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N fate and transport under variable cropping history and fertilizer rate on loamy sand and clay loam soils: I. Calibration of the LEACHMN model

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Abstract

The need for efficient use of agricultural chemicals and their potential adverse impact on critical water resources have increased the use of simulation models of the soil and plant system. Nevertheless, there is currently little or no agreement concerning model validity and applicability in varied soils and environments. The research version of LEACHMN (the N subroutine of LEACHM) was calibrated using field data including soil physical, hydraulic, and chemical properties, and maize (*Zea mays* L.) N uptake collected from a 3-yr nitrate leaching experiment. The field site consisted of plot-size lysimeters on clay loam and loamy sand soils with N fertilizer rates of 22, 100 and 134 kg N ha^{-1}. The calibration involved adjusting nitrification, denitrification, and volatilization rate constants to optimize the fit between predicted and measured data. When calibrated for each treatment-year combination and soil type, the model simulations of soil profile NO_3–N distribution were generally successful. The N transformation rate constants yielded by the calibration efforts were similar or close to those used in other model simulation studies. At both sites, the calibrated rate constants for the first year (following sod plowdown) were different from those for the subsequent two years. Denitrification rate constants were consistently higher for the clay site than for the sand site, while the nitrification rate constants were lower. N rate of application appeared not to affect the rate constants within each year-site combination, suggesting that cropping history and soil type had the greatest effect on N transformation rates.

Introduction

Concern has increased about the potential for lake, stream, and aquifer contamination by chemicals applied to farmlands. Studies using tile lines and lysimeters to collect drainage water have been conducted to address fertilizer N use efficiency, nitrate leaching, and water quality related issues (Angle et al., 1993; Magdoff et al., 1984; Randall et al., 1997; Roth and Fox, 1990; Saragoni et al., 1991). These studies are useful for assessing the impact of agricultural management practices on groundwater quality. However, the application of most of these research results may still remain inadequate primarily because of the complexity associated with nitrate dynamics in the soil-plant-atmosphere system and water flow through the soil profile (Kladivko et al., 1991; van Es et al., 1991). Addiscott et al. (1991) concluded that, as many physical, chemical and biological processes affecting soil nitrate can happen practically at once, any attempt at a simultaneous description of the process requires an explicit, often computer-based, model.

One of the uses to which models are frequently put is the prediction of nitrate leaching and other processes in circumstances in which they cannot be measured (Addiscott et al., 1991). Notable recent N modeling research include that by Addiscott and Whitmore (1987); Bergstrom and Jarvis (1991); Bergstrom et al. (1991); Hutson and Wagenet (1991); Molina et al. (1983) and Ramos and Carbonell (1991). Other research has focused on simulating organic matter transformations (Van der Linden et al., 1987; Wolf and van Keulen, 1989); crop yield and N uptake (Clay et al., 1985b); manure-N dynamics (Borg et al., 1990); and tillage effects (Clay et al., 1985a). Nitrogen models range in degree of sophistication from

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simple empirical equations to complex mechanistic computer simulation models (Bergstrom et al., 1991). As model predictions improve, they may guide application of water and agricultural chemicals, or be used as regulatory tools (Pennell et al., 1990). It is necessary to understand which types of mathematical models should be used to describe specific processes and to establish criteria for model validity (Saleh et al., 1990).

LEACHM (Hutson and Wagenet, 1992) is a process-based, one-dimensional model that simulates water and solute movement, and related chemical and biological processes, in the unsaturated soil. LEACHMN, the version of LEACHM that addresses N dynamics, was selected in this study because it has subroutines to calculate water flow, NO_3 leaching, evapotranspiration, heat flow, N transformations and uptake, and plant growth. The major N transformation processes modeled by LEACHMN are:

(1) a mineralization reaction for each organic pool, including urea,

$$\mathrm{d}Ni/\mathrm{d}t = -k_{\mathrm{mi}}Ni \tag{1}$$

where *Ni* represents the concentration of humus-N, litter-N, faeces-N or urea-N in the soil, and k_{mi} are first-order rate constants;

(2) nitrification, which proceeds at a potential rate $k_{\mathrm{nit}}N_{\mathrm{NH4}}$ decreasing as a maximum NO_3^-/NH_4 concentration ratio $r_{\max}$ (Johnsson et al., 1987) is approached,

$$\mathrm{dNH_4}/\mathrm{d}t = -k_{\mathrm{nit}}\max(O, (N_{\mathrm{NH_4}} - N_{\mathrm{NO_3}}/r_{\max})); \tag{2}$$

(3) denitrification, which follows Michaelis–Menten kinetics,

$$\mathrm{d}N_{\mathrm{NO_3}}/\mathrm{d}t = -k_{\mathrm{denit}}N_{\mathrm{NO_3}}/(N_{\mathrm{NO_3}} + \mathrm{C_{sat}}), \tag{3}$$

where k_{denit} is a potential rate and c_{sat} is a half-saturation constant;

(4) volatilization, a first-order process of NH_4 loss from the surface layer,

$$\mathrm{d}N_{\mathrm{NH_4}}/\mathrm{d}t = -k_{\mathrm{volat}}N_{\mathrm{NH_4}}. \tag{4}$$

The constants k_{mi}, k_{nit} and k_{denit} are adjusted for temperature and water content effects (Johnsson et al., 1987). A Q_{10}-type response is assumed for temperature, while rate constant values decrease on either side of an optimum range of water content, except for denitrification, which increases with increasing water content.

Maize N uptake simulation is based on root distribution and a logistic N uptake curve. Annual N uptake (total uptake from emergence to harvest) is an input requirement, and also sets the maximum simulated N uptake. The water flow may be simulated based on field-measured values of hydraulic conductivity and soil water retention (research version of the model), or predicted values of these properties through pedotransfer functions based on bulk density and particle size information (management version). Equations and descriptions of the processes in the model are presented in Borg et al. (1990) and Hutson and Wagenet (1992).

