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Numerical Modeling of Nitrate in a Flood-Irrigated Pecan Orchard

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Pecan [(*Carya illinoinensis* (Wangenh.) K. Koch] is an important specialty crop in New Mexico. This research quantifies soil water and soil nitrate-nitrogen (NO_3–N) (mg L^{-1} of soil) variations with depth, root NO_3–N (kg ha^{-1}) uptake, and NO_3–N (kg ha^{-1}) balance for the 100-cm soil profile during two growing seasons in a flood-irrigated pecan orchard. Nitrate-nitrogen was determined six times during the growing seasons of 2015 and 2016. The HYDRUS-1D model was used to optimize the water flow parameters using measured volumetric soil water content (θ). Model calibration and validation for NO_3–N included the optimization of reaction parameters for nitrification and denitrification of each soil layer. The results showed that the model simulated θ well (0.44 ≤ d [index of agreement] ≤ 0.73) at different depths during both calibration (2009) and validation (2010) periods. Generally, HYDRUS-1D simulated soil profile NO_3–N concentrations that were correlated with measurements at all depths during both years. Total root NO_3–N uptake showed a significant increase of 72% in 2016 compared with 2015. The NO_3–N balance showed that ~40% of applied NO_3–N per year was denitrified, which was the main contributor to the NO_3–N loss from the soil profile during both years. Nitrate-nitrogen leaching below the soil profile was 32 and 26% of applied NO_3–N in 2015 and 2016, respectively. The fertigation rate was much higher than the plant demand during both years, and it should be decreased to reduce NO_3–N losses.

Abbreviations: DOY, day of year; Ea, actual evaporation; Ep, potential evaporation; RLD, root length density; SCF, soil cover fraction; Ta, actual transpiration; TDR, time-domain reflectometry; Tp, potential transpiration.

Core Ideas

- **Pecan is a vitally important specialty crop in the southwestern United States.**
- **No study is available on modeling temporal variability of NO_3–N transport in pecan orchards.**
- **Hydrus-1D predicted well water and NO_3–N variability by depth for a heavy textured soil.**
- **NO_3–N balance identified denitrification contributing to major loss.**
- **Nitrogen management in pecan orchards should take into account on and off years to decrease leaching.**

Pecan [*Carya illinoinensis* (Wangenh.) K. Koch] is a vitally important specialty crop in New Mexico, which is one of the largest producers of pecans in the United States. Mature pecan trees require a lot of water to grow, with evapotranspiration ranging between 1000 and 1300 mm per season under flood irrigation (Miyamoto, 1983). Irrigation water applied to mature pecan orchards in the Mesilla Valley, NM, has fluctuated from 1870 to 1940 mm per season (Sammis et al., 2004). Increasing acreage under pecan orchards in the arid southwestern United States has put pressure on available water resources. Moreover, the amount of fresh water for irrigation is becoming scarce because of low precipitation, high evaporation rates, and continued drought in the southwestern United States. Water availability for irrigation can be a major deterrent to pecan productivity, and more attention to water conservation is needed.

Nitrogen (N) is an essential element for plant growth, and pecan needs N fertilizer during the nut enlargement and nut filling stages (Byford, 2005a). Nitrogen application rates are usually much higher than rates for other nutrients (Wells, 2013), which increases the risk of N leaching in irrigated pecan orchards. The recommended rate of N fertilizers is ~200 kg ha^{-1} (Byford, 2005b). Excess N fertilization in ir-

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rigated fields contaminates groundwater (Böhlke, 2002; Cepuder and Shukla, 2002) because NO_3–N is a weakly absorbed ion that moves quickly through soil (González–Delgado and Shukla, 2014; Spalding and Exner, 1993). Leaching of NO_3–N to groundwater is affected by type of irrigation system (Sharma et al., 2012a) and by soil texture, and it can be high in arid and semiarid areas such as southern New Mexico, especially in surface-irrigated areas with sandier soils (Al-Jamal et al., 1997; Sharma et al., 2012b). However, not many accounts are available of NO_3–N leaching from irrigated fields in southern New Mexico. For example, Sharma et al. (2012b) reported that NO_3–N loadings below the root zone under furrow-irrigation systems were highest for onion (*Allium cepa* L.), followed by chili pepper (*Capsicum annuum* L.) and cotton (*Gossypium* spp.).

Measurements of water and NO_3–N in pecan orchards are limited because they are time- and labor intensive and because the cost of instrumentation and analysis can be high (van der Laan et al., 2010). On the other hand, solute transport in and out of the root zone can be simulated using a variety of numerical models. Among these models are the Nitrate Leaching and Economic Analysis Package (Shaffer et al., 1991) and the Agriculture Production Systems Simulator (McCown et al., 1996). These models can also provide deeper insight into the transport behavior as well as leaching of the applied chemicals and fertilizers toward the groundwater table with irrigation. Several successful applications of the HYDRUS model are also available in the literature (e.g., Dabach et al., 2015; Deb et al., 2011b; Kandelous and Šimůnek, 2010; Ramos et al., 2011; Skaggs et al., 2010; Tafteh and Sepaskhah, 2012). The HYDRUS model has been applied in diverse scenarios of different land uses and management systems as well as for different irrigation and fertigation practices (e.g., Crevoisier et al., 2008; Deb et al., 2015; Ebrahimian et al., 2011, 2013; Hanson et al., 2006; Kurtzman et al., 2013; Levy et al., 2017; Phogat et al., 2014; Ramos et al., 2012; Siyal et al., 2012). For example, Li et al. (2015) applied HYDRUS to optimize fertilizer management practices in a direct-seeded rice field and reported high performance of the model in simulating the N transport and transformation. Additionally, Turkeltaub et al. (2018) used the HYDRUS-1D model to investigate recharge and nitrate transport through the deep vadose zone of the Loess Plateau and reported future vulnerability of groundwater to contamination at a regional scale.

