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Assessment of LEACHN and a simple compartmental model to simulate nitrogen dynamics in citrus orchards

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Abstract

A simple compartmental model using a tipping bucket approach for the water dynamics coupled with a nitrogen-carbon transformations model has been adapted to simulate the soil nitrogen and water balance in mature orange groves on a daily step. This model has been compared with the more mechanistic LEACHN model (the N module of the LEACHM model), which uses Richards' equation to simulate soil water movement in unsaturated conditions, the convection-dispersion equation for solute transport, and that, in addition to including evapotranspiration, N transformations and N plant uptake as in the compartmental model, it also considers gaseous losses due to denitrification and ammonia volatilization, that are not considered in the compartmental model. This comparison was made using data from a three-year experiment in a citrus orchard with two nitrogen fertilization rates. After calibration using the first year data, a reasonable match between simulated and measured values in both models was observed for soil water storage in the whole profile for the validation period (2nd and 3rd year), but the agreement was not so good for the soil mineral nitrogen content. In spite of the differences in the nature and in the complexity of the two models, the soil water dynamics and drainage were well simulated during the whole period by both models. However, the LEACHN model predicted nitrate leaching better than the compartmental model, probably because it considers the nitrogen cycle in a more detailed way. This work is the first calibration and performance evaluation of

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the LEACHN model for citrus in the Mediterranean area and the results obtained in this study indicate that this model can be a valid tool to evaluate the effects of irrigation and N management on nitrate leaching. The compartmental model has a lower data requirement and calibration is less complex than the LEACHN model and, therefore, may be more appealing for advisory N management purposes.

1. Introduction

Nitrogen is an important nutrient in agricultural systems but inadequate management of nitrogen fertilizers and irrigation, especially in areas of intensive agriculture under irrigation and with important inputs of nitrogen fertilizer, may result in major environmental problems such as nitrate leaching or nitrous oxide emissions to the atmosphere (Alva et al., 2006; Neeteson and Carton, 2001; Quiñones et al., 2007). Nitrate pollution of groundwater is a worrying problem in many irrigated areas in Spain (MMA, 2006). Ground water is used for irrigation in 27% of the irrigated agricultural land, and also provides 40% of the drinking water. In some areas of the coastal plain in the Valencia region nitrate concentration in groundwater is greater than 100 mg NO_3^- L^{-1} (MMA, 2004). In this region there are 178000 ha of citrus, representing about 32% of the cultivated land, of which about 77000 ha are sweet orange with a fruit production of about 1.9 Mt year^{-1}. The most common irrigation system in this area is flood irrigation although drip irrigation is increasing. The irrigation water use for this crop in this region is about 750 - 900 mm year^{-1} (Castel et al., 1987). With respect to nitrogen fertilization, some authors have established that the annual nitrogen requirement of citrus in the Valencia region is between 600 - 800 g N tree^{-1} (Primo-Millo and Legaz, 1993), approximately equivalent to 240 – 300 kg N ha^{-1}, that is somewhat higher than the 200 – 250 kg N ha^{-1} year^{-1} recommended by the Valencian Code of Good Agricultural Practices (VCGAP) (DOGV, 2010) for citrus under flood irrigation. However, there is still a large variation in the nitrogen fertilization rates applied by farmers.

Different studies dealing with nitrate leaching in citrus have quantified the losses of nitrate for different fertilization practices (Lamb et al., 1999; Paramasivam et al., 2001; Ramos et al., 2002). These studies show that for nitrogen application rates up to 400 kg N ha^{-1} year^{-1}, nitrate leaching rate was, in most cases, less than 100 kg N ha^{-1} year^{-1}. In general, nitrate leaching losses increased with fertilizer nitrogen application rate and the amount of water drained, and accounted for up to 33% of the total applied nitrogen. Although in different agricultural systems there seems to be a direct relationship between nitrogen inputs and the increasing concentration of nitrate in groundwater (Babiker et al., 2004; Bouwer, 1990; Canter, 1996), nitrogen transport is difficult to measure, since it is affected not only by water flow but also by all the N transformations that take place in soil (mineralization, immobilization, denitrification, plant uptake, etc.).

To attain higher nitrogen use efficiency, it is necessary to improve both nitrogen fertilization and irrigation management. Computer simulation models can help in this improvement because they integrate the different processes affecting the nitrogen dynamics in the soil-plant system. Some nitrogen models in the soil-plant system are LEACHM (Wagenet and Hutson, 1989), SOILN (Hoffmann and Johnsson, 1999), STICS (Brisson et al., 1998) and WAVE (Vanclooster et al., 1996). These models, after calibration, allow the estimation of nitrate leaching, soil mineral nitrogen and water content for different crops under different conditions of irrigation, rainfall and fertilization, being an inexpensive and rapid technique to evaluate the effects of various agricultural management practices on nitrate leaching (Cannavo et al., 2008; Kersebaum et al., 2007).

The LEACHM model has been widely used and validated for several annual crops (Jabro et al., 1995; Webb and Liburne, 1999). However, it has hardly been used with perennial plants. Harrison et al. (1999) used the LEACHM model for evaluating the long-term impacts of alternative citrus nitrogen and water management practices on the Central Florida Ridge. Alva et al. (2006) used the LEACHM model to estimate the N budget components for different nitrogen and irrigation practices for citrus in sandy soils in Florida.

In this paper it is assumed that a simpler model capable to obtain good predictions of water and soil nitrogen dynamics in citrus orchards, would be more appealing for advisory purposes. From a practical point of view, the main problem of using simulation models such as LEACHM is that many experimental data are needed for their calibration (Jung et al., 2010) and this is probably the reason why they are barely used for irrigation and N fertilization management in commercial orchards. Thus, simpler models with fewer data requirements could be of interest for estimating the water and nitrogen needs in farmer fields and at a regional scale (Nendel, 2009). For this reason, a compartmental model developed by Contreras et al. (2009) that combines a simple soil water capacity module with an analytical model for the carbon and nitrogen dynamics developed by Porporato et al. (2003) was selected. This later model was applied in the broad-leafed savannah at Nylsvley (S. Africa) (D’Odorico et al., 2003) coupled with an existing stochastic soil moisture model and provided good results.

The two main goals of this study were (1) to adapt the LEACHN and the compartmental models to be used on citrus orchards, and (2) to calibrate them and assess their performance using data from a 3-year experiment with two N fertilization treatments. This work constitutes the first calibration and validation of LEACHN model in citrus orchards in the Mediterranean area.

2. Material and methods

2.1. LEACHN model for citrus

LEACHN is the nitrogen module of the LEACHM model. LEACHM (Leaching Estimation And Chemistry Model) is a process-based, one-dimensional model that simulates water and solute movement, and related chemical and biological processes, in the unsaturated soil (Wagenet and Hutson, 1989). A summary of the main terms of water and nitrogen balance and their treatment by the LEACHN model is presented in Table 1. The model describes the one-dimensional water flow in the unsaturated zone using the Richards' equation. Solute transport is modeled by the convection-dispersion equation, and the main processes described in the nitrogen module are mineralization, nitrification, denitrification and volatilization.

Input data for the LEACHN model include soil physical and chemical properties for the different soil layers as well as weather and crop data. The soil physical properties include: bulk density, hydraulic conductivity and water retention curve parameters. The water flow routine in LEACHN uses equations proposed by Campbell (1974) to relate volumetric water content, pressure potential and hydraulic conductivity. The evapotranspiration calculation is based on the method proposed by Childs and Hanks (1975) using weekly data of the class A pan evaporation E_o, the pan coefficient k_p, and a crop coefficient k_c. Potential crop evapotranspiration is calculated as $E_o \cdot k_p \cdot k_c$. Soil chemical properties required by the model include: initial organic carbon, organic and inorganic nitrogen contents, and rate constants for the N-transformation processes.