The LEACHM model has been evaluated in several model simulation studies. Lotse et al. (1992) used LEACHMN to predict leachate nitrate concentrations, soil nitrate distribution, and plant uptake in non-manured and manured field sites (Duffield silt loam and Clarksburg silt loam) in southern Pennsylvania. They performed sensitivity analyses of the N transformations of the model. Jabro et al. (1994) tested LEACHM predictions of bromide leaching against field measured data in southeastern Pennsylvania. They concluded that the model performed adequately under preferential flow conditions, perhaps because the infiltration rate at eaach site was used as a model input. In their evaluation study of LEACHMN, Jemison et al. (1994b) found that when calibrated for each treatment and year, LEACHMN-predicted and observed NO_3–N leaching losses were similar, but predictions were not satisfactory without such calibration.

The primary objective of this study was to calibrate the LEACHMN model for nitrification, denitrification, and volatilization rate constants using measured data from a 3-yr field study involving sod plowdown followed by maize production under three N fertilizer rates on clay loam and loamy sand soils. The performance of the calibrated model in simulating nitrate leaching and maize N uptake is discussed in a companion paper (Sogbedji et al., 2000c).

Materials and methods

Experimental sites

The study was conducted at the Cornell University Experimental Farm at Willsboro, New York (44° 22′ N, 73° 26′ W) on two experimental sites of different soil types at a distance of approximately 1 km. One site is on a Muskellunge sandy clay loam (fine, mixed, frigid, Aeric Ochraqualf) with a total silt plus clay content of approximately 69% at 0.18 m depth and values above 80% at 0.35–1.30 m depth. The soil developed from glacio-lacustrine parent material, and is somewhat poorly drained in its natural state. The other site is on a Stafford fine sandy loam (mixed, mesic typic Psammaquent), a somewhat poorly drained soil formed in glacial outwash material with a total sand content of approximately 85% at 0.18 m depth. It is underlain by a glacio-lacustrine clay at depths ranging from 0.6 to 1.5 m.

Each site contains 16 plots in a four-by-four pattern (Figure 1), each of which is surrounded by 0.8 mm-thick impermeable pvc geomembrane to a depth of 1.8 m to make them hydrologically independent. On the clay loam, plots were of 18 × 18 m size and included perimeter drains which drained to a central drain line (Figure 1). On the loamy sand, plots were 14 × 14 m and, because of their smaller size and higher hydraulic conductivity, included only a central drain line. All drain lines were installed at 0.9 m depth. Since each plot was underlain by a very slowly-permeable clay layer, they functioned effectively as plot-size lysimeters (Figure 2). The central drain line of two adjacent plots extended towards each other outside the plot boundaries into a manhole midway between the two plots, allowing for sampling of drainage water (Figure 1). Within each manhole, valves were installed at the end of each drain line, permitting the imposition of two hydrologic regimes on the plots: a dry regime in which the drains were left unobstructed, and a wet regime in which the valves were completely closed. In this study, only data from plots with the dry hydrologic regime (eight for each soil type) were used (Figure 1), as the other treatments did not allow for continuous drain sampling.

Crop, soil and drainage water management

A 3-year-old alfalfa (*Medicago sativa*) sod was moldboard plowed in the fall of 1991 on the clay loam, and maize was planted after disking on May 13, 1992. On the loamy sand, a 20-year grass sod (primarily fescue, *Festuca rubra*) was moldboard plowed in the Spring of 1992, and maize was similarly planted after disking on May 13, 1992. For the second and third years (1993 and 1994) of the study, the clay and sand sites were again fall-plowed and spring-plowed, respectively, and maize was planted on May 11, 1993, and May 12, 1994 at both sites. In each of the three years, maize (CV. Funk G4070) was planted at the density of 70 000 plants ha^{-1}. Cornell University-recommended crop management practices were used.

Three fertilizer rates were applied to the plots at each site. A low rate consisting of only starter fertilizer (22 kg N ha^{-1}), an intermediate rate based on a pre-sidedress nitrate test (PSNT, Magdoff, 1991), and a high rate of 134 kg N ha^{-1} (22 kg N ha^{-1} starter plus 112 kg N ha^{-1} sidedress). The intermediate, PSNT-based, N rate was 100 kg N ha^{-1} (22 kg N ha^{-1} as starter plus 78 kg N ha^{-1} as sidedress) in five out of six site-year combinations. In 1992 on the clay loam following alfalfa plowdown, the PSNT-recommended sidedress rate was zero (i.e. identical to the starter-only treatment). In the quantitative analysis of this experiment, the PSNT-based rate was therefore considered fixed at 100 kg N ha^{-1} with missing data for one site-year. The highest rate was Cornell University's recommended rate for those soil types in fourth-year continuous maize, and therefore was intended to represent an eventual maximum N recommendation. All starter N fertilizer applications were banded at planting. All sidedressed N was delivered as urea ammonium nitrate (UAN) 8 cm below the soil surface between alternate maize rows by a John Blue (Huntsville, Alabama) injector approximately 6 weeks after planting.

The two hydrologic regimes and three fertilizer N rates were crossed in a spatially-balanced complete block design (van Es and van Es, 1993) with three replicates for each combination, except the 22 kg N ha^{-1} treatment which was replicated twice at each site (Figure 1).

During the course of the study, drain line flow rate was determined and effluent samples were obtained at least weekly when drains were flowing and more intensively (up to every 4 h) during the growing season.

The LEACHMN model input data

Input data required for the research version of LEACHMN include soil physical and chemical properties for various depth increments, and weather and crop data. The soil physical properties include: saturated hydraulic conductivity, bulk density, and water retention curve. The soil chemical properties include: soil initial organic carbon, NO_3–N, and total N. The soil profile was segmented into 9 layers of 0.1 m thick.

