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Simulation of Leaching Losses in the Nitrogen Cycle

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Abstract: The CERES (Crop Estimation through Resource and Environment Synthesis) family of crop models predicts cereal growth, development, and yield. CERES simulates nitrogen (N) as a yield-limiting macronutrient. Because N leaching is an economic and environmental concern, this study evaluated if CERES

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can be used to predict N leaching under different N management scenarios: background leaching in unfertilized corn (*Zea mays* L.), alfalfa (*Medicago sativa* L.) residue mineralization, and till versus no-till management. Data were collected during a 7-yr field experiment on tillage practices in a maize–alfalfa–maize succession. Sensitivity analyses were performed for decomposition rates of the different residue pools and the relative proportions of carbohydrate, cellulose, and lignin in the residues. During the last 5 yr, under corn, CERES accurately simulated nitrate leaching from the no-till lysimeters. Nitrate leaching was underestimated in the tillage treatments, possibly because CERES does not simulate tillage. The model is not very sensitive to the decomposition rates and to the composition of the residues.

Keywords: CERES, DSSAT, mineralization, modeling, nitrogen balance, residues, tillage

Software availability: The CERES models (Crop Estimation through Resource and Environment Synthesis) are the cereal component of the software package DSSAT (Decision Support System for Agrotechnology Transfer). DSSAT is a product of the IBSNAT (International Benchmark Sites Network for Agrotechnology Transfer) project, sponsored by the U.S. Agency for International Development during 1982–1992. DSSAT has since been maintained and developed by a network of volunteers at universities and research organizations. Currently, DSSAT is available from ICASA (International Consortium for Agricultural Systems Applications), 2440 Campus Rd., Box 527, Honolulu, HI 96822, USA; phone +1 808 956 7531; fax +1 808 956 2711; e-mail icasa@icasa.net. An order form is available on the World Wide Web at http://www.icasa.net/dssat/order.html (verified 19 March 2005). The modifications to DSSAT that were necessary for this research are available free of charge from the senior author.

INTRODUCTION

CERES (Crop Estimation through Resource and Environment Synthesis) is a family of crop–soil–atmosphere models that predict cereal growth, development, and yield (Jones and Kiniry 1986). CERES models include components that simulate nitrogen (N) balances in both soils and plants. Because of the risk of groundwater contamination by nitrates, N management in the soil–plant system has become an important component of modern agronomy. Because of its many successful applications and its relatively long existence, the CERES family of models is used by numerous scientists and extension agents. Although CERES has mostly been used for yield prediction, their use could be expanded if multiple scenarios of N management could be predicted. Vigil, Kissel, and Smith (1991) tested an early version of CERES for the amount of mineralized N and N recovered from residues by sorghum and wheat. The model demonstrated reasonable fit with measured data after calibration of critical parameters. Gerakis (1994) tested the N component of CERES with data from a controlled water table experiment in lysimeters by reporting reasonable agreement between model predictions and the cumulative N outflow from lysimeters. Quemada and Cabrera (1995) and Quemada, Cabreara, and McCraken (1997) reported that CERES predictions of soil N originating from residue mineralization is sensitive to the decomposition rates and relative proportions of the carbohydrate, cellulose, and lignin fractions of the residues.

The first objective of this work was to evaluate how well CERES predicts N leaching under different N management scenarios: background leaching from a corn crop without fertilizer, leaching from alfalfa residue mineralization, and leaching from a tilled and non-tilled agroecosystem.

The second objective was to evaluate how sensitive the leaching prediction is to N mineralization parameters: decomposition rates of the different residue fractions and the relative proportion of each fraction in the composition of residues.

MATERIALS AND METHODS

Model Overview

CERES is a family of functional, deterministic, crop–soil–atmosphere models. The CERES models are an important component of the Decision Support System for Agrotechnology Transfer (DSSAT), a product of the International Benchmark Sites Network for Agrotechnology Transfer (IBSNAT, Tsuji, Uehara, and Balas 1994).

The CERES models have been tested worldwide. Entenmann and Allison (1991) tested CERES for corn leaf area, dry matter, phenology, and soil water nitrate content and found good agreement, overall. Jintrawet et al. (1991) successfully simulated yield of nonphotosensitive rice cultivars and heading and maturity dates of photosensitive ones. Kiniry and Jones (1986) presented test results for corn phenology, leaf area index, biomass, grain number, grain yield, total N uptake, grain N concentrations, and grain N uptake. Correlations between measured and simulated values were statistically significant. Vigil, Kissel, and Smith (1991) tested the model for amount of mineralized N and N recovered from residues by sorghum and wheat. The model showed reasonable fit after calibration of critical parameters. The CERES models have also been used for 1) risk analysis and multicriteria optimization of production (Alocilja and Ritchie 1990; Martin 1992); 2) site-specific irrigation management (Ritchie and Amato 1990); and 3) assessment of global climate change, in conjunction with climate models (Adams et al. 1990).

The CERES models simulate the effects of cultivar, planting density, weather, soil water, and N on crop growth, development, and yield. They do not simulate the effects of pests, nutrients (except N), catastrophic weather, or tillage. Yet, users may adapt and extend the model to suit specific needs. The models simulate multiyear crop rotations (Tsuji, Uehara, and Balas 1994). The generic CERES version includes corn, wheat (*Triticum aestivum, T. durum*), sorghum (*Sorghum bicolor*), pearl millet (*Pennisetum typhoides*), and barley (*Hordeum vulgare*) models.

The CERES models require minimum inputs of soil and weather data, which are routinely collected in most parts of the world or can be reasonably estimated (Ritchie and Crum 1989; Ritchie, Godwin, and Singh 1990; Ritchie 1998). The soil profile is divided into layers; therefore, values for soil properties must be specified for each layer. Weather inputs are daily values.

A typical run of CERES includes the following steps: reading of daily weather data; simulation of soil temperature; and simulation of soil water balance, N transformations, plant growth and phenology. This sequence is repeated for every day of the simulation for the duration of a season or throughout the year.

