Soil-Test N Recommendations Augmented with PEST-Optimized RZWQM Simulations

R. W. Malone,* D. B. Jaynes, and L. Ma USDA–ARS
B. T. Nolan USGS
D. W. Meek and D. L. Karlen USDA–ARS

Improved understanding of year-to-year late-spring soil nitrate test (LSNT) variability could help make it more attractive to producers. We test the ability of the Root Zone Water Quality Model (RZWQM) to simulate watershed-scale variability due to the LSNT, and we use the optimized model to simulate long-term field N dynamics under related conditions. Autoregressive techniques and the automatic parameter calibration program PEST were used to show that RZWQM simulates significantly lower nitrate concentration in discharge from LSNT treatments compared with areas receiving fall N fertilizer applications within the tile-drained Walnut Creek, Iowa, watershed (>5 mg N L^{-1} difference for the third year of the treatment, 1999). This result is similar to field-measured data from a paired watershed experiment. A statistical model we developed using RZWQM simulations from 1970 to 2005 shows that early-season precipitation and early-season temperature account for 90% of the interannual variation in LSNT-based fertilizer N rates. Long-term simulations with similar average N application rates for corn (*Zea mays* L.) (151 kg N ha^{-1}) show annual average N loss in tile flow of 20.4, 22.2, and 27.3 kg N ha^{-1} for LSNT, single spring, and single fall N applications. These results suggest that (i) RZWQM is a promising tool to accurately estimate the water quality effects of LSNT; (ii) the majority of N loss difference between LSNT and fall applications is because more N remains in the root zone for crop uptake; and (iii) year-to-year LSNT-based N rate differences are mainly due to variation in early-season precipitation and temperature.

Among the most promising tools available for determining precise N requirements are soil mineral N tests (Schroder et al., 2000). The pre-side-dress nitrate test (PSNT) combined with a split application of N was proposed by Magdoff et al. (1984) and has been found effective for determining if corn (*Zea mays* L.) will benefit from side-dress N (Klapwyk and Ketterings, 2006; Bundy and Andraski, 1995). The PSNT can help reduce N loss while maintaining acceptable corn yields (Sogbedji et al., 2000; Meisinger and Delgado, 2002). The PSNT in the form of the late-spring nitrate test (LSNT) was recommended for corn N fertilization in Iowa (Blackmer et al., 1997). The LSNT protocol involves applying a nominal rate of N fertilizer before corn emergence followed by measuring residual soil nitrate in the top 30 cm of soil during early crop growth and side-dressing additional fertilizer based on soil nitrate concentrations.

Although soil testing methods such as the LSNT are promising tools, adoption by farmers is limited because of little time between soil testing and fertilizer application; higher labor, equipment, and soil sampling costs; and potential prediction errors in N application rates. Much of the LSNT-determined N rate variability is weather related. Using the agricultural system model LEACHMN, Sogbedji et al. (2001) concluded that economic optimum N rates were minimally affected by field variability from drainage class but strongly affected by annual variation in early-season precipitation. Field results confirm that plant available N is most strongly influenced by rainfall early in the growing season (Kay et al., 2006). Also, increasing soil temperature is usually associated with increasing soil organic matter decomposition (Kirschbaum, 1995), and thus higher plant available N can be expected during years with higher early-season temperature. Agricultural system models such as the Root Zone Water Quality Model (RZWQM) can accurately simulate variation among year-to-year crop yield and field N dynamics due to fluctuations such as weather after thorough calibration (Ma et al., 2007b; Li

J. Environ. Qual. 39:1711–1723 (2010)
doi:10.2134/jeq2009.0425
Published online 12 July 2010.
Supplementary data files available online for this article.
Received 24 Oct. 2009.
*Corresponding author (rob.malone@ars.usda.gov).

R.W. Malone, D.B. Jaynes, D.W. Meek, and D.L. Karlen, USDA–ARS, National Laboratory for Agriculture and the Environment, Ames, IA; L. Ma, USDA–ARS, Agricultural Systems Research Unit, Fort Collins, CO; B.T. Nolan, USGS, Reston, VA. Assigned to Associate Editor Christopher Green.

Abbreviations: AR, autoregressive; CN1, northernmost control subbasin; CN2, southernmost control subbasin; CS, corn–soybean rotation with corn planted in 1997; EF, Nash–Sutcliffe efficiency; FWNC, flow-weighted nitrate concentration; LSNT, late-spring nitrate test; MIN, minimum N fertilizer rate; NLIM, nonlimiting N fertilizer rate; PBIAS, percent bias; PSNT, pre-side-dress nitrate test; RSR, ratio of root mean square error to the standard deviation of measured data; RZWQM, Root Zone Water Quality Model; SC, soybean–corn rotation with soybean planted in 1997; TR1, subbasin with the LSNT treatment.

et al., 2008; Thorp et al., 2007). These models may help our understanding of N rate predictions under long-term weather scenarios (Magdoff, 1991; Sogbedji et al., 2001). Therefore, application of thoroughly tested agricultural system models will increase our understanding of annual soil nitrate variation and help stimulate adoption of side-dress fertilizer management operations such as the LSNT.

An experiment first described by Jaynes et al. (2004) investigated the LSNT within a 366-ha subbasin of the tile-drained Walnut Creek watershed in Iowa. They compared the LSNT to primarily fall applied N fertilizer treatments in adjacent subbasins. These watershed data have been utilized previously for development, testing, and application of the agricultural systems models ADAPT and SWAT (Gowda et al., 2008; Saleh et al., 2007; Du et al., 2005). Also, Bakhsh et al. (2004a,b) applied RZWQM to a nearby field within the Walnut Creek watershed that did not include the LSNT subbasin.