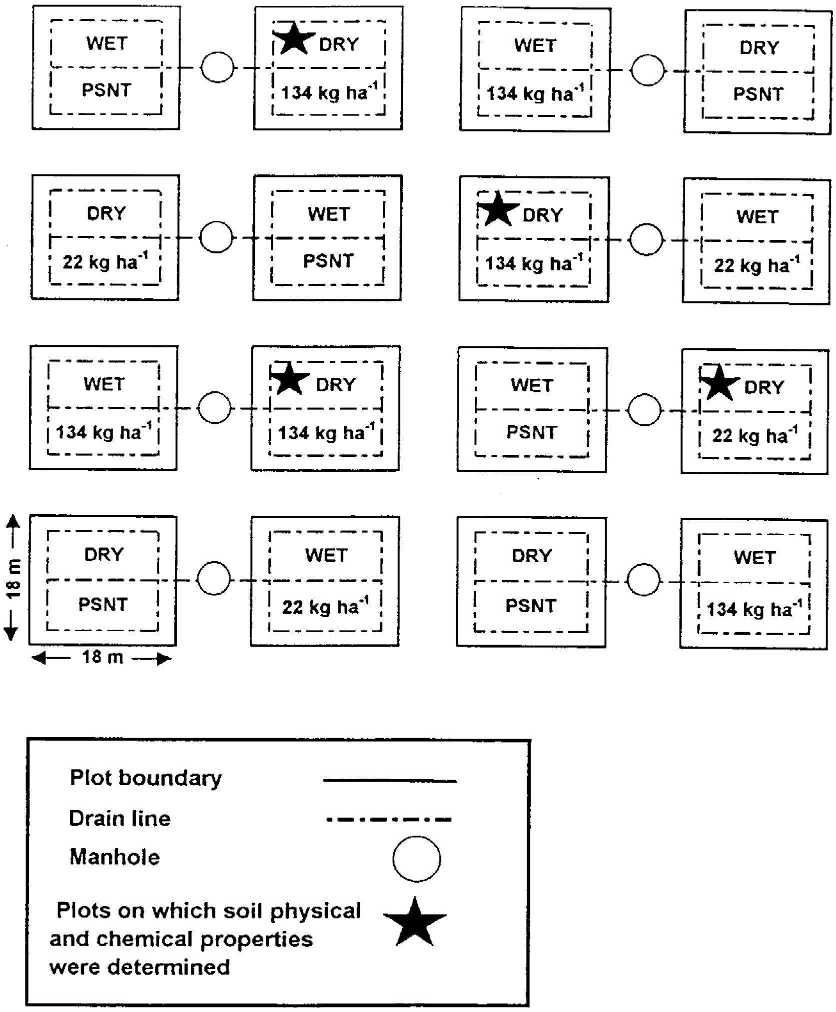

Figure 1. Plot lay out and experimental design for the clay loam site. For the loamy sand site, plot lay out and experimental design were identical except for the size of the plot (14 × 14 m).

At each of the two sites, four of the eight plots were selected (Figure 1) on which soil physical properties were determined. From each of the selected plots, undisturbed cores were collected at each depth increment using a tractor-mounted Giddings hydraulic soil coring and sampling device (Giddings Machine Co., Fort Collins CO 80522, USA). On the clay loam, a 1 m long × 5 cm dia. soil tube with a butyrate plastic liner was used. This was pushed into the soil to obtain a single continuous sample which was then sectioned into samples of 10 cm length. On the loamy sand, excavations of the profile were made to appropriate depths and the machine was used to take the undisturbed samples with a Uhland-type sampler and aluminum sample rings (76 mm inner dia. 76 mm height).

At both sites, composites of 32 soil subsamples were collected at depth intervals of 0–15, 15–30, 30–60 and 60–90 cm to determine initial soil NO_3–N, total N and organic C contents. The model-required soil properties and the used methodologies are presented in Table 1. The water flow model in LEACHMN requires equations relating volume fractional water content, pressure potential and hydraulic conductivity. Currently, the model uses functions based on those proposed by Campbell (1974), and has a subroutine to calculate the Campbell's water retention equation parameters from measured values of bulk density and saturated hydraulic conductivity.

Crop information required to predict plant N uptake include planting, emergence, maturity and harvest

Table 1. Measurement methods for soil physical and chemical properties used for LEACHMN

Soil properties	Measurement methods
Chemical properties	
Initial soil nitrate content	Cornell University Nutrient Analysis
Initial total soil N content	Laboratories (1989)
Initial organic carbon content	Wet oxidation diffusion procedure (Synder and Trofymow, 1984)
Physical properties	
Water retention curve	Pressure plate method (Klute, 1986)
Bulk density	Core methods (Blake and Hartge, 1986)
Hydraulic conductivity	Constant head methods (Klute and Dirksen, 1986)
Particle size distribution	Pipet methods (Gee and Bauder, 1986)

Table 2. LEACHMN parameter input values used in the simulations

Parameter *	Input values
Partition coefficient, NH_4–N	3.0 L kg^{-1}
Partition coefficient, NO_3–N	0.0 L kg^{-1}
Denitrification half saturation constant	10 mg L^{-1}
Litter mineralization rate constant	0.01 day^{-1}
Humus mineralization rate constant	7×10^{-5} day^{-1}
Q10 factor	2.0
C:N ratio for biomass and humus	10.0
Maximum NO_3/NH_4^- ratio in solution to control nitrification rate	8.0

*All parameter values in the simulations came from Wagenet and Hutson (1992), Jansson and Anderson (1988) or Johnsson et al. (1987).

dates, rooting depth and annual N uptake which were collected for each plot at the two experimental sites (Table 2). Maize N uptake was estimated from silage yield (kg ha^{-1}) multiplied by the N content. For silage yield, two 6-m long rows of maize from the center of each plot were harvested, a subsample of three plants per plot was oven dried at 65°C to determine moisture content, and yields were adjusted to 65% dry mass (kg ha^{-1}). A subsample of the dried matter was ground and analyzed for total Kjeldahl-N analysis (Cornell University Nutrient Analysis Laboratories, 1989).

Daily precipitation, total weekly potential evapotranspiration, mean weekly air temperature, and mean weekly amplitude of air temperature were measured at the research farm meteorological station managed by the Northeast Regional Climate Center at Cornell University.

