C_S}$ is the solution electrical conductivity (dS m$^{-1}$), $E_{C_{TD}}$ is the electrical conductivity estimated using TDR (dS m$^{-1}$) and $\theta$ is the soil water content (cm$^3$ cm$^{-3}$). The $R^2$ value (0.960) was better, but the errors remained high (0.536 and 0.400 dS m$^{-1}$ for RMSE and MAE, respectively), reflecting a relatively poor adjustment.

Potassium nitrate solution concentrations were correlated next with the electrical conductivity ($E_{C_S}$) by preparing different potassium concentrations (0.02–2.00 mg cm$^{-3}$) in solution with deionized water. The following correlation was obtained (Fig. 8):

$$C_{NO_3^-} = 0.8699E_{C_S} - 0.0634$$

(18)

where $C_{NO_3^-}$ is the potassium nitrate concentration in solution (mg cm$^{-3}$). Since our study focused on potassium transport, we needed to separate the potassium and nitrate concentrations as shown Fig. 9. This produced the following correlation (having an $R^2$ of 0.987):

$$C_{K^+} = 0.3760C_{NO_3^-} + 0.0281$$

(19)

where $C_{K^+}$ is the potassium concentration in solution (mg cm$^{-3}$).

Fig. 10 compares indirectly measured potassium concentrations using TDR and direct measurements, as reflected by an $R^2$ value of 0.995, RMSE and MAE were 0.038 and 0.030 dS m$^{-1}$, respectively.

3.2. Potassium breakthrough curve

Fig. 11 shows the measured potassium breakthrough curve, plotted in terms of dimensionless concentration (from 0 for the initial concentration to unity for the inlet concentration) versus the number of pore volumes (PV) of solution leached through the column. The use of dimensionless time is useful since it eliminates the effects of travel distance and flow velocity, which are specific to any one experiment (Skaggs and Leij, 2002):

$$R^2 = 0.923$$

Fig. 7. Correlation between the electrical conductivity of soil solution and the electrical conductivity measured by TDR.
where $\phi$ is the soil porosity (decimal), $V_s$ is the soil column volume (cm$^3$) and $V_c$ is the volume collected (cm$^3$) from each point of breakthrough curve. From the fitted dimensionless transport data, a column Peclet number of 4.90, a retardation factor ($R$) of 1.79, the values of 4.08 cm for the longitudinal dispersivity ($\lambda_L$) and 0.289 cm$^3$ g$^{-1}$ for the distribution coefficient ($K_d$), which we used subsequently in the HYDRUS-2D simulations.

3.3. Simulations of soil water content

The average soil water content of the first (0–25 cm) layer of the containers as measured with eight TDR probes (observed data) and of the eight observation nodes (simulated data) as calculated with HYDRUS-2D, are shown in Fig. 12. Similar data are provided for the second (25–50 cm) layer. HYDRUS-2D overestimated volumetric water contents of the first layer before and at the time of the irrigations until about day 101, with simulated values varying between 0.16 and 0.27 cm$^3$ cm$^{-3}$, compared to the observed data between 0.16 and 0.23 cm$^3$ cm$^{-3}$. The maximum simulated value was above of field capacity, which did not occur with the observed data.

However, after this period, the model simulated smaller water contents before irrigation until day 210. One plausible explanation is the assumption in HYDRUS-2D of having a constant crop rooting system in time, because the model has no options to change the root system each day or during a certain period. This may well be an important limitation. For example, Assouline (2002) noted temporal changes in root growth and distribution of drip-irrigated corn, which also depended on the drip irrigation rate within 28-day periods, while Roberts et al. (2009) illustrated these effects for successive crops of cantaloupe and broccoli and Mguidiche et al. (2015) for potato. Fig. 12 shows that after day 210 simulated water contents became very similar to the observed data before irrigation, varying from 0.16 to 0.17 cm$^3$ cm$^{-3}$.

Simulations of the second layer mostly agreed better with the data, especially during the middle and later parts of the experiments when simulated water contents varied between about 0.18 to 0.30 cm$^3$ cm$^{-3}$ and observed values between 0.15 and 0.28 cm$^3$ cm$^{-3}$. Notable differences between simulated and observed data remained between day 60 and the first irrigation on day 80. These changes can be explained in part by small differences in the coordinates of the TDR probes and the observation nodes in the model, in addition to the differences in root growth, distribution and water uptake observed experimentally and simulated with the model.