Monitoring volumetric soil water content (θ) and N variations, which are key factors in crop productivity, is essential for gaining a deeper understanding of soil–plant–atmosphere–water relations. Simulations can provide additional information, such as on N leaching, which may cause groundwater contamination. However, there are no studies reporting NO_3–N leaching in irrigated pecan orchards of southern New Mexico, and most available studies are only for lighter-textured soils. To the best of our knowledge, there are only two studies that focused on modeling water fluxes in the root zone of a flood-irrigated pecan tree (Deb et al., 2011a, 2013b). This research was therefore conducted (i) to determine soil water and NO_3–N dynamics within and below the root zone, (ii) to simulate water and NO_3–N variations and root NO_3–N uptake using HYDRUS-1D, and (iii) to compute the NO_3–N balance during two growing seasons in a pecan orchard.

MATERIALS AND METHODS

Study Site

Field measurements of θ were performed from April to December 2009 and from March to December 2010 in a pecan orchard located at the Leyendecker Plant Science Research Center of New Mexico State University. The site is 14.5 km south of Las Cruces (32°11′ 56.66″N, 106° 44′ 30.50″W) at an elevation of 1174 m asl. The area of the orchard is 1 ha, with seven rows of 30-yr-old ‘Western Schley’ pecan trees planted in a rectangular pattern (29 trees in each row). The row and tree spacings in the orchard were 7 and 8 m, respectively. The average tree height, trunk diameter at breast height, and tree crown width were 10.9 ± 0.2, 0.7 ± 0.0, and 7.1 ± 0.5 m, respectively. Tree canopy was divided into four quadrants; in one of the quadrants, time-domain reflectometry (TDR) sensors with an accuracy ±2% (CS 616; Campbell Scientific, Inc., Logan, UT) were installed to continuously record diurnal θ under the canopy (2-m distances from tree trunk in the no tilled part) at depths of 10, 20, 40, 60, and 80 cm. Other quadrants were used for identifying root distribution and soil physical and chemical properties.

The orchard has been under similar management regarding tillage operations since 2007. The tillage operations include chiseling at 40-cm depth once per year before first irrigation, disking at 10- and 25-cm depths four times per year, and cultivating at 5- and 10-cm depths two to three times per year, followed by land leveling. All tillage operations were done outside of the canopy area between tree rows. The orchard is flood irrigated, and a total of 5, 6, 9, and 10 irrigations were applied at the site during 2009, 2010, 2015, and 2016, respectively. In 2009 and 2010, pecans were subjected to water stress treatments, and that is why only five irrigations were made in 2009 and six in 2010. The irrigation was scheduled approximately once every 20 d from the beginning of the growing season until June. After that, it was done once every 15 d until mid-October. The fertigation was scheduled by the farm manager. To determine volume of water per application, the rate of inflow was multiplied with the duration of pumping. The groundwater table was 7 m below the soil surface, and the sources of irrigation were surface water and groundwater. The soil is classified as Harkey (coarse-silty, mixed, calcareous, thermic Typic Torrifluvents)-Glendale (fine-silty, mixed, calcareous, thermic Typic Torrifluvents). Nitrogen and zinc are the two nutrients most often required by pecan trees annually; the type and amounts of fertilizers applied are given in Table 1.

Numerical Modeling

The HYDRUS-1D model (version 4.16.0110) was used to simulate the one-dimensional movement of soil water and solutes in variably saturated porous media (Šimůnek et al., 2016). The orchard was flood irrigated; therefore, it is reasonable to use the HYDRUS-1D model. However, for this study, we have used average root length density (RLD) from three different quadrants of a pecan tree. The HYDRUS-1D model uses the Richards equation (Eq. [1]) to predict the redistribution of water in soil:

$$\frac{\partial\theta}{\partial t}=\nabla(K\nabla H)-S_r \qquad [1]$$

where θ is the volumetric soil water content ($cm^3\ cm^{-3}$), K is the unsaturated hydraulic conductivity ($cm\ d^{-1}$), H is the hydraulic head (cm), S_r is a sink term that represents the volume of water removed from a unit volume of soil per unit time attributable to plant water uptake ($cm^3\ cm^{-3}\ d^{-1}$), ∇ is the spatial gradient operator, and t is time (d). The van Genuchten–Mualem functional relationships are used as follows (Mualem, 1976; van Genuchten, 1980):

$$\theta(\psi)=\begin{cases}\theta_r+\dfrac{\theta_s-\theta_r}{[1+(|\alpha_v\psi|^n)]^m} & \psi<0;\ \theta_s\psi\geq 0\end{cases} \qquad [2]$$

$$K(\psi)=K_s S_e^l[1-(1-S_e^{1/m})^m]^2 \qquad [3]$$

where θ_s is the saturated θ ($cm^3\ cm^{-3}$), θ_r is the residual θ ($cm^3\ cm^{-3}$), ψ is the soil water pressure head, α_v is the reciprocal of the air entry ψ (cm^{-1}), m is $1 - 1/n$ ($n > 1$), n is the pore size distribution index (unitless), S_e is the effective saturation (unitless) given as $S_e = [\theta(\psi) - \theta_r]/(\theta_s - \theta_r)$, l is the pore-connectivity parameter (unitless), and K_s is the saturated hydraulic conductivity ($cm\ d^{-1}$). Root water uptake was simulated according to Feddes et al. (1978), with the sink term (S_r) accounting only for the water stress. The uncompensated root water uptake model was used (with a ω_c value of 1) (Šimůnek and Hopmans, 2009).