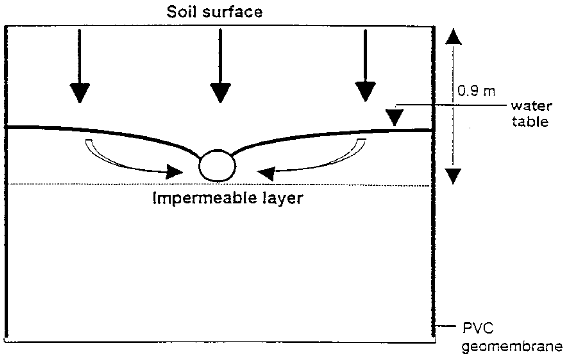

Figure 2. Cross-sectional view of a lysimeter plot (on the loamy sand).

Hutson and Wagenet (1991) performed sensitivity analyses of the LEACHMN model, and discussed how assumptions regarding rate constant values influenced simulated residual nitrate distributions and organic N one year after incorporation of organic matter (litter) in the profile. They reported in the LEACHMN manual (Hutson and Wagenet, 1992), similarly to Lotse et al. (1992), that the model output was affected by slight increases or decreases in nitrification, denitrification and volatilization rates, but it was less sensitive to changes in the mineralization rate and suggested a default value for humus mineralization rate constant. Their default value for humus mineralization rate constant (Table 2) was used in this study, as the context of their sensitivity analyses in terms of organic source of N was reasonably similar to the context of this study.

All model parameter input values (Table 2) except those adjusted in the calibration procedure were selected from Hutson and Wagenet (1992), Jansson and Anderson (1988), or Johnsson et al. (1987). The model was calibrated for each treatment in each of the three years of the study at both sites. The calibration was done based on measured mean values of growing season soil profile nitrate distribution under each N treatment at each site. At both sites, soil NO_3–N was monitored monthly during the three growing seasons at depth intervals of 0–15, 15–30, 30–60 and 60–90 cm in 1992 and 1993, and 0–15 and 15-30 cm in 1994. Soil profile NO_3–N was determined calorimetrically by automated hydrazine reduction (Cornell Nutrient Analysis Laboratories, 1987, 1989) for each depth interval from the composite of four cores per plot.

Model calibration

With the collected input data under each N treatment in each year at each of the two experimental sites, multiple runs of the model were performed in which the specific rate constants were adjusted. Simulations covered the growing season of each of the three years of study at both sites. The calibration consisted of slight increases or decreases of each rate constant within an expected range of values during each run, and was completed when adjustments to the specific rate constants no longer reduced the difference between measured mean and simulated values of soil profile NO_3–N distribution or increased the coefficients of correlation. Graphical and statistical methods (Loague and Green, 1991) were used to assess the calibrated model simulations' accuracy. Measured mean and simulated values of soil profile NO_3–N distribution were plotted on 1:1 scale to examine their trends. The statistical measures included root mean square error (RMSE) and normalized root mean square error (NRMSE) defined as:

$$\mathrm{RMSE} = \Big[\sum_{i=l}^{n}(\text{measured} - \text{predicted})^2/n\Big]^{0.5}$$

$$\mathrm{NRMSE} = \mathrm{RMSE}/\text{measured grand mean}$$

where n is the number of observations.

No adjustment was performed for the model-predicted soil water retentivity parameters, as these were determined directly from undisturbed field soil cores. In the simulations, the free drainage boundary conditions option of the model was used. This assumes that once the bottom layer of the profile is at saturation, any further water percolate from the profile that reaches this layer is subject to drainage. In this study, the bottom boundary conditions of the experimental plots did not exactly match this principle of the model in simulating water flow to a drain line, as a two-dimensional water flow to the drain line and some deep percolation (although presumably small) occurred at the bottom of the plots. These effects on measured drainage water flow rate and volume were assumed to be minor because: (1) a dense clay layer underlies the experimental plots at each site (Figure 2), which causes most percolating water to exit the plots through the drain lines; (2) the maximum horizontal distance to the drain lines was small (3 and 6.8 m for the clay loam and loamy sand, respectively), which minimizes the time effect of two-dimensional flow at the bottom of the plots. When plotted against time, measured and LEACHMN-predicted drainage water flow rates at both sites (Figure 3) followed a similar trend in time and space in each of the three years of study, indicating that the presumed effects of the bottom boundary conditions of the experimental plots were insignificant.

Results and discussions

LEACHMN input data

At both sites, the saturated hydraulic conductivity (geometric mean values) varied between depth increments and the variability appeared to be higher on the loamy sand than on the clay loam (Table 3). As a general trend at both sites, values were consistently highest for the top 0.40 m compared to the other depth increments of the 0.90 m soil profile, and lowest for the bottom layers. This pattern in the distribution of the saturated hydraulic conductivity was supported by the soil texture data (Table 3), as being the result of a high clay content layer at the bottom of the soil profile at each site. Overall, the saturated hydraulic conductivity values were consistently higher on the loamy sand site than on the clay loam (Table 3). Saturated water content and water retentivity were lower on the loamy sand compared to those on the clay loam. Nevertheless, for the bottom layer, saturated water content and water retentivity appeared to be similar for the two soil types, indicating the presence of a dense clay layer at the bottom of the 0.90 m soil profile at each site. Bulk density values were lowest for the top layer at the two sites (Table 3), and for the remaining depth intervals of the soil profile, values were generally similar for the clay site, but varied slightly for the loamy sand site due to layering in the glacial outwash material.

Plant N uptake varied between treatments and years at both sites (Table 4). On the loamy sand, N uptake mean values were consistently lowest, intermediate, and highest for the 22, 134 and 100 kg N ha^{-1} treatments, respectively. Differences between the 100 and 134 kg N ha^{-1} rates were nonsignificant. For the 1992 and 1993 years, N uptake values were identical, but lower compared to those in 1994 under each of the three treatments. On the clay loam, plant N uptake consistently increased with increasing N rate, and was consistently highest, intermediate, and lowest in 1992, 1994 and 1993, respectively. Among soil types, plant N uptake did not display any consistent pattern. However, N uptake was higher on the clay loam in 1992 than on the loamy sand, presumably as the result