RMSE values of observed versus simulated data were 0.027 and 0.030 cm$^3$ cm$^{-3}$ and MAE values 0.023 and 0.024 cm$^3$ cm$^{-3}$ for the first and second layer, respectively. These values compare closely with results of other investigations (Crevoisier et al., 2008; Ghazouani et al., 2008).
HYDRUS-2D provides relatively accurate results also for subsurface drip irrigation with sugarcane.

Fig. 13 shows the maps of observed and simulated water content at different dates during the experiments. The isolines had a very similar structure on day 2, one day after 1st irrigation. However, the model overestimated soil water contents by producing a maximum value of about 0.40 cm$^3$ cm$^{-3}$ compared to 0.36 cm$^3$ cm$^{-3}$ observed experimentally. Only the isolines with 0.18 cm$^3$ cm$^{-3}$ were close. RMSE and MAE were 0.048 and 0.043 cm$^3$ cm$^{-3}$, respectively. These values were higher than those of the average water content per day in each layer.

On day 83, one day before 2nd irrigation, the observed isolines were relatively horizontal with the water content showing lower value in a homogeneous fashion from the container bottom to the soil surface. HYDRUS-2D produced more concentrated isolines on the left side near the soil surface, with simulated water contents being higher than the observed values along the entire profile. The concentrated isolines near the dripper are indicative of the locally higher root distribution and hence water uptake. RMSE and MAE were 0.051 and 0.046 cm$^3$ cm$^{-3}$, respectively.

Higher observed and simulated values water contents occurred on the lower left side at day 84 (irrigation day). Nevertheless, the model overestimated all water contents in the soil profile on this day, with numerical results being the least accurate as reflected also by RMSE and MAE values of 0.067 and 0.062 cm$^3$ cm$^{-3}$, respectively. Days 86 and 233, two days after irrigation, showed similar behavior as day 84 with RMSE values of 0.051 and 0.050 cm$^3$ cm$^{-3}$ and MAE of 0.046 and 0.043 cm$^3$ cm$^{-3}$, respectively.

The observed isolines were relatively horizontal and the simulated isolines vertical on day 226, five days before irrigation. The model underestimated the lower water contents (0.12 cm$^3$ cm$^{-3}$) and overestimated the higher values (0.30 cm$^3$ cm$^{-3}$). RMSE and MAE were 0.062 and 0.056 cm$^3$ cm$^{-3}$, respectively. The same behavior of day 226 was present in days 230 (one day before irrigation) and 240 (last observed day) with RMSE of 0.060 and 0.059 cm$^3$ cm$^{-3}$, respectively, and MAE of 0.052 cm$^3$ cm$^{-3}$ for both.

The best HYDRUS-2D simulations were obtained using the measured soil hydraulic properties. We also ran the model using hydraulic properties based on Rosetta (Schaap et al., 2001) and the Carsel and Parrish (1988) pedotransfer functions. Fig. 14 compares results using these pedotransfer functions with the measured properties. For the first layer, simulations with the Rosetta function produced similar RMSE and MAE values (0.029 and 0.022 cm$^3$ cm$^{-3}$, respectively) compared to using the measured hydraulic properties. However, RMSE and MAE for the second layer were 0.041 and 0.036 cm$^3$ cm$^{-3}$, these values were higher than those for the measured properties. Simulations with Rosetta underestimated the water contents near days 125–200, especially during the drying events before the mid-season irrigations.

Results with the class pedotransfer functions by Carsel and Parrish (1988) were even less accurate, giving RMSE and MAE of 0.038 and 0.030 cm$^3$ cm$^{-3}$ for the first layer, and 0.050 and 0.044 cm$^3$ cm$^{-3}$ for the second layer, respectively, compared to the simulations using the measured properties. One reason may be that the pedotransfer functions by Carsel and Parrish (1988), and to a lesser extent also those by Schaap et al. (2001), were derived nearly exclusively using temperate region soils data, and hence may not be overly applicable to the tropical soil used in our study.