Agricultural system models continue to be used to quantify the management effects on nitrate fate. For example, ADAPT was used to evaluate the effect of timing and amount of N application in south-central Minnesota and central Iowa (Nangia et al., 2008; Gowda et al., 2008); DRAINMOD-NII was used to evaluate the effect of drainage design and management (Luo et al., 2010); RZWQM was used to evaluate the effect of N application rates in central Iowa (Bakhsh et al., 2004a; Thorp et al., 2007); and RZWQM was used as part of a larger study of several management practices to briefly evaluate the effect of soil testing in northeastern Iowa (Malone et al., 2007). Missing from this research is watershed-scale testing and application of RZWQM and thorough evaluation of the model simulated response to the LSNT compared to fall applied N fertilizer.

A common aspect of previous studies involving RZWQM is that the model was generally calibrated manually. This generally involves manually adjusting model parameters and then running long-term simulations to allow C/N pool sizes to equilibrate. This is performed in an iterative fashion to try to match model results with observed soil water, field N dynamics, and plant growth for the period after C/N equilibration (Hanson et al., 1999).

Automatic parameter estimation (calibration) programs such as PEST may be an improvement over manual calibration. These methods specify an objective function based on data-model goodness-of-fit where user-defined model parameters are automatically adjusted until the objective function reaches a minimum (e.g., Doherty, 2004; Doherty and Johnston, 2003). Using automatic calibration methods such as PEST helps provide an objective, defensible, and repeatable way to calibrate models with many parameters (Rose et al., 2007). Robust optimization packages also usually allow much easier, efficient, and accurate model fit to field measurements than manual calibration (Doherty and Johnston, 2003). Nolan et al. (2010b) used PEST to calibrate RZWQM for conditions that did not include artificially drained soils.

Our objectives are to use field data described by Jaynes et al. (2004) (i) to objectively calibrate RZWQM using the automatic parameter optimizer program PEST and compare the effects of the LSNT on nitrate leaching from RZWQM-simulated and observed data and (ii) to use the optimized model to investigate the long-term LSNT effects on field N dynamics compared to single spring and fall N applications, which includes investigating the effects of year-to-year weather variability on LSNT-determined N application rates.

Materials and Methods

Field Experiment

Figure 1 shows the Walnut Creek watershed located in central Iowa (41°55′ to 42°00′ N; 93°32′ to 93°45′ W). Weather and cropping patterns have been monitored within the 5130-ha watershed since 1991. Details of the location, geology, soils, climate, land use, and farming practices are found in Hatfield et al. (1999a) and the associated references. Details of the LSNT-treatment and control subbasins within the watershed are found in Jaynes et al. (2004); we briefly describe them here. Crop cover for fields in each subbasin were determined by ground surveys (1991–1998), supervised classification of Landsat photos (1998–1999; USGS, http://landsat.usgs.gov), or cropland data layers (2000–2007; USDA National Agricultural Statistics Service, 2009). To avoid adding unnecessary complexity to the analysis and RZWQM simulations, we do not simulate fields with crops other than corn and soybean [*Glycine max* (L.) Merr.] (e.g., alfalfa [*Medicago sativa* L.], oat [*Avena sativa* L.], and pasture).

The LSNT treatment was implemented for 4 yr (1997–2000) on 16 fields (300 ha) of a 366-ha subbasin within the larger watershed and designated TR1 to retain the terminology of Jaynes et al. (2004). Simple corn–soybean rotations from 1991 through 2000 were practiced on 69% of the TR1 area (TR1_CS for corn in 1997; TR1_SC for soybean in 1997). Including three more fields with some years of consecutive corn before 1997 (Supplementary Table 1SI) represents 99% of TR1 long-term management. In 2001, several fields categorized as TR1_CS and TR1_SC planted a second consecutive year of corn (Fig. 2), which we assumed had little effect on our simulations.

The adjacent subbasins CN1 and CN2 were selected as controls for a paired watershed research design. We use CN2 for

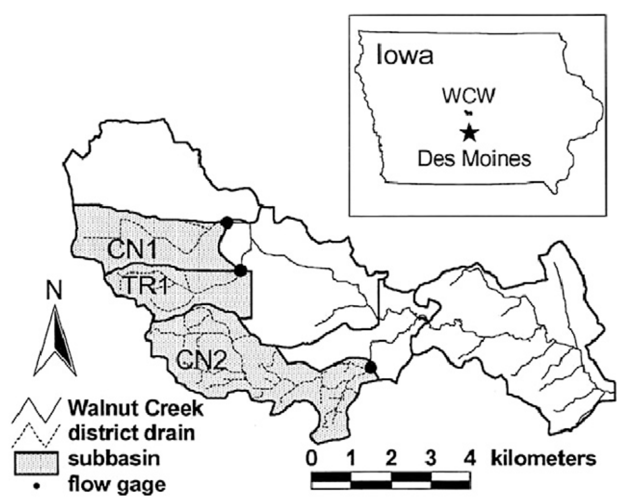

Fig. 1. Walnut Creek watershed. Location of Walnut Creek watershed (WCW) within the state of Iowa (inset), and the location of the stream, district drains, discharge gaging stations, control subbasins (CN1 and CN2), and treatment subbasin (TR1) within WCW. From Jaynes et al. (2004).

the calibration watershed for reasons listed below. Crop rotations for 39 fields within CN2 (715 ha) were identified. Corn–soybean rotations from 1991 through 2000 were practiced on 491 ha (69%) of CN2, which we categorized CN2_CS and CN2_SC. Including four more fields with some years of consecutive corn (Supplementary Table 1SI) represent 82% of CN2.. Fifty-four hectares of CN2 practiced simple corn–soybean rotations through 1999 but changed in 2000 to continuous corn, continuous soybean, or undetermined. Assuming this change had little effect on our simulations results in six rotations representing 89% of CN2 long-term management.