The HYDRUS-1D model provides simulations of multiple solutes, which can be either independent of each other or linked using the first-order degradation (or hydrolysis) pathway, which can be applied to N species. The solute transport equation describes advective-dispersive transport in the liquid phase and diffusive transport in the gaseous phase. In this study, urea, NH_4–N, and NO_3–N were the N species considered in simulations. The following set of equations is used in HYDRUS-1D to predict movement of N species:

$$\frac{\partial\theta c_1}{\partial t}=\nabla.(\theta D\nabla c_1)-\nabla.(qc_1)-\mu_a\theta c_1-S_r c_1 \qquad [4]$$

$$\frac{\partial\theta c_2}{\partial t}+\rho\frac{\partial s_2}{\partial t}=\nabla.(\theta D\nabla c_2)-\nabla.(qc_2)-\mu_{vol}\theta c_2-\mu_{nit}\theta c_2+\mu_a\theta c_1-S_r c_2 \qquad [5]$$

$$\frac{\partial\theta c_3}{\partial t}=\nabla.(\theta D\nabla c_3)-\nabla.(qc_3)-\mu_{dnit}\theta c_3+\mu_{nit}\theta c_2-S_r c_3 \qquad [6]$$

where c_1, c_2, and c_3 are liquid phase concentrations ($mg\ cm^{-3}$) of urea, NH_4–N, and NO_3–N, respectively; D is the dispersion coefficient ($cm^2\ d^{-1}$); q is the volumetric flux density ($cm\ d^{-1}$); ρ is the bulk density of the soil ($g\ cm^{-3}$); s_2 is the adsorbed concentration of NH_4–N ($g\ g^{-1}$), which is a linear function of c_2 using the distribution coefficient of NH_4–N (k_d); μ_a is the first-order rate constant (d^{-1}) representing hydrolysis of urea to NH_4–N; μ_{vol} is the first-order rate constant (d^{-1}) representing volatilization of NH_4–N to NH_3–N; μ_{nit} is the first-order reaction rate constant (d^{-1}) representing nitrification of NH_4–N to NO_3–N; and μ_{dnit} is the first-order reaction rate constant (d^{-1}) representing denitrification of NO_3–N.

Table 1. Dates of irrigation, fertigation, and amounts in the pecan orchard during 2009, 2010, 2015, and 2016. During each irrigation, 13.29 cm of water were applied.

Irrigation/ fertigation	Type	N applied	Total applied N
		— kg ha^{-1} —	
14 May 2009	urea (46% N)	51.75	
21 June 2009	urea (46% N)	103.5	
2 Aug. 2009	ammonium sulfate (21% N)	35.5	
2 Sept. 2009		–	
10 Oct. 2009		–	190.75
7 Apr. 2010	urea (46% N)	129.4	
27 May 2010	urea (46% N)	51.75	
22 June 2010	urea (46% N)	103.5	
18 July 2010		–	
23 Aug. 2010	ammonium sulfate (21% N)	35.5	
7 Oct. 2010		–	320.15
23 Mar. 2015		–	
21 Apr. 2015	urea (46% N)	129.4	
17 May 2015	urea (46% N)	51.75	
9 June 2015	urea (46% N)	103.5	
28 June 2015		–	
23 July 2015		–	
23 Aug. 2015	ammonium sulfate (21% N)	35.5	
15 Sept. 2015		–	
8 Oct. 2015		–	320.15
21 Mar. 2016		–	
12 Apr. 2016	UAN† (32% N)	118.8	
19 May 2016	UAN (32% N)	118.8	
7 June 2016	UAN (32% N)	118.8	
23 June 2016		–	
17 July 2016		–	
12 Aug. 2016		–	
28 Aug. 2016		–	
21 Sept. 2016	UAN (32% N)	118.8	
14 Oct. 2016		–	475.2

† Urea-ammonium nitrate.

Measurements and Model Inputs

Soil physical properties, including particle size, bulk density, and saturated hydraulic conductivity, are presented in Table 2. Diurnal variations of θ at five depths (10, 20, 40, 60, and 80 cm) were measured using five TDR sensors installed horizontally. The θ values were recorded every 10 min using a CR10X datalogger connected to an AM16/32B multiplexer. Measured θ values obtained by TDR sensors were calibrated by the gravimetric method (Deb et al., 2013a). For HYDRUS-1D modeling, the average RLD was obtained by depth from the northwest, southwest, and southeast quadrants of the pecan canopy. The rooting depth and RLD (cm root cm^{-3} of soil) distribution for this flood-irrigated pecan orchard were reported in Deb et al. (2013a). Briefly, there were no roots below the 80-cm soil depth. The RLD was higher at

Table 2. Soil physical properties at the study field.

Soil depth	Particle size distribution			Bulk density	K_s†
	Sand	Silt	Clay		
cm		%		Mg m^{-3}	cm min^{-1}
0–20	22.84 ± 1.92	51.00 ± 1.47	26.16 ± 0.71	1.53 ± 0.04	0.001 ± 0.000
20–40	10.84 ± 1.29	59.00 ± 1.29	30.16 ± 0.82	1.28 ± 0.05	0.001 ± 0.001
40–60	49.34 ± 12.99	37.25 ± 10.88	13.41 ± 3.59	1.24 ± 0.08	0.0174 ± 0.0108
60–100	37.84 ± 11.52	51.00 ± 10.74	11.16 ± 2.00	1.11 ± 0.05	0.0097 ± 0.0028

† Saturated hydraulic conductivity.

0- to 40-cm depths than at the 40- to 80-cm depths. Root length density accounts for 60 to 74% of the total RLD within the 0- to 40-cm depth. Replicated soil samples were collected 4 to 5 d after the scheduled irrigation from canopy area. The NO_3–N (mg kg^{-1} of soil) (EPA 353.2) was measured six times (February, June, and October in 2015 and 2016), with three sample replications. Using bulk density, NO_3–N in mg kg^{-1} of soil was converted to mg L^{-1} (of soil). Measurements of NO_3–N were performed at five depths (10, 30, 50, 70, and 90 cm). Initial values of the van Genuchten soil water parameters, including θ_s, θ_r, α_v, and n, were estimated using the neural network prediction module in HYDRUS-1D for each soil depth interval. The initial value of Parameter l was assumed to be 0.5 (Mualem, 1976).