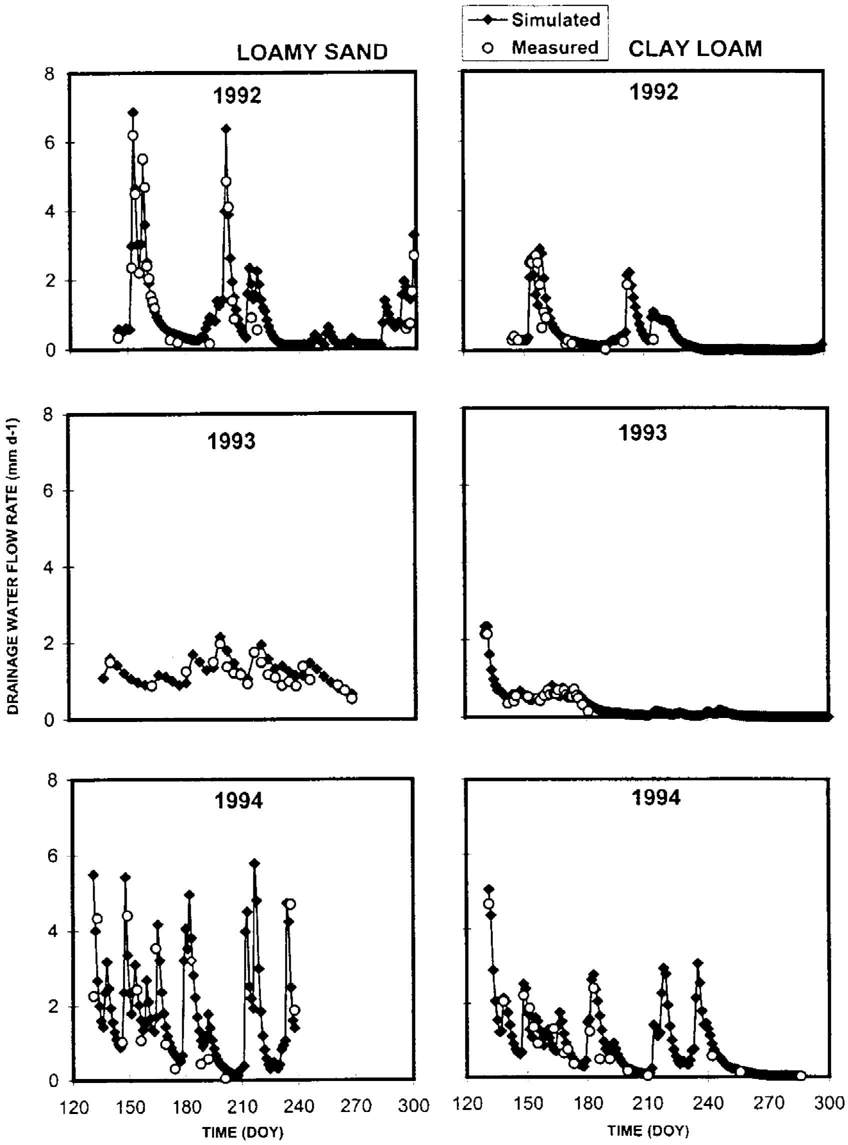

Figure 3. Measured and LEACHMN-predicted values of drainage water flow rate for clay loam and loamy sand.

of higher initial soil NO_3–N on the clay loam due to recent sod plowing (Table 5).

Initial soil NO_3–N greatly varied between treatments, years, and sites (Table 5). In 1992, initial NO_3–N was higher than that in the other two years at both sites because of sod plowdown. On the clay loam, initial soil NO_3–N consistently decreased from 1992 to 1994, but did not follow any trend on the loamy sand.

Model calibration

The calibrated N transformation rate constants and associated N fluxes are presented in Table 6. The rate constants were similar or close to those used in other model evaluation studies. Hutson and Wagenet (1992) suggested values of 0.20 and 0.10 d^{-1} for nitrification and denitrification, respectively, in the LEACHM manual. Johnsson et al. (1987) and Jansson and Anderson (1988) in their work with the SOILN model used 0.10 and 0.20 d^{-1} for their denitrification rate constant, and 0.20 d^{-1} for their nitrification

Table 3. Physical properties for the clay loam and loamy sand as used in the model simulations

Depth (cm)	Bulk density (Mg m^{-3})	Particle size (%)			Saturated hydraulic Conductivity (mm d^{-1})	Campbell equation retentivity parameters		Water content, m^3 m^{-3} at pressures (kpa)					
		Sand	Silt	Clay		a	b	1	10	40	100	300	1500
Clay loam													
5	1.16	44.5	17.1	38.4	5471	−0.26	7.40	0.47	0.34	0.32	0.23	0.19	0.17
15	1.43	42.3	15.3	42.4	7413	−0.30	12.00	0.40	0.36	0.34	0.28	0.24	0.22
25	1.53	29.3	16.8	53.9	1360	−4.89	12.00	0.43	0.39	0.38	0.35	0.31	0.27
35	1.49	12.2	26.4	60.8	1176	−4.89	12.00	0.45	0.43	0.41	0.39	0.34	0.31
45	1.51	4.8	27.5	67.7	446	−4.89	12.00	0.42	0.40	0.38	0.36	0.34	0.31
55	1.51				905	−4.89	12.00	0.45	0.43	0.42	0.41	0.37	0.34
65	1.52	6.6	24.1	69.3	109	−4.89	12.00	0.45	0.42	0.41	0.40	0.38	0.34
75	1.55				52	−4.89	12.00	0.44	0.42	0.41	0.39	0.35	0.32
85	1.57	3.2	16.4	80.4	446	−4.89	12.00	0.45	0.43	0.41	0.39	0.37	0.34
Loamy sand													
5	1.25	79.8	10.1	10.1	10163	−0.52	3.87	0.45	0.25	0.21	0.15	0.08	0.07
15	1.52	80.6	10.0	9.4	24614	−0.95	4.38	0.38	0.25	0.22	0.10	0.09	0.08
25	1.55	86.9	5.8	7.3	5346	−0.60	4.61	0.35	0.23	0.21	0.09	0.07	0.06
35	1.69	84.8	5.5	9.7	5228	−0.26	5.00	0.28	0.17	0.15	0.09	0.07	0.06
45	1.51	73.8	12.0	14.2	826	−0.01	8.20	0.32	0.24	0.22	0.17	0.14	0.12
55	1.50				4314	−0.16	7.72	0.35	0.25	0.23	0.18	0.14	0.13
65	1.54	50.3	20.9	28.8	3554	−1.10	8.10	0.41	0.30	0.29	0.25	0.21	0.16
75	1.56	20.7	32.0	43.7	289	−4.90	12.00	0.44	0.41	0.40	0.36	0.32	0.29
85	1.44	6.7	20.6	72.7	136	−4.90	12.00	0.44	0.42	0.41	0.38	0.35	0.31