Farmers in CN2 were assumed to add N fertilizer in the fall at 165 kg N ha^{-1} before the 1999 corn planting seasons (1991–1998) and 185 kg N ha^{-1} thereafter (Jaynes et al., 2004). When a second consecutive year of corn was planted, we assumed 200 kg N ha^{-1} fertilizer application. The LSNT program consisted of applying 56 kg N ha^{-1} shortly before planting. Around late May to mid-June, soil samples were taken and analyzed for nitrate content to determine the required rate of N to apply by side-dressing. Nitrogen fertilizer rates were calculated using the formula $y = 1.121 \times 8 \times (25 - x)$ (Blackmer et al., 1997), where x is the average nitrate concentration (mg N ha^{-1}) in the soil, y is the N fertilizer rate in kg N ha^{-1}, the factor 8 is considered a first approximation for the conversion rate between fertilizer N application and resulting soil N concentration, 25 is the required soil N concentration for full yield, and 1.121 converts the recommendation from pound per acre to kilogram per hectare. The total N rates determined with the LSNT (measured soil nitrate concentration, x) for 1997, 1998, 1999, and 2000 were 168, 118, 174, and 96 kg N ha^{-1}. Rates and timing of N application for TR1 before 1997 and after 2000 were assumed to be the same as the two control watersheds.

To confirm that the LSNT program was meeting plant N requirements, 12 to 16 row check strips were strategically placed within a very small fraction of subbasin TR1 to determine corn yield under different N application strategies. One strip received only the preplant application of approximately 56 kg N ha^{-1} (MIN), whereas another received a nonlimiting N rate (>220 kg N ha^{-1}; NLIM). A third strip received the LSNT rate. Details on the procedure to analyze corn response to LSNT in the Walnut Creek watershed are found in Karlen et al. (2005).

The fields within each subbasin were extensively drained by subsurface tiles that had been installed over the past 120 yr. The field tiles drained into subsurface drainage district pipes that drained each subbasin. The partially submerged district drains were instrumented to measure flow rate as they emptied into Walnut Creek (Fig. 1) by simultaneously measuring water depth and velocity using Flowtote meters (Marsh-McBirney, Frederick, MD). Water samples were taken manually once a week at the flow gauge on each subbasin and automatically during runoff events. All water samples were refrigerated until analysis. Nitrate was analyzed by quantitative reduction to NO_2 and measuring the NO_2 concentration colorimetrically with a Lachat Autoanalyzer (Zellweger Analytics, Lachat Instrument Division, Milwaukee, WI). The method had a quantitation limit of 1.0 mg N L^{-1} as NO_3. Flow-weighted average NO_3 concentrations were computed by summing the product of the weekly/daily NO_3 concentration and total weekly/daily discharge.

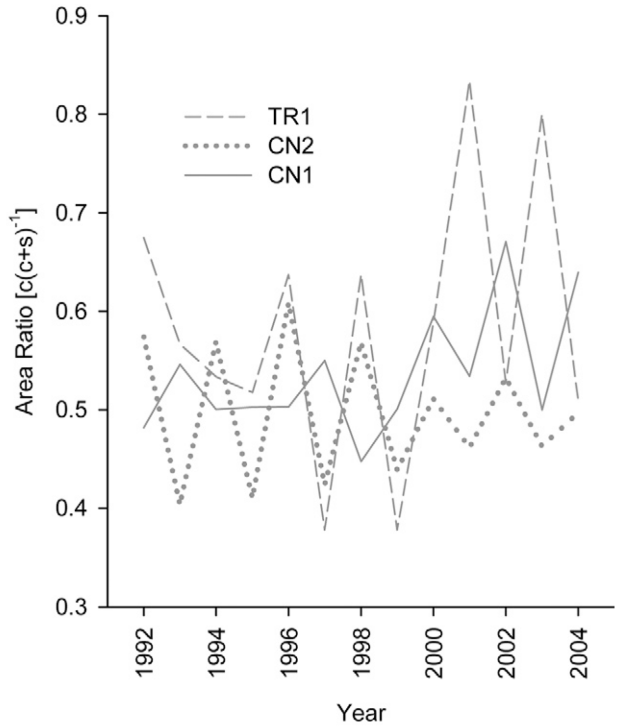

Fig. 2. Ratio of corn area to corn (c) and soybean (s) area in the three subbasins. TR1, CN2, and CN1 are the subbasin with the Late Spring Nitrate Test (LSNT) treatment, the southernmost control subbasin, and the northernmost control subbasin.

RZWQM Description

The RZWQM simulates water infiltration into the soil matrix using the Green-Ampt equation and water redistribution using the Richards' equation. Soil hydraulic properties are described with a modification of the Brooks-Corey equation. Tile drainage is simulated by the Hooghoudt's steady state equation in RZWQM. These hydrologic processes as implemented in RZWQM have been described elsewhere (e.g., Malone et al., 2003; Ma et al., 2007a).

A comprehensive description of the carbon and nitrogen dynamics in RZWQM is found in Ma et al. (2001, 2007a); we describe the first-order decomposition of soil organic C here:

$$r_i = -k_i C_i$$

where r_i is the decay rate of the ith pool (mg C kg^{-1} d^{-1}); i is the soil organic C pool (RZWQM has five soil organic C pools: slow surface residue, fast surface residue, fast humus, intermediate humus, and slow humus); C_i is the C concentration (mg C kg^{-1} soil); and k_i is a first-order rate coefficient (s d^{-1}):

$$k_i = f_{\mathrm{aer}}\left(\frac{k_{\mathrm{b}}T}{h_{\mathrm{p}}}\right)A_i\exp\left(-\frac{E_{\mathrm{a}}}{R_{\mathrm{g}}T}\right)\frac{[O_2]}{[H^{kh}\gamma_1^{kh}]}P_{\mathrm{het}} \qquad [1]$$