Regarding solute transport parameters, urea and NO_3–N were assumed to be present only in the dissolved phase (k_d = 0 cm^3 g^{-1}). Ammonium-nitrogen was considered to adsorb to the solid phase using a k_d value of 3.5 cm^3 g^{-1} for all soil depths (Hanson et al., 2006). The longitudinal dispersivity was considered equal to one-tenth of the profile depth for all soil depth intervals (Cote et al., 2003; Hanson et al., 2006; Phogat et al., 2012). Molecular diffusion was neglected because it was considered negligible relative to hydrodynamic dispersion (Deb et al., 2015; González-Delgado and Shukla, 2014). The first-order decay coefficient μ_a for urea was considered to be 0.38 d^{-1} for all soil depth intervals (Hanson et al., 2006). The nitrification and denitrification rates were initially set to be the same at all soil depth intervals (μ_{nit} = 0.2 d^{-1} and μ_{dnit} = 0.02 d^{-1}) and were adjusted for each soil depth interval according to observed data. Volatilization of NH_4–N and subsequent NH_4–N transport by gaseous diffusion were neglected in this study. Under flood irrigation, urea is reported to be washed into soils and is not available to be nitrified significantly (Hu et al., 2008). The last term in Eq. [4], [5], and [6] represents passive root nutrient uptake, which is directly coupled with root water uptake by convective mass flow of water. Unlimited passive uptake of NO_3–N was considered by specifying the c_{max} value larger than dissolved simulated concentrations, which allowed all dissolved nutrients to be taken up by plant roots with root water uptake (Šimůnek and Hopmans, 2009). For root water uptake, the piece-wise model of Feddes et al. (1978) was chosen. All critical ψ values for a deciduous fruit from the HYDRUS-1D database were used in this study (Deb et al., 2011a, 2013b).

The HYDRUS-1D model requires separate values of potential evaporation (Ep) and potential transpiration (Tp) with time. The soil cover fraction (SCF) was determined monthly in the pecan orchard (Samani Majd et al., 2013). Meteorological parameters were taken from a climate station located at the Leyendecker Plant Science Research Center. The HYDRUS-1D model calculated the daily reference evapotranspiration (ET_0) based on the Penman–Monteith equation and then divided it into Ep and Tp using measured SCF. The Feddes et al. (1978) reduction function reduces Tp to actual transpiration (Ta), and the absolute value of the minimum allowed pressure head at the soil surface (hCritA) value limits Ep to actual evaporation (Ea).

Model performance was assessed using the following quantitative measures (Shen et al., 1998; Willmott, 1981):

$$\text{RMSE} = \sqrt{\frac{\Sigma_{i=1}^{N}(S_i - M_i)^2}{N}} \quad [7]$$

$$d = 1.0 - \frac{\Sigma_{i=1}^{N}(S_i - M_i)^2}{\Sigma_{i=1}^{N}(|S_i - M_{\text{avg}}| + |M_i - M_{\text{avg}}|)^2} \quad [8]$$

where d is the index of agreement between measured and simulated values, N is the number of paired measured and simulated values, S_i is the ith simulated value, M_i is the ith measured value, M_{avg} is the average of measured values, and RMSE is the mean difference between measured and simulated results.

Initial and Boundary Conditions

The initial water content was based on observed θ (0.33 cm^3 cm^{-3}) for all soil depth intervals. The initial NO_3–N and NH_4–N concentrations were determined separately for each depth interval based on measured data before the start of the growing season. The transport domain was considered to be urea free at the beginning of the fertigation simulation. An atmospheric boundary condition with a potential surface water layer was considered at the soil surface for water flow, defined by potential evaporation, potential transpiration, and rainfall. In this study, the soil profile was assumed to be 100 cm deep, and the water table was 7 m below the soil surface. Therefore, the boundary condition at the bottom of the transport domain was assumed as free drainage. The top and bottom boundary conditions for solute transport were set as "Concentration Flux BC" and "Zero Concentration Gradient," respectively.

RESULTS AND DISCUSSION

HYDRUS-1D Calibration and Validation for Water Flow

All measured θ values in 2009 were used to calibrate water flow in HYDRUS-1D and to obtain optimized water flow parameters by inverse modeling. The HYDRUS-1D model uses

Table 3. Optimized parameters of the calibrated flow and nitrogen species transport model.

Material no.	Depth interval	Water flow parameters†				N reaction parameters‡	
		θ_r	θ_s	*n*	K_s	μ_{nit}	μ_{dnit}
	cm	– cm^3 cm^{-3} –			cm d^{-1}	—— d^{-1} ——	
1	0–20	0.09	0.46	1.11	5	0.13	0.015
2	20–40	0.1	0.42	1.11	5	0.11	0.017
3	40–60	0.15	0.34	1.4	25	0.22	0.006
4	60–100	0.24	0.37	1.4	25	0.21	0.002

† θ_r, residual volumetric soil water content; θ_s, saturated volumetric soil water content; *n*, pore size distribution index (unitless); K_s, saturated hydraulic conductivity.

‡ μ_{nit}, first-order reaction rate constant representing nitrification of NH_4–N to NO_3–N; μ_{dnit}, first-order reaction rate constant representing denitrification of NO_3–N.

the Marquardt–Levenberg optimization algorithm (Marquardt, 1963) to optimize VG parameters, which is an effective method for nonlinear least squares fitting (Kool et al., 1985, 1987; van Genuchten, 1981). The model calibration started with optimizing water flow parameters for Material 1, followed by parameters for sequentially deeper soil materials. The parameters that were shown to be the most sensitive were optimized for each soil layer (Table 3). Water flow parameters were optimized using measured θ values for a 247-d period from day of year (DOY) 91 through DOY 337 (1 April–3 December) in 2009 for each material separately. HYDRUS-1D were validated using measured θ values for a 233-d period from DOY 132 through DOY 364 (12 May–30 December) in 2010. During HYDRUS-1D calibration and validation, model simulations of daily average θ at depths of 10, 20, 40, 60, and 80 cm were statistically compared with measured values using the above-mentioned quantitative measures.