rate constant. Jemison et al. (1994) in their evaluation of the LEACHMN model used values ranging from 0.10 to 0.40 and 0.02 to 0.005 d^{-1} for their nitrification and denitrification rate constants, respectively. Little or no information was available on volatilization rate constants. The value of 0.40 d^{-1} for ammonia volatilization from the surface was suggested in the LEACHM manual (Hutson and Wagenet, 1992). Jemison (1991) used values of 0.0 d^{-1}, and values ranging from 0.00127 to 0.00154 d^{-1} were used by Chin and Kroontje (1963) in laboratory experiments evaluating volatile loss of NH_3 from urea. Our values of 0.2 d^{-1} for the first year, and 0.0 d^{-1} for the two other years were the best fit values for the conditions of this study.

On a soil type basis, nitrification and denitrification rates on the loamy sand were different from those on the clay loam, while volatilization rate was not affected by soil type. Notably, denitrification rates were much higher for the clay loam than for the loamy sand (3-yr average of 0.15–0.17 and 0.07 d^{-1} respectively, Table 6). The higher denitrification rates for the clay loam presumably reflect the greater potential for anaerobic conditions.

At both sites, the rate constants were generally similar for each site-year combination (Table 6), which suggests that they were minimally affected by the N rates of application used in this study. The rate constants were similar for the 1993 and 1994 years, and different from 1992. Higher denitrification and volatilization and lower nitrification rates were estimated for 1992 compared to those for 1993 and 1994. This yearly effect on the rate constants presumably resulted from cropping history. In 1992, the first year following sod plowdown at both sites (alfalfa on the clay loam and grass on the loamy sand), high denitrification and volatilization and low nitrification rate constants were needed to optimize the fit between simulated and measured values of the soil profile NO_3–N distribution due to high initial (May) soil NO_3–N levels. In the subsequent years (1993 and 1994), soil NO_3–N levels decreased, and, as a result, low denitrification and volatilization and high nitrification were estimated to better match simulated soil profile NO_3–N to meas-

Table 4. Required crop data in the LEACHMN model to simulate maize N uptake

	Planting	Emergence	Maturity	Harvest	Loamy sand		Clay loam	
					Rooting depth (cm)†	N uptake (kg ha^{-1})	Rooting depth (cm)	N uptake (kg ha^{-1})
1992								
Treatments								
22 kg N ha^{-1}						126		158
100 kg N ha^{-1}	05/13/92	05/23/92	09/20/92	10/12/92	65	179	55	178
120 kg N ha^{-1}						166		210
1993								
Treatments								
22 kg N ha^{-1}						126		103
100 kg N ha^{-1}	05/20/93	06/01/93	09/29/93	10/16/93	65	176	55	142
120 kg N ha^{-1}						166		186
1994								
Treatments								
22 kg N ha^{-1}						141		151
100 kg N ha^{-1}	05/12/94	05/23/94	09/20/94	10/10/94	65	197	55	159
120 kg N ha^{-1}						186		208

†Rooting depth determined from neutron moisture measurements.

Table 5. Initial (May) soil NO_3–N (kg ha^{-1}) in the top 0.90 m soil profile under each N treatment in 1992, 1993 and 1994 for the clay loam and loamy sand

Year	Clay loam			Loamy sand		
	22 kg N ha^{-1}	100 kg N ha^{-1}	134 kg N ha^{-1}	22 kg N ha^{-1}	100 kg N ha^{-1}	134 kg N ha^{-1}
1992	377	377	377	103	103	103
1993	100	41	64	60	59	33
1994	18	19	43	48	60	53

ured values. The yearly effect (primarily as a result of variation in initial soil N content) on the rate constants suggests an apparent problem with the model in adjusting rate constants (particularly denitrification rate) according to substrate supply. This agrees in part with Lotse et al. (1992), Jabro et al. (1993) and Jabro et al. (1995) who reported that the sub-routine controlling N transformation processes and associated rate constants in LEACHMN appears to inadequately perform according to water content, oxygen and substrate supply, and temperature.

The LEACHMN model satisfactorily predicted growing season soil profile nitrate distribution with the use of the calibrated N transformation rate constants (Figures 4 and 5). The correlation coefficients between measured and simulated values for all the calibrated data sets were high, ranging from 0.71 to 0.98, the RMSEs were low, and the prediction errors (NRMSE) varied between 14 and 37% with most values below 30% (Figures 4 and 5). The simulations' accuracy, however, varied among years and sites. In 1992 at both sites in general, and particularly on the loamy sand, the model slightly overestimated soil NO_3–N early in the growing season, especially in the top 0.5 m of the soil profile, and predicted depletion of soil NO_3–N from the root zone by the end of the growing season (Figures 4 and 5). Due to the high initial soil NO_3–N of the experimental sites, high denitrification rate constants were estimated for the subsequent period. This was accentuated by the fact that the model underestimated maize N uptake early in the growing season (Figure 6). Since the model balances N in the soil through deni-

Table 6. LEACHMN rate constants adjusted to optimize fit between predicted and measured growing season soil profile NO_3–N distribution and associated nitrification, denitrification and volatilization N fluxes for 1992, 1993 and 1994 on the loamy sand and clay loam