The Nitrogen Component in CERES

Model simulation of soil N and crop growth interact in a feed forward and feedback relationship. If there is a soil deficit relative to plant demand, CERES calculates N stress coefficients that impact plant growth and development. In turn, plant growth and development affect the demand for N. A set of options allows crop simulation with unlimited N supply, which suppresses the simulation of the N budget. The N budget is also suppressed when the water balance is suppressed, because simulation of the N cycle requires knowledge of water fluxes and soil water content. Figure 1 is a flowchart of the N-related modules (subroutines) in CERES, in the approximate calling sequence. Module names are in uppercase. The N component of CERES is explained fully by Godwin and Jones (1991).

Modifications to CERES, Version 3.5

Several subroutines of CERES, version 3.5, had to be modified to meet the objectives of this study. Some routines responded erratically in preliminary runs because of the very low soil N concentrations in the test data. Other subroutines were modified so that model output files could be easily imported and evaluated in a spreadsheet or graphing package. The lack of an adequate graphing utility in DSSAT necessitates the use of a separate software package for plotting results. The modifications of the CERES source code and of the input and output files are described in the appendix.

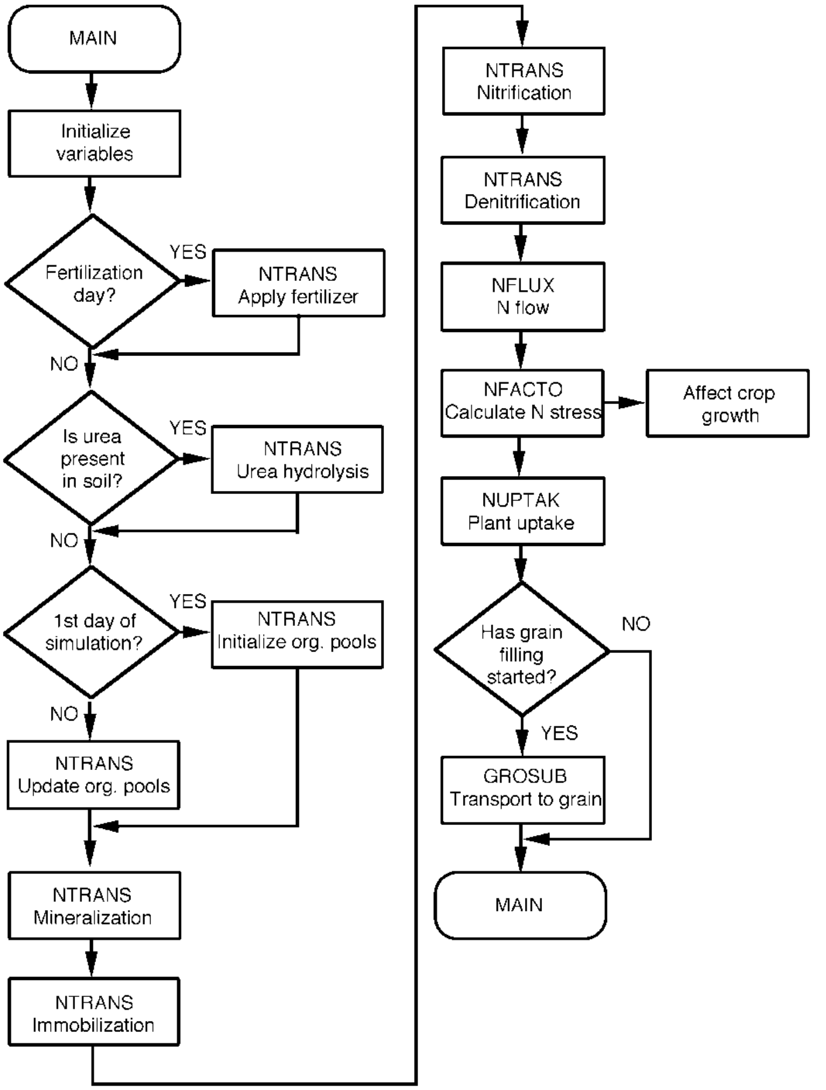

Figure 1. Flowchart of the N balance in the CERES models. Module (subroutine) names are in uppercase. The full description is in Godwin and Jones (1991).

Field Testing

Nitrogen-conserving agricultural systems are increasingly sought by agricultural environmentalists. The leaching of nitrates through the soil profiles in corn production is responsive to tillage systems and N fertilizer inputs. Corn N fertilization tends to augment NO_3 leaching when applications are in excess of plant uptake (Gast, Nelson, and Randall 1978; Angle et al. 1993). Total NO_3 losses by deep leaching appear to be slightly higher for conventional tillage than no-tillage soils, through soil profiles under corn production (Randall and Ivaragarapu 1995; Weed and Kanwar 1996).

On the other hand, Rasse and Smucker (1999) suggest that tillage management is not the only decisive factor controlling NO_3 leaching from the fields. Alfalfa stands may increase N availability to the subsequent crop through mineralization of alfalfa residues. Alfalfa absorbs considerable quantities of N and fixes N (Lamb et al. 1995). Rasse and Smucker (1999) found that 2 years after planting, alfalfa crowns and roots stored at least 97 to 133 kg ha^{-1} of total N. However, a mineralization burst from spray-killed or plowed-under alfalfa, during its rapid decomposition, leads to high levels of NO_3 leached to the groundwater if its decomposition is not timed to match crop consumption (Campbell et al. 1994; Philipps and Stopes 1995; Rasse and Smucker 1999).

Baseline leaching of nitrate nitrogen (NO_3-N) through profiles of medium-textured loam soils under unfertilized corn can also be significant. Rasse and Smucker (1999) report that 21 to 25 kg ha^{-1} of NO_3-N was leached annually from unfertilized corn. Knowledge and prediction of this baseline leaching is important in managing N fertilizer.

Based on this information, we decided to simulate an experiment where three potential factors in fertilizer management could be observed: background leaching of zero N fertilization, alfalfa mineralization, and tillage.