where A_i is the rate constant for pool i, $[O_2]$ is O_2 concentration in the soil water with assumption that oxygen in soil air is not limited (moles O_2 per liter pore water), H is the hydrogen ion concentration (moles H per liter pore water), γ_1 is the activity coefficient for monovalent ions ($1/\gamma_1^{kh} = 3.1573 \times 10^3$

if pH > 7.0, and $1/\gamma_1^{kh} = 1.0$ if pH ≤ 7.0), kh is hydrogen ion exponent for decay of organic matter (= 0.167 for pH $\leq$ 7.0 and = –0.333 for pH > 7.0), P_{het} is the population of aerobic heterotrophic microbes (no. of organisms per g soil, minimum 50,000, default value 100,000), k_b is the Boltzman constant (1.383×10^{-23} J K^{-1}), T is soil temperature (K), h_p is the Planck constant (6.63×10^{-34} J s), R_g is the universal gas constant (1.99×10^{-3} kcal mol^{-1} K^{-1}), E_a (= 15.1 + 12.3 U, U is ionic strength mole]) is the apparent activation energy (kcal mol^{-1}), and f_{aer} is a soil aeration factor estimated from Linn and Doran (1984):

$$f_{aer} = 0.0075\ P_\theta;\ P_\theta \leq 20$$

$$f_{aer} = -0.253 + 0.203\ P_\theta;\ P_\theta < 20\ P_\theta < 59$$

$$f_{aer} = 41.1\ \exp(-0.0625\ P_\theta);\ P_\theta \geq 59$$

where P_θ is water-filled pore space.

A fraction of decayed organic materials is transferred between carbon pools: slow residue to intermediate residue, fast residue to fast humus, fast humus to intermediate humus, and intermediate humus to slow humus. This decay process is described in detail in Ma et al. (2001), and these four transformation coefficients were calibrated along with the recommended initialization procedure suggested by Ma et al. (2010). Nitrogen conservation is observed during organic matter decay, and transformation is based on the C-to-N ratio of each carbon pool (e.g., fast humus). Nitrogen is released as NH_4 during the decay process and may be nitrified to NO_3. Figure 3 shows the effect of temperature and water-filled pore space on the decay rate coefficient (k_i) for fast humus, where k_i increases with increasing temperature and is highest with P_θ of 59% (see Eq. [1]).

Model Input and Optimization

Meteorological model input included daily minimum and maximum temperatures, wind speed, solar radiation, relative humidity, and hourly precipitation. Nitrate and NH_4 ions were added to precipitation at concentrations of 1.0 and 0.5 mg L^{-1} (0.23 and 0.39 mg N L^{-1}), which are the approximate average annual concentrations for Iowa (from the National Atmospheric Deposition Program website, http://nadp.sws.uiuc.edu/). To reduce spatial variation effects caused by selecting one gauge for rainfall input, we used the median weekly rainfall as the most representative gauge for rainfall input to RZWQM from several gauges throughout the watershed (e.g., Hatfield et al., 1999b). The "representative" rain gauge was used for each week's RZWQM breakpoint rainfall input. Solar radiation and humidity were checked using procedures described by Allen (1996). These included comparing hourly relative humidity against 100%. Daily solar radiation was compared against clear sky radiation and monthly solar radiation compared to temperature estimated radiation. From the two Walnut Creek watershed weather stations where data were collected, the radiation and humidity values that best reflected these quality checks were used for RZWQM input. In addition, solar radiation was included from the Iowa Environmenal Mesonet station west of Ames, IA (http://mesonet.agron.iastate.edu; 42°1′ N, 93°47′ W). The weather data quality

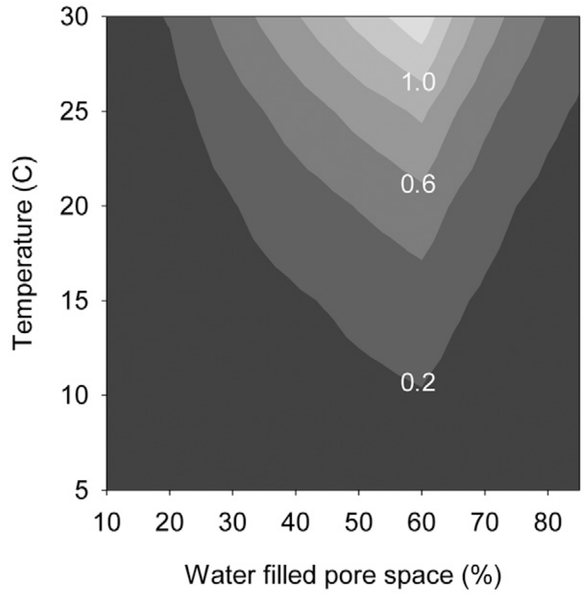

Fig. 3. Decay rate coefficient ($k_i \times 100$) for fast humus as a function of temperature and water filled pore space of soil, estimated using Eq. [1] (contour intervals of 0.2). Constant values are used for Eq. [1] variables except temperature and water filled pore space. (e.g., $P_{het} = 1 \times 10^{-6}$, $A_i = 2.5 \times 10^{-7}$, $U = 0.1$, $[O_2]^*[H^{kh*}\gamma^{kh}]^{-1} = 5 \times 10^{-3}$; other constants are listed in text).

control procedure is described more thoroughly in Malone et al. (2010).