Soil type	Year	Nitrification (d^{-1})	Denitrification (d^{-1})	Volatilization (d^{-1})	Nitrified N (kg ha^{-1})	Denitrified N (kg ha^{-1})	Volatilized N (kg ha^{-1})
LOAMY SAND							
Treatment							
22 kg ha^{-1}	1992	0.200	0.200	0.200	125.0	38.0	2.0
	1992	0.400	0.004	0.000	112.0	28.0	0.0
	1994	0.400	0.003	0.000	114.0	18.0	0.0
3-yr average		0.333	0.069	0.060			
100 kg ha^{-1}	1992	0.200	0.200	0.200	200.0	49.8	3.2
	1993	0.380	0.004	0.000	177.0	53.0	0.0
	1994	0.400	0.004	0.000	188.0	27.0	0.0
3-yr average		0.326	0.070	0.060			
134 kg ha^{-1}	1992	0.200	0.200	0.200	221.0	56.8	4.0
	1993	0.380	0.004	0.000	212.0	41.0	0.0
	1994	0.390	0.004	0.000	214.0	24.7	0.0
3-yr average		0.323	0.070	0.060			
CLAY LOAM							
Treatment							
22 kg ha^{-1}	1992	0.200	0.260	0.200	201.0	64.0	10.4
	1993	0.200	0.100	0.000	196.0	70.0	0.0
	1994	0.300	0.080	0.000	144.0	23.0	0.0
3-yr average		0.233	0.150	0.060			
100 kg ha^{-1}	1992	–†	–	–	–	–	–
	1993	0.200	0.130	0.000	275.0	122.0	0.0
	1994	0.270	0.100	0.000	221.0	34.0	0.0
2-yr average		0.235	0.115	0.000			
134 kg ha^{-1}	1992	0.200	0.280	0.200	354.0	2270.0	19.5
	1993	0.200	0.130	0.000	261.0	33.0	0.0
	1994	0.270	0.100	0.000	255.0	41.6	0.0
3-yr average		0.223	0.170	0.060			

†Treatment not applied.

trification, volatilization, leaching and plant N uptake, end-of-season soil NO_3–N levels were predicted to be low.

In 1993 and 1994, simulations were more accurate (Figures 4 and 5). In these years, early-season soil profile NO_3–N was reduced and denitrification rate constants were estimated to be lower (Table 6). As a result, NO_3–N losses by denitrification at the end of the growing season were reduced, which provided a better match between predicted and measured values compared to results of 1992, especially on the loamy sand.

In evaluating the LEACHMN model, Jemison et al. (1994) calibrated the model based on NO_3–N leaching losses. They found significant discrepancies between simulated and observed data as a result of two factors: the model's incapacity to accurately predict maize uptake of N early in the growing season, and its one-dimensional characteristic that does not allow solute diffusion from flow pathways. Results of this

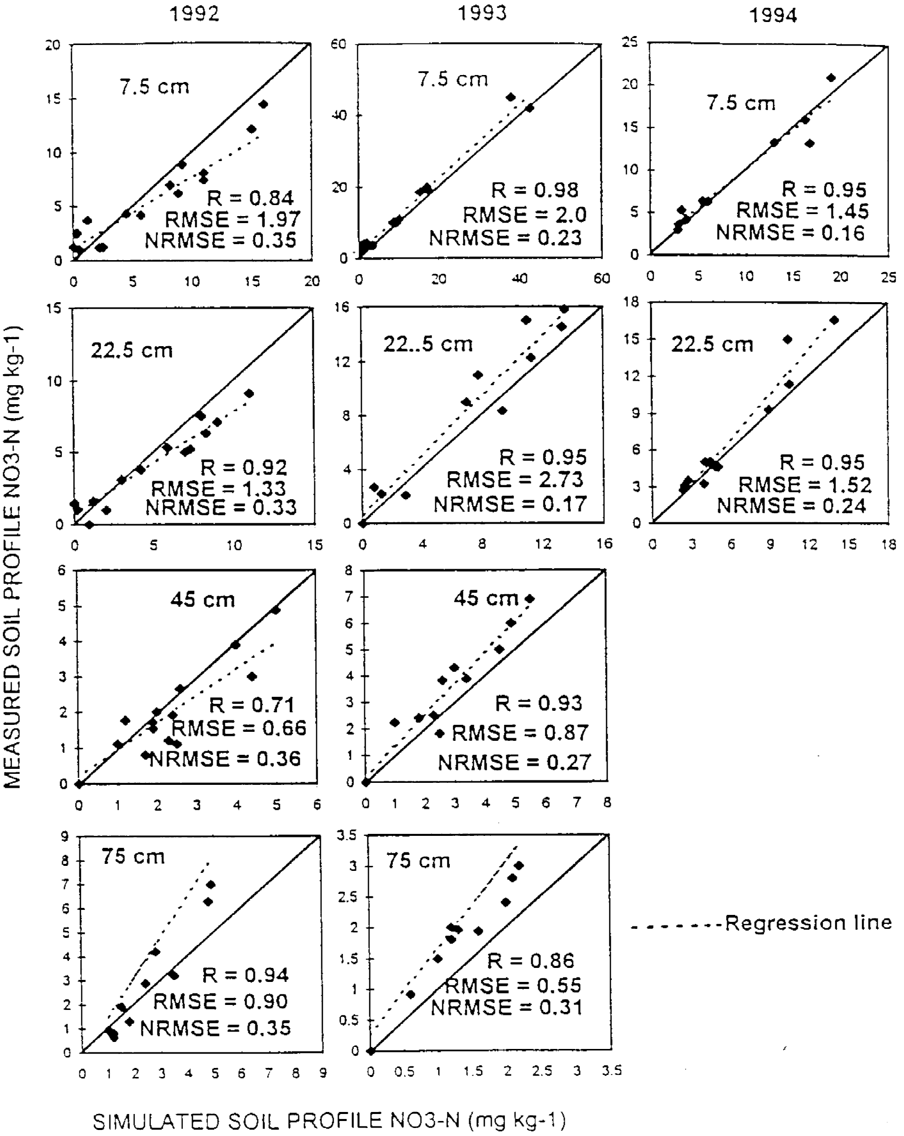

Figure 4. 1:1 scale plot and regression of measured and LEACHMN-predicted values of soil profile NO_3–N under the three N treatments on the loamy sand in 1992, 1993 and 1994.

study showed that the model slightly overestimated soil NO_3–N early in the growing season in the surface 0.5 m and underestimated it by the end of the growing season in the first year, but simulations were more accurate in the following years.