To apply LEACHN to citrus orchards, the nitrogen plant uptake module had to be modified since, in its original form, LEACHN only considers N uptake in annual crops. The model requires the potential annual N uptake by the crop, but since it calculates this uptake on a daily basis, it is necessary to obtain the potential daily values. These were estimated based on the seasonal uptake pattern measured by Legaz and Primo (1988). According to these authors the maximum monthly N uptake in the Valencia region is in July (about 43 kg N ha^{-1}) and the minimum is in January (about 3 kg N ha^{-1}). The seasonal N uptake pattern observed by Legaz and Primo (1988) was transformed in a cumulative curve throughout the year, and the potential N uptake for a given day was calculated as a fraction (FTNU) of the total annual uptake using the following polynomial regression model:

$$\mathrm{FTNU} = -1.1447\ \mathrm{FGS}^6 + 3.6476\ \mathrm{FGS}^5 - 4.2331\ \mathrm{FGS}^4 + 2.1291\ \mathrm{FGS}^3 - 0.4314\ \mathrm{FGS}^2 + 0.033\ \mathrm{FGS}, \qquad (1)$$

where FGS is the fraction of the year passed from the 1^{st} of January till that day. This regression model, had a coefficient of determination (R^2) of 0.98, and satisfies that when FGS is zero FTNU is also zero, to eliminate the possible negative values for N uptake.

2.2. Compartmental model

This model computes the soil nitrogen balance in a mature orange grove on a daily step and is described in Contreras et al. (2009). The model resulted from the coupling of a compartmental model of the nitrogen dynamics in the soil, developed by Porporato et al. (2003), with a simple soil water capacity model described in Lidón et al. (1999). A summary of the main terms of water and nitrogen balance and their treatment by the compartmental model is presented in Table 1.

The water module uses a ‘tipping bucket’ approach in the root soil profile, which is a simplified scheme for calculating soil water content, which requires a relatively small number of input parameters in comparison to a scheme using Richards’ equation (Emerman, 1995). Several modifications were made to implement a soil profile consisting of three layers of different thickness, layer 1 (0-30 cm), layer 2 (30-60 cm) and layer 3 (60-80 cm), according to the scheme shown in Fig. 1. Changes in the calculation of the different components of water balance with respect to the original one-layer model are as follows: a) percentage of the root distribution in each soil layer has to be given as an input and this is used when calculating root water uptake from each layer; b) irrigation and rainfall inflow is considered only in the first layer; c) if the water content of the first layer exceeds maximum allowed soil water storage, then this excess is considered runoff; d) if the water content exceeds field capacity, then this excess of water drains into the underlying layer; and e) drainage from a layer is a water input to the layer below (Contreras et al., 2009).

The nitrogen module considers five N pools and their relations are described in Contreras et al. (2009). The model assumes that nitrogen losses by volatilization and denitrification are similar to the atmospheric deposition and biological fixation, and none of these are considered. This simplifying assumption has also been used by other authors (Jeuffroy and Recous, 1999). Other assumptions are: a) mineral nitrogen inputs for rainfall, irrigation and fertilizers are inputs only for the first layer; b) the inputs to the following layer are only due to mineralization and nitrate leaching from the above layer; c) the calculated nitrogen uptake is compared with the potential daily uptake of N for an adult orange tree, and the lower of these two values is taken.

2.3. Field experiment

Data used to calibrate and validate the two simulation models were obtained from a three year experiment conducted in a commercial citrus orchard in the Valencia province of Spain (39º30'18''N, 0º23'01''W, 14 meters above sea level). The main objective of the experiment was to evaluate the effects of different N fertilization rates on fruit yield and nitrate leaching. Table 2 summarizes the main characteristics of the field experiment, while selected physical and chemical properties of this soil are shown in Table 3. In this paper, data are from two N fertilizer treatments: N1 (150 kg N ha^{-1} year^{-1}), and N2 (300 kg N ha^{-1} year^{-1}) that correspond to rates about 75 kg N ha^{-1} lower and higher, respectively, than that recommended by the VCGAP (200-250 kg N ha^{-1} year^{-1}).

Nitrate leaching at a given depth and for a period was calculated as the product of the drainage for this period and the mean nitrate concentration of the soil solution to the depth considered. Drainage was calculated by a chloride balance (Lidón et al., 1999), since this method has some advantages over the water balance method. In the latter approach any reduction in evapotranspiration produced by water deficits or other causes (nutrient deficiencies, pests, etc.) are difficult to assess. The chloride balance method is not influenced by these factors and it is relatively simple to use. In this method the main Cl^- inputs considered are the irrigation water and, in some cases, potassium fertilisers, and the main outputs are: drainage, plant uptake, and change in soil content. Chloride uptake by citrus trees was estimated from Lidón et al. (1999) and was considered to be uniform throughout the year. There are two major sources of uncertainty in this balance: 1) the high variability in the soil chloride content, and 2) the assumption of a linear change in the chloride concentration of the draining soil solution at the bottom plane of the soil layer considered in the balance from the beginning to the end of the period considered. Ramos (1988) and Lidón et al. (1999) reviewed the application of this method for drainage estimation and concluded that the effects of a high spatial variability of chloride content in soil are less important when the chloride input is large relative to the amount of chloride in the soil profile, and that at depths greater than about 60 cm, the variation of chloride concentration with time can be considered approximately linear for periods of 1-2 months. Evapotranspiration was calculated by a water balance in which drainage was obtained by a chloride balance, and runoff was assumed to be zero (this assumption is reasonable, since the irrigation units were leveled basins surrounded by ridges about 15 cm high).

2.4. Models calibration and validation

Calibration of both models was performed using data from the higher N rate fertilizer treatment, N2, for the first year. First, the water module was calibrated and, after this, the nitrogen module parameters were adjusted as described below. Data from the first year were used for calibration because during this year there were more soil mineral data available for the irrigation and fertilization season, and this provided a wider range of water and nitrogen contents.

Some assumptions were made in the use of both models. For the citrus orchard used in the experiment, a potential annual N uptake of 200 kg N ha^{-1} was assumed. Although this parameter has a great influence on the other components of the nitrogen balance, especially when soil water and mineral nitrogen are not limiting, it was decided not to calibrate it because this assumed value is very close to that measured by Legaz and Primo (1988) for citrus trees of similar age and size in the same Mediterranean area. Also, it was assumed that the soil organic C content was in equilibrium since the experimental orchard had trees 20 years old, and a relatively constant management over the time. In addition, since citrus are perennial plants, it was considered that the leaf litter input kept constant the soil organic matter content during the simulation period. Leaf litter input to the soil surface was taken as 2350 kg C ha^{-1} year^{-1} with a C/N ratio of 28, representing an annual input of 85 kg N ha^{-1} year^{-1} (Harrison et al., 1999). The C/N ratio of the plant residues annually added to the soil as litterfall, microbial biomass and litter were estimated from Moreno (2001), Ferrer et al. (2006) and Brady and Weil (2002).

For the water module of the LEACHN model the parameters used were those proposed by Lidón et al. (1999) for this same orchard, with minor changes. A free-draining lower boundary was assumed, since the depth of the groundwater was 3-4 meters as indicated by the water level of nearby wells. The pan coefficient to calculate evapotranspiration was set to $k_p = 0.815$ (Doorenbos and Pruitt, 1977) and the monthly values of k_c for citrus in the Valencia region were based on Castel et al. (1987), and are given in Lidón et al. (1999). The fraction of ground cover by the trees was taken as 0.85. The root resistance parameter was varied until a good fit of the simulated water content in the soil profile was obtained. Root distribution with soil depth was assumed to follow the pattern described by Ayers and Wescott (1985) for water uptake by plants, but slight modifications were introduced to obtain a good fit of the simulated water content in the soil profile to the measured values. The saturated hydraulic conductivity (k_s) of the soil layers was calculated following Ahuja and Nielsen (1991). Some other parameters of the water retention curve could have been changed instead, but it was decided to vary only k_s, since this parameter is the main factor determining drainage flux in a low permeability layer where water content is often close to saturation. Soil hydraulic and crop parameters used in

LEACHN are presented in Table 4.