Model Performance during the Calibration and Validation for Water Flow

Figures 1 and 2 illustrate differences between measured and simulated daily mean θ at five depths (10, 20, 40, 60, and 80 cm) during the calibration (DOY 91 through DOY 337, 2009) and validation (DOY 132 through DOY 364, 2010) periods. Generally, there was good agreement between measured and simulated θ during both calibration and validation periods (in the calibration period in particular). For instance, during the calibration period, RMSE fluctuated between 0.03 and 0.04 cm^3 cm^{-3}, and *d* fluctuated between 0.57 and 0.73 (Fig. 1). During the validation period, RMSE varied between 0.04 and 0.06 cm^3 cm^{-3}, and *d* varied between 0.44 and 0.66 for different soil depths (Fig. 2). Other studies also reported good agreement between measured and predicted θ (Abbasi et al., 2003, 2004; Deb et al., 2013b; Ebrahimian et al., 2011, 2012; Saito et al., 2006). The HYDRUS-1D model simulated both rapid rises in θ immediately after irrigation (Table 1) and gradual declines during drying periods. Model-predicted θ_s matched well ($0.01 \leq$ RMSE ≤ 0.03) with measured values at all depths except for 60 and 80 cm during the calibration period (Fig. 1) and 40 and 60 cm during the validation period (Fig. 2). However, some underpredictions during the validation period at the depth of 60 cm were likely associated with the soil water retention behavior of the heavy-textured soil as well as measurement errors associated with sensors. Differences between simulated and measured θ were also reported by Abbasi et al. (2004) and Deb et al. (2012, 2013b), among others.

HYDRUS-1D Calibration and Validation for Solute Transport

Calibration and validation of the solute transport model is complicated because several parameters need to be simultaneous-

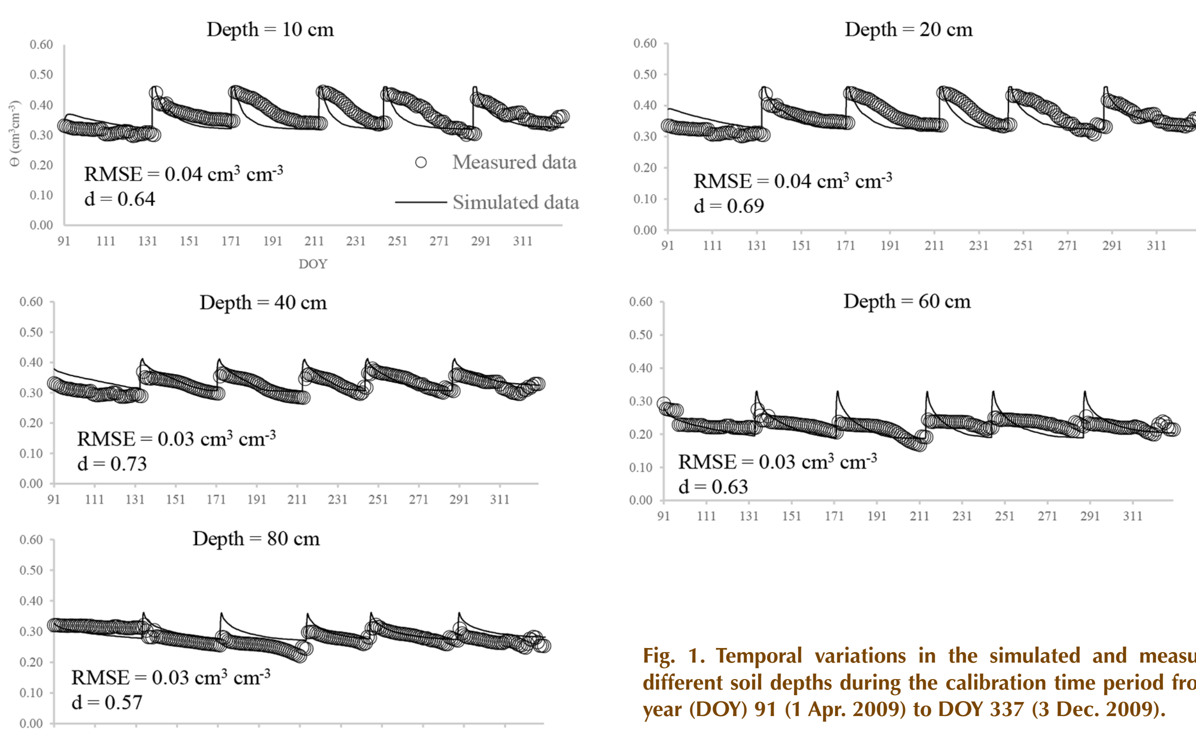

Fig. 1. Temporal variations in the simulated and measured θ at different soil depths during the calibration time period from day of year (DOY) 91 (1 Apr. 2009) to DOY 337 (3 Dec. 2009).