Most notable, again, are the very low water content values (especially in the second layer) near the middle and end of the simulations. Simulated water contents were then only 0.09 to 0.16 cm$^3$ cm$^{-3}$ during pre-irrigation drying, thus causing apparent water stress problems for the sugarcane crop. One reason of the lower water contents with the pedotransfer functions is the very low value of the wilting point (and of the residual water content), which contributed to a rapid reduction in the water content of the lower layers, also in view of the adopted bottom boundary condition.
3.4. Simulations of potassium concentrations in soil solution

Fig. 15 compares observed and simulated average potassium concentrations of the 0–25 and 25–50 cm layers. HYDRUS-2D overestimated potassium concentrations of the first layer during most of the experimental period. Accurate results were obtained at the beginning, but the model slightly underestimated the concentrations in some periods, such as between days 94–106 and isolated days as 109, 127, 219 and 233.

Most notable is that simulated potassium concentrations generally

![Graphs showing observed and simulated soil water content during sugarcane development.](image)

**Fig. 12.** Observed and simulated soil water content during sugarcane development.

![Spatial distribution of observed and simulated water contents (cm³ cm⁻³) in the soil profile at selected dates.](image)

**Fig. 13.** Spatial distribution of observed and simulated water contents (cm³ cm⁻³) in the soil profile at selected dates.
remained constant between the fertigation periods as if the model did not consider any leaching from the container, or other sinks like potassium uptake by the sugarcane roots. These results point to the need to understand and describe relevant root solute uptake processes and parameters to be used by HYDRUS-2D, including root growth and dynamic root distributions as discussed by Assouline (2002), Mguidiche et al. (2015) and Roberts et al. (2009). Simulated data in the first layer ranged from 0.08 to 0.25 mg cm⁻³ and observed data from 0.09 to 0.24 mg cm⁻³. Results reflect a less than optimal performance of the model relative to the observed data.

Simulated potassium results for the second layer intercalated between fluctuated between underestimation and overestimation relative to the observed data. Simulated concentrations during the fertigation applications were far below the observed data, while remaining practically constant in between the applications, and then higher than the observed data. This suggest that potassium uptake by roots was passive and constant in each interval after the fertigation applications, as seen for the 0–25 layer, leading to concentrations that remained constant in time.

In experimental initial conditions, it is important to notice that sodium concentration presents in chemical analyze was higher than potassium concentration. One could presume that sodium influenced potassium dispersion because its lower atomic radius (280 pm) and higher ionization energy (496 kJ mol⁻¹) as compared to potassium (227 pm and 419 kJ mol⁻¹, respectively), which would have caused more spreading of potassium through the flow domain (Andrade, 2009). This sodium influence and potassium dispersion were not considered in the simulations by the model.

The RMSE and MAE values for the first layer was 0.065 and 0.053 mg cm⁻³, respectively, and for second layer of 0.135 and 0.105 mg cm⁻³, respectively. Similar values were found by others (Doltra and Muñoz, 2010; Ramos et al., 2011; Phogat et al., 2014; Wang et al., 2014; Karandish and Šimůnek, 2017). However, all those studies were carried out for nitrate leaching in temperate soils, and not of potassium. This demonstrates the importance of our study on potassium dynamics in a tropical soil, including potential contamination of underlying groundwater.

Fig. 14. Soil water contents measured by TDR and simulated by HYDRUS-2D using the measured hydraulic properties, the pedotransfer function ROSETTA and soil catalog (Carsel and Parrish, 1988).

Fig. 16 shows the distributions of observed and simulated potassium concentration at different dates. The isolines showed difference behavior in day 83, one day before 1st fertigation, in that the observed isolines were mostly horizontal with the potassium concentrations declining steadily between the container bottom and the soil surface. HYDRUS-2D, on the other hand, showed far more vertical isolines on the left side, with lower concentrations. RMSE and MAE were 0.037 and 0.030 mg cm⁻³, respectively. On day 86, the model overestimated the observed data on the left side close to dripper and underestimated the measurements in the lower left side. The statistical parameters (RMSE and MAE) were 0.180 and 0.135 mg cm⁻³, respectively.