Soil hydraulic parameters required by the compartmental model were initially estimated using Saxton et al. (1986) approach. For the calibration of the water module of this model, the guidelines given by Lidón et al. (1999) for each soil layer (0-30 cm, 30-60 cm and 60-80 cm) were followed. Minimum soil water content was initially set equal to a typical water content value measured in the soil profile just before irrigation. The maximum soil water storage held against gravity was taken as the average soil water content measured 3-5 days after irrigation. The initial maximum soil water storage estimate was taken as the water content at saturation in the first 50 cm, plus 5 cm to account for the possibility of water ponding due to ridges in the irrigation basins. All these values were then adjusted to improve the fit between predicted and measured soil water content in each layer and drainage, using data measured in periods with large soil water changes during first year. Initial values of root distribution before calibration followed the distribution used in different studies, but the root distribution was slightly modified from that used in the LEACHN model to better fit the experimental data. Other parameters used in the compartmental model and not subject to calibration are listed in Table 5.

To find the most influential parameters of nitrogen dynamics determining the soil mineral nitrogen content in the LEACHN model, a sensitivity analysis was performed following Sogbedji et al. (2001, 2006). Multiple runs of the model were performed in which changes of each parameter selected were made. The ammonium and nitrate soil content and nitrate leaching were affected by changes in the potential annual N uptake and by changes in the rate constants for mineralization, nitrification, ammonia volatilization from surface, and denitrification. The measured mineral nitrogen content in each layer was the variable used in the calibration process for N parameters. The sensitivity analysis showed that the most important parameters were: potential annual N uptake, native organic matter mineralization rate constant, synthesis efficiency factor and humification fraction, ammonia volatilization, denitrification, nitrification and litter mineralization rate constants. Adjustment of the selected parameters followed the order: the humification fraction, the rates of nitrification, denitrification and mineralization of litter, and finally the rate of mineralization of humus and the synthesis efficiency factor.

In the compartmental model respiration and humification fraction, microbial biomass death rate and partition nitrogen coefficients were obtained from D’Odorico et al. (2003). For the nitrogen module the calibration process was started with those parameters with a similar meaning in the LEACHN model and they were varied to obtain the best fit with the measured soil nitrogen mineral content.

Calibration of a given parameter was finished when further adjustments no longer reduced the difference between measured and simulated data using the root mean squared error (RMSE) given by

$$RMSE = \sqrt{1/N \sum_{i=1}^{N} (D_i)^2} \qquad (2)$$

where D_i is the difference between the measured value (Y_i) and the corresponding value calculated by the model ($\hat{Y}_i$), and N is the total number of values of soil water and mineral nitrogen content. This procedure was performed for each soil layer starting with the top layer.

To assess the accuracy of the calibrated model, simulated values were plotted against the corresponding measured values on a 1:1 graph, and the correlation coefficient (r) and the mean difference between simulated and measured data were used as criteria to evaluate the model predictions. In addition, other indices have been computed such as the relative root mean square error (RRMSE) and the agreement index (AI) described in Wallach (2006) and given by,

$$RRMSE = \frac{RMSE}{\bar{Y}} \qquad (3)$$

$$AI = 1 - \frac{\sum_{i=1}^{N}\left(Y_i - \hat{Y}_i\right)^2}{\sum_{i=1}^{N}\left(\left|\hat{Y}_i - \bar{Y}\right| + \left|Y_i - \bar{Y}\right|\right)^2} \qquad (4)$$

where $\bar{Y}$ is the average of the Y_i values.

Validation of both models was performed using data from the second and third years of treatment N2, and from the three years for treatment N1. For this purpose, measured values of the soil water content of the different layers and the amount of water stored in the whole soil profile, drainage, soil mineral N content, and nitrate leaching were compared with the simulated values. The statistical indices listed above were then obtained.

3. Results and discussion

3.1. Models calibration

The calibrated water parameters, N transformation rate constants and other adjusted parameters are presented in Table 6. Differences between some parameter values for both models are due to the different meanings they have in each model. For example, in the compartmental model the rates of litter and humus decomposition and the nitrification depend on soil moisture and the microbial biomass content, whereas in the LEACHN model nitrogen mineralization rates depend upon the rate of decomposition of the organic C pools, the N content of these pools, and the C/N ratio of the decomposition products, and nitrification proceeds at a potential rate decreasing until a given maximum NO_3^-/NH_4^+ concentration ratio is achieved (Johnsson et al., 1987).

After calibration, simulated and measured soil water storage values for the three soil layers were, in general, close in both models (Table 7), but the LEACHN model overestimated soil water content, whereas the compartmental model tended to underestimate it (Fig. 2). Both models gave a high correlation coefficient (r) and agreement index (AI) in the surface layer (0-30 cm), probably because this layer has the highest temporal variation, and this improves the calibration. The fit obtained in the second and third layers is not as good as in the surface layer, probably due to a lower range of variation of soil water content that made calibration less accurate (Fig. 2). On the whole profile, the prediction error (RRMSE) was 11% for the LEACHN model and 8% for the compartmental model, with a correlation coefficient similar in both models. The high values of the *AI* for LEACHN and for compartmental model indicate a good match between simulated and measured data for the calibration period.

For the calibration period, soil water storage simulated by LEACHN was more responsive to water application than in the compartmental model (Fig. 3), and the influence of the hydraulic properties of a given layer on the water content of another layer was also greater in the LEACHN model. This is due to the different treatment of water dynamics in both models: while in the compartmental model, the water exceeding field capacity value is attributed immediately to drainage, in the LEACHN model water flow is determined by Richards' equation, that uses the hydraulic conductivity as a key variable, and soil water content changes in the lower soil layers after an irrigation or rainfall event can take several days. These effects on soil water flow in the LEACHM model might explain the overestimation of water storage values at the end of the irrigation period and the beginning of the rainy season, if the assigned saturated hydraulic conductivity for the 60 – 80 cm layer was lower than the real value. The calculated k_s for the deepest soil layer, following Ahuja and Nielsen (1991), was very low, and this resulted in much lower drainage values in comparison to those obtained by chloride balance. To correct for this, the k_s for this layer was increased to obtain a better fit between the simulated and measured soil chloride content during the first year, since soil chloride content depends on drainage. The compartmental model does not account for these hydraulic conductivity effects, but despite this and although its calibration was simpler, the results were acceptable.

For the soil mineral nitrogen content (Table 7 and Fig. 2), although RRMSE showed that the agreement between measured and simulated data was not as good as for soil water content, the AI indicated that the agreement for the whole profile was good and similar for both models. The worst fit occurred again in the third layer, as shown by the low agreement index obtained for this layer. In this layer the main process governing the N dynamics is nitrate leaching that depends strongly on the water flow, and the calibration of the N transformation parameters is less important.

The lower agreement between observed and simulated values for the soil nitrogen content in both models is not surprising since there are many processes involved in the nitrogen cycle (including water movement). In addition, in the compartmental model the temperature and soil moisture effects on some parameters are not taken into account. In the 60 – 80 cm soil layer, differences between measured and simulated N content values were larger in both models, reflecting probably the accumulation of simulation errors when going from the upper to the deeper soil layers, as well as the difficulties in calibrating the hydraulic parameters for these layers for the reasons mentioned before.

3.2. Models validation

In the validation test both models predicted soil water content even better than in the calibration period, but for soil mineral nitrogen content the agreement between measured and simulated values was worse than for water, and slightly better for the N2 treatment (Table 7), probably because calibration used N2 treatment data. Fig. 3 shows the measured and simulated soil water storage and cumulative drainage at 80 cm for both models in the whole period. In this case, there are no differences between N treatments because the water input was the same in both treatments. It can be seen that both models fit the data well in the first year of the validation period, but that in the last year the LEACHN model underestimates drainage.

A comparison of the measured and simulated soil water balance components values is presented in Table 8. It can be observed that the simulated cumulative ETc for the 3-year period and the annual values were close to the measured values in both models, except for the third year in the LEACHN model where there was an overestimation of about 10%. Simulated drainage was within 14% from the measured values for the two models in the first two years, and only in the third year the LEACHN model underestimated drainage grossly. Although drainage obtained by chloride balance method has some uncertainties (see Lidón et al., 1999), these are mitigated in this case because the chloride balance is calculated from several points (3 points per tree, 2 trees per treatment, and 2 treatments), and because soil was sampled several times throughout the year. This provided a chloride balance for each sampling period, and annual drainage was obtained as the sum of drainage in each period.