The main components of RZWQM include hydrology, nutrient dynamics, and plant growth. Most of the input parameters were the same or similar to Thorp et al. (2007) and/or Ma et al. (2008). Parameters that were adjusted from these values or RZWQM default are listed in Table 1 and Supplementary Table 2SI. "Adjusted parameters" (e.g., saturated hydraulic conductivity, Ksat; Supplementary Table 2SI) were manually or PEST adjusted before the final model optimization described below; brief justifications for the final values are reported in the table comments. One reason important soil parameters such as Ksat and air-entry pressure were not included in the formal PEST optimization is that the RZWQM solution to Richards' equation failed to converge with certain combinations of soil parameters. Numerical approximation is required to solve Richards' equation due its nonlinearity, the complex nature of pressure head–hydraulic conductivity–water content relations, and the heterogeneous nature of soil systems. A robust solution to Richards' equation is desirable but not currently possible for certain reasonable sets of constitutive relations, parameter values, and environmental conditions (e.g., Miller et al., 1998).

The subbasin CN2 was used for optimization because it had similar annual proportions of corn and soybean as TR1 in the LSNT treatment years (1997–2000; Fig. 2) and we wanted to avoid using the LSNT subasin (TR1) for calibration. Optimized parameters determined from CN2 were used for TR1; thus only management (N application and crop rotations) changed among RZWQM simulated subbasins.

Data have been collected on all three subbasins through the present, but we terminate the calibration and testing at July 2001 (2001.5) because several fields transitioned to continuous corn in 2001 (Fig. 2). If we continued model testing after 2001.5, several more fields would have to be simulated and

Table 1. PEST-calibrated parameters.

Parameter		Value	Comments
slow r to intermediate h		0.86	Interpool organic matter transformation coefficients; r is residue, h is humus. More detail provided by Thorp et al. (2007) and the associated references.
fast r to fast h		0.40	
fast h to intermediate h		0.43	
intermediate h to slow h		0.74	
LHG		3.62E-06	The LHG is the lateral hydraulic gradient which controls flow out of the system below the subsurface drain (Ma et al., 2007a).
SRGF	15–30	0.81	SRGF is corn soil root growth factors for 15–30, 30–45, 45–60, 60–90 cm; the values for soybean were maintained as in Thorp et al. (2007).
	30–45	0.23	
	45–60	0.10	
	60–90	0.01	
PSD	0–2	0.19	PSD is pore size distribution index for the four different soil depth horizons (0–2, 2–20, 20–130, and 130–268 cm); values are within range listed by Rawls et al. (1982).
	2–20	0.20	
	20–130	0.15	
	130–268	0.08	
N2	0–2	2.19	N2 is the unsaturated hydraulic conductivity curve slope for the four different soil depth horizons; N2 = a2+2, where a2 is the pore size distribution index; Malone et al. (2004); Russo and Bresler (1980); Kutilek and Nielsen (1994).
	2–20	2.20	
	20–130	2.15	
	130–268	2.08	

composited, which for our objectives would unnecessarily complicate the analysis. We use a decimal system to briefly designate monthly results and to force January and December to have their fractional parts as 0.0 and 0.9. For example, 2001.5 is July 2001 and 2001.9 is December 2001 [2001+ (7 – 1)/12 = 2001.5; 2001+ (12–1)/12 = 2001.9].

We used the parameter estimation software PEST for RZWQM optimization in conjunction with the PEST utility software PAR2PAR and TSPROC (Doherty, 2004; Doherty and Johnston, 2003). In estimating model parameter values, PEST minimized a multicriteria objective function composed of four components representing different observation groups. These were the summed weighted squared differences between observed and RZWQM simulated monthly water quality values from 1993 to 2001.5 and 1997 to 2000 annual corn yield, specifically (i) monthly N loss in drain flow, (ii) monthly drain flow amount, (iii) monthly flow-weighted nitrate concentration (FWNC) in drain flow, and (iv) annual corn yield from the nonlimiting and minimum (NLIM and MIN) N treatments. The use of multiple criteria must be accompanied by a suitable selection of relative weights (w_i) when calculating the overall objective function. Weights were chosen so that no criterion was allowed to dominate the objective function: 2.0, 2.0, 1.0, and 0.015 were used for N loss, drain flow, FWNC, and corn yield, respectively. We also removed monthly N loss, drain flow amount, and FWNC from the optimization for months with very low drain flow (e.g., <1.0 mm) by selecting a weighing function of zero for those months. The Gauss–Marquardt-Levenberg optimization methodology that underlies PEST and similar programs has been criticized for being too easily trapped in local objective function minima. Using an objective function that combines multiple criteria and suitable relative weights reduces the problem of local minima (Doherty and Johnston, 2003). The objective function [$\Phi(\beta)$] based on parameter set (β) can be summarized as

$$\begin{aligned}\Phi(\beta) = &\sum_{i=1}^{n1}[w_{\mathrm{nl},i}(P_{\mathrm{nl},i} - O_{\mathrm{nl},i})]^2 \\ &+\sum_{i=1}^{n2}[w_{\mathrm{df},i}(P_{\mathrm{df},i} - O_{\mathrm{df},i})]^2 \\ &+\sum_{i=1}^{n3}[w_{\mathrm{nc},i}(P_{\mathrm{nc},i} - O_{\mathrm{nc},i})]^2 \\ &+\sum_{i=1}^{n4}[w_{\mathrm{cy},i}(P_{\mathrm{cy},i} - O_{\mathrm{cy},i})]^2\end{aligned}$$

where subscript i = monthly or annual ith observation, O = observed values, P = simulated values, w = observation weights, subscript nl = N loss, subscript df = drainflow, subscript nc = flow-weighted nitrate concentration, subscript cy = corn yield, and $n1$–4 = number of observations associated with each observation group.

Input parameters formally calibrated by PEST were soil root growth factors for corn at four depths (15–30, 30–45, 45–60, and 60–90 cm), the four interpool transformation coefficients for the organic matter pools, the lateral hydraulic gradient, and the pore-size distribution index for the surface three horizons. Model parameters for different components (crop growth, hydrology, N dynamics) were optimized simultaneously because they interact. For example, N uptake by corn is often the largest component of the annual nitrogen budget, and N uptake is sensitive to both N mineralization and root growth factors.