MATERIALS AND METHODS

A corn–alfalfa–corn sequence was studied from 1991 to 1998 as part of a long-term field experiment investigating N supply and tillage effects on soil–plant interactions. Field plots, 40 by 27 m each, were established in 1986 in a randomized complete block design in a Kalamazoo loam soil (fine loamy, mixed, mesic Typic Hapludalf) at the Long-Term Ecological Research (LTER, http://www.lter.kbs.msu.edu) site of the Kellogg Biological Station (KBS, http://www.kbs.msu.edu) in southwestern Michigan. Soil horizons are a loamy Ap from 0 to 0.30 m, which overlays a clay loam Bt1 from approximately 0.30 to 0.55 m, then a Bt2 enriched in coarse material from approximately 0.55 to 0.75 m, underlaid by a coarse sandy glacial outwash parent material. Treatments, replicated four times, consisted of 1) conventional tillage and no fertilization (CT-NF), 2) no tillage and no fertilization (NT-NF), 3) conventional tillage and fertilization (CT-F), and 4) no tillage and fertilization (NT-F). Undisturbed monolith stainless steel lysimeters, 1.2 by 1.8 m on surface area and 2.1 m deep, were installed in two NT-NF and two CT-NF plots in 1990. Figure 2 shows a cross section of a lysimeter.

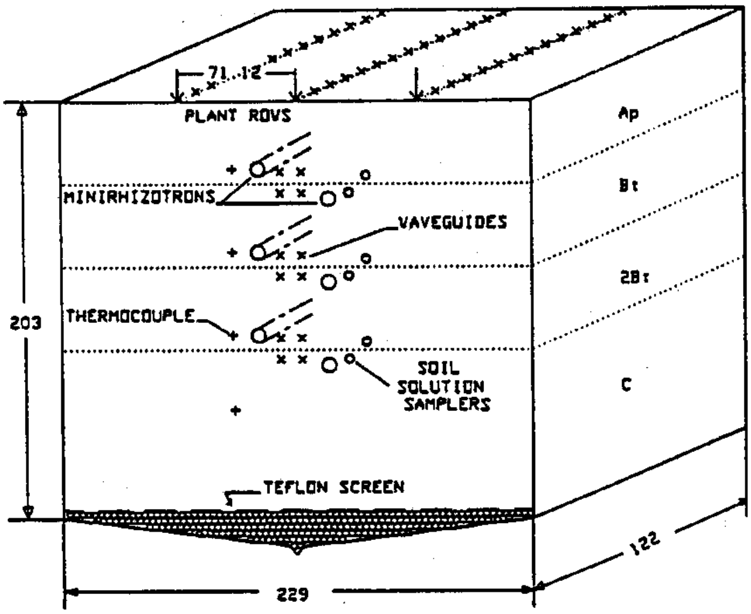

Figure 2. Diagrammatic representation of a natural soil profile lysimeter with a surface area of $2.79\,m^2$ and a total volume of $5.67\,m^3$, encased in stainless steel and lined at the base with Teflon® screen, 120-micron openings, located above a layer of pea-sized gravel that facilitates natural drainage through the port at the bottom of the lysimeter. The natural soil profile is located above the Teflon screen. Minirhizotrons, suction soil solution samplers, time domain reflectometry wave guides, Teflon gas sampling tubes, 0.03 mm ID, are located 2 cm above and 2 cm below each interface of the natural soil horizons.

The lysimeters, which were identically managed to the field plots, were manually tilled (where applicable), planted, and harvested. Crops were planted at high density in the lysimeters and later thinned to guarantee a uniform plant density matching field conditions. Total biomass per lysimeter was recorded and, as for field plots, subsamples were taken for moisture content and total N analyses. Table 1 lists the rotation species, cultivar, and planting and harvesting dates.

Table 2 lists the soil properties. Figure 3 is initial soil N for the 1991 and 1996 growing seasons. The lysimeters were not fertilized prior to September 1990, at which time approximately 10 times the normal application rate of nitrate ammonia fertilizer was unintentionally applied. Because of the uncertainty in the applied fertilization in 1990 (Aiken 1992), measurements of N leaching in the period from 2 May 1991 to 1 May 1993 were not compared with the simulations. Further details of the experiment are in Ostrom et al. (1998) and Rasse and Smucker (1999).

Table 1. Rotation species, cultivar, and start and end date of cultivation

Rotation species and cultivar	Start date	End date
Corn (Pioneer 3704)	16 May 1991	30 Sep. 1991
Corn (Pioneer 3704)	8 May 1992	30 Oct. 1992
Corn (Great Lakes 450)	8 May 1993	22 Oct. 1993
Corn (Pioneer 3573)	6 May 1994	22 Aug. 1994
Alfalfa (Pioneer 5246)	1 Sep. 1994	2 May 1996
Corn (Pioneer 3573)	13 May 1996	4 Sep. 1996
Corn (Pioneer 3573)	10 June 1997	18 Nov. 1997

Statistical Measures

Agreement between measured and simulated cumulative N leaching was compared graphically and with the normalized RMSE (root mean square error). The RMSE estimates the variation, expressed in the same units as data, between simulated and measured values (Loague and Green 1991; Xevi, Gilley, and Feyen 1996). The RMSE tests the accuracy of the model, which is how much simulated values approach a corresponding set of measured values (Loague and Green 1991). The RMSE can also be expressed as a coefficient of variation, by dividing it by the mean of the measured values. This normalized RMSE (NMRSE) is defined as:

$$\mathrm{NRMSE} = 100\frac{1}{\bar{y}}\left[\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2\right]^{1/2} \tag{1}$$

where y_i is the ith observed value, $\hat{y}_i$ is the ith simulated value, n is the number of comparisons, and $\bar{y}$ is the mean of observations.

For the sensitivity analysis, decomposition rates for the carbohydrate, cellulose, and lignin fractions were varied 50% more than and 50% less than the default rates (Table 3). These ranges are similar to the adjustments that Quemada, Cabrera, and McCraken (1997) proposed to the default rates of CERES. The NRMSE and total NO_3-N leaching were compared. To calculate the effect of the composition of residues, the carbohydrate content was varied 50% more than and 50% less than the default content (Table 3). These ranges are similar or exceed the range of the carbohydrate content encountered in various plant residues (Quemada, Cabrera, and McCracken 1997). We chose to vary the carbohydrate because it is the most dynamic fraction of fresh organic matter.