Simulated runoff was relatively small in all cases (less than 6% of total water input). In the compartmental model runoff is calculated from the maximum soil water storage, while in the version of LEACHN model used in this paper runoff is the water that cannot infiltrate in the time step considered. Although runoff was not measured it is unlikely that it was important because of the ridges (about 10 – 15 cm high) surrounding the irrigation units that prevent the generation of runoff, except when heavy rains occur. In the soil water balance (Table 8), the variation of soil water storage is small relative to the other terms, and can be considered negligible for long periods of time.

An estimate of irrigation efficiency was obtained calculating the ratio evapotranspiration/applied irrigation water, during a long period of the main irrigation season, when the rains were not significant. Very high values were obtained (even higher than 100%) indicating that irrigation applied by the farmer was lower than required (221 – 413 mm as compared to 450 – 520 mm that is considered normal in this period (Castel et al., 1987)). These water deficits must have induced a reduction in actual evapotranspiration during some period in summer, and therefore an upward water flow from the soil layers below the 80 cm depth (soil moisture in the 80-150 cm soil layer was always greater than that of the 60-80 cm layer (data not shown)).

For the validation period both models reproduced relatively well the measured values of soil mineral nitrogen content in both N treatments, although a slight underestimation was observed in the N1 treatment (Fig. 4). The errors associated with both models (RRMSE) for the N1 and N2 treatments were similar, but the agreement indices for N1 were lower than for N2 (Table 7).

The main components of the N budget for the two N treatments are given in Table 9. Simulated plant uptake was the major N output term, accounting for 72 – 77% of the total N output for treatment N1 and 61 – 63% for treatment N2. For treatment N1, simulated plant uptake was greater than total input (in fertilizer and irrigation water) indicating that the citrus trees had to use part of the initially available soil mineral nitrogen and that produced by mineralization. The differences in the N plant uptake in both models are probably due to the different soil nitrogen content simulated by both models, to the different algorithms used for N plant uptake, and to the differences in the simulated evapotranspiration. In the LEACHN model N uptake (nitrate and ammonium) occurs in the transpiration stream but it cannot exceed the potential N uptake. If this uptake does not satisfy the plants requirements, then a diffusive component for nitrate only is calculated. In the compartmental model N plant uptake is calculated solely as a function of N concentration in the soil solution and root water uptake.

Mineralization values estimated by both models were, on average, about 100 and 125 kg N ha^{-1}

year^{-1} for the compartmental and LEACHN models, respectively. These values are within the range measured by Dou et al. (1997) for the 20-yr-old citrus trees growing in Florida with sandy soils and organic matter content ranging from 10 – 27 g kg^{-1}, and those reported by Lidón et al (2006) in an area close to the experimental plot, with a similar soil but cultivated with vegetable crops. These results indicate that mineralization provides a significant portion of the annual N requirement. The steady state assumption for the humus compartment considered in this paper is supported by results in the compartmental model, which simulated only a 0.6% reduction in the initial content of soil organic nitrogen over three years, whereas the LEACHN model simulated this reduction was of 1.5%, indicating that to achieve equilibrium in soil N humus content, it would be necessary to increase the fraction of litter that is transformed into humus.

Gaseous losses of N by NH_3 volatilization simulated by the LEACHN model represented 9% and 11% of applied N in the N1 and N2 treatments, respectively. These values are within the range reported by Alva et al. (2006) for a citrus grove fertilized with ammonium nitrate and urea and with a fine sand soil with a pH of 6.0 for the surface layer. The low denitrification values simulated by the LEACHN model are consistent with the experimental conditions: well-drained soils, with only a few days of irrigation or heavy rains during which some gaseous losses could occur (Paramasivam et al., 1999).

Measured nitrate leaching represented about 30% of the total nitrogen input in both N treatments for the whole period. Since both treatments had the same drainage, because the water input was the same for both N treatments, the leaching differences observed reflect the different nitrogen input in each treatment (Fig. 4). Nitrate leaching increased with N fertilization, and was well predicted by the LEACHN model, but the compartmental model overestimated it by 60% and 49% in treatments N1 and N2, respectively. Looking at the simulated leaching for the different years for the compartmental model, it becomes apparent that it is in the second year when the differences between measured and simulated values are greater. This is also observed with the LEACHN model but much less pronounced (Table 9), and there are not clear reasons for this overprediction in both models. With respect to the differences in nitrate leaching between the two models, it is possible that these are due to the higher drainage simulated by the compartmental model and to a higher availability of soil nitrate in this model, probably because it does not consider volatilization nor denitrification losses. However, the LEACHN model simulated a higher mineralization than the compartmental model, and this would increase nitrate leaching, contrary to what is observed. Despite these differences in nitrate leaching, both models gave similar total N losses.

These results indicate that the LEACHN model predicted nitrate leaching better than the compartmental model, probably because it considers the nitrogen cycle in a more detailed way and includes processes such as volatilization, denitrification and accounts also for temperature effects on the N related rate constants.

3.3. Using the models to improve N management

Once calibrated and validated both models, different fertilization and irrigation management practices were assessed considering only the environmental aspects (nitrate leaching and gaseous nitrogen emissions), since agronomic effects on yield or tree growth are not included in both models, and can only be estimated indirectly by looking at the simulated soil mineral N availability and the N uptake, that can be lower than the potential uptake and, therefore, limit yield and growth.

Table 10 shows the scenarios considered, in which irrigation rate, N fertilizer rate, the chemical form of nitrogen used and the number of fertilizer applications were varied. Nitrate leaching, N plant uptake and other N losses, as volatilization and denitrification, obtained in each of the scenarios are compared with results obtained with conventional management (N2 in field experiment). The simulation period included the three year period used in the evaluation of the models.

The results show that the variation in the irrigation rate (± 10%) produced changes in drainage and therefore in nitrate leaching (Fig. 5). Increasing irrigation causes increased nitrate leaching (9%), whereas reducing irrigation decreased it by 6-8% without affecting N plant uptake.

The decrease in the N fertilizer rate affected different outputs of nitrogen balance. A reduction of 10% in N rate produced a similar reduction of nitrate leaching, in both models (Fig. 5, Sc3), but this did not affect N plant uptake. In this case, the LEACHN model also predicted a reduction of volatilization (12%) and denitrification (15%). Using ammonium nitrate instead of ammonium sulphate did not affect nitrate leaching but reduced volatilization (6%). Increasing the number of N applications and reducing the total N rate resulted in a greater nitrate leaching reduction. Using the N fertilizer rate recommended by the current regional legislation (DOGV, 2008) reduced nitrate leaching by 19% (Fig. 5, Sc7), while N plant uptake was barely affected.

The combined effect of the reduction in irrigation and nitrogen rates resulted in an important nitrate leaching reduction of 17 – 25% (Fig. 5, Sc6 and Sc10), similar to the sum of the reduction caused by irrigation and fertilization separately, in both models.

Additional examples on the use of the LEACHN model for N management in citrus orchards in the Valencia region are given in Lidón and Paches (2005).

4. Conclusions

Two different models to simulate water and nitrogen dynamics in a soil profile have been adapted for their use on citrus orchards and assessed using data from a three-year field experiment with two nitrogen application rate treatments in a commercial citrus orchard in the region of Valencia (Spain): a compartmental model using a tipping bucket approach for the water dynamics and a transport model based on the solution of physical equations governing the movement of water and solutes in soils.

After calibration, the compartmental and LEACHN models gave relatively good estimations of soil water content in the whole period. The compartmental model predicted drainage better than the LEACHN model, and the simulated evapotranspiration was similar in both models. With respect to the soil mineral N, the LEACHN model predicted well the measured values for the calibration period in the soil profile (0-80 cm), but for the validation years, this agreement decreased in both N treatments. The compartmental model gave good predictions for the soil mineral nitrogen content, but overpredicted nitrate leaching.