The distributions for days 127 (the day of fertigation) and 130 (three days after fertigation) were very similar to those on day 86, but with the model now overestimating the potassium concentrations in nearly the entire soil profile. Day 127 showed the worst performance of all plots, having RMSE and MAE values of 0.284 and 0.207 mg cm⁻³, respectively. RMSE and MAE for day 130 were 0.117 and 0.088 mg cm⁻³, respectively.

Subsequent plots in Fig. 16 were for irrigations without fertigation (days 226, 230, 233 and 240). The higher observed concentrations (0.32 to 0.26 mg cm⁻³) were now in the 25–40 cm layer in day 226 and the higher simulated concentrations (0.24 to 0.21 mg cm⁻³) in the 20–50 cm layer with RMSE and MAE of 0.078 and 0.063 mg cm⁻³, respectively. The highest potassium concentrations obtained with HYDRUS-2D remained in the same layer at day 230, but with
overestimated values. On this day, the higher observed concentrations started at the 25 cm depth, showing RMSE and MAE of 0.080 and 0.070 mg cm\(^{-3}\), respectively. The model underestimated the higher concentrations on day 233, with the concentrations slowly decreasing from a depth of 35 cm until the bottom of the container, suggesting some leaching with the now potassium-free irrigation water. RMSE and MAE were 0.109 and 0.086 mg cm\(^{-3}\), respectively, and the higher observed concentrations (0.26 to 0.22 mg cm\(^{-3}\)) started in 20 cm depth. A similar behavior of days 230 and 233 was present in day 240 (last observed day) with RMSE and MAE of 0.072 and 0.060 mg cm\(^{-3}\).
respectively.

We further show in Fig. 17 how the calculated potassium concentrations in the soil profile were affected by using the measured hydraulic properties and estimated (Table 3) using pedotransfer functions (Rosetta Lite by Schaap et al. (2001) and the Carsel and Parrish (1988) class pedotransfer functions). The pedotransfer functions overestimated potassium concentrations in the 0–25 cm layer almost the entire experimental period. Results of measured and estimated hydraulic properties were close in the interval of days 92–108. However, the concentrations were underestimated by the functions from day 219. The first layer showed RMSE and MAE values were 0.066 and 0.055 mg cm\(^{-3}\), when we used the Rosetta (actually very similar to those of the measured properties: 0.065 and 0.053 mg cm\(^{-3}\), respectively). RMSE and MAE were 0.082 and 0.068 mg cm\(^{-3}\) for the pedotransfer functions of Carsel and Parrish (1988).

Calculations for the 25–50 cm layer using the pedotransfer functions were nearly identical to the results using measured hydraulic properties. RMSE and MAE were the same for measured properties and the Rosetta function (0.135 and 0.105 mg cm\(^{-3}\), respectively), while those for the Carsel and Parrish functions were only minimally larger (0.137 and 0.106 mg cm\(^{-3}\), respectively). These results suggest that the relatively poor results for potassium fate and transport were not caused by the hydraulic properties but rather by incomplete or inaccurate knowledge of root growth and root distribution, and related water and solute uptake processes and its parameters.

4. Conclusions

The present research concerned a combination of observed and simulated data involving subsurface drip irrigation under sugarcane to evaluate HYDRUS-2D performance in water and potassium dynamics. Soil water contents monitored by TDR were predicted reasonably well through the technique calibration, but potassium concentrations had a non-consistent adjustment between variables. Parameters statistical indicated a favorable capacity of HYDRUS-2D model to simulate soil water content. The measured hydraulic properties were found to generally lead to better water content predictions that the estimated functions. The Rosetta function actually produced very similar results as the measured properties for the first (0–25 cm) layer, but performed less well for the second (25–50 cm) layer. The Carsel and Parrish (1988) function, by comparison, performed relatively poorly for both layers. For the potassium concentrations, a less than optimal performance was obtained with HYDRUS-2D using both the measured hydraulic properties as well as the pedotransfer functions, thus suggesting that overall model performance for potassium was not related to proper estimation of the hydraulic properties. A better understanding and accurate determination of potassium concentration in soil profile, uptake parameters, schematization of the spatial and temporal crop root system should be necessary for improve simulations and observed data. The inability of HYDRUS-2D to accurately estimate potassium concentrations hence should not be viewed as a limitation of the model as such, but rather a limitation of our understanding of selected crop growth processes and root functioning.

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