Table 2. Soil properties of the four lysimeters

B.L.	Hor.	LL	DUL	Sat.	H.F.	H.C.	B.D.	O.C.	Cl.	Silt	C.F.	N	pH	CEC
Lysimeter 2														
10	Ap	0.18	0.29	0.41	1.00	3.1	1.47	1.28	19	38	10	0.07	6.5	10.0
30	Ap	0.18	0.29	0.41	1.00	3.1	1.47	1.28	19	38	10	0.07	6.5	10.0
43	Btu	0.18	0.29	0.41	0.40	3.1	1.47	0.32	22	38	10	0.03	6.5	10.0
56	Btl	0.13	0.22	0.38	0.80	3.1	1.55	0.07	12	06	10	0.03	6.0	10.0
68	Bt2u	0.11	0.16	0.36	1.00	3.1	1.61	0.02	08	05	10	0.01	6.0	10.0
80	Bt2l	0.11	0.16	0.36	0.40	3.1	1.61	0.02	04	02	10	0.01	6.0	3.0
100	C	0.12	0.14	0.33	0.10	3.1	1.70	0.01	03	02	10	0.01	5.6	3.0
203	C	0.12	0.14	0.33	0.00	3.1	1.70	0.01	03	02	10	0.01	5.6	3.0
Lysimeter 6														
10	Ap	0.25	0.34	0.41	1.00	4.0	1.47	1.28	19	38	5	0.07	6.5	10.0
22	Ap	0.26	0.35	0.41	1.00	4.0	1.47	1.28	19	38	5	0.07	6.5	10.0
31	E	0.26	0.35	0.41	1.00	4.0	1.47	1.28	22	47	5	0.04	6.5	10.0
41	Btu	0.24	0.35	0.43	0.90	4.0	1.40	0.32	23	44	5	0.04	6.5	10.0
51	Btm	0.24	0.35	0.38	0.70	4.0	1.55	0.22	25	19	5	0.04	6.0	10.0
61	Btl	0.24	0.35	0.38	0.80	4.0	1.55	0.07	21	17	5	0.04	6.0	10.0
75	Bt2u	0.15	0.21	0.36	0.40	4.0	1.61	0.02	19	12	5	0.02	6.0	10.0
89	Bt2l	0.10	0.16	0.36	0.10	4.0	1.61	0.02	07	04	5	0.02	6.0	3.0
102	Bt3u	0.11	0.13	0.33	0.00	4.0	1.70	0.02	07	05	5	0.01	6.0	3.0
115	Bt3l	0.11	0.13	0.33	0.00	4.0	1.70	0.01	04	03	5	0.01	6.0	3.0
120	Bt/E	0.10	0.13	0.33	0.00	4.0	1.70	0.01	01	01	5	0.01	5.6	3.0
203	C	0.11	0.13	0.33	0.00	4.0	1.70	0.01	03	02	5	0.01	5.6	3.0

(*continued*)

Table 2. Continued

B.L.	Hor.	LL	DUL	Sat.	H.F.	H.C.	B.D.	O.C.	Cl.	Silt	C.F.	N	pH	CEC
Lysimeter 9														
10	Ap	0.29	0.40	0.41	1.00	1.1	1.47	1.28	19	38	5	0.08	6.5	10.0
22	Ap	0.29	0.40	0.41	1.00	1.1	1.47	1.28	19	38	5	0.08	6.5	10.0
28	E	0.29	0.40	0.41	1.00	1.1	1.47	1.28	27	38	5	0.03	6.5	10.0
49	Bt	0.16	0.25	0.43	1.00	1.1	1.40	0.07	27	28	5	0.03	6.0	10.0
51	Bt2u	0.19	0.25	0.38	0.50	1.1	1.55	0.02	18	09	5	0.02	6.0	10.0
55	Bt2l	0.19	0.25	0.38	0.40	1.1	1.55	0.02	09	06	5	0.02	6.0	3.0
70	Bt3u	0.15	0.21	0.36	0.10	1.1	1.61	0.02	07	05	5	0.01	6.0	3.0
85	Bt3l	0.12	0.15	0.33	0.00	1.1	1.61	0.01	04	02	5	0.01	6.0	3.0
89	Bt/E	0.12	0.13	0.33	0.00	1.1	1.70	0.01	04	02	5	0.01	5.6	3.0
203	C	0.11	0.13	0.33	0.00	1.1	1.70	0.01	03	02	5	0.01	5.6	3.0
Lysimeter 13														
10	Ap	0.23	0.34	0.41	1.00	2.0	1.47	1.28	19	38	5	0.09	6.5	10.0
22	Ap	0.23	0.34	0.41	1.00	2.0	1.47	1.28	19	38	5	0.03	6.5	10.0
28	E	0.23	0.34	0.41	0.80	2.0	1.47	1.28	20	49	5	0.03	6.5	10.0
45	Btu	0.23	0.34	0.41	0.80	2.0	1.47	0.32	26	40	5	0.03	6.5	10.0
63	Btl	0.25	0.36	0.38	0.80	2.0	1.55	0.07	16	07	5	0.03	6.0	10.0
75	Bt2u	0.19	0.26	0.36	0.70	2.0	1.61	0.02	14	06	5	0.03	6.0	10.0
86	Bt2l	0.17	0.21	0.36	0.80	2.0	1.61	0.02	07	04	5	0.03	6.0	3.0
100	C	0.12	0.14	0.33	0.20	2.0	1.70	0.01	03	01	5	0.02	5.6	3.0
203	C	0.12	0.13	0.33	0.00	2.0	1.70	0.01	03	01	5	0.02	5.6	3.0

Notes: B.L.: bottom of layer (cm). Hor.: horizon. LL: lower limit of water availability ($cm^3\ cm^{-3}$). DUL: drained upper limit of water availability ($cm^3\ cm^{-3}$). Sat.: saturated water content ($cm^3\ cm^{-3}$). H.F.: soil hospitality factor. H.C.: saturated hydraulic conductivity ($cm\ h^{-1}$). B.D.: soil bulk density ($Mg\ m^{-3}$). O.C.: organic C (%). Cl.: clay content (%). Silt: silt content (%). C.F.: coarse fragment content (%). N: N content (%). CEC: cation exchange capacity ($\mu mol\ L^{-1}$).