Conclusions

LEACHMN, the version of LEACHM that addresses N dynamics in the soil-plant-atmosphere system was calibrated for its critical N transformation rate constants including nitrification, denitrification, and volatilization rates for a clay loam and loamy sand under maize. When calibrated for each N treatment-year combination and soil type, the model satisfactorily predicted growing season soil profile nitrate distributions. Slight discrepancies occurred however between measured and predicted data, primarily as a result of the model's incapacity to accurately simulate maize N uptake and the high initial soil nitrate of the experimental sites due to sod plowdown. A more sophisticated mechanism for maize N uptake simulation is

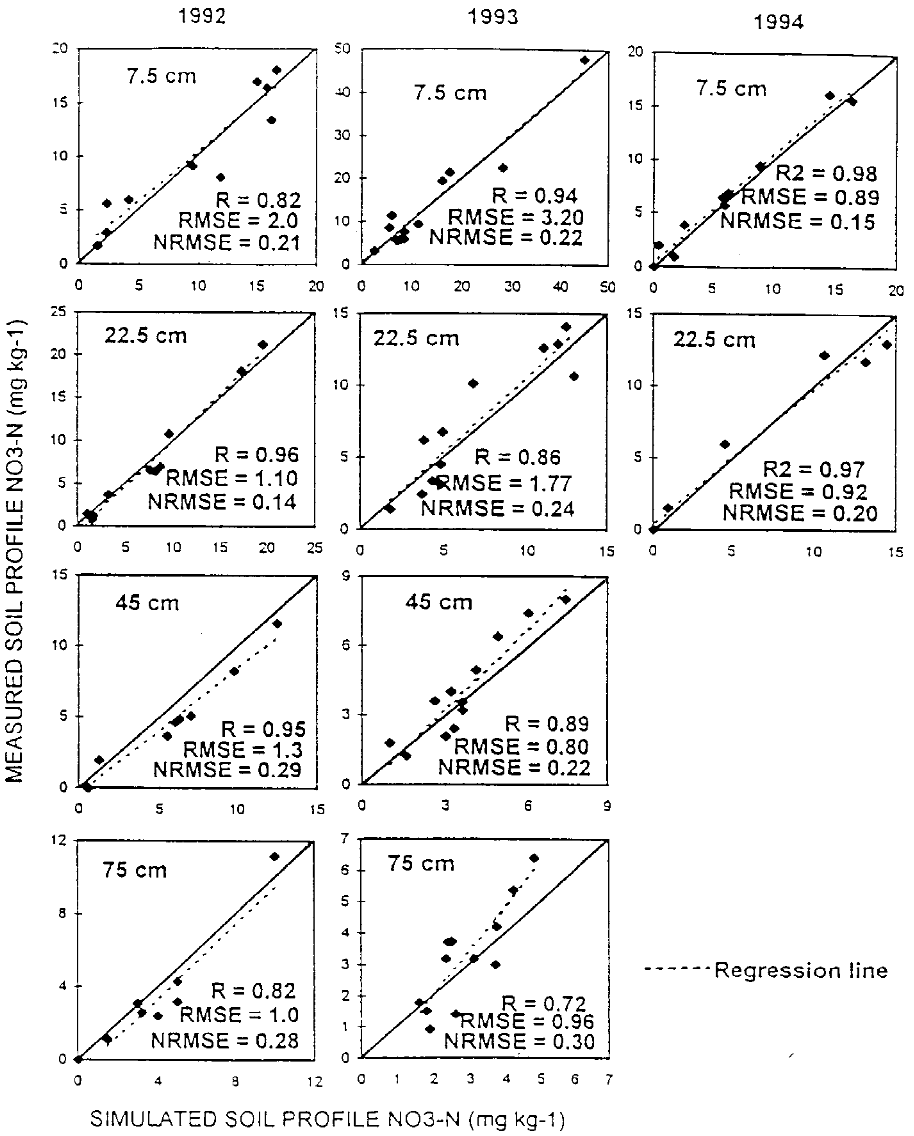

Figure 5. 1:1 scale plot and regression of measured and LEACHMN-predicted values of soil profile NO$_3$–N under the three N treatments on the clay sand in 1992, 1993 and 1994.

needed to increase the model's accuracy. In addition, refinement of the model's sub-routine for rate constant adjustment may contribute the improvement to its predictions.

Results indicated that N application rates used in this study minimally affected the calibrated N transformation rates, while cropping history and soil type have greater effects on the N transformation rates. This implies that single N transformation rate constants can be applied to estimate N fate and transport within a given soil type and cropping practice. Rate coefficients need to be adjusted for different soil types and when crop conversions occur.

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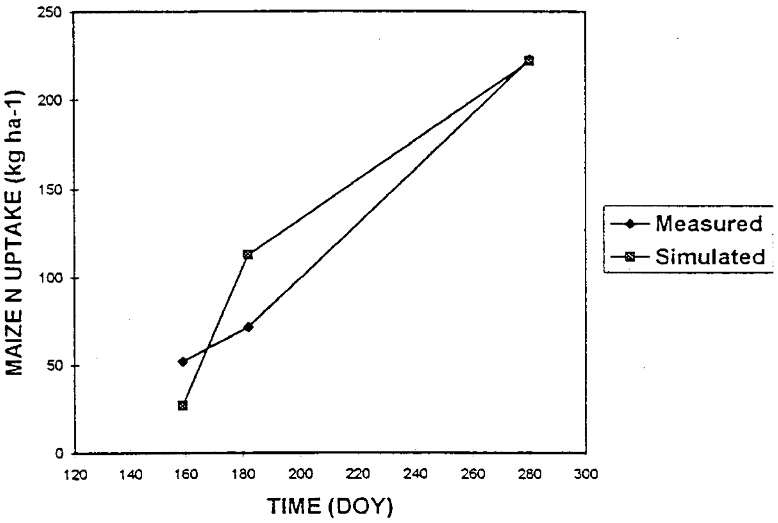

Figure 6. Measured and LEACHMN-predicted maize N uptake.

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