Calibration of the compartmental model is easier than that of LEACHN and this is important if the model is to be used as an advisory tool for crop management in commercial orchards. Improvement of the compartmental model could be done by: a) introducing some algorithms to simulate the N gaseous losses (ammonia volatilization and denitrification), b) modifying the tipping bucket approach to allow for a temporal delay in the water flow from one soil layer to the other and to avoid abrupt changes of drainage in time, and c) accounting for the temperature effects on the nitrogen transformation parameters. The compartmental model has been implemented in a Matlab code and is available for further test and research on request to the authors. The comparison of the observed and predicted values of drainage and nitrate leaching demonstrates that both models, once calibrated, can be used to evaluate different management strategies of irrigation and fertilization to achieve the goal of reducing nitrogen pollution from agricultural sources without reducing yield.

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Table 1
Main characteristics and processes related to water and nitrogen balance and their treatment by the LEACHN and compartmental models.

Processes	LEACHN	Compartmental model
Water related		
Evapotranspiration	Potential ET and considering soil water content, root resistance and root density	Potential ET corrected as a function of soil water content and a minimum soil water storage below which plants cannot extract water
Water flux	Richards' equation; water content and hydraulic conductivity based on Campbell's equation	A function of maximum soil water storage held against gravity. No lateral water flux to or from soil is assumed
Soil hydraulic parameters	The Campbell's coefficients estimated according to Hutson and Wagenet (1991) and saturated hydraulic conductivity estimated by Ahuja and Nielsen method (1991)	Estimated after Saxton et al. (1986) and Lidón et al. (1999)
Runoff	A function of maximum infiltration and the rate of water application	A function of maximum soil water storage
Nitrogen related		
Input	Rainwater, irrigation, fertilization, organic amendments	Rainwater, irrigation, fertilization, organic amendments
Nitrogen pools	Humus, litter, organic amendments, urea, ammonium and nitrate	Humus, litter, microbial biomass, ammonium and nitrate
Plant uptake	A function of N concentration in soil solution and root water uptake	A function of N concentration in soil solution and root water uptake
Mineralization	First order kinetics	Nonlinear kinetics
Nitrification	Depends on a given potential rate and the actual NO_3^-/NH_4^+ ratio	Nonlinear kinetics
Denitrification	First-order process with respect to nitrate concentration	Not considered
N rate constants adjustment	Temperature (Q_{10}), water content	Water content
Leaching	Convection-dispersion equation	Determined by concentration in soil solution and drainage
Adsorption	Adsorption isotherm	Not considered
Volatilization	First order kinetics with respect to ammonium concentration	Not considered

Table 2
Characteristics of the experimental plot.

Crop	
Scion	*Citrus sinensis* L. Osbeck cv. Navelina
Rootstock	*Citrus aurantium* L.
Planting density	453 trees/ha (4.8 m between rows and 4.6 m within rows)
Typical yields	35 to 45 t ha^{-1}
Soil type	Xerofluvent
Tillage	
1 and 3th year	rototiller and cultivator to break the soil surface crust
2 year	non tillage
Irrigation	
Method	flood irrigation in basins (3.5 x 112 m^{2})
Period	April to October (8-10 irrigations)
Average water applied	58 mm (with tillage); 32 mm (non tillage)
Measuring method	Rectangular sharp-crested weir
Fertilizer treatments	
Rate	N1: 150 kg N ha^{-1} year^{-1}; N2: 300 kg N ha^{-1} year^{-1}
Number applications	3 (about April, June and August)
Chemical form	ammonium sulphate
Soil sampling	
Number of samples	three points/tree, in two trees per treatment (Lidón et al., 1999)
Depth	0-30, 30-60 and 60-80 cm
Frequency	6-7 times per annual season
Soil analysis	
Gravimetric moisture	drying the sample at 105 ºC
Nitrate	ultraviolet spectroscopy (Sempere et al., 1993)
Ammonium	Berthelot method (Keeney and Nelson, 1982)
Chloride	saturated paste extract and a Corning Chloride Analyzer 926
Meteorological data	IVIA station (4 km away from experimental site)
Water analysis (average)	
Nitrate in rainfall	5 mg NO_3^- L^{-1}
Chloride in rainfall	12 mg Cl^- L^{-1}
Nitrate in irrigation	83 mg NO_3^- L^{-1} (groundwater), 17 mg NO_3^- L^{-1} (surface water)
Chloride in irrigation	136 mg Cl^- L^{-1} (groundwater), 125 mg Cl^- L^{-1} (surface water)
Others	
N uptake and litter fall	Estimated form Legaz and Primo(1988); Quiñones et al. (2003)

Table 3

Soil physical and chemical properties of the experimental plot.

	Depth (cm)		
Soil properties	0 – 30	30 – 60	60 – 80
Texture (%)			
Sand	67	35	24
Silt	17	35	39
Clay	16	30	37
Textural class (USDA)	sandy loam	clay loam	clay loam
Organic C (g C kg^{-1})	9.0	8.0	8.0
Organic N (g N kg^{-1})	1.0	0.9	0.9
pH (KCl)	7.5	7.5	7.5
CEC ($cmol_c$ kg^{-1})	8.8	12.1	-
Bulk density (Mg m^{-3})	1.25	1.51	1.73

Table 4

Soil hydraulic, crop and nitrogen related parameters values used in LEACHN.

Parameter	Value
Soil hydraulic	
Water retention parameters	
Air entry value (kPa) [a]	-0.840 / -1.960 / -3.070
Exponent in Campbell’s equation [a]	3.59 / 5.91 / 9.33
Crop	
Roots distribution (%) [a]	51 / 40 / 9
Maximum ratio of actual to potential transpiration	1.1
Root resistance	125
Ground cover fraction	0.85
Annual N uptake (kg ha^{-1})	200
Nitrogen [b]	
Partition coefficient NH_4^+-N (L kg^{-1})	2.6
Partition coefficient NO_3^--N (L kg^{-1})	0.0
C/N ratio (biomass and humus)	10
Q_{10}	2.0
Base temperature at which rate constants apply (ºC)	20.0
High end of optimum water content range, air-filled porosity	0.08
Lower end of optimum water content (kPa)	-300
Minimum matric potential for transformations [c] (kPa)	-1500
Relative transformation rate at saturation	0.6
Ammonia volatilization (day^{-1})	0.5
Denitrification half-saturation constant (mg L^{-1})	10.0
Limiting NO_3^-/NH_4^+ ratio in solution for nitrification	8.0

[a] Values for the three soil layers 0-30, 30-60 and 60-80 cm, respectively

[b] All parameter values in the simulations taken from Wagenet and Hutson (1989) or Harrison et al. (1999)

[c] Mineralization, nitrification and volatilization

Table 5

Crop and nitrogen parameters values used in the compartmental model and not subject to calibration.

Parameter	Value
Roots distribution (%)[a]	65 / 30 / 5
Ground cover (%)	0.85
Pan coefficient k_p	0.815
C/N ratio litter	28
C/N ratio humus	10
C/N ratio microbial biomass	8
Microbial biomass death rate (day^{-1})	0.00137

[a] Values for the three soil layers 0-30, 30-60 and 60-80 cm, respectively.

Table 6

Water related parameters, N transformation rate constants obtained after calibration for soil water and mineral nitrogen content.

Variable	LEACHN[a]	Compartmental model[a]
Sat. hydraulic conductivity (mm d^{-1})	4400 / 500 / 132	–
Water storage (mm)		
L_{max}	–	110 / 117 / 70
L_{min}	–	19 / 40 / 37
L_{fc}	–	60 / 60 / 43
L_{crit}	–	34.2 / 60/ 43
Synthesis efficiency factor	0.30	–
Respiration factor	–	0.50
Humification fraction	0.45	0.30
Mineralization rate constants (day^{-1})		
Litter[b]	(2.0 /2.0 /2.0) x 10^{-3}	(0.6 / 4.0 / 4.0) x10^{-3}
Humus[b]	(9.0 / 1.0 / 4.0) x 10^{-5}	(6.8 / 0.04 / 2.0) x10^{-5}
Nitrification rate constants[b] (day^{-1})	(6.0 / 6.0 / 6.0) x 10^{-1}	(6.0 / 0.7 / 0.5) x10^{-1}
Denitrification rate constants (day^{-1})	0.2 / 0.3 / 0.001	–

[a] Values for the three soil layers 0-30, 30-60 and 60-80 cm, respectively.