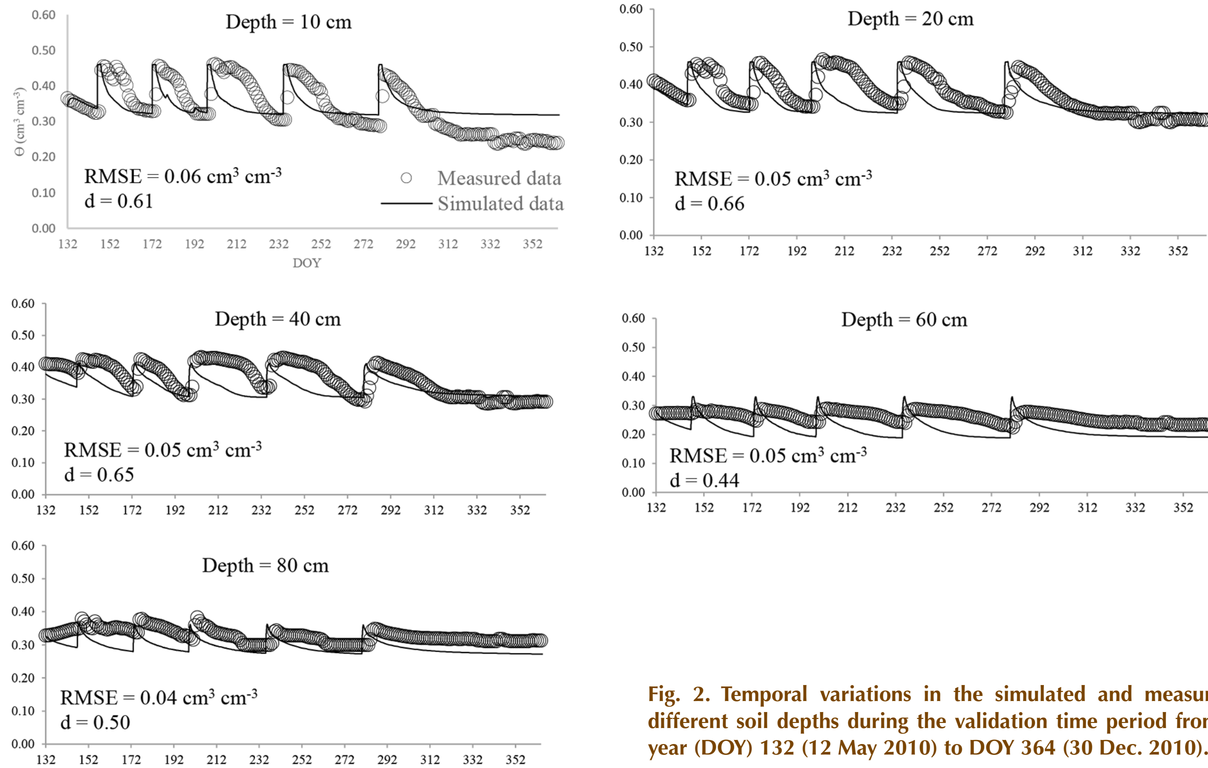

Fig. 2. Temporal variations in the simulated and measured θ at different soil depths during the validation time period from day of year (DOY) 132 (12 May 2010) to DOY 364 (30 Dec. 2010).

ly specified. Optimized water flow parameters (Table 3) and measured NO_3–N concentration profiles during 2015 were used for calibration. In this study, nitrification and denitrification parameters were adjusted and optimized for each soil depth separately (Table 3). Remaining parameters, listed in the Measurements and Model Inputs section, were obtained from published studies (Cote et al., 2003; Hanson et al., 2006; Phogat et al., 2012). The measured NO_3–N concentration profiles during 2016 were used for model validation. The RMSE and *d* values were calculated from measured and simulated NO_3–N concentration profiles to assess the performance of the model input parameters.

Model Performance during the Calibration and Validation for Solute Transport

Simulated and measured depth distributions of NO_3–N concentrations during two growing seasons, which represented calibration and validation periods, are presented in Fig. 3. Generally, Fig. 3 illustrates that the optimized set of solute transport/reaction parameters considered in model simulations (Table 3) was reasonable and applicable for simulating the N transport and transformations in the pecan orchard. Fluctuations in the measured and simulated NO_3–N concentration profiles at specified times showed that HYDRUS-1D simulated well ($0.36 \leq d \leq 0.79$) the patterns of NO_3–N concentration profiles for both 2015 and 2016 (Fig. 3). Predictions of depth distributions of NO_3–N concentrations were the best at all depths during the calibration period of June 2015, with $d = 0.74$ (Fig. 3b). However, simulated NO_3–N values had a relatively low *d* value and high RMSE during the validation period of June 2016 (Fig. 3e). The model simulated very well ($0.99 \leq \text{RMSE} \leq 5.16$) NO_3–N concentrations below the rooting zone (~60 cm for pecan) in all months during both years (Fig. 3). Because root nutrient uptake occurs in the rooting zone, NO_3–N below the rooting zone could leach to the groundwater. To the best of our knowledge, there are no studies on simulating NO_3–N concentrations in pecan orchards. However, the HYDRUS-1D model showed good agreement between the measured and simulated NO_3–N in bare soil (Wang et al., 2010). The HYDRUS-1D model was reported to perform well on simulating water and N leaching in furrow-irrigated rapeseed and maize under different rates of fertilizer applications ($0.094 \leq \text{NRMSE} \leq 0.11$ for deep percolation and $0.14 \leq \text{NRMSE} \leq 0.18$ for NO_3–N leaching) (Tafteh and Sepaskhah, 2012).

Root NO_3–N Uptake

Simulated cumulative Ea, Ta, and cumulative root NO_3–N uptake during two growing seasons are shown in Fig. 4. Actual evaporation and Ta were almost similar during both years due to similar irrigation schedules (Fig. 4). Root nutrient uptake was based on the assumption that all uptake was passive, through the root water uptake pathway only. Therefore, an increase in Ta caused an increase in root NO_3–N uptake (Fig. 4). A comparison of root NO_3–N uptake in 2015 and 2016 showed an increase of ~27 kg ha^{-1} in 2016, which was in agreement with ~48% more N fertilizer applied in 2016 than 2015 (Table 1). More N uptake was reported for rapeseed and maize at higher N application rates (Tafteh and Sepaskhah, 2012). The growing season of 2016 was the alternate bearing or "off" year, when a higher fertilizer application and soil N increased root NO_3–N uptake in June 2016 (Fig. 4b; DOY 154–183). A 48% increase in N fertilizer application (Table 1) resulted in a 72% increase in NO_3–N uptake in 2016 compared with that in 2015 (Fig. 4; Table 4).