We used the utility PAR2PAR together with PEST to keep root growth factors for deeper layers less than shallower layers, to maintain pore size distribution index within a factor of 0.7 to 1.4 for adjacent soil layers, and to adjust soil parameters that are calculated on the basis of pore size distribution index (e.g., unsaturated hydraulic conductivity parameters). We used the PEST utility TSPROC to process the daily RZWQM simulated runoff and tile drainage from the corn and soybean fields of the control subbasin (CN2_CS and

CN2_SC) into proportional monthly composite N loss in drain flow and drain flow amount (DFX) using the formula

$$\mathrm{DFX} = \sum_{i=1}^{n} (T_i + RO_i) f_i \qquad [2]$$

where T is daily tile flow amount (cm) or N loss in tile flow (kg N ha^{-1}), RO is daily runoff amount (cm) or N loss in runoff (kg N ha^{-1}), i represents the crop rotation (e.g., CN2_CS or CN2_SC), n is the number of rotations (e.g., 2), and f is the fraction of subbasin area in a given rotation (0.526 for CN2_SC and 0.474 for CN2_CS). Note that the fractions were determined as CN2 area in SC or CS divided by sum of area in SC and CS [e.g., 258/(258+233)]. Monthly values for DFX were then computed followed by monthly FWNC in drain flow {[(N loss in drainflow, kg N ha^{-1}) ×10]/ drainflow amount, cm}. We use the term *drain flow* as the sum of subsurface (tile) drainage and runoff because the watershed samples included both, which was partly due to the many surface inlets into the subsurface drainage system. Annual simulated runoff was sensitive to snowmelt; therefore, before the final formal PEST optimization we adjusted the fraction of infiltrated snowmelt to 0.7 (default was 0.8) to achieve accurate simulated annual runoff compared to runoff calculated using hydrograph separation at the exit of the 5130-ha watershed.

To summarize, our optimization scheme involved:

1. PEST adjusted the user-defined model parameters;
2. PAR2PAR calculated the appropriate RZWQM parameters based on PEST parameter adjustments in step 1;
3. RZWQM input files were updated for the six scenarios (CN2_CS, CN2_SC, NLIM_CS, NLIM_SC, MIN_CS, MIN_SC);
4. RZWQM was run for each scenario from 1985 to 2001;
5. daily model output for nitrate N loss in tile flow, N loss in runoff, tile flow amount, and runoff amount was converted to monthly values for CN2_CS and CN2_SC using the PEST utility TSPROC;
6. monthly simulated values of step 5 were used to proportionally compute composite N loss in drain flow and drain flow amount using Eq. [2];
7. the weighted objective function was computed; and
8. steps 1–7 were repeated until optimization criteria met. Nolan et al. (2010a, b) discusses application of PEST to optimize RZWQM in more detail.

One of the advantages of optimizing RZWQM parameters using PEST is efficiency. Formal calibration of 12 parameters required less than 300 parameter perturbations. Running the six scenarios for a parameter set requires about 15 min or 75 h for 300 parameter perturbations. Nolan et al. (2010a) discusses further application of PEST with RZWQM simulations such as parameter sensitivity analysis and uncertainty analysis of RZWQM predictions.

Model Performance and Testing

Compositing only two RZWQM simulated rotations for PEST optimization of water quality and hydrology output (CN2_SC and CN2_CS) resulted in acceptable calibrations and covered 69% of the watershed management. Including more fields would have added considerable time and complexity to the PEST optimization. To test calibrated model performance however, four to six rotations per watershed were composited (Supplementary Table 1SI). Two rotations for each subbasin were simple corn–soybean rotations with corn in even or odd years. We composited the daily simulated tile drainage and runoff from each subbasin proportionally using a modification of Eq. [2] and then computed the monthly value.

To evaluate the calibrated RZWQM simulated hydrology, nitrate loss, and nitrate concentration for 1993 to 2001 across the two subbasins, we use the quantitative statistics Nash–Sutcliffe efficiency (EF), percent bias (PBIAS), and ratio of the root mean square error to the standard deviation of measured data (RSR):

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(P_i - O_i\right)^2} \qquad [3]$$

$$\mathrm{EF} = 1 - \left[\sum_{i=1}^{n}(P_i - O_i)^2 \Big/ \sum_{i=1}^{n}(O_i - \overline{O})^2\right] \qquad [4]$$

$$\mathrm{RSR} = \frac{\mathrm{RMSE}}{\mathrm{STDEV(obs)}} = \left[\sqrt{\sum_{i=1}^{n}\frac{1}{n}(P_i - O_i)^2} \Big/ \sqrt{\sum_{i=1}^{n}\frac{1}{n}(O_i - \overline{O})^2}\right] \qquad [5]$$

$$\mathrm{PBIAS} = \left[\sum_{i=1}^{n}(O_i - P_i)100 \Big/ \sum_{i=1}^{n}(O_i)\right] \qquad [6]$$

where $\bar{O}$ is the mean observed values, P_i is the model estimated values, O_i is the observed values, and n is the number of data pairs. Model simulations can be considered satisfactory under a monthly time step if (Moriasi et al., 2007): EF > 0.5, RSR < 0.7, PBIAS is within ±25% for streamflow, and PBIAS is within ±70% for N loss. The values of RMSE and EF when model estimates perfectly match observed data are 0 and 1.0, respectively. An EF value less than zero indicates that the average of observed measurements was a better estimator than the model.

We will only briefly discuss hydrology and crop simulations. Our main purpose in the model testing is to determine if RZWQM responds to LSNT treatments compared to fall N application. Therefore, we briefly report and discuss model comparisons to observed data such as the individual treatment drain flow, crop production, and nitrate loss, but the observed and RZWQM simulated FWNC difference between LSNT and control watershed is the most important comparison.