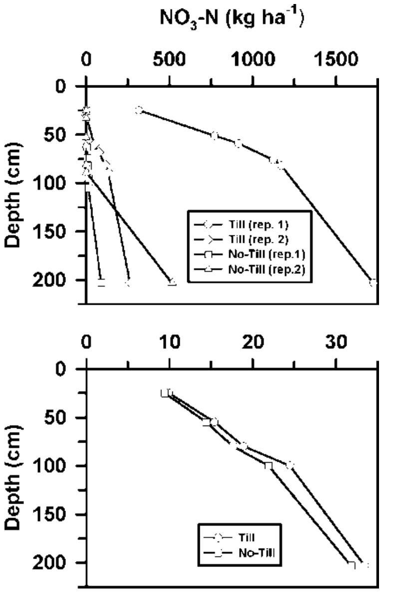

Figure 3. Initial cumulative soil N with depth on 2 May 1991 and 2 May 1996. The 1991 plot shows the high N pulse caused by the unintended fertilization in Sep. 1990.

Data Utilization

The drainage and leaching data from the LTER lysimeters had been collected and stored over the years by different investigators in various formats. The first task was to locate and combine all the data into a few uniform digital files. Same-type measurements were converted to common units, matching the observation depths among the four lysimeters, outlier data were removed, and data gaps were filled. The criteria for removing outlier observations and filling in missing values were as follows:

For some dates, there were drainage volume measurements, but no NO_3-N concentration measurements. Missing effluent NO_3-N concentrations were interpolated. Interpolation was simply the averaging of the NO_3-N concentrations before and after the missing date.

For some dates, there were NO_3-N concentration measurements but no drainage volume measurements. Because the missing drainage measurement could not be guessed, those NO_3-N concentrations were averaged with the next date that had both NO_3-N concentration and drainage volume measurement.

Occasionally, there was a note in the data records that the container that collected the effluent overflowed. In these cases, it was assumed that the drainage volume for that date was equal to the container capacity ($0.058\,m^3$ for 1991–94, $0.056\,m^3$ for 1996–98).

Table 3. Values used in sensitivity analyses of model parameters

	Decomposition rates (d^{-1})			Relative proportions		
Parameter set	Carbohydrates	Cellulose	Lignin	Carbohydrates	Cellulose	Lignin
Default set	0.2	0.050	0.0095	0.20	0.70	0.10
Decomposition rates +50%	0.3	0.075	0.0143	0.20	0.70	0.10
Decomposition rates −50%	0.1	0.025	0.0048	0.20	0.70	0.10
Carbohydrate content +50%	0.2	0.050	0.0095	0.30	0.65	0.05
Carbohydrate content −50%	0.2	0.050	0.0095	0.10	0.75	0.15

Sometimes, instead of two concentrations, one for each replicate lysimeter, only the mean was recorded. In these cases, we used the mean concentration to represent each replicate.

Soil water content measurements from 27 June 1997 to 10 February 1998 were discarded because they were higher than the calculated total soil porosity. Total soil porosity was calculated from measured bulk density:

$$e = 1 - \frac{\rho b}{\rho d} \tag{2}$$

where e is total soil porosity, ρb is soil bulk density, and ρd is soil particle density equal to $2.65\,\mathrm{Mg\,m^{-3}}$, the mineral density of quartz.

Weather data from the Kalamazoo airport, about 25 km from the experiment site, was used. These precipitation data were consistent with drainage records. Temperature for 2 days had to be corrected because minimum temperature was recorded higher than maximum temperature.

Measured drainage was sometimes erratic. Drainage volume for all lysimeters should be approximately the same over a long period of time, because the same amount of rain falls on all lysimeters. However, the large error bars in the later period of drainage measurements (Figure 4) suggest problems. A known problem is missing drainage measurements between 4 March and 28 May 1997.

Therefore, measured concentrations times simulated drainage volume to calculate total NO_3-N leaching were used. Using the conservative approach of a water balance model in which every item of the water balance is accounted for, the error possibly is relatively small. With lysimeters, we have nonrepresentative lower boundary conditions but conservative measurements most of the time. With direct measurements or estimates of the hydraulic gradient and conductivity, the possible errors are high considering spatial variability and the disturbance of the system with the instruments. If one uses estimates of the hydraulic dynamics, that is only a model also. Once the soil water limits were calibrated (as described in the next section), we believe that simulated drainage more accurately represents actual drainage in our experiment. For that, indirect and direct evidence is provided. The indirect evidence is the soil water contents, a series of "snapshots" in time of the soil water status (Figures 5–7). The direct evidence is that for two periods (2 May 1993 to 30 April 1994 and 1 May to 31 August 1994), simulated drainage is in good agreement with the measured data (Figure 4).

Calibration of Soil Water Limits

Approximately 1 year of TDR measurements of soil water content (2 May 1993 to 30 April 1994) was used to calibrate the soil water limits. The soil water

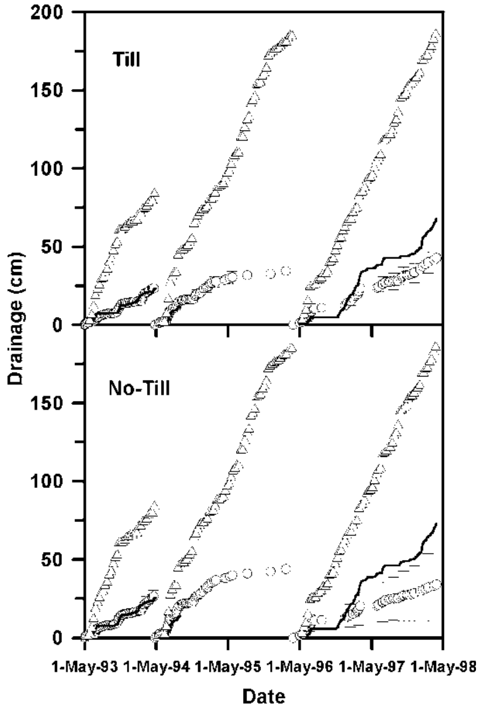

Figure 4. Simulated cumulative drainage (lines), measured cumulative drainage (circles), and cumulative precipitation (triangles). For clarity, cumulative precipitation is plotted every 10 d. For measured cumulative drainage, every other measurement is plotted. Vertical error bars are ± 1 SD for $n = 2$. Large error bars during the third period in the no-till treatment indicate problems with drainage measurements. Also, there is a lack of drainage data between 4 Mar. and 28 May 1997.