[b] Although the original units of the compartmental model are different, they have been transformed to those used by the LEACHN model to facilitate comparison.

Table 7

Statistics for the comparison between observed and simulated values for soil water storage (mm) and mineral nitrogen content (kg N ha^{-1}) for the calibration and validation periods in both models.

	Calibration period								**Validation period**	
	0-30 cm		**30-60 cm**		**60-80 cm**		**0-80 cm**		**0-80 cm**	
Statistics	**LEACHN**	**Compartm.**	**LEACHN**	**Compartm.**	**LEACHN**	**Compartm.**	**LEACHN**	**Compartm.**	**LEACHN**	**Compartm.**
Water										
Mean difference	-0.7	0.2	-3.1	2.7	9.1	10.1	-5.0	2.4	-4.0	0.6
RMSE	4.0	5.4	6.8	3.6	9.8	11.0	12.6	9.1	13.7	10.1
RRMSE	0.13	0.18	0.14	0.07	0.20	0.22	0.11	0.08	0.11	0.08
AI	0.95	0.94	0.76	0.91	0.55	0.49	0.87	0.93	0.91	0.95
Nitrogen (N2)										
Mean difference	18.9	6.1	-6.0	-6.5	-4.8	0.8	8.1	0.4	-37.5	-14.8
RMSE	22.8	10.4	6.6	13.8	9.5	7.7	18.4	20.0	68.2	76.2
RRMSE	0.43	0.20	0.24	0.50	0.41	0.33	0.18	0.19	0.36	0.40
AI	0.85	0.97	0.90	0.80	0.33	0.19	0.91	0.93	0.76	0.73
Nitrogen (N1)										
Mean difference	–	–	–	–	–	–	–	–	23.5	15.0
RMSE	–	–	–	–	–	–	–	–	41.5	45.3
RRMSE	–	–	–	–	–	–	–	–	0.39	0.42
AI	–	–	–	–	–	–	–	–	0.61	0.65

Table 8

Water balance components measured and simulated (mm).

Water balance component	Measured		Compartmental model		LEACHN model	
	Periods [a]	**Total (three years)**	**Periods [a]**	**Total (three years)**	**Periods [a]**	**Total (three years)**
***Input*[b]**						
Rainfall	388 / 460 / 222	1070	388 / 460 / 222	1070	388 / 460 / 222	1070
Irrigation	221 / 303 / 413	937	221 / 303 / 413	937	221 / 303 / 413	937
Total input	609 / 763 / 635	2007	609 / 763 / 635	2007	609 / 763 / 635	2007
Output						
ET	489 / 630 / 566 [c]	1685 [c]	471 / 575 / 566	1613	499 / 629 / 626	1754
Drainage	128 / 110 / 78	316	123 / 125 / 68	316	122 / 100 / 20	242
Runoff	–	–	37 / 39 / 0	76	5 / 3/ 3	11
Total output	617 / 740 / 644	2001	631 / 739 / 634	2005	626 / 732 / 649	2007
Change						
Δ Soil water	-8 / 23 / -9	6	-22 / 24 / 1	3	-18 / 31 / -14	-1

[a] 31 May 91 – 10 April 92 / 11 April 92 – 5 April 93/ 6 April 93– 3 March 94

[b] Rainfall and Irrigation data are inputs to both models and equal to the measured values.

[c] Calculated by water balance assuming that runoff is negligible

Table 9

Nitrogen balance for the low (N1) and high (N2) fertilization rate treatments (kg N ha^{-1}).

N balance component	Measured		Compartmental model		LEACHN model	
	Periods [a]	Total (three years)	Periods [a]	Total (three years)	Periods [a]	Total (three years)
N1 treatment						
Input						
Rainfall	4 / 5 / 2	11	4 / 5 / 2	11	4 / 5 / 2	11
Irrigation	25 / 10 / 16	51	25 / 10 / 16	51	25 / 10 / 16	51
Fertilizer	30 / 170 / 150	350	30 / 170 / 150	350	30 / 170 / 150	350
Mineralization	–	–	75 / 119 / 116	310	119 / 133 / 123	375
Output						
Plant uptake	–	–	152 / 182 / 162	496	169 / 205 / 199	573
Leaching	44 / 42 / 37	123	49 / 98 / 49	196	45 / 62 / 13	120
Volatilization	–	–	–	–	5 / 18 / 18	41
Denitrification	–	–	–	–	3 / 8 / 1	12
Change						
Δ Nmin	-11 / 20 / 31	40	-67 / 24 / 73	30	-45 / 25 / 59	39
N2 treatment						
Input						
Rainfall	4 / 5 / 2	11	4 / 5 / 2	11	4 / 5 / 2	11
Irrigation	25 / 10 / 16	51	25 / 10 / 16	51	25 / 10 / 16	51
Fertilizer	80 / 320 / 300	700	80 / 320 / 300	700	80 / 320 / 300	700
Mineralization	–	–	62 / 63 / 91	216	118 / 133 / 123	374
Output						
Plant uptake	–	–	109 / 335 / 318	514	173 / 204 / 200	577
Leaching	68 / 73 / 77	218	72 / 171 / 82	325	66 / 126 / 36	228
Volatilization	–	–	–	–	10 / 37 / 36	83
Denitrification	–	–	–	–	7 / 22 / 4	33
Change						
Δ Nmin	-11 / 21 / 160	170	-57 / 38 / 158	139	-29 / 77 / 165	213

[a] 31 May 91 – 10 April 92 / 11 April 92 – 5 April 93/ 6 April 93– 3 March 94

Table 10

Different scenarios evaluated with LEACHN and compartmental model in a three year period.

Scenario	Management	N rate fertilization (kg N ha^{-1} $year^{-1}$)	Number of applications	Chemical form [a]	Irrigation (mm) (three years)
Sc0	Conventional fertilization and irrigation	300	3	AS	937
Sc1	Conventional fertilization and increased irrigation (+10%)	300	3	AS	1031
Sc2	Conventional fertilization and reduced irrigation (-10%)	300	3	AS	843
Sc3	Reduced fertilization (-10%)	270	3	AS	937
Sc4	Reduced fertilization (-10%) and two chemical forms	270	3	AS - AN	937
Sc5	Reduced fertilization (-10%), two chemical forms and increased number of applications	270	4	AS - AN	937
Sc6	Reduced fertilization (-10%) and reduced irrigation (-10%)	270	3	AS	843
Sc7	Rate fertilization according to VCGAP	230	3	AS	937
Sc8	Rate fertilization according to VCGAP and two chemical forms	230	3	AS - AN	937
Sc9	Rate fertilization according to VCGAP, two chemical forms and increased number of applications	230	4	AS - AN	937
Sc10	Rate fertilization according to VCGAP and reduced irrigation (-10%)	230	3	AS	843

[a] AS = ammonium sulphate; AN = ammonium nitrate; VCGAP = Valencian Code of Good Agricultural Practices

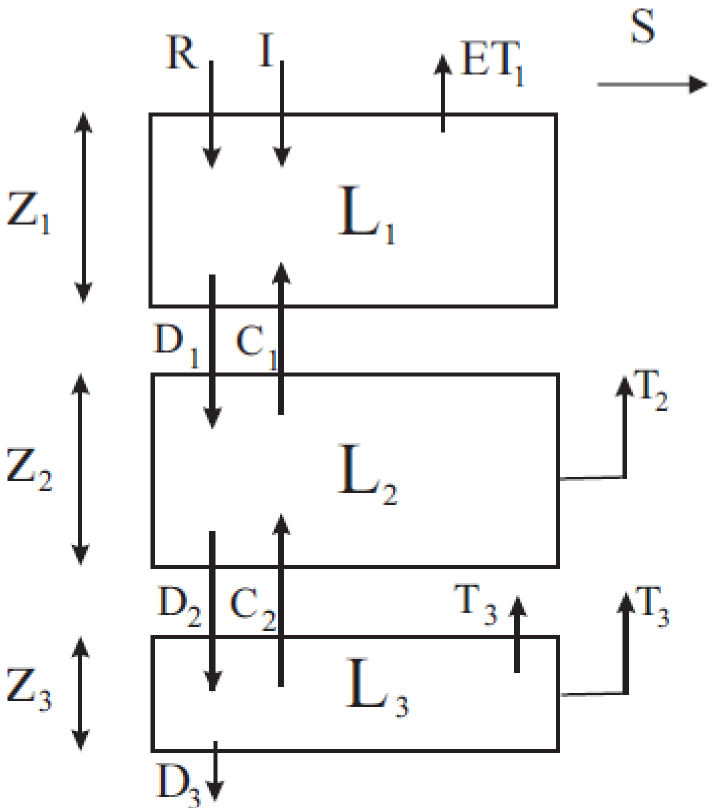

Fig. 1. Three layers soil water module. R indicates rainfall, I irrigation, S runoff, ET_1 evapotranspiration in layer one, T_2 and T_3 transpiration in layers two and three, L_1, L_2 and L_3 soil water content in each layer, D_1 D_2 and D_3 drainage in each layer and C_1 and C_2 capillary rise.