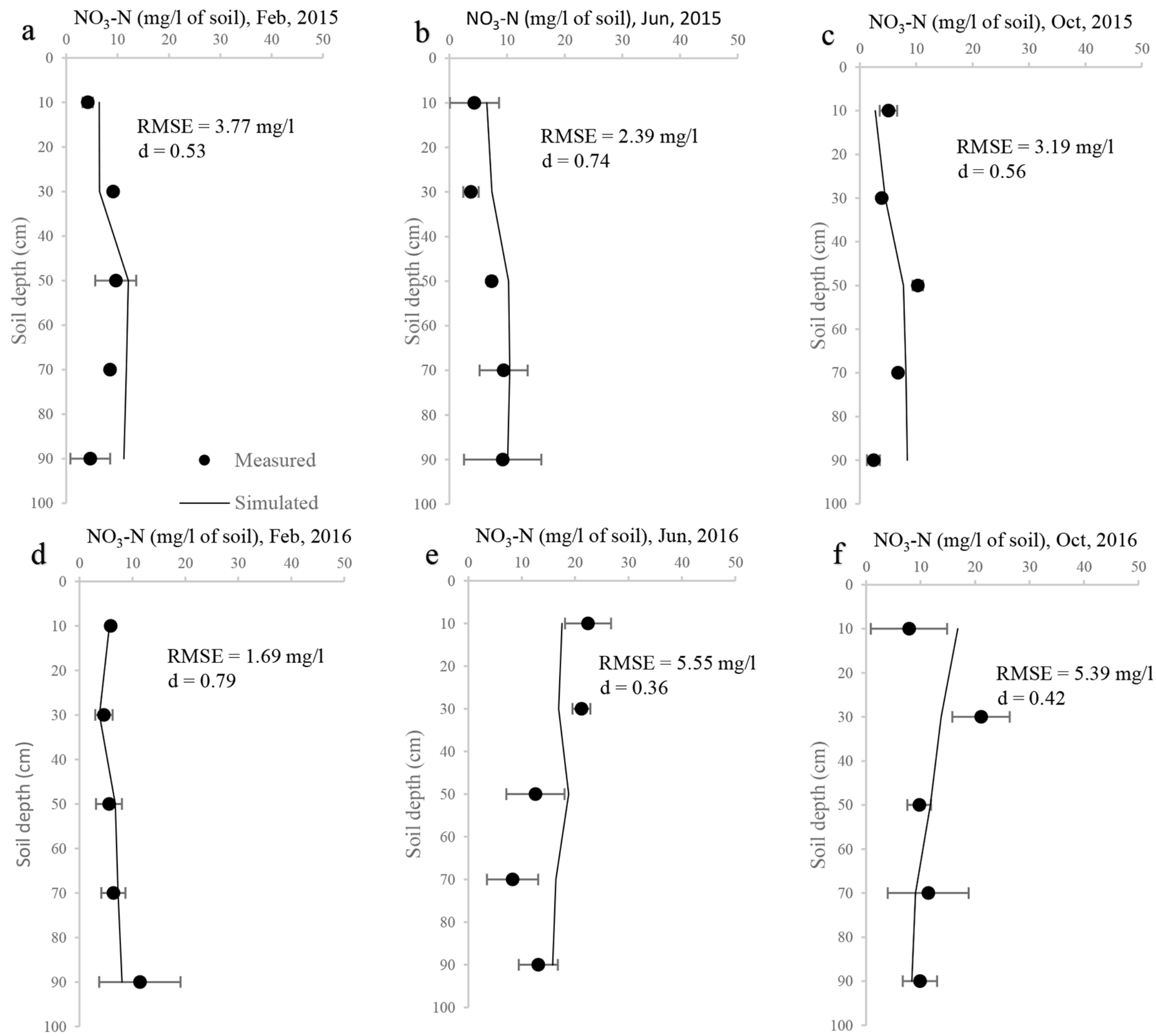

Fig. 3. Simulated and measured NO_3–N concentration profiles for days of soil sample collections during the calibration (a, b, c) and validation (d, e, f) periods of 2015 and 2016, respectively.

The N demand of pecan is high in June during the nut enlargement period and stays high during the subsequent nut filling stages (Acuña-Maldonado et al., 2003). The timing of fertilizer applications influences N absorption and partitioning as well as nut yield; therefore, fertilizer application during the entire growing season should be taken into consideration. The first N application should be done before the bud break because absorption apparently takes place during dormancy, followed by rapid N absorption during the shoot and leaf development (Acuña-Maldonado et al., 2003). A 5-yr study assessed in pecan orchards showed that applying just 125 kg ha^{-1} N per year (less than one-third the average N rate applied in our study) led to roughly 80 kg ha^{-1} of total N uptake (Acuña-Maldonado et al., 2003). The high N uptake efficiency could be explained by the difference in the type of irrigation system (drip irrigation vs. flood irrigation). Obviously, fertilizer management is more efficient in drip irrigation compared with flood irrigation.

NO_3–N Balance

The importance of the NO_3–N balance is to gain deeper understanding about fertilizer efficiency and fertilizer losses due to various processes. Table 4 shows simulated cumulative components of the NO_3–N balance (kg ha^{-1}) across the 100-cm soil profile during 2015 and 2016. The two inputs of NO_3–N were from applications of NO_3–N fertilizers and nitrification of NH_4–N to NO_3–N as a result of urea fertilizer applications (Table 1). From Table 4, all components of NO_3–N outputs were different between years because of differences in the amount and type of fertilizer applications (Table 1). Denitrification had a large contribution to the NO_3–N loss from the soil profile in both years, accounting for ~40% of applied NO_3–N each year (Table 4). Nitrate-nitrogen leaching accounted for 32 and 26% of applied NO_3–N in 2015 and 2016, respectively. To reduce NO_3–N leaching, more frequent but lighter applications of N fertilizers are highly recommended in flood-irrigated orchards. The soil NO_3–N storage increased on average by 14.15 kg ha^{-1} during both years. Total NO_3–N balance errors with HYDRUS simulations were <1% during both years.