limits are basic soil properties that the model uses to simulate the soil water balance. The drained upper limit (θ_d) is the highest, field-measured, water content of a soil after thorough wetting and draining until drainage becomes practically negligible. The θ_d corresponds closely to water content at "field capacity" and to matric suction in the range of 10 to 33 kPa. The lower limit, θ_l, is the lowest, field-measured, volumetric water content of a soil after plants stop extracting water because of premature death or dormancy as a result of water deficit. The lower limit corresponds closely to the water content at the "permanent wilting point" and to matric suction of 1.5 MPa (Ritchie, Gerakis, and Suleiman 1999). The potentially plant-extractable water (θ_p) is the difference between the θ_d and the θ_l.

From the rapid drop in soil water content after rainfall events, it was estimated that most of the gravitational water was drained in 1 day. We set θ_d equal to the measured water content on 22 March 1994, 1 day after a major precipitation event (21.3 mm). It is possible that the gravitational

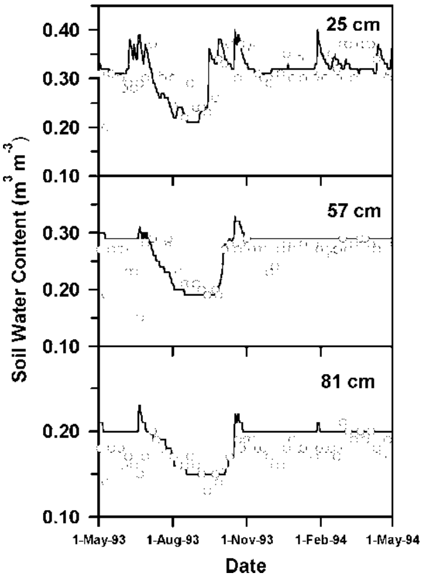

Figure 5. Calibration of soil water content for the till treatment, by layer. Markers are observed; lines are simulated values.

water was not all drained in 1 day. In the same soil, Huang (1995) observed a decline in water content for as long as 4 days after a major precipitation event. However, the soil was not covered, and the lysimeters were planted with crops. We cannot rule out significant soil and plant evaporation losses, in addition to deep drainage.

We fine-tuned θ_d to closely match measured to simulated soil water contents (Figures 5 and 6). The criterion to minimize was the NRMSE at three depths: 25, 57, and 81 cm, but mostly the NRMSE of the total profile water to the 81-cm depth. The minimum NRMSE that we achieved for the individual depths was 22%, and for the total profile water to the 81-cm depth was 10%. This means that predictions for individual depths are more erratic than for the whole profile. Apparently the errors caused by the discretization of the soil profile into layers are smoothed out during integration of the water content over the whole profile (Figure 7).

Part of the NRMSE for the whole profile can be explained because the measured soil water content at 25 cm was used to represent the 0–25 cm depth. This overestimated soil water content. Surface soil is more likely to be drier than at the 25-cm depth because of evaporation.

The potentially plant-extractable water was estimated according to Ritchie, Gerakis, and Suleiman (1999). We set the lower limit to the difference between the measured θ_d and the estimated θ_p. This was in part because of the difficulty in accurately measuring the lower limit of soil water availability in Michigan, where it often rains during the summer.

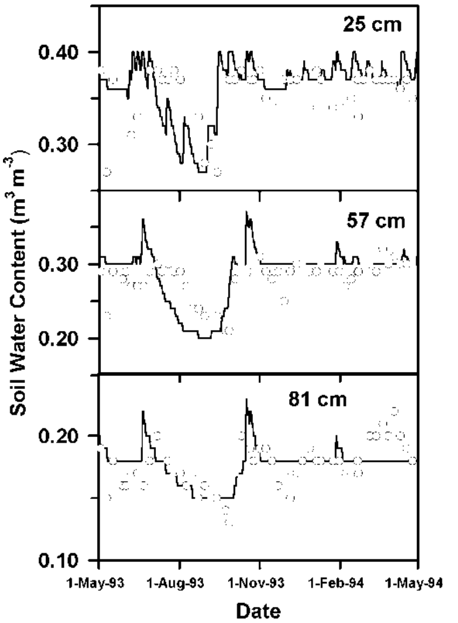

Figure 6. Calibration of soil water content for the no-till treatment, by layer. Markers are observed; lines are simulated values.

Also, it is not possible to optimize the soil water limit inputs for both till and no-till treatments. This is because the model does not simulate the effect of tillage. Experimental results using the same soil show that soil water content in the no-till treatments is maintained at higher levels throughout the growing season (Huang 1995; Rasse and Smucker 1999). This may be because the no-till treatment has less crusting of the soil surface and facilitates infiltration.

RESULTS AND DISCUSSION

Figure 8 shows observed versus simulated NO_3-N leaching with time for the two treatments, till and no till.