One method to examine paired watershed data was described by Jaynes et al. (2004, 2001). We modified this to determine if RZWQM responded to LSNT (TR1) compared to the control watershed (CN2). Our adaption of this method involved fitting a Gompertz function to both the RZWQM and the observed difference in monthly FWNC between the LSNT and control subbasin. A Gompertz function describes a time series with asymptotic decline or growth, nitrate concentration differences in our case. We also included an autoregressive (AR) residual component to correct for the effects of residual autocorrelation. Nonlinear regression was used to fit the Gompertz function to the nitrate concentration differences. A lag1 residual AR component was added to this trend and the combined model simultaneously fitted to the data using an iterative least squares method and "Fair" weighting to reduce outlier effects (e.g., Heiberger and Becker, 1992). Residual lag values were assumed missing at the start of the time sequence and after breaks in the time series caused by periods of low drain flow (<1 mm mo^{-1}).

The Gompertz function with the AR residual component can be described by the following:

$$\text{LSNT} - \text{control} = A + C\exp\{-1\exp[-b(x-m)]\} + a1r_{(x-1)} + r_x \quad [7]$$

where A is the upper boundary, C is the difference between the lower and upper boundary, b is the rate of monthly N concentration decline (mg N L^{-1} mo^{-1}), x is the number of months since December 1992 (in January 1993, $x = 1$), m is the month of maximum decrease ($x = 50$ to 70), $a1$ is the lag1 residual coefficient, and r is the residual or error.

Long-Term RZWQM Simulations

The field experiments for this research compared the LSNT protocol to primarily fall-applied N fertilizer (Jaynes et al., 2004). We used the calibrated and tested RZWQM to study long-term effects of three N treatments: (i) LSNT with a single 50 kg N ha^{-1} application at corn planting followed by soil testing to determine a side-dress N application rate 35 d after corn emergence (about mid-June); (ii) a single fall application of 150.7 kg N ha^{-1} about 40 d after soybean harvest (about mid-November); (iii) a single spring application of 150.7 kg N ha^{-1} at corn planting (2 May). The 150.7 kg N ha^{-1} rate was chosen for fall and spring application rates because it was the average RZWQM determined LSNT rate from the long-term simulations. Fertilizer was applied as injected anhydrous ammonia. Historical weather data near the watershed were used for the simulations (1 Jan. 1960 through 31 Dec. 2005). Although the model runs began in 1960, N mass balance and regression analysis used only the model results from 1970 through 2005, which allowed time for soil C/N initialization.

To help improve our understanding of the relationship between long-term LSNT rate and weather variables before soil testing, multivariate regression was performed using temperature and rainfall as predictors and LSNT rate determined by RZWQM from 1970 through 2005 as the dependent variable. The regression analysis included power and interactive weather predictors (e.g., temperature × precipitation, temperature$^{0.1}$, precipitation^3). Power regression was used because weather variables such as temperature and precipitation may have a nonlinear effect on N application rate determined from soil testing. The interaction terms were included because variables such as precipitation may affect soil determined N rate differently at high and low temperature. We used stepwise, k-fold cross-validation, and leave-one-out cross-validation for selection of variables. The final set of variables is mechanistically plausible and tested using both k-fold and leave-one-out cross-validation.

The k-fold was used in the event of serial correlation of weather variables used in the regression (temperature and precipitation), where the data were split into 6 blocks of 30 observations for model calibration and 6 omitted values for model validation. The data used for cross-validation were 1970 to 2005 RZWQM predicted N rate and the predictands for the regression equation (see predictand definition below). The equation with the final set of included variables produced the lowest predictand residual sum of squares (cross-validation PRESS statistic) and lowest mean square error (MSE) for all the steps in the regression procedure. Predictand is the predicted value for the observations omitted from the calibration blocks. The 6 validation blocks for k-fold were 1970 to 1975, 1976 to 1981, 1982 to 1987, 1988 to 1993, 1994 to 1999, and 2000 to 2005. This cross-validation technique is described more thoroughly in Malone et al. (2009).

Multivariate regression, nonlinear regression, and cross-validation were performed using SAS v. 9.1 (SAS Institute, Cary, NC).

Results and Discussion

Model Testing: Yield

Corn yield was simulated within 500 kg ha^{-1} (±5%) of observed values for 11 of 12 observations. These corn yield calibration scenarios included the three different N application types (LSNT, NLIM, MIN) over the 4-yr period of the LSNT treatment (1997–2000; Fig. 4a). The average observed and RZWQM annual yield difference between minimum (MIN) and LSNT-determined N application were 994 and 1234 kg ha^{-1}, confirming that RZWQM corn yield predictions responded to N application rates. The least-accurate simulation was for 1998 NLIM, which is underpredicted by about 1200 kg ha^{-1}. The 1998 June rainfall was the second-highest monthly precipitation next to the flood year of July 1993. Both July 1993 and June 1998 received more than 30 cm of precipitation. The poor RZWQM-predicted corn yield in 1998 is attributed to simulation of excessive water logging.

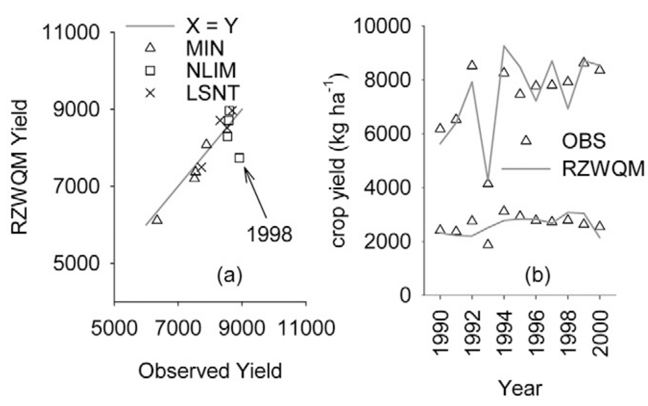

Fig. 4. Annual crop yield. (a) Observed and Root Zone Water Quality Model (RZWQM) simulated corn yield. The three treatments are nonlimiting N fertilizer applied (NLIM; 220 kg N ha^{-1} for RZWQM), Late spring nitrate test (LSNT), and minimum application of 56 kg N ha^{-1}, MIN. (b) Observed (OBS) crop yield from USDA National Agricultural Statistics Service for Story County, Iowa; RZWQM simulations for fall N application.