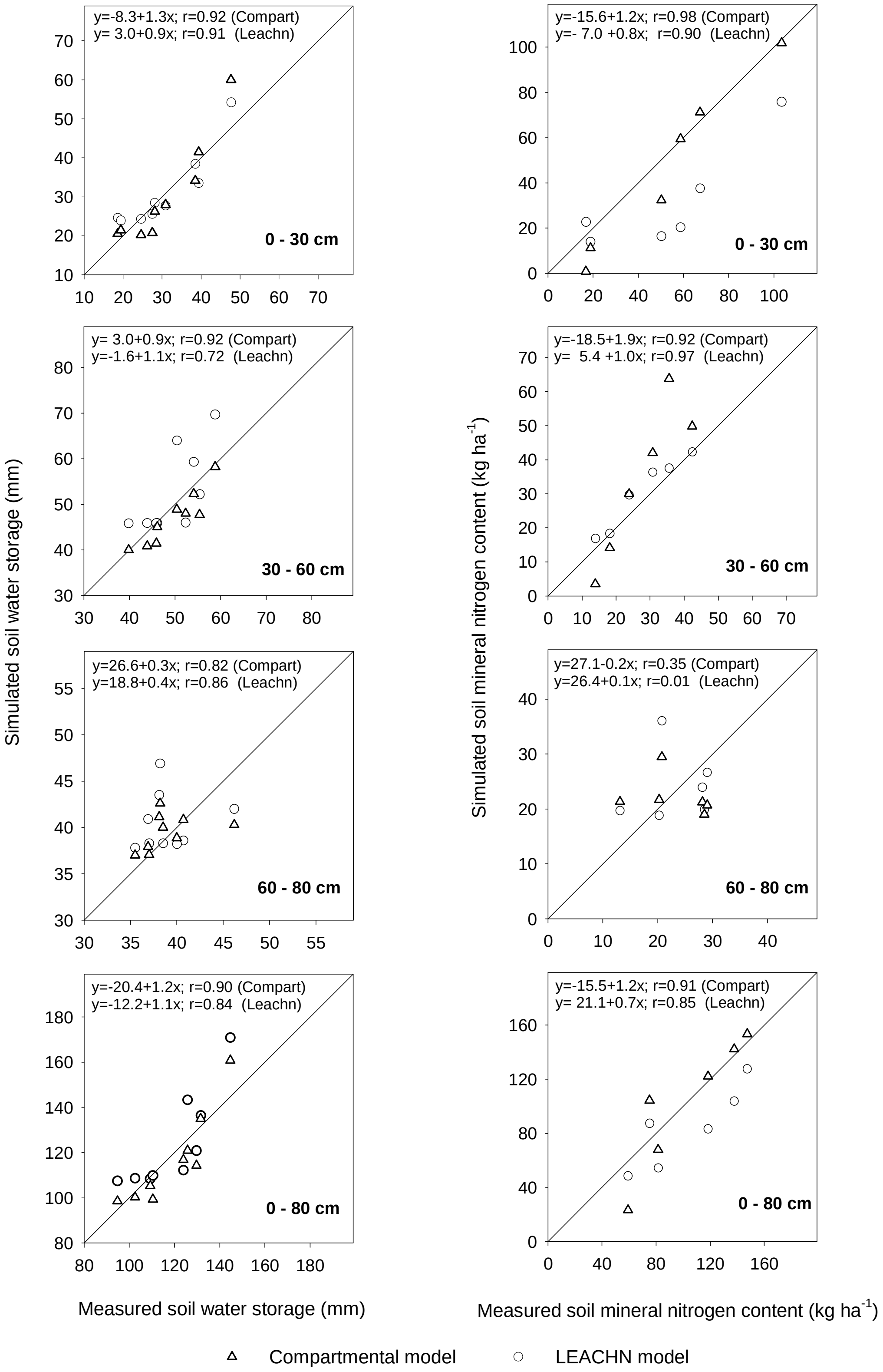

Fig. 2. 1:1 plot and regression of measured and simulated soil water storage (left) and soil mineral nitrogen values (right) in each soil layer after model calibration (using data from first year and high nitrogen fertilizer rate, N2).

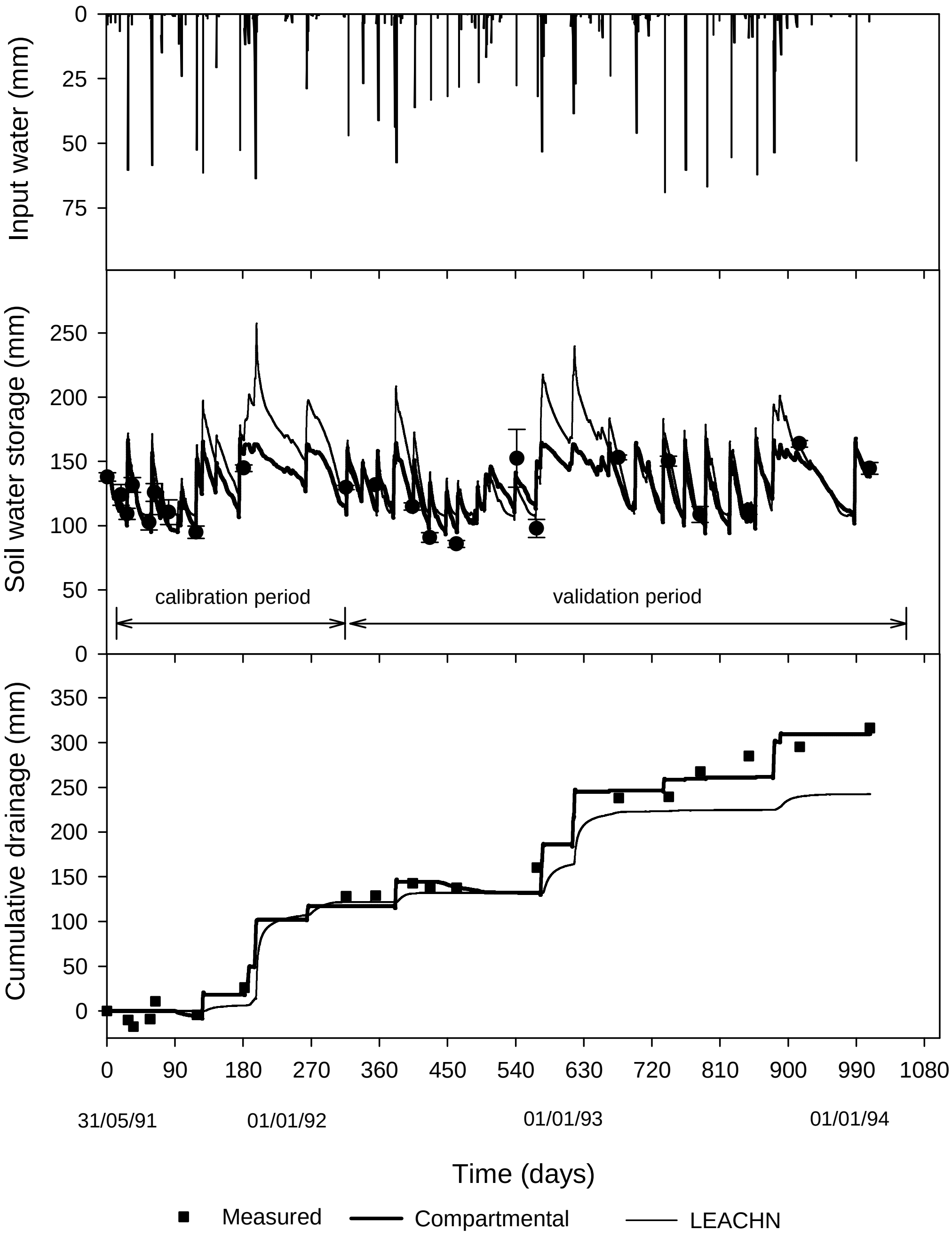

Fig. 3. Soil water storage and cumulative drainage measured at 80 cm depth and simulated with LEACHN and with the compartmental model during the calibration period (first year) and validation period (second and third year). At the top, water input by rainfall and irrigation. Each data of soil water content is the average of four points (see table 2). Vertical bars represent the standard error.