Background leaching in the unfertilized corn for two periods (2 May 1993 to 30 April 1994 and 1 May to 31 August 1994) was fairly well simulated, although the end values are somewhat overestimated. Unless a mass balance is performed on N, it is difficult to say which model component is responsible for the small discrepancy. Between 9 and 11 kg ha^{-1} of measured NO_3-N escaped through drainage during the 12-month period of 2 May 1993 to 30 April 1994, a useful quantity to consider when calculating fertilizer recommendations to farmers. This is the annual baseline NO_3-N loss

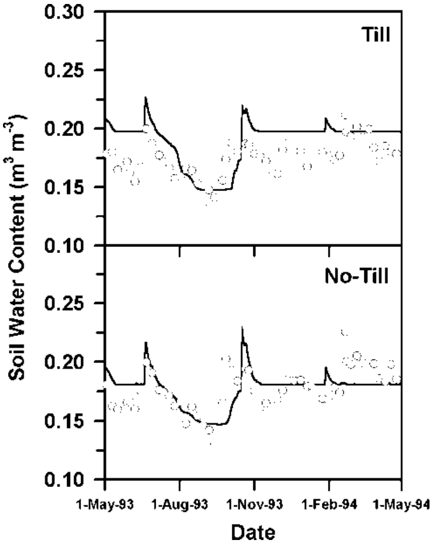

Figure 7. Calibration of soil water content for the till and no-till treatments, for the soil profile 0 to 81 cm. Markers are observed; lines are simulated values. Some of the errors caused by the discretization of the soil profile in the model are reduced when soil water is integrated with depth. Integrated soil water content may be overestimated because the 25-cm-depth measurement also represents the drier soil surface.

that cannot be further reduced, unless there is a cover crop during the winter. This loss results from the continuous mineralization of plant residues and soil organic matter.

Background leaching for the 1994 growing season was only simulated until 31 August 1994. On 1 September 1994, alfalfa was planted. It is expected that the alfalfa cover crop reduces the N leaching losses after the corn crop, because it absorbs some of the N released through the mineralization of corn roots and residues. Therefore, it was expected that the background leaching for the 12-month period of 1 May 1994 to 30 April 1995 would be less than for the previous 12-month period, 2 May 1993 to 30 April 1994. Because the CERES models do not simulate alfalfa, the possible reduction in background leaching effected by the alfalfa cover crop cannot be simulated.

During alfalfa mineralization (2 May 1996 to 27 March 1998) the mean, cumulative NO_3-N leached from the no-till treatment was accurately simulated (Figure 8). In the till treatment, leaching was underestimated, probably because CERES does not simulate tillage. The difference in N leaching between till and no-till treatments began approximately at the tillage date (8 May 1996) to the 22-cm depth. These results strongly suggest that simulation of tillage may improve the predictive capabilities of CERES with respect to N leaching by adjusting the water content for each

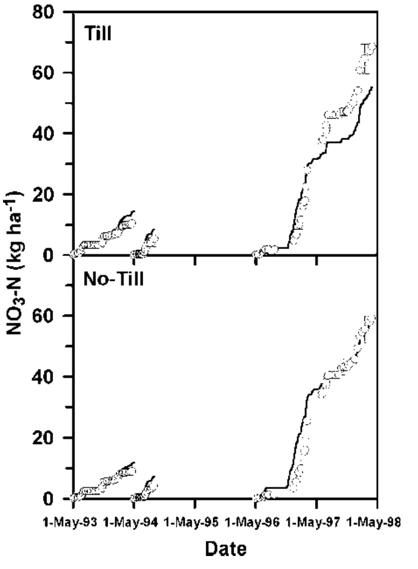

Figure 8. Comparison of observed versus simulated cumulative NO_3-N (nitrate nitrogen) leaching for the till and no-till treatments. Vertical error bars are ± 1 SD for $n = 2$. Comparison during the third period suggests that simulation of tillage may improve the predictive capabilities of CERES with respect to NO_3-N leaching.

lysimeter. Huang (1995) has shown that no-till systems maintain more and better connected macropores. Tillage disrupts macropore continuity. The implications are twofold: First, water drains faster through a well-connected macropore network. Second, in no-till systems, the residence time of water in the soil is less. Nitrate that already is in the interaggregate solution has less time to come in contact with the fast-moving drainage water. As a result, we expect less NO_3 leaching from no-till systems.

Sensitivity analysis results (Table 4) suggest that varying the decomposition rates of the residues or the carbohydrate content by 50% does not substantially affect the prediction of N leaching. CERES does not respond much to changes in decomposition rates with respect to leaching. This seemingly negates the high importance that Quemada and Cabrera (1995) and Quemada, Cabrera, and McCracken (1997) place on the accuracy of these parameters, although we think that there is no real disagreement. Quemada, Cabrera, and McCraken (1997) and Quemada and Cabrera (1995) simulated N mineralization. If mineralized N is taken up at a sufficiently high rate by the plants, the effect on leaching should be insignificant, unless N is released too fast and finds its way to the groundwater before it can be taken up. The decomposition rate and carbohydrate content in fresh organic matter does not affect how much total N will be available but rather how soon it will be available. This is because the C:N ratio in all three fresh

Table 4. Results from sensitivity analyses of model parameters

Parameter set	NRMSE (%)	Total NO_3-N leached ($kg\,ha^{-1}$)	Difference in total NO_3-N leached compared to default parameter set (%)
Default set	138	349	0
Decomposition rates +50%	137	362	+4
Decomposition rates −50%	139	330	−5
Carbohydrate content +50%	138	356	+2
Carbohydrate content −50%	138	343	−2

Notes: Period simulated is 1 Jan. 1993 to 31 Aug. 1994 and 2 May 1996 to 27 Mar. 1998.
NO_3-N: nitrate nitrogen.
NRMSE: normalized root mean square error.

organic matter pools in CERES is the assumed to be the same. Consequently, it is concluded that the user can work with default generic values for crop residue and does not need cultivar-specific soil organic matter mineralization parameters to accurately estimate potential N leaching losses over long periods of time.

Also, the version of CERES evaluated by Quemada, Cabrera, and McCracken (1997) and Quemada and Cabrera (1995) used a higher decomposition rate for carbohydrates. The decay rate, $0.8\,d^{-1}$, originally reported by Seligman and van Keulen (1981), has since been revised. The current version of CERES has a default rate of $0.2\,d^{-1}$. This is closer to the first-order rate constants reported in the literature for easily decomposable materials (Paul and Van Veen 1978; Verberne et al. 1990; Bowen et al. 1993; Vanotti, Bundy, and Peterson 1997).