The crop yield simulations from 1990 to 2000 suggest that RZWQM accurately responded to yearly weather effects (Fig. 4b). The simulated yield is presented along with the average annual crop yield for Story County, Iowa (USDA National Agricultural Statistics Service, 2009). Among the least-accurate simulations was 1998 corn yield, which was underpredicted by about 1000 kg ha^{-1} (Fig. 4b). The soybean yield was simulated fairly well, with the largest discrepancy in 1993, where yield was overpredicted by 632 kg ha^{-1} (Fig. 4b). The simulated and observed corn yield in 1993 was very low because of excessive rain (64 cm precipitation for May–July); unlike the RZWQM–maize model, the RZWQM–soybean model does not simulate water logging.

Model Testing: Drain Flow

The annual average simulated and observed drain flows for the three watersheds were within 3 cm of each other (1993–2001.5; Table 2, Fig. 5). These simulations showed acceptable model indicators with PBIAS <16%, RSR <0.42, and EF >0.80 (Table 2). The EF is greater than the evaluation data of Thorp et al. (2007; EF = 0.78), where the management was better known and the soil more homogenous. We adjusted the snowmelt infiltration factor to optimize surface runoff, which results in good simulated average annual runoff of 5.4 cm with an EF of 0.86 for 1992 through 2001; average observed runoff was 5.6 cm (more detailed runoff results not shown).

For the most part, the model adequately responded to monthly drain flow with an EF of 0.62 and 0.84 for TR1 and CN2 (Table 2). Supplementary Fig. 1SI shows TR1 monthly drain flow; note that TR1 had the lowest EF. An EF of 0.5 can be considered acceptable for monthly drain flow (Moriasi et al., 2007).

Model Testing: Nitrogen

The annual and monthly N loss in subsurface drain flow was simulated acceptably for TR1 and CN2 with PBIAS within ±20%, EF >0.5, and RSR <0.7 (Table 2; Fig. 5). The annual and monthly FWNC in subsurface drain flow showed little bias (< ±11%). But the EF was <0.1 and the RSR was >0.9 for both watersheds (Table 2). Although the EF is low, it is higher than other recent RZWQM evaluations where the specific management was more precisely known and soils more homogenous (e.g., Thorp et al., 2007; Li et al., 2008). Despite low EF values, Li et al. (2008) and Thorp et al. (2007) concluded that the calibrated model was acceptable for estimating the relative effects of different management under different conditions on nitrate loss in subsurface drainage.

The annual and monthly FWNC simulations with the lowest EF was CN2 (Table 2) and among the least-accurate simulated FWNC for this watershed was 1996.8 (Fig. 5). Although the N loss and FWNC were underpredicted in 1996.8 for TR1, CN2 appears the more inaccurate (Fig. 5). We simulated spring N application for all watersheds in 1997 rather than fall 1996 applications because of the wet conditions (Jaynes et al., 2004). Some fields may have received fall N application, which would increase the simulated FWNC and N loss. The observed FWNC and N loss suggest that CN2 had management that resulted in higher N loss than TR1.

Another poorly simulated FWNC for both watersheds was 1999.8 (Fig. 5). The observed and simulated drain flow was <3 cm in 1999.8 (Fig. 5). For the most part, the poor simulated FWNC was caused by the highest monthly drain flow of 1999.8 to be simulated snowmelt in 2000.08 (February 2000) when the monthly simulated FWNC was zero (Supplementary Fig. 1SI).

Model Testing: Nitrate Concentration Difference between LSNT and Control Watershed (TR1-CN2)

Figure 6 shows the monthly time series of paired nitrate concentration differences for the watersheds. The Gompertz function with the AR residual component accounted for more than 70% of the variation in observed and RZWQM simulated concentration differences (Supplementary Table 3SI). Figure 7 also shows that for the most part, annual RZWQM simulations responded to FWNC differences compared with the observed differences (R^2 = 0.62). The poorest simulated annual difference was because snowmelt in 2000.08 drives the annual RZWQM simulated FWNC; therefore, little simulated difference was found between the two subbasins. The 2000.08

Table 2. Statistics summary (1993–2001.5).†

Value	Units	CN2 drainflow	CN2 FWNC	CN2 N loss	TR1 drainflow	TR1 FWNC	TR1 N loss
					Annual		
PBIAS	unitless	−12.23	13.33	−1.57	−9.39	3.29	−11.26
RSR	unitless	0.30	1.44	0.33	0.31	0.99	0.60
RMSE	‡	4.77	4.01	5.15	5.33	2.45	9.03
EF	unitless	0.91	−1.08	0.89	0.90	0.03	0.64
RZWQM	‡	22.83	12.39	27.21	22.72	11.53	25.36
OBS	‡	20.35	14.29	26.79	20.77	11.92	22.80
					Monthly		
PBIAS	unitless	−12.32	11.56	0.20	−9.97	1.54	−9.19
RSR	unitless	0.40	1.09	0.45	0.61	0.98	0.61
EF	unitless	0.84	−0.20	0.80	0.62	0.04	0.63

† CN2, southern-most control subbasin; TR1, subbasin with the late-spring nitrate test treatment; FWNC, flow-weighted nitrate