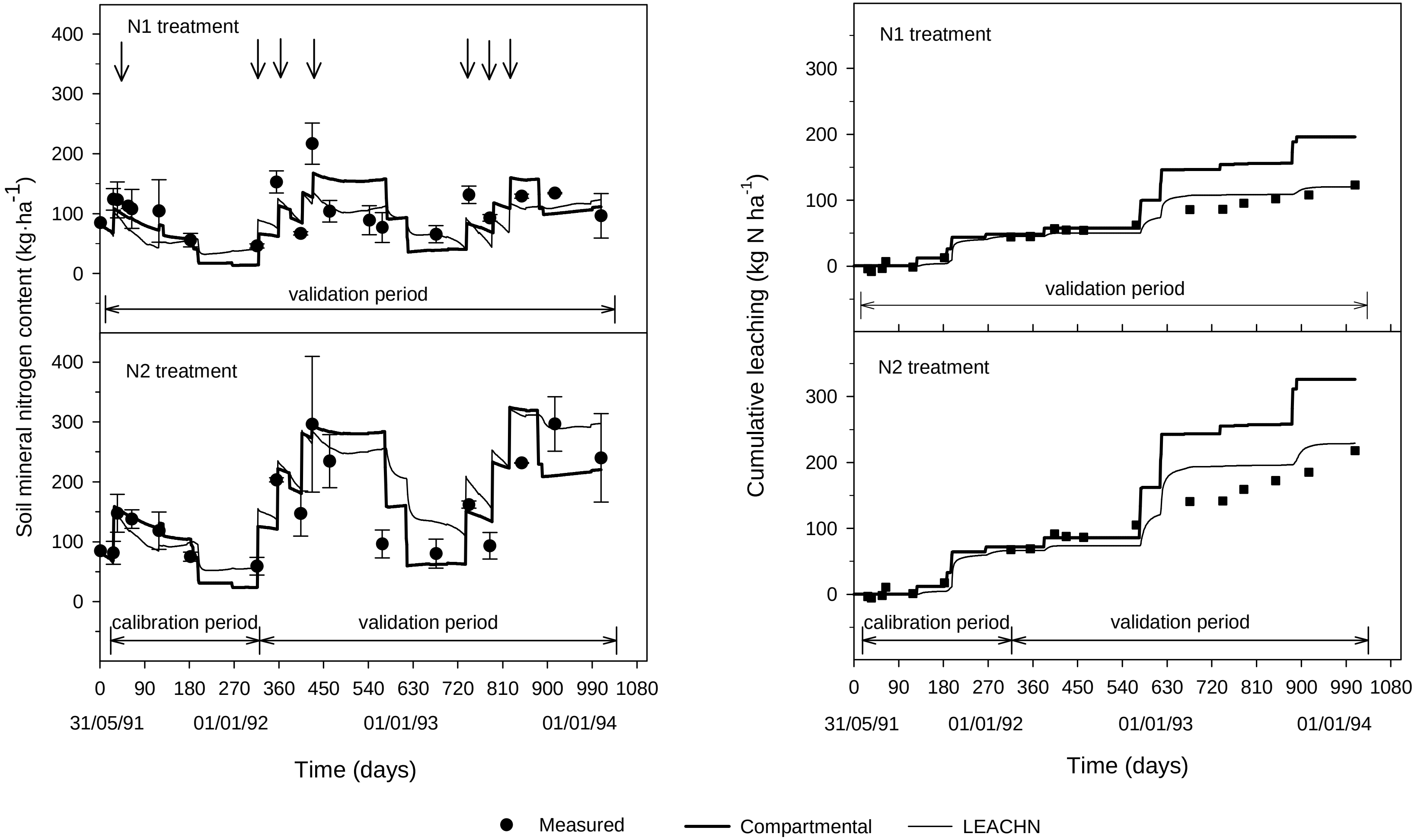

Fig. 4. Mineral nitrogen content in the soil profile and cumulative nitrate leaching at 80 cm soil depth measured and simulated with the LEACHN and the compartmental models during the calibration and validation periods in treatments N1 and N2. The arrows indicate the fertilizer applications in both treatments. Each data of Nmin is the average of two points (see table 2). Vertical bars represent the standard error.

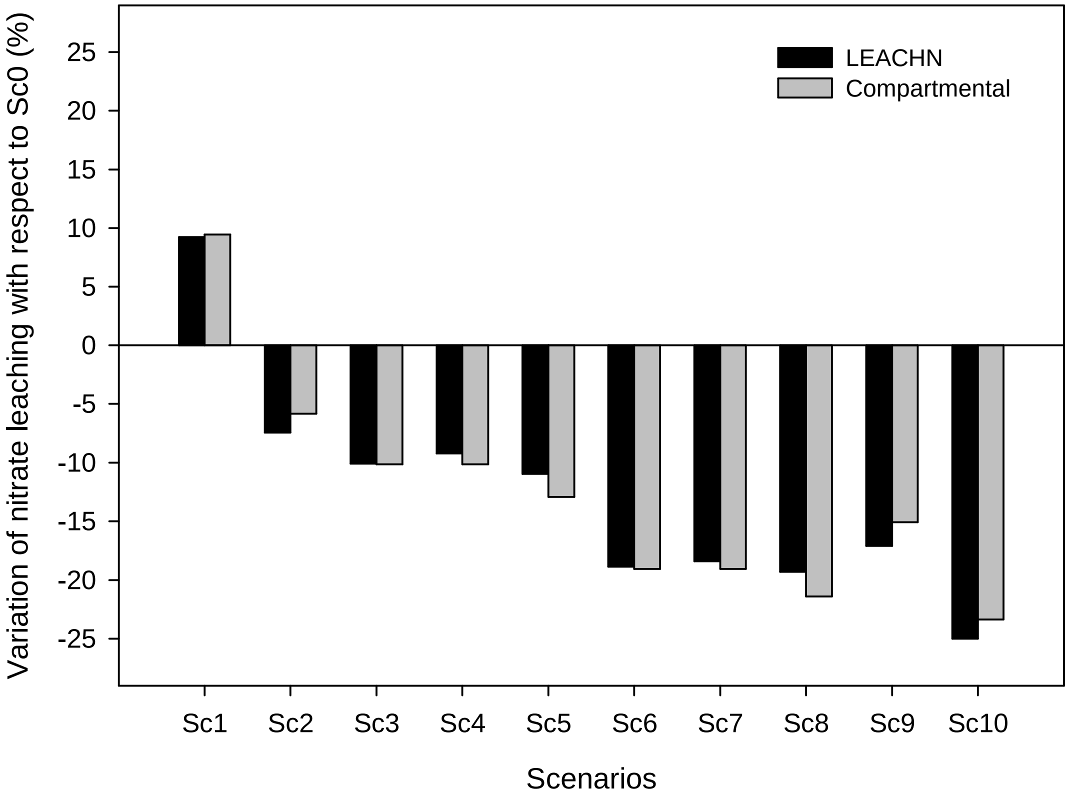

Fig. 5. Variation in nitrate leaching simulated with both models under the different fertilization and irrigation management scenarios assessed (see Table 10).