There is a caveat in such sensitivity analysis; the default mineralization rates used in CERES are for nonlimiting conditions of mineralization. Seldom are field conditions nonlimiting. The actual rate that the model uses is potentially reduced by temperature, soil water content, and C:N ratio factors. Therefore, different calibration studies are not necessarily comparable. Some may adjust the default rate constant to a higher value simply to compensate for an environmental deficit factor. Ideally, calibration studies should use the same data sets, or report the effective rate constants, after accounting for the environmental modifications. The latter is impractical because the effective rate constants vary daily.

Experience from this study reveals the following advantages of applying CERES to simulate the N balance.

Speed of Execution

Because of the daily time step, simulation of a growing season lasts only seconds on a modern computer. The relatively large soil-depth increments (a few centimeters each) contribute to the speedy simulation of the soil water and N processes, arguably at the expense of some precision in the results. Because measurements are also prone to error at small scale, due to soil spatial variability, we do not consider this a serious drawback.

Simplicity

A model is an abstract representation of reality, and so it includes only the components that are thought to be relevant for the purposes of the model. The CERES models are simple enough so that they can be realistically modified by others. The addition of a tillage component would strengthen the model for the purpose of studying the water and N balance, without seriously detracting from its simplicity.

Data Requirements

CERES are typical "functional" models that are founded on capacity concepts (e.g., the water-storage capacity of the soil) rather than dynamic rate concepts. Capacity variables often are less spatially variable than rate variables (Addiscott and Wagenet 1985). Where possible, functional models use rational empiricisms to integrate almost minute-by-minute variations in variables such as solar radiation, air temperature, and rainfall into daily values. Thus, functional models demand less data and computing power than mechanistic models, without seriously compromising accuracy (Ritchie and Johnson 1990). Because of its modest input requirements, CERES is easier to independently test by others. A detailed protocol developed for data collection ensures that all modelers use data of the same quality and format (Tsuji, Uehara, and Balas 1994).

The main drawback in using the current version of CERES is the somewhat old-fashioned interface and lack of a built-in, user-friendly plotting capability. The output files had to be manipulated extensively to import them into a spreadsheet (for quick evaluation of the results) and into the plotting software (to generate publication-quality figures).

CONCLUSIONS

CERES can be a useful aid to agronomists to predict the N budget of the crop–soil system and manage fertilizer. Fertilizer recommendations can be more accurate when the baseline leaching potential and residue contributions from previous crops can be predicted. CERES cannot evaluate the effect of tillage management; the addition of a tillage component in CERES will further increase its usefulness. Sensitivity analyses showed that to predict long-term N leaching, CERES does not require an exact knowledge of mineralization parameters of either surface or incorporated alfalfa residues.

APPENDIX: MODIFICATIONS TO CERES VERSION 3.5

CERES Routines

The following routines are part of the CERES program, that is, the science core of the DSSAT cereal models.

IPIBS

The unit of variable ROWSP (row spacing) was changed from centimeters to meters so that the light interception is calculated correctly.

OPNIT

We increased the width of the inorganic N output column to print larger numbers.

OPDAY

We suppressed the printing of headers in the N, water, and plant growth output files so that files are more rapidly imported to a spreadsheet and increased the accuracy of the TLCH (total N leaching) variable to display four significant digits in the output. The model was forced to print a zero LAI (leaf area index) when the crop is not growing. We replaced PESW (potentially extractable soil water) with TSW (total soil water) in the water output file.

OPDONE

We suppressed the printing of a blank line at the end of the output files for water, N, and plant growth. The blank line was confusing to the spreadsheet programs that were importing the output files.

NTRANS

We placed a zero lower boundary to variable B2 (ammonium nitrified in a given layer) because it could become negative if ammonium dropped below $0.5\,mg\,kg^{-1}$.

NUPTAK

We placed a zero lower boundary to variable RNH4U (potential ammonium uptake) because it could become negative if ammonium dropped below $0.5\,mg\,kg^{-1}$. We placed a zero lower boundary to UNO3 and UNH4 (plant uptake of nitrate and ammonium) to avoid negative values.

PHASEI

In CERES, transpiration continued even after physiological maturity. We reset LAI to zero at maturity so that transpiration stops.

Input Program Routines

The following modifications are in the input program, that is, the ancillary program in DSSAT that handles the input data.

IPSLIN

We set minimum initial N to 0.5 mg kg^{-1} in all soil layers. We increased minimum allowable soil NO_3 from 100 to 200 mg kg^{-1} to avoid an error message. These limits are rather high. We have measured NO_3 as low as 40–60 mg kg^{-1} in the soils that we used to test the model. However, the daily time step of the model is rather large. Simulated removals of soil NO_3 can exceed 100 mg kg^{-1} in 1 day, due mostly to leaching and plant uptake. A more permanent and scientifically appropriate solution would be to limit the large daily fluctuations of soil N at the process level.

IPFILX

We deleted unused variable ECONO from the list of the arguments of the subroutine.

OPIBS3

We suppressed the printing of headers in the N, water, and plant growth output files so that they could be more rapidly imported to a spreadsheet.

OPHEAD

We increased the width of the output file headers for total initial soil nitrate because we increased the accuracy of total initial soil nitrate by one decimal place.

Input Files

The following modifications concern the DSSAT input files:

Soils Description File

We set variable SLRO (runoff curve number) to zero to prevent runoff because the test lysimeters were built with raised edges that prevented runoff.

Residue Parameter File

If residue is applied on the first day of simulation, it becomes part of the initial conditions' residue amount. The problem is that CERES (subroutine NTRANS) always uses the default residue decomposition parameters, which are those of the first residue type, RE001, in parameter file SOILN980.SOL. The way around this problem is to temporarily modify the residue decomposition parameters of residue type RE001 so that the model uses them as default parameters.

Output Files

The initial condition values (left column) in the N balance summary file (NBAL.OUT) are true only for the first crop in the rotation. This is because CERES reads initial conditions information only once, on the first day of simulation. The initial conditions for subsequent crops must be ignored.

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