CONCLUSIONS

The HYDRUS-1D model was used to optimize selected water flow and solute transport parameters needed to simulate

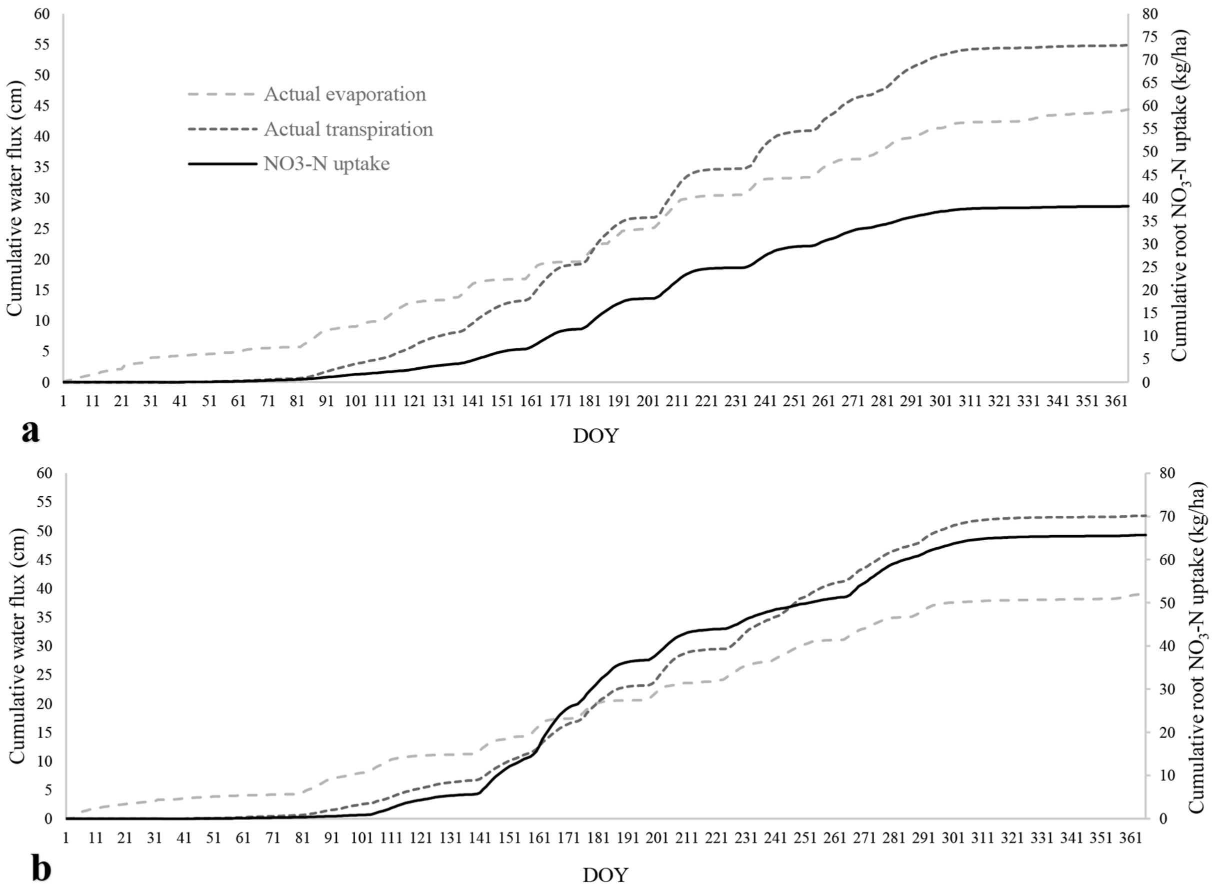

Fig. 4. Simulated cumulative water fluxes (total actual evaporation and transpiration) (cm) and cumulative NO_3–N (kg ha^{-1}) removed from the flow domain by root uptake during the time periods day of year (DOY) 1 (1 January) to DOY 365 (31 December) in (a) 2015 and (b) 2016.

depth distributions of soil water and NO_3–N, root NO_3–N uptake, and the NO_3–N balance during two growing seasons in a flood-irrigated pecan orchard. In general, the model simulations of temporal variations of θ matched well with the corresponding measurements at various depths, especially during the calibration period ($0.57 \leq d \leq 0.73$). The model was calibrated and validated for the NO_3–N transport, and nitrification and denitrification parameters were optimized for each soil depth interval. Concentrations of NO_3–N simulated by HYDRUS-1D agreed well with corresponding measurements in most depths, especially in deeper depths, during both years, with $d > 0.5$ during the calibration period. Total root NO_3–N uptake was 72% higher in 2016 than in 2015 due to excessive N fertilizer applications in 2016 compared with 2015. Leaching of NO_3–N below the rooting zone (60 cm) indicated a potential of groundwater pollution by NO_3–N leaching. The NO_3–N balance for the 100-cm soil profile corresponded well with differences in the amount and type of the fertilizer applications. Denitrification accounted for most of the NO_3–N loss (40% of NO_3–N input each year) from the soil profile. An average of 29% of applied NO_3–N was leached during both years. This research demonstrated that, to decrease NO_3–N leaching, N management strategies should consider the alternative bearing of pecan and adjust fertilizer application rates accordingly.

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Table 4. Cumulative components of the NO_3–N balance across the 100-cm soil profile during 2015 and 2016.

Year	Input NO_3–N	Leaching	Denitrification	Root uptake	Change in soil storage	Total NO_3–N balance error
			kg ha^{-1}			
2015	+172.92	–56.03	–68.67	–38.2	–11.64	–1.62
2016	+254.43	–66.86	–105.47	–65.69	–16.65	–0.24

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