ROOT ZONE WATER QUALITY MODEL SENSITIVITY ANALYSIS USING MONTE CARLO SIMULATION

L. Ma, J. C. Ascough II, L. R. Ahuja, M. J. Shaffer, J. D. Hanson, K. W. Rojas

ABSTRACT. *Performing a sensitivity analysis for a mathematical simulation model is helpful in identifying key model parameters and simulation errors resulting from parameter uncertainty. The Root Zone Water Quality Model (RZWQM) has been evaluated for many years, however, detailed sensitivity analyses of the model to various agricultural management systems and their representative input parameters are lacking. This study presents results of RZWQM output response sensitivity to selected model input parameters. Baseline values for the parameters were measured for an experiment on a manured corn field in eastern Colorado. Four groups of model input parameters (saturated hydraulic conductivity, organic matter/nitrogen cycling, plant growth, and irrigation water/manure application rates) were selected and three model output responses (plant nitrogen uptake, silage yield, and nitrate leaching) were used to quantify RZWQM sensitivity to selected model input parameters. A modified Monte Carlo sampling method (Latin Hypercube Sampling) was used to obtain parameter sets for model realizations. The model parameter sets were then analyzed separately using linear regression analysis. In general, RZWQM output responses were most sensitive to plant growth input parameters and manure application rates. The plant nitrogen uptake and silage yield model output responses were less sensitive to nitrogen cycling and irrigation rate input parameters than those observed in previous field experiments. This finding may warrant further study on the effects of water and nitrogen stresses on crop growth. Finally, the results showed that model output responses were more sensitive to the average saturated hydraulic conductivity of the entire soil profile than to the saturated hydraulic conductivity of individual soil layers.*

Keywords. *RZWQM, Modeling, Sensitivity analysis, Monte Carlo analysis, Water quality.*

In order to correctly use mathematical simulation models, sensitivity analysis is needed to identify sources of simulation errors, key parameters, and parameter precision required (Fontaine et al., 1992; Larocque and Banton, 1994; Ferreira et al., 1995). Sensitivity analysis may also be used to infer statistical consequences due to parameter uncertainty and to find programming errors (Gwo et al., 1996). A sensitivity analysis is usually conducted by varying (perturbing) model parameter values (Nearing et al., 1990), adding or removing model parameters (Ma and Selim, 1997), or running the model under dynamic conditions (Ma et al., 1998). Results from a sensitivity analysis may be site and condition specific (Ferreira et al., 1995).

In most sensitivity analyses, model parameters are allowed to vary around their base values independently (Tiscareno-Lopez et al., 1993, 1994; Barnes and Young, 1994) or dependently (Silberbush and Barber, 1983). The range of the perturbation may be a specific percentage (Barnes and Young, 1994; Ferreira et al., 1995) or determined from experimental measurements (Fontaine et al., 1992; Gwo et al., 1996). The most common form of sensitivity analysis is independent parameter perturbation (IPP) in which parameters are varied individually by a fixed percentage around a base value (Ferreira et al., 1995). An example of this approach is first-order analysis (Haan and Zhang, 1996), which is best applicable to linear systems. More recent approaches vary multiple parameters simultaneously based on underlying probability distributions of the parameters, such as the traditional Monte Carlo simulation (Shaffer et al., 1988; Tiscareno-Lopez et al., 1993, 1994), Latin Hypercube Sampling (Gwo et al., 1996; Ellerbroek et al., 1998), Plackett-Burman screening design (Fontaine et al., 1992), and Fourier amplitude sensitivity testing (Fontaine et al., 1992). Model output responses to parameter perturbation may be quantified by percentage change of selected output variables (Barnes and Young, 1994; Ferreira et al., 1995), relative change of output versus input (Nearing et al., 1990; Larocque and Banton, 1994), sensitivity coefficients from linear regression analysis (Fontaine et al., 1992; Tiscareno-Lopez et al., 1993, 1994; Gwo et al., 1996), and graphic response curves or probability distributions (Franti et al., 1996; Haan and Zhang, 1996; Baffaut et al., 1997; Ellerbroek et al., 1998). The overall model response may be obtained by taking the average response of selected output variables (Nearing et al., 1990).

In this study, the Latin Hypercube Sampling (LHS) technique was used to perform a sensitivity analysis on the

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Root Zone Water Quality Model (RZWQM) (RZWQM Development Team, 1998). LHS is a modified Monte Carlo method that has been shown to be more efficient than traditional Monte Carlo simulation in sampling parameters with a given distribution (McKay et al., 1979; Gwo et al., 1996). For example, suppose there are K input variables or parameters, X_k, (k = 1, 2, . . . , K), and each X_k has a distribution. To sample M vectors of import variables, each distribution is divided into M intervals, each interval is sampled with a probability of 1/M and a total of M values are obtained for variable X_k (X_{kj}, j = 1, 2, . . . , X_{kM}). To produce vectors of the input variables, one of the values of X_1 is randomly selected and matched with a randomly selected value of X_2, and so on, through X_K. This matching procedure is repeated on the rest of sampled values of X_k until all the values are exhausted. The resulting M vectors of the K input variables may be used to study the sensitivity of selected RZWQM (or other model) output responses from multiple simulation runs.

The comparability of LHS results with traditional Monte Carlo simulation results can be difficult to see in practice. Certainly in the limit of a large number of observations, there is a statistical equivalence between the results of an LHS sensitivity analysis and those produced by a representative Monte Carlo analysis. However, when a smaller sample size is used (either for LHS or Monte Carlo analysis), several factors can combine to obscure that equivalence. For Monte Carlo, a small sample size can allow unintended correlations to be introduced to the sampled data set (the insufficient number of samples does not allow randomness to reduce those correlations), or the sample set may not cover the entire range of a distribution (dependent on the particular random number sequence that was generated). For LHS, a small sample size should not cause unintended correlations or result in poor distribution coverage. Rather, if the results of an LHS analysis with few samples (say, 100) are compared with the results of a Monte Carlo analysis with many samples (say, 100,000), the statistical agreement between those analyses may not be as good as expected. This is particularly true when sampling one or more distributions that have very long tails (e.g., normal or lognormal variables with large standard deviations, among others), and can be especially noteworthy when examining statistics such as the mean or standard deviation (as opposed to order statistics such as the median). Furthermore, LHS can be more sensitive to the random seed value than traditional Monte Carlo techniques. This also can obscure the equivalence between the Monte Carlo and LHS sensitivity results that might be expected.

RZWQM studies have been conducted previously for macropore flow (Ahuja et al., 1993), pesticide transport (Ma et al., 1996; Ellerbroek et al., 1998,), and tile drainage (Singh and Kanwar, 1995a,b; Walker, 1996) model components. A RZWQM sensitivity analysis for east-central Illinois agricultural conditions was performed by Walker et al. (2000) to identify model input parameters with the greatest influence on simulated tile drain flow, tile nitrate, and crop yield. A goal of this research was to avoid duplicating prior RZWQM studies, therefore, three preliminary steps were conducted before performing the actual sensitivity analysis. First, model input variables that vary in a predetermined manner were chosen. Based on previous experience (Ahuja et al., 1993; Walker, 1996; Ellerbroek et al., 1998; Ma et al., 1998), four sets of model input parameter groups were identified: (1) saturated hydraulic conductivity; (2) organic matter/nitrogen (N) cycling parameters; (3) plant growth parameters; and (4) irrigation water and manure application rates. RZWQM output sensitivity to each set of input parameter groups was determined independently to avoid interactions among different simulation processes. Second, baseline values for the model input parameters were selected. An experimental data set on manure management in an eastern Colorado corn field was used to obtain the values (Ma et al., 1998). RZWQM was calibrated for this data set by varying crop residue-soil organic matter inter-pool mass transfer coefficients and evaluating their effect on crop yield. The calibrated model successfully predicted manure effects on corn yield, plant nitrogen (N) uptake, and nitrate (NO_3-N) leaching (Ma et al., 1998). Third, critical RZWQM output responses were identified in order to quantify overall model sensitivity. Three model outputs, plant N uptake, silage yield, and NO_3-N leaching beyond the root zone, were selected because of their probable overall response to the input parameters.

The general objectives of this study were to evaluate the performance of RZWQM and to identify key (sensitive) model input parameters under eastern Colorado conditions in terms of corn production and NO_3-N leaching. Because of the complexity of RZWQM, a secondary intent was to provide guidance towards calibration of RZWQM and identification of potential sources of RZWQM simulation errors.

FIELD EXPERIMENT DESCRIPTION

Input parameter baseline values for the sensitivity analysis were obtained from a field experiment designed to study residual effects of manure on irrigated corn production in eastern Colorado (Ma et al., 1998). Over the past decade, the field had a history of receiving beef cattle manure (44.8 Mg ha^{-1}) as fertilizer every autumn after the harvest of silage corn. No inorganic fertilizer was applied. The experimental plots were on a Vona sandy loam soil (coarse loamy, mixed, mesic, *Ustollic Haplargid*). The water table was approximately 8 m below the ground surface. The field was irrigated in alternate furrows with ditch water containing 1.3 ppm NO_3-N. Each irrigation event lasted 12 h with a total application amount of 20 cm. The farmer irrigated infrequently—usually only four to six times during the months of July and August.

Soil organic matter content, soil pH, and soil texture were measured by the Colorado State University Soil, Water and Plant Testing Laboratory. The modified Walkey and Black method was used to measure soil organic matter content (Allison, 1965), and soil texture was measured with the hydrometer method (Gee and Bauder, 1986). Soil bulk density was measured using the core method (Blake and Hartge, 1986) with a 3.8-cm cylindrical sampler, and 33-kPa soil water content was estimated using the ceramic pressure plate method (Gardner, 1986). A summary of the soil physical properties by layer is listed in table 1. Weather data were obtained from a weather station 0.4 km southwest of the experiment site. Dates for agricultural management practices such as manure application,

Table 1. Soil physical properties by layer from a field experiment designed to study residual effects of manure on irrigated corn production in eastern Colorado

Soil Physical Property	Soil Layer				
	1	2	3	4	5
Soil depth (cm)	0-30	30-60	60-90	90-120	120-150
Bulk density (g cm^{-3})	1.4	1.5	1.5	1.5	1.5
Organic matter (%)	1.7	0.7	0.6	0.3	0.3
Sand (%)	63	61	41	64	48
Silt (%)	15	15	28	16	28
Clay (%)	22	24	31	20	24
33 kPa water content (cm^3 cm^{-3})	0.227	0.222	0.279	0.188	0.279
Soil classification	Sandy clay loam		Clay loam	Sandy loam	Loam

irrigation, tillage, and planting and harvesting were recorded and are listed in table 2 for years 1993-1996.

THE ROOT ZONE WATER QUALITY MODEL (RZWQM)

The Root Zone Water Quality Model has been discussed in detail in the literature (Ma et al., 1998; RZWQM Development Team, 1998; Ahuja et al., 1999). The model was developed to simulate the physical, chemical, and biological processes in the root zone as affected by agricultural management practices. Modeling of selected processes is illustrated here to provide a background for the input parameter groups chosen for the sensitivity analysis.

SATURATED HYDRAULIC CONDUCTIVITY

Soil properties (Ma et al., 1998) for the eastern Colorado experimental data set included soil bulk density, soil texture, and soil water content at 33 kPa. Measured field values were used in this sensitivity analysis; however, emphasis is placed here on RZWQM output response to saturated hydraulic conductivity (K_{sat}, cm/h) because of its importance in water and chemical movement (Singh et al., 1996; Singh and Kanwar, 1995a,b). RZWQM estimates K_{sat} from effective porosity, ϕ_e, using (Ahuja et al., 1989):

$$K_{sat} = 764.5\ \phi_e^{3.29} \tag{1}$$

$$\phi_e = \theta_s - \theta_{1/3} \tag{2}$$

where θ_s and $\theta_{1/3}$ are soil water content at saturation and 33 kPa suction. The range of values tested was calculated from equations 1 and 2 using soil water contents at saturation and 33 kPa suction, as given by Rawls et al. (1982). K_{sat} baseline and testing range values are shown in table 3. Testing ranges for K_{sat} and other input variables were determined using maximum and minimum values based on a combination of expert opinion and literature review. LHS was used to sample K_{sat} values for individual soil layers in order to identify an unusual RZWQM output response sensitivity to a particular soil layer. Values of K_{sat} were assumed to be lognormally distributed for all soil layers (Ellerbroek et al., 1998).

Brooks-Corey input parameters were also obtained from Rawls et al. (1982). RZWQM output response sensitivity to these parameters was not studied for two reasons. First, a sensitivity analysis study examining the Brooks-Corey parameters has previously been conducted (Walker, 1996). Second, it is extremely difficult, if not impossible, to randomly sample these parameters without affecting the integrity of the Brooks-Corey equations. Other soil property-related processes such as macropore and tile

Table 2. Management practices for 1993 to 1996 from a field experiment designed to study residual effects of manure on irrigated corn production in eastern Colorado

Management Practice	Timing	Method	Specific Information
Planting & harvesting	15 April 1994 & 10 Sept 1994 22 April 1995 & 15 Sept 1995 20 April 1996 & 14 Sept 1996		Corn always planted with 76 cm row spacing at a rate of 8000 to 8700 seeds/ha Corn always harvested for silage
Manure & Fertilizer	15 October 1993 15 October 1994 15 October 1995	Surface broadcast	No inorganic fertilizer was applied Nitrogen applied with manure at a rate of 582 kg/ha
Irrigation	14, 25 June 1994 7, 17, 29 July 1994 18 Aug 1994 13 July 1995 2, 16, 31 Aug 1995 20 May 1996 29 June 1996 12, 26 July 1996 10, 25 Aug 1996	Furrow irrigation	20 cm/event
Tillage	17 Oct 1993	Moldboard plow	15 cm of effective tillage depth (same for all)
	15 days before planting 1993	Field cultivator	10 cm of effective tillage depth (same for all)
	2 days before planting 1993	Field cultivator	
	21 May 1994	Field cultivator	
	17 Oct 1994	Moldboard plow	
	15 days before planting 1994	Field cultivator	
	2 days before planting 1994	Field cultivator	
	13 June 1995	Field cultivator	
	2 July 1995	Field cultivator	
	17 Oct 1995	Moldboard plow	
	15 days before planting 1995	Field cultivator	
	2 days before planting 1995	Field cultivator	
	13 June 1996	Field cultivator	
	2 July 1996	Field cultivator	

Table 3. Baseline values, testing ranges, and probability distributions of model input parameters selected for RZWQM sensitivity analysis

Simulated Process Group	Model Input Parameter		Unit	Baseline Value	Testing Range	Distribution
Soil physical properties	K_{sat}: saturated hydraulic conductivity,	1st layer:	cm/h	7.449	9.5×10^{-5} to 11.3	Lognormal
		2nd layer:	cm/h	4.643	9.5×10^{-5} to 11.3	Lognormal
		3rd layer:	cm/h	1.657	3.1×10^{-3} to 10.2	Lognormal
		4th layer:	cm/h	7.574	8.5×10^{-2} to 47.2	Lognormal
		5th layer:	cm/h	1.657	7.4×10^{-3} to 25.6	Lognormal
Organic matter/N cycling	k_{nit}: nitrification rate constant		s/day/org.	1.0×10^{-9}	0.1×10^{-9} to 10×10^{-9}	Lognormal
	k_{den}: denitrification rate constant		s/day/org.	1.0×10^{-13}	0.1×10^{-13} to 10×10^{-13}	Lognormal
	k_{SRP}: decay rate constant for the SRP		s/day	1.67×10^{-7}	0.167×10^{-7} to 16.7×10^{-7}	Lognormal
	k_{FRP}: decay rate constant for the FRP		s/day	8.14×10^{-6}	0.814×10^{-6} to 81.4×10^{-6}	Lognormal
	k_{FHP}: decay rate constant for the FHP		s/day	2.5×10^{-7}	0.25×10^{-7} to 25×10^{-7}	Lognormal
	k_{IHP}: decay rate constant for the IHP		s/day	5.0×10^{-8}	0.5×10^{-8} to 50×10^{-8}	Lognormal
	k_{SHP}: decay rate constant for the SHP		s/day	4.5×10^{-10}	0.45×10^{-10} to 45×10^{-10}	Lognormal
	k_{dhet}: death rate constant for heterotrophs		s/day	5.0×10^{-35}	0.5×10^{-35} to 50×10^{-35}	Lognormal
	k_{dnit}: death rate constant for nitrifiers		s/day	4.77×10^{-40}	0.477×10^{-40} to 47.7×10^{-40}	Lognormal
	k_{dden}: death rate constant for denitrifiers		s/day	3.4×10^{-33}	0.34×10^{-33} to 34×10^{-33}	Lognormal
Plant growth	N_{max}: maximum active daily N uptake rate		g/plant/day	0.5	0.0 to 3.3	Normal
	R_1: photorespiration rate		percentage	0.08	0.0 to 0.525	Normal
	SLW: specific leaf weight		g/LAI	9.0	0.0 to 27.3	Normal
	A_p: photosynthesis reduction factor at propagules		percentage	0.9	0.708 to 1.0	Normal
	A_s: photosynthesis reduction factor at seed stage		percentage	0.8	0.48 to 1.0	Normal
Irrigation water and manure application rates	W: amount of water irrigated each event		cm	20	0.0 to 40	Normal
	M: amount of manure applied each year		Mg/ha	44.8	0.0 to 89.6	Normal

drainage flow were not measured at the eastern Colorado experimental site; thus RZWQM output responses for these processes are not included in the sensitivity analysis.

ORGANIC MATTER/N CYCLING

RZWQM differentiates various organic materials according to their physical status and chemical properties (Ma et al., 1998; RZWQM Development Team, 1998; Shaffer et al., 1999). A fast (FRP) and a slow residue pool (SRP) are identified according to their composition. Three humus pools are also distinguished based on their half-lives in the soil: (1) a fast humus pool (FHP) with a half-life of five years; (2) an intermediate humus pool (IHP) with a half-life of 20 years; and (3) a slow humus pool (SHP) with a half-life of 2000 years. Each pool is characterized with a specific carbon/nitrogen (C/N) ratio and a first-order decay constant. Materials from an organic matter pool may be transferred into other pools, assimilated into microbial biomass, or emitted as CO_2 (Ma et al., 1998). During these transformations, nitrogen is conserved and CO_2 is used as sink/source for carbon to maintain the C/N ratios of each pool. RZWQM also simulates nitrification and denitrification processes. A zero-order nitrification equation and a first-order denitrification equation are currently used.

Organic matter/N cycling in the soil system is mediated by three types of microorganisms, namely heterotrophic decomposers, nitrifiers, and denitrifiers. These three microorganism pools dynamically respond to soil nutrient contents, soil pH, soil aeration, and soil temperature. Microbial growth rates are proportional to the rates of reactions that they are catalyzing. Microbial death rates are proportional to their biomass.

The decay rate of each organic matter pools is described by (Shaffer et al., 1999):

$$R_i = k_i \, f_1 \, (T, O_2, pH, P_{het}) \, C_i \tag{3}$$

where R_i and C_i are the decay rate and carbon concentration of organic matter pool i (i = FRP, SRP, FHP, IHP, and SHP), respectively. f_1 is a function of soil temperature (T), soil aeration (O_2), pH, and the population of heterotrophic decomposers (P_{het}). Nitrification rate (R_{nit}) is simulated by:

$$R_{nit} = k_{nit} \, f_2 \, (T, O_2, pH, P_{nit}) \tag{4}$$

The denitrification rate (R_{den}) is expressed as:

$$R_{den} = k_{den} \, f_3 \, (T, O_2, pH, P_{den}) \, C_{NO_3} \tag{5}$$

where k_{nit} and k_{den} are nitrification and denitrification constants, and f_2 and f_3 are modifiers depending on soil temperature, soil aeration, pH, and microbial populations. P_{nit} and P_{den} are populations of nitrifiers and denitrifiers. C_{NO_3} is concentration of NO_3. The death rates (D_i) of microbial populations (P_i) are assumed to be first-order kinetics:

$$D_i = k_{di} \, f_{4i} \, (T, O_2, pH) \, P_i \tag{6}$$

where k_{di} is the death constant for microbial population P_i [i = het, nit, and den) and f_{4i} is the corresponding modifier for soil environment. In this study, 10 rate constants were selected for sensitivity analysis: the five decay constants (k_{SRP}, k_{FRP}, k_{FHP}, k_{IHP}, and k_{SHP}), nitrification constant (k_{nit}), denitrification constant (k_{den}), and the three microbial death constants (k_{dhet}, k_{dnit}, and k_{dden}). The baseline and testing range values of the organic matter/N cycling parameter set are shown in table 3. The parameter test ranges were determined by multiplying (maximum value) and dividing (minimum value) the baseline values by 10. Each organic matter/N cycling parameter is assumed to be lognormally distributed.

PLANT GROWTH

The generic plant growth model was developed by Hanson (1999). It simulates both plant growth and plant population development. Seven phenological growth stages, dormant, germinating, emergence, four-leaf, vegetative, reproductive, and senescence, are identified in the model. Plants in any stage can remain alive in the current stage, pass to the next stage, or die depending on environmental fitness. A modified Leslie probability matrix is used to calculate plant population development (Hanson, 1999). Nitrogen uptake by plants is passive if the amount of uptake to the plants through water transpiration meets plant nitrogen demands, otherwise, active plant N uptake occurs according to the Michaelis-Menton equation (Hanson, 1999).

Five RZWQM plant growth and N uptake parameters were recommended by Hanson et al. (1999) for calibration: (1) maximum active daily N uptake rate (N_{max}); (2) photorespiration rate as a percentage of daily photosynthate (R_1); (3) biomass needed to obtain a leaf area index of 1.0, or specific leaf weight (SLW); (4) leaf photosynthesis reduction factor at propagule stage as a percentage of maximum daily photosynthesis rate (A_p); and (5) leaf photosynthesis reduction factor at seed production stage as a percentage of maximum daily photosynthesis rate (A_s). Hanson et al. (1999) provides ranges and standard errors for each of the parameters using model calibration results from field experiments in Colorado, Iowa, Minnesota, Nebraska, and Ohio. The baseline and testing range values of the plant growth parameter set assimilate the results of Ma et al. (1998) and Hanson et al. (1999) and are listed in table 3. Each plant growth parameter is assumed to be normally distributed.

WATER AND MANURE APPLICATION RATES

Average irrigation water and manure application rates were used in the evaluation of RZWQM by Ma et al. (1998). However, irrigation water and manure applications were not uniform in the field, especially when alternative furrow irrigation was used. In the eastern Colorado field experiment, an average of 20 cm of water was applied during each irrigation event. Since alternative furrow irrigation was used, some portion of the field received no water. Therefore, a test range of irrigation water application variability of 0 to 40 cm with a baseline value of 20 cm was used (table 3). Likewise, a test range for manure application variability of 0 to 89.6 Mg ha^{-1} with a baseline value of 44.8 Mg ha^{-1} was used (table 3). Both variables are assumed to be normally distributed since no measurement was conducted on the spatial distribution of water and manure applications in the field. The assumption of a normal distribution should have minimal effect on the sensitivity analysis results (Fontaine et al., 1992; Haan and Zhang, 1996).

RZWQM SENSITIVITY ANALYSIS

In this study, three RZWQM output responses, plant N uptake, silage yield, and NO_3-N leaching below the root zone (i.e., beyond 1.5 m), were selected because of their practical interest for agricultural production and environmental quality. RZWQM output responses to each group of model input parameters of saturated hydraulic conductivity, organic matter/N cycling, plant growth, and irrigation water and manure application rates were quantified by linear regression analysis (Fontaine et al., 1992; Tiscareno-Lopez et al., 1993, 1994; Gwo et al., 1996) as:

$$Y = b_0 + b_1X_1 + b_2X_2 + \ldots + b_nX_n \qquad (7)$$

where Y is a model output, X_i is the *ith* model parameters, and b_i is the corresponding coefficient. A normalized sensitivity coefficient (β_i) can be defined as:

$$\beta_i = b_i\, S_{xi}/S_Y \qquad (8)$$

where S_{xi} and S_Y are the standard deviations of X_i and Y, respectively. A sensitivity coefficient value of 1.0 means that one standard deviation change in the model parameter will lead to a standard deviation change in the model output (Tiscareno-Lopez et al., 1993, 1994). An implication of linear regression analysis (along with the LHS method) is the analog to analyzing experimental data collected from an underlying statistical distributions with due consideration of experimental errors (Gwo et al., 1996).

Sensitivity of the selected model output responses was analyzed individually for each group of model input parameters, keeping the other parameter group input variables constant. However, since we are using a relative sensitivity coefficient that is independent of sample distribution (Fontaine et al., 1992), sensitivity results should be comparable across groups. LHS was used to generate 100 parameter sets each for the saturated hydraulic conductivity, plant growth, and irrigation water and manure application rates parameter groups; 200 parameter sets were generated for the organic matter/N cycling parameter group. This resulted in a total of 500 computer runs of the model. Table 4 shows the minimum number of runs needed for a confidence size greater than or equal to ±10% of the mean simulated output response for a simple Monte Carlo analysis according to Shaffer (1988). The number of simulation runs conducted for this study was generally much larger than needed, except for the irrigation water and manure application rates parameter group. However, since LHS is a much more efficient sampling technique than traditional Monte Carlo simulation, the total number of simulation runs should be adequate.

For each input parameter set generated using LHS, RZWQM was initialized for the organic matter pools by running the model for 12 years prior to the 1993-1996 actual simulation period. A 12-year initialization run was suggested by Ma et al. (1998) to obtain steady-state conditions for the faster soil organic pools. Model initialization is also beneficial when conducting a sensitivity analysis in order to obtain steady-state conditions as affected by model input parameters only (Larocque and Banton, 1994). Table 4 lists the sampling means, standard deviations, and the minimum and maximum values of each parameter generated using the LHS technique. LHS requires inputs of mean value (μ) and standard error (σ) for each distribution, and samples are taken between $\mu - 3.09\sigma$ and $\mu + 3.09\sigma$ (Iman and Shortencarier, 1984). It was difficult to obtain standard errors for some RZWQM input parameters in this study (e.g., saturated hydraulic conductivity and many of the parameters related to organic matter/N

Table 4. Statistics for LHS generated RZWQM input parameters and general simulation results for N uptake, silage yield, and NO_3-N leaching

Simulated Process Group	Model Input Parameter	Mean	S.D.	Maximum	Minimum	Estimated Min. Runs*
Soil physical properties	K_{sat}, 1st layer:	0.242	1.150	11.30	0.0002	
	2nd layer:	0.247	1.157	11.30	0.0004	
	3rd layer:	0.390	0.60	3.87	0.0074	
	4th layer:	3.468	5.037	41.60	0.131	
	5th layer:	1.085	2.385	21.00	0.0107	
	Simulated N uptake (kg N/ha)	298.187	26.578	359.00	250.00	4
	Simulated silage yield (kg/ha)	25929.64	2168.78	28787.82	17612.77	3
	Simulated NO_3-N leaching (kg N/ha)	178.48	83.58	256.36	0.0025	85
Organic matter/N cycling	k_{nit}:	1.309×10^{-9}	1.063×10^{-9}	6.94×10^{-9}	0.115×10^{-9}	
	k_{den}:	1.325×10^{-13}	1.167×10^{-13}	10.0×10^{-13}	0.146×10^{-13}	
	k_{SRP}:	2.191×10^{-7}	1.786×10^{-7}	11.5×10^{-7}	0.175×10^{-7}	
	k_{FRP}:	10.801×10^{-6}	9.523×10^{-6}	81.40×10^{-6}	0.998×10^{-6}	
	k_{FHP}:	3.307×10^{-7}	2.90×10^{-7}	25.00×10^{-7}	0.25×10^{-7}	
	k_{IHP}:	6.569×10^{-8}	5.421×10^{-8}	36.60×10^{-8}	0.706×10^{-8}	
	k_{SHP}:	5.971×10^{-10}	5.28×10^{-10}	45.00×10^{-10}	0.484×10^{-10}	
	k_{dhet}:	6.597×10^{-35}	5.614×10^{-35}	45.10×10^{-35}	0.708×10^{-35}	
	k_{dnit}:	6.319×10^{-40}	5.553×10^{-40}	47.7×10^{-40}	0.625×10^{-40}	
	k_{dden}:	4.456×10^{-33}	3.638×10^{-33}	23.5×10^{-33}	0.361×10^{-33}	
	Simulated N uptake (kg N/ha)	310.515	14.426	334.00	198.00	1
	Simulated silage yield (kg/ha)	27498.823	544.129	27897.64	22582.47	1
	Simulated NO_3-N leaching (kg N/ha)	239.955	37.828	324.85	71.91	10
Plant growth	N_{max}:	1.559	0.573	3.30	0.0547	
	R_1:	0.197	0.103	0.446	0.001	
	SLW:	12.105	4.903	27.30	1.25	
	A_p:	0.879	0.056	1.00	0.731	
	A_s:	0.810	0.109	1.00	0.510	
	Simulated N uptake (kg N/ha)	264.323	80.476	371.00	43.50	37
	Simulated silage yield (kg/ha)	19551.62	6758.959	30915.22	2994.28	47
	Simulated NO_3-N leaching (kg N/ha)	295.881	83.48	521.74	21.123	32
Irrigation water and manure application rates	W:	20.02	6.583	40.00	2.67	
	M:	44797.29	14313.27	78920.00	9669.00	
	Simulated N uptake (kg N/ha)	307.49	48.34	360.67	117.00	10
	Simulated silage yield (kg/ha)	26925.02	1672.29	28309.46	16550.6	2
	Simulated NO_3-N leaching (kg N/ha)	251.48	129.07	593.43	0.0233	102

* Number of computer runs needed for confidence size ≤ ±10% of mean simulated outputs.

cycling). In these cases, model input parameters were sampled from their individual distributions within the test ranges defined in table 3.

Results and Discussion

RZWQM Output Responses to Saturated Hydraulic Conductivity

Mean saturated hydraulic conductivities (K_{sat}) for soil layers 1 to 5 generated using LHS were 0.242, 0.247, 0.390, 3.468, and 1.085 cm/h (table 4), which are much lower than the values of 7.449, 4.643, 1.657, 7.574, and 1.657 cm/h (table 3) estimated from measured bulk density and 33 kPa water content of the soil (Ma et al., 1998). However, the estimated values are still within the LHS ranges. Linear regression analysis (table 5) indicates that plant N uptake, silage yield, and NO_3-N leaching are weakly correlated to K_{sat} (coefficient of correlation $r \leq 0.326$). Corresponding sensitivity coefficients (β_i) are generally small ($\beta_i \leq 0.224$). The eastern Colorado field experimental location may be an inadequate test of K_{sat} effects on model output responses because of the low yearly precipitation (~22 cm/year) and infrequent irrigation events (only four to six yearly). Calculated plant N uptake, silage yield, and NO_3-N leaching sensitivity coefficients for the average K_{sat} of the soil profile (all

Table 5. Sensitivity coefficients (β_i) calculated for RZWQM output response to perturbations in model input parameters

Simulated Process Group	Model Input Parameter	Plant N Uptake	Silage Yield	NO_3-N Leaching
Soil physical properties	K_{sat}, 1st layer:	+0.1323	+0.1573	+0.1125
	2nd layer:	–0.01915	+0.01716	+0.07723
	3rd layer:	–0.1632	–0.03096	+0.07499
	4th layer:	+0.2242	+0.03229	–0.1560
	5th layer:	+0.1275	–0.005478	–0.1006
	All layers:	–0.1478	+0.2987	+0.4906
	r	0.326	0.164	0.241
Organic matter/N cycling	k_{nit}:	–0.03299	+0.009228	–0.01883
	k_{den}:	–0.2293	–0.1866	–0.2338
	k_{SRP}:	–0.06288	+0.09159	+0.1127
	k_{FRP}:	+0.2361	+0.1698	+0.2165
	k_{FHP}:	–0.1508	+0.06592	+0.07682
	k_{IHP}:	+0.04404	+0.01555	+0.1532
	k_{SHP}:	+0.1745	+0.02564	+0.2056
	k_{dhet}:	–0.4826	–0.5502	–0.6518
	k_{dnit}:	–0.05938	–0.02425	–0.02392
	k_{dden}:	+0.2647	+0.1978	+0.2543
	r	0.680	0.648	0.815
Plant growth	N_{max}:	+0.07091	–0.001944	–0.07285
	R_1:	–0.4351	–0.5144	+0.3787
	SLW:	–0.7333	–0.7829	+0.8316
	A_p:	–0.03862	–0.001877	–0.1180
	A_s:	–0.006375	+0.03824	+0.03469
	r	0.854	0.936	0.926
Irrigation water and manure application rates	W:	–0.2674	+0.004373	+0.1967
	M:	+0.8734	+0.7053	+0.9531
	r	0.914	0.706	0.973

layers, 0-150 cm) are –0.1478, +0.2987, and +0.4906, respectively (table 5). Sensitivity coefficients for silage yield and NO_3-N leaching are higher than the sensitivity coefficients calculated for each individual soil layer. Therefore, RZWQM output responses appear to be more closely related (sensitive) to the average soil profile K_{sat} than to the K_{sat} of an individual soil layer. Plant N uptake and silage yield output responses were less sensitive to average K_{sat} than NO_3-N leaching, which may reflect a weak response of plant growth to water stresses. In addition, plant N uptake was negatively correlated to average K_{sat}. This may suggest that less N was available at high saturated hydraulic conductivity due to leaching.

RZWQM OUTPUT RESPONSES TO ORGANIC MATTER/N CYCLING

Organic matter/N cycling parameter mean values generated using LHS sampling (table 4) are closer to the baseline values (table 3) than the K_{sat} LHS generated values. Table 5 shows that model output responses are least sensitive to nitrification rate constant (k_{nit}) and death rate of nitrifiers (k_{dnit}) parameters, and the most sensitive to the death rate of heterotrophs (k_{dhet}) parameter (one standard deviation change in k_{dhet} results in 0.48 to 0.65 standard deviation decrease in model output responses). Linear regression analysis shows a moderate correlation between all RZWQM output responses and the organic matter/N cycling parameters ($r \geq 0.648$). Furthermore, all model output responses are negatively related to the denitrification constant (k_{den}) and death rate of nitrifiers (k_{dnit}) parameters, suggesting more N was available for plant uptake and leaching as these parameters decrease in value. Conversely, all RZWQM output responses are positively related to the death rate of denitrifiers (k_{dden}). Silage yield and NO_3-N leaching are positively related to the five residue/humus pools decay rate constants (k_{SRP}, k_{FRP}, k_{FHP}, k_{IHP}, and k_{SHP}); whereas, plant N uptake responds in an inconsistent fashion to perturbations in the decay rate constants (table 5).

RZWQM OUTPUT RESPONSES TO PLANT GROWTH PARAMETERS

Plant growth parameter mean values generated using LHS sampling (table 4) are generally higher than baseline values (table 3). Linear regression analysis in table 5 shows a very strong correlation between all RZWQM output responses and the plant growth parameters ($r \geq 0.854$). The specific leaf weight (SLW) is the most sensitive plant growth input parameter for all model output responses, followed by the photorespiration rate (R_1). Higher SLW results in a lower leaf area index, therefore lower silage yield and plant N uptake are simulated. Increasing the photorespiration rate causes less biomass accumulation and lower plant N uptake to be simulated. These results agree with previous evaluation of the RZWQM plant growth component (Hanson et al., 1999). RZWQM output responses are relatively insensitive to the remaining plant growth input parameters ($\beta_i \leq 0.118$). A possible reason for RZWQM output response insensitivity to maximum daily nitrogen uptake (N_{max}) may be due to the relatively high values tested (baseline value of 0.5 with a test range of 0.0 to 3.3). Generally, setting N_{max} equal to 0.05 in RZWQM suffices N demand for most crops (Ma et al., 1998). Since the photosynthesis reduction factors (A_p and A_s) are more related to grain yield during the productive growth stage, and less to plant biomass, their small effect on silage yield would be expected.

RZWQM OUTPUT RESPONSES TO WATER/MANURE APPLICATION RATES

Water and manure application rate mean values generated using LHS sampling (table 4) are nearly the same as the baseline values (table 3). The high standard deviation of simulated silage yield and NO_3-N leaching (table 4) suggests that RZWQM is very sensitive to changes in water and manure application rates. Linear regression analysis shows a moderate to strong correlation between all RZWQM output responses and water and manure application rates ($r \geq 0.706$) (table 5). Correlation is especially high for the plant N uptake and NO_3-N leaching model output responses, however, further analysis shows that manure application rate is the decisive parameter responsible for the strong correlation. As presented in table 5, sensitivity coefficients for all RZWQM output responses were much higher for manure application rate than for irrigation application rate, further suggesting that RZWQM output responses are much less sensitive to variations in water application rate. These results agree with those reported by Martin and Watts (1999), who evaluated RZWQM for the MSEA project. Plant N uptake was negatively correlated to irrigation water application rate ($\beta = -0.2674$). However, as shown by Ma et al. (1998), a peak plant N uptake is observed as irrigation application rate increases from 0 to 40 cm/event.

ADDITIONAL IMPLICATIONS OF SENSITIVITY ANALYSIS RESULTS

The above sensitivity analysis results demonstrate variability in RZWQM output responses as affected by perturbations (uncertainty) in model input parameters and non-uniformity in water and manure application rates. As with other agricultural water quality models, RZWQM was developed based on a limited understanding of the physical system. Many processes (biological, chemical, and physical) are simulated in a rather simplified manner. As a result, model parameters are assumed to be constant with due consideration of various environmental factors (e.g., water, temperature, solar radiation, etc.). In reality, many of the assumed parameter constants may change spatially and temporally because of processes not considered in the model or inability to simulate a particular process at present. It is important to remember that linear regression analysis can only determine overall (average) model output sensitivity to perturbations in input parameters within the specified testing ranges. Graphical display may still be required to reflect the nonlinear behavior of model output responses. Presenting sensitivity analysis results in this manner may provide additional practical insight into the consequences of parameter uncertainty and confidence intervals for the selected model output responses.

Figures 1 to 4 show cumulative probability distributions of RZWQM-predicted (simulation years 1993 to 1996) plant N uptake, silage yield, and NO_3-N leaching for each group of RZWQM input parameters. All the distributions failed normal and lognormal Chi-square and Kolmolgorov-

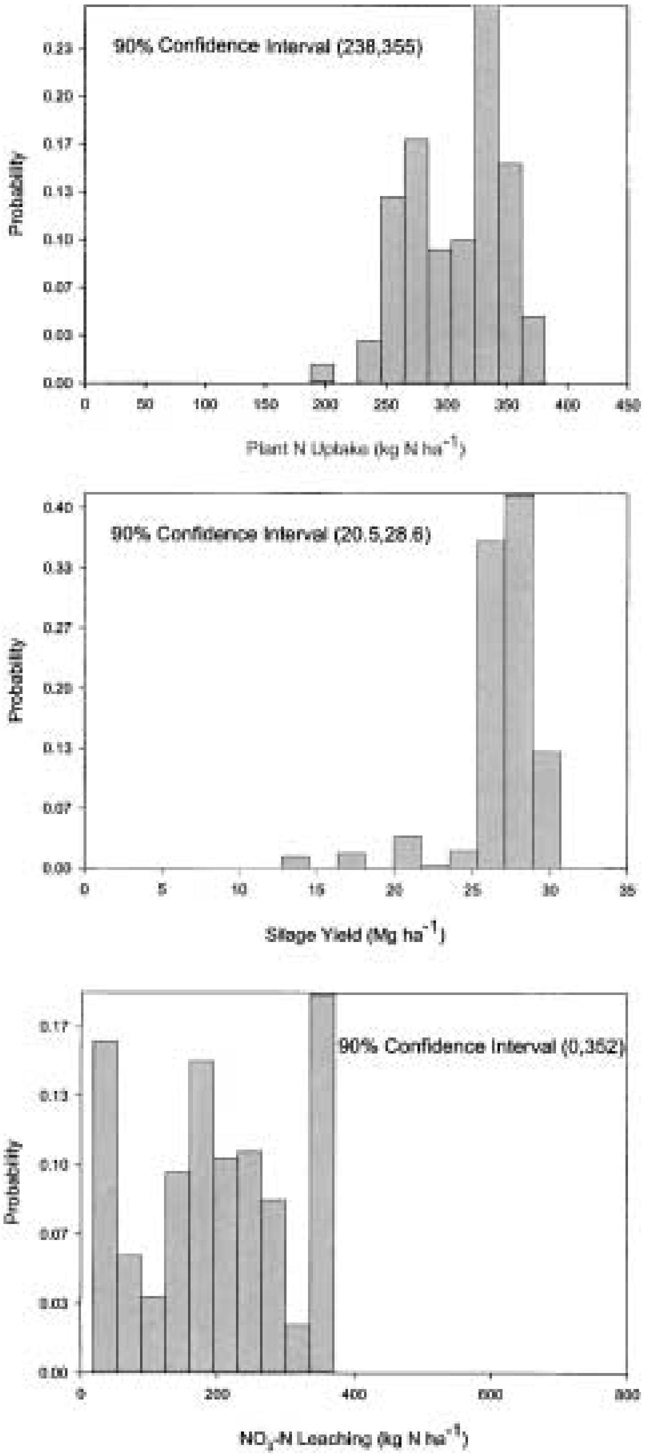

Figure 1–Probability distributions of plant N uptake, silage yield, and NO_3-N leaching beyond the root zone due to variation in saturated hydraulic conductivity, K_{sat}.

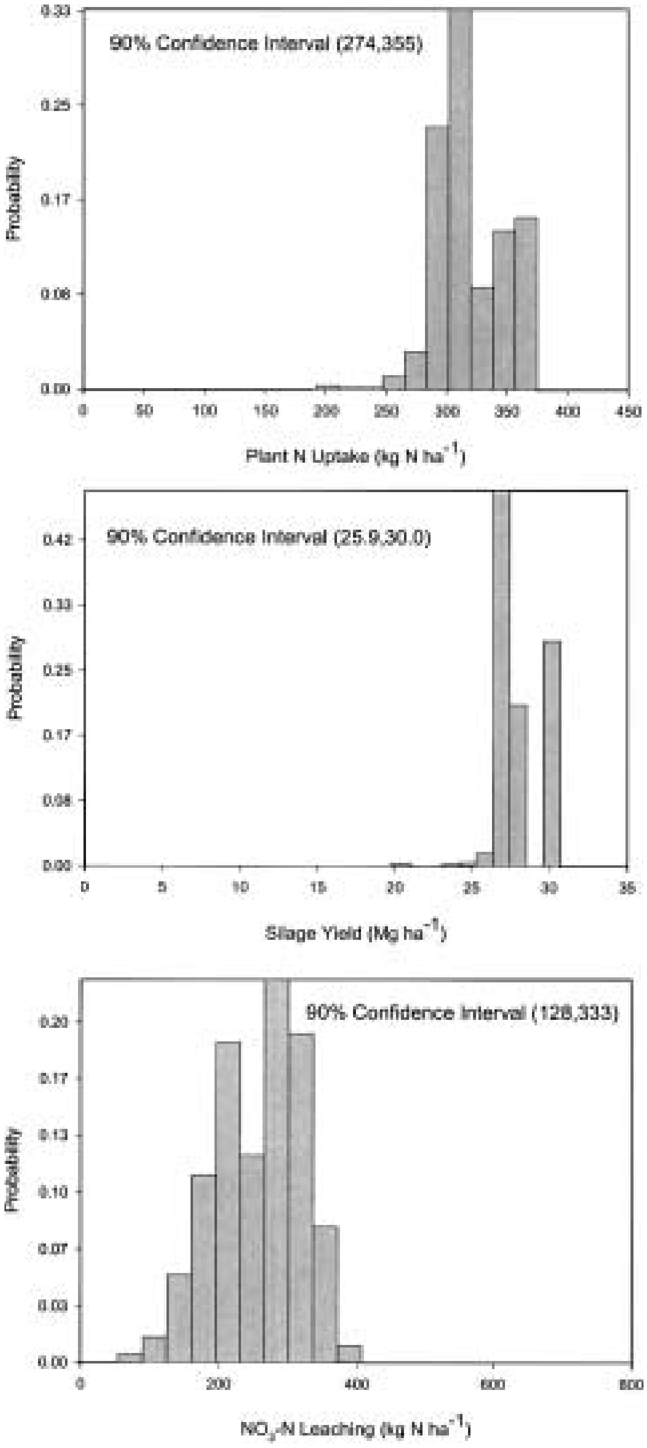

Figure 2–Probability distributions of plant N uptake, silage yield, and NO_3-N leaching beyond the root zone due to variation in organic matter/N cycling parameters.

Smirnoff hypothesis tests. Confidence intervals (90% level) based on probability counts are also shown in figures 1 to 4. Sensitivity to model input parameters is reflected in the distribution shape, i.e., the narrower the distributions in figures 1 to 4, the less sensitive RZWQM output responses are to variations within the input parameter groups. Plant N uptake is most sensitive to plant growth parameters that directly relate to biomass accumulation (table 5 and fig. 3). Silage yield is also most sensitive to plant growth parameters (fig. 3). Based on the spatial variability of manure and water application rates, the amount of NO_3-N leached out of the root zone ranged from 0 to 755 kg N ha^{-1} (fig. 4). The worst scenario for NO_3-N leaching arises from a combination of high irrigation and manure application rates (fig. 4, table 5).

It is interesting to compare observed experimental results with the probability distributions in figure 4,

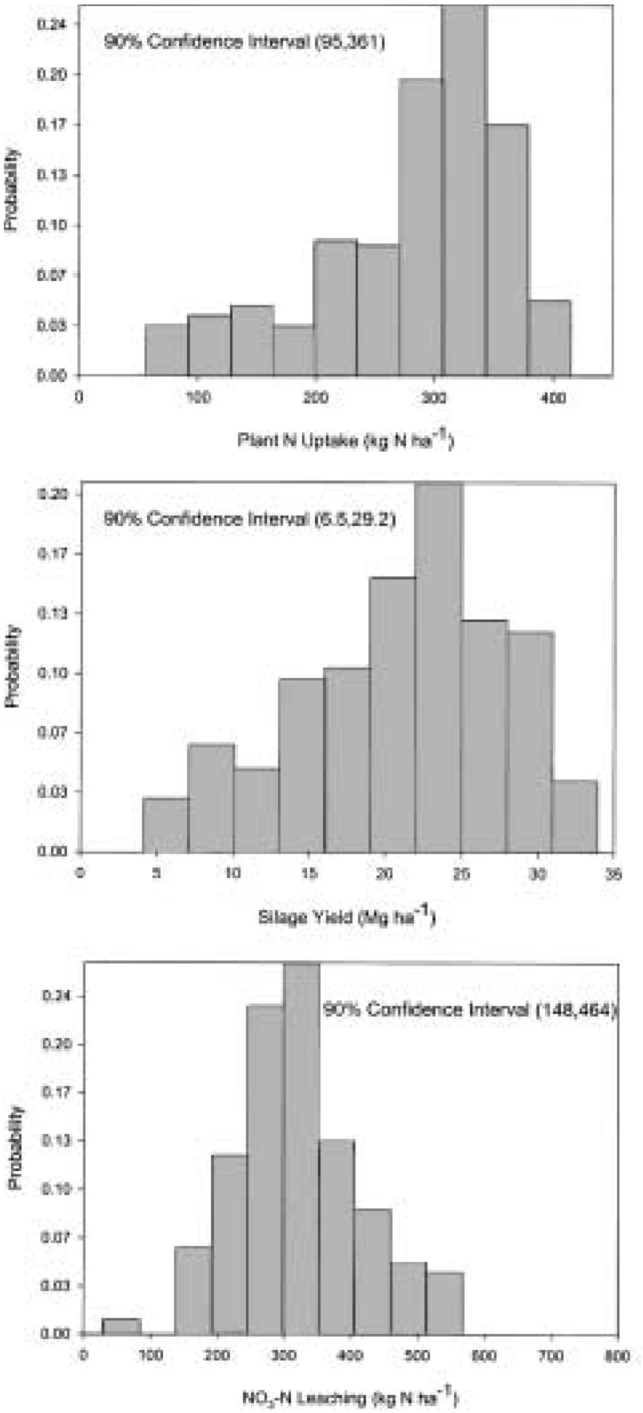

Figure 3–Probability distributions of plant N uptake, silage yield, and NO_3-N leaching beyond the root zone due to variation in plant growth parameters.

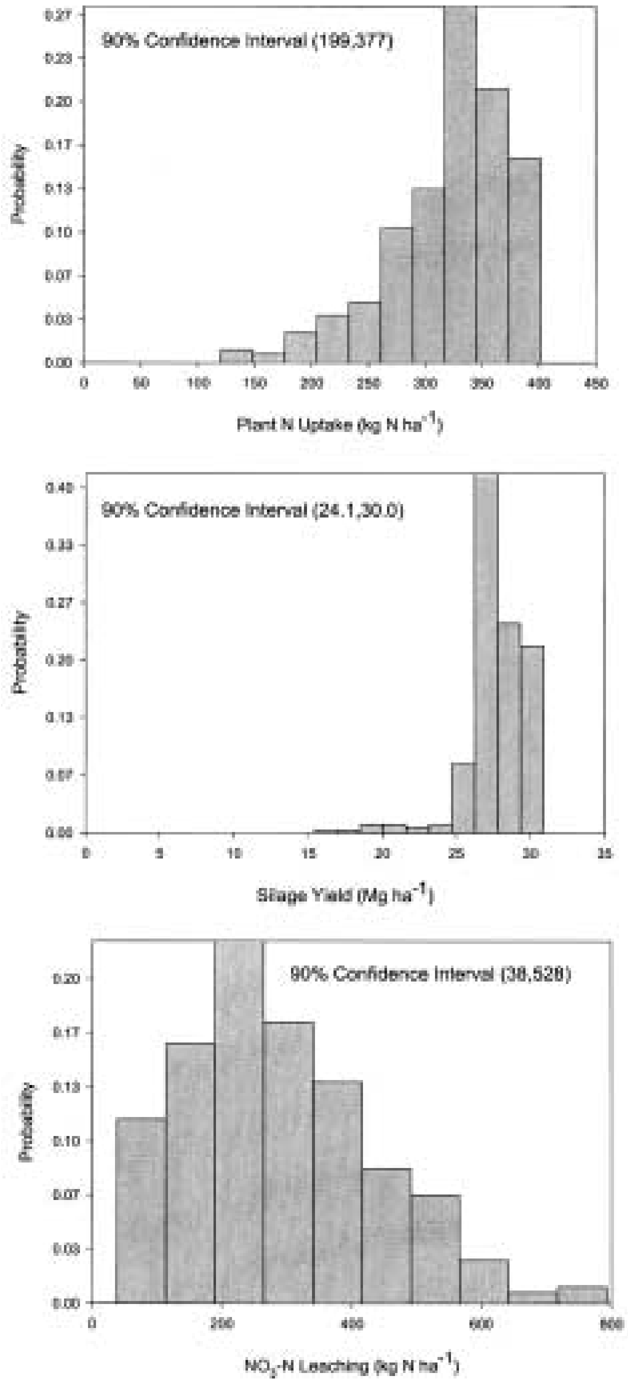

Figure 4–Probability distributions of plant N uptake, silage yield, and NO_3-N leaching beyond the root zone due to variation in water and manure application rates.

assuming that experimental error was due to improper characterization of spatial variability in water and manure application rates. Measured silage yields for the eastern Colorado field experiment were 25.1, 30.9, and 24.3 Mg ha^{-1} for 1994, 1995, and 1996, respectively, which are within or close to the 90% confidence interval of 24 to 30 Mg ha^{-1}. Yields for 1994 and 1996 were closer to the mean (25.1 Mg ha^{-1}) than that of 1995 (fig. 4). Although the high yield in 1995 (30.9 Mg ha^{-1}) was probably due to an unusually wet spring (Ma et al., 1998), this yield may also be explained by possible bias in sampling location. Measured plant N uptake based on silage N content was 245, 361, and 211 kg N ha^{-1} for 1994, 1995, and 1996, respectively, which are within the 90% confidence interval of 199 to 377 kg ha^{-1}. The high N uptake in 1995 was not accurately simulated by Ma et al. (1998), however, sensitivity analysis results in figure 4 indicate there is a high probability for plant uptake of more than 300 kg N ha^{-1} in the manured field.

Model output responses to the most sensitive input parameters in each group are graphically presented in

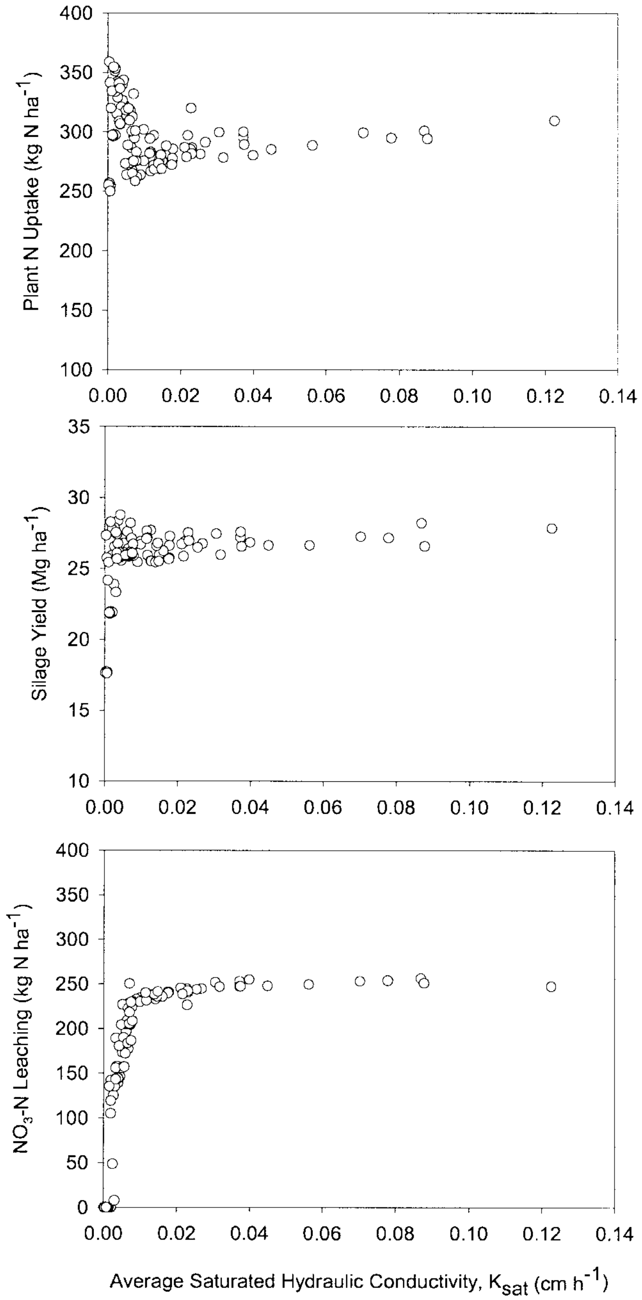

Figure 5–Simulated responses of plant N uptake, silage yield, and NO_3-N leaching beyond the root zone to average saturated hydraulic conductivity, K_{sat}, in the soil profile.

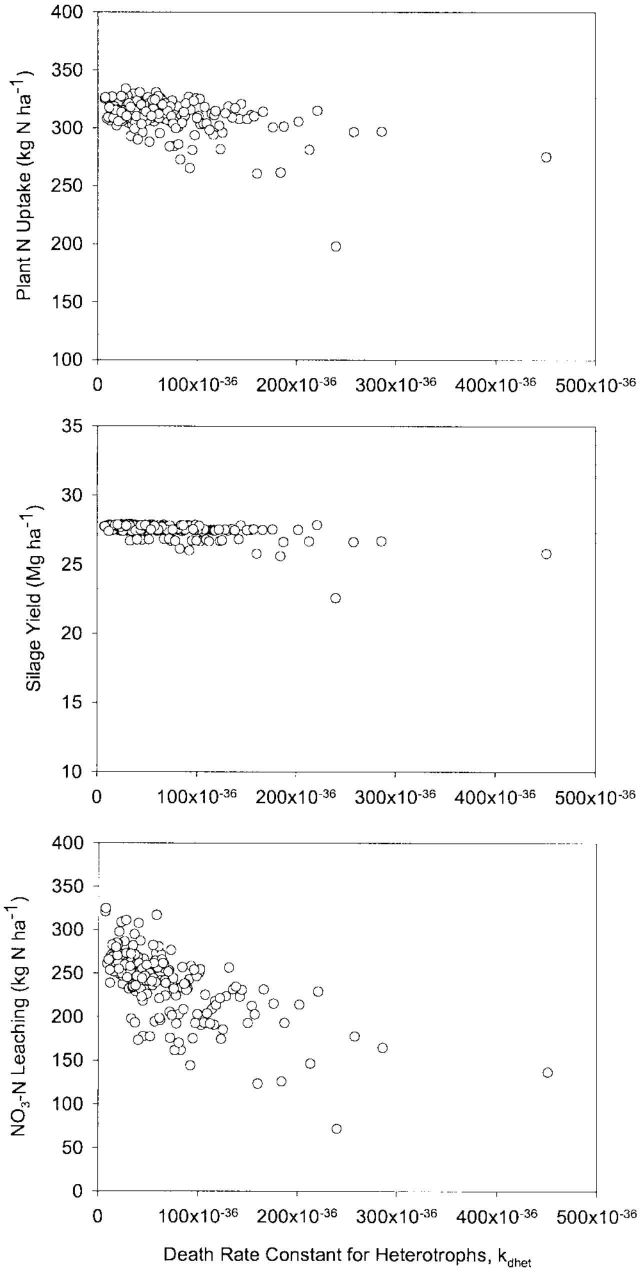

Figure 6–Simulated responses of plant N uptake, silage yield, and NO_3-N leaching beyond the root zone to the death rate constant for heterotrophs, k_{dhet}, with other organic matter/N cycling parameters varied.

figures 5 to 8 to show nonlinear behavior in RZWQM. The nonlinear response curves indicate variability resulting from other input parameters in the group. Figure 5 shows the model output responses for the 1993-1996 simulation years to the average soil profile K_{sat}. A decreasing trend in plant N uptake and an increase in NO_3-N leaching was simulated for increasing K_{sat} up to 0.01 cm h^{-1}. Therefore, K_{sat} affects N availability in the soil profile but only at very low K_{sat} values. Silage yield is very weakly related to the average K_{sat}, however. Figure 6 presents model output responses to the most sensitive N cycling input parameter, death rate of the heterotrophs, with random variation of other nutrient parameters presented in table 4. Generally, there is a decreasing trend in plant N uptake and NO_3-N leaching; whereas, silage yield is not sharply affected (fig. 6). The heterotroph death rate affects N supply to the system by limiting the number of organic matter decomposers. Model output responses are highly correlated to SLW (fig. 7) because of its dominant role in simulating LAI, which is in agreement with previous studies (Hanson et al., 1999). Manure application rate has a dominant effect on plant N uptake, silage yield, and NO_3-N leaching (fig. 8) as anticipated simply because additional N is added to the system as the manure application rate increases. A plateau was observed for both plant N uptake and silage yield, which was expected and has been confirmed in previous field studies (Cerrato and Blackmer, 1990; Overman et al., 1994). NO_3-N leaching increased

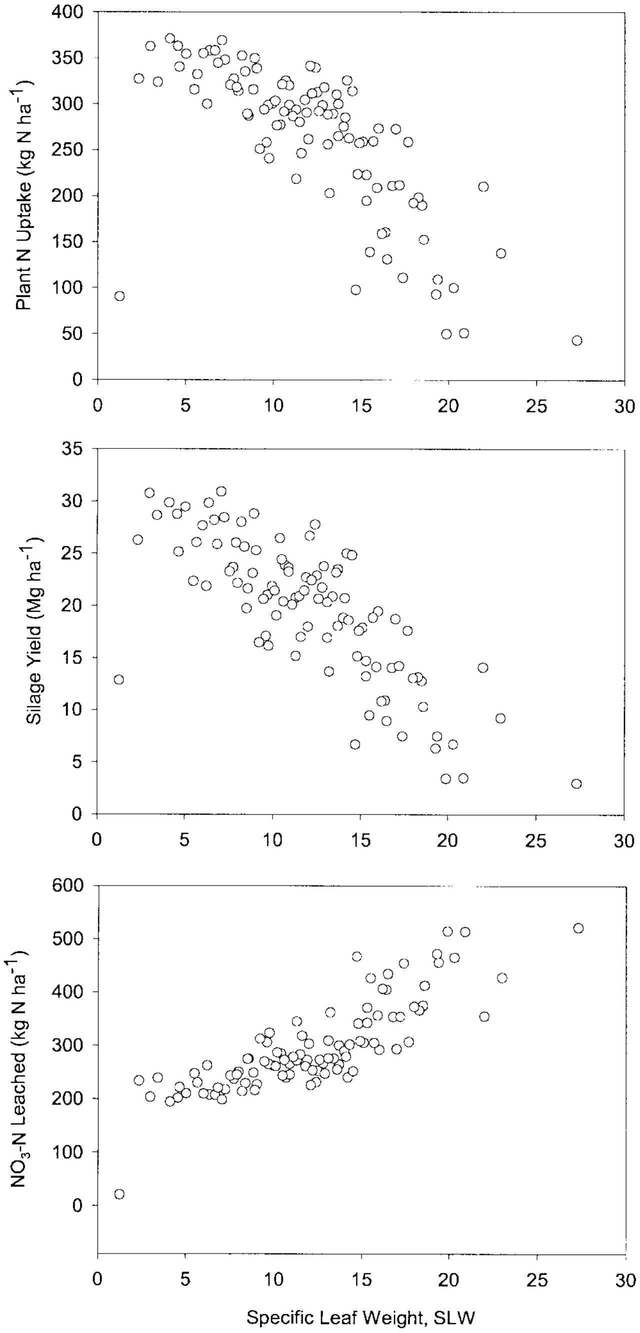

Figure 7–Simulated responses of plant N uptake, silage yield, and NO_3-N leaching beyond the root zone to specific leaf weight, SLW, with other plant growth parameters varied.

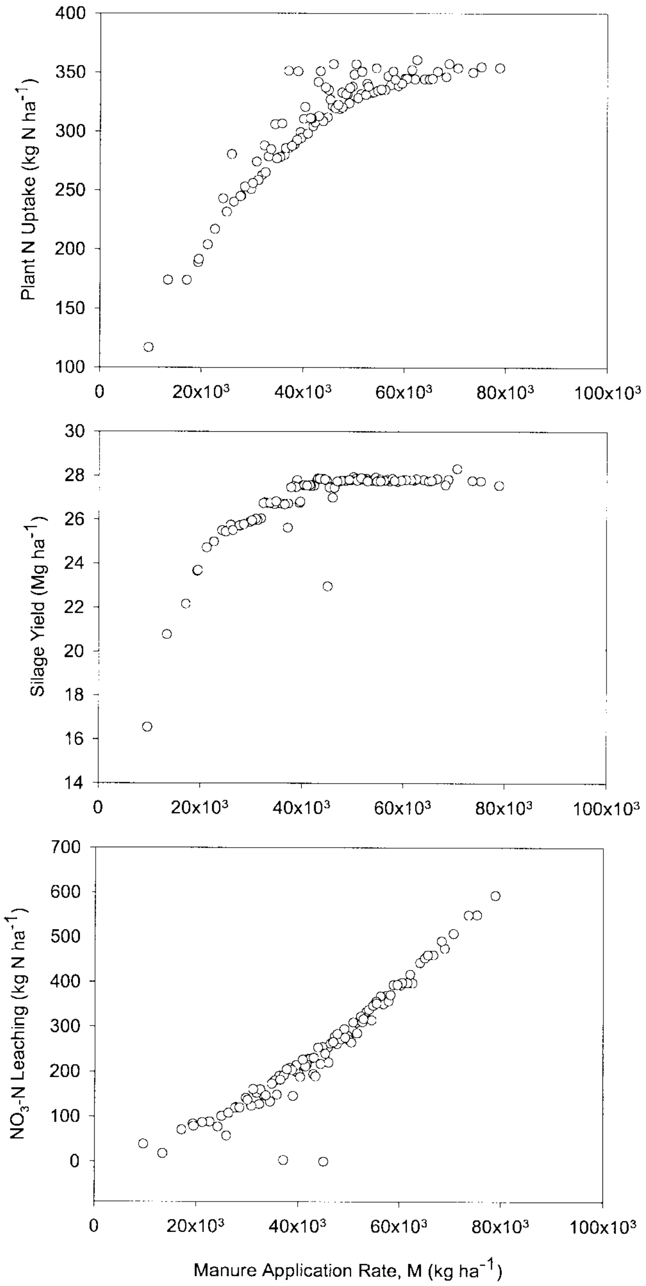

Figure 8–Simulated responses of plant N uptake, silage yield, and NO_3-N leaching beyond the root zone to manure application rate, M, with water irrigation rate, W, varied.

linearly with manure application rate as plant N uptake approached a maximum value.

SUMMARY AND CONCLUSIONS

The purpose of this study was to conduct a sensitivity analysis for selected RZWQM input parameters. Results of this study may be used to identify key model parameters and confidence intervals that need to be carefully determined due to possible parameter variability. These results may also point out weaknesses in the model that warrant further development; however, care should be taken in their interpretation. For example, we did not consider a possible suppressing effect on silage yield at very high N concentrations, i.e., silage yield may decrease at very high manure application rates. Similarly, manure application may affect the pH of soil, the supply of other micro-nutrients, and change the environment for microorganisms. The interdependency of various soil processes (parameters) may also add uncertainty to the sensitivity analysis results.

In this study, we assumed lognormal distributions for saturated hydraulic conductivity and organic matter/N cycling input parameters, and normal distributions for plant growth parameters and water/manure application rates. These assumptions are arbitrary to some extent, and depend on the definition of parameter variation. For example, saturated hydraulic conductivity (K_{sat}) is generally lognormally distributed spatially in a field, but if we consider K_{sat} distribution due to experimental measurement errors, it is normally distributed. However, parameter distribution assumptions have been shown not to have significant effect on sensitivity analysis results (Haan and Zhang, 1996, Fontaine et al., 1992).

As demonstrated by the calculated sensitivity coefficients, the selected RZWQM output responses are most responsive to manure application rate, death rate of heterotrophs (k_{dden}), photorespiration rate as a percentage of daily photosynthate (R_1), and specific leaf weight (SLW). Since RZWQM output responses are not highly correlated to the K_{sat} of each individual soil layer, accurate (model) delineation between soil layers may not be critical. Spatial variability of water irrigation has less effect on plant N uptake, silage yield, and NO_3-N leaching than uneven distribution of manure on the field. This effect may be even less important when lateral water flow is considered.

Finally, the linear regression analysis does not consider the interactions between model parameters, which is valid only for independent input variables. However, in the case of dependency, the interaction between parameters may be important and the interpretation of sensitivity coefficients should be adjusted. One example is the interaction between water and manure application rates. As shown in figure 8, simulated plant N uptake, silage yield, and NO_3-N leaching responded to manure application rates in distinct patterns, although irrigation rates were varied from 0 to 40 cm/event. However, RZWQM output responses to irrigation rate were very much scattered (data not shown) given a simultaneously random variation in manure application rate from 0 to 89.6 Mg ha^{-1}; whereas, the three output variables responded to irrigation rate in distinguishable trends when only irrigation rates were varied (Ma et al., 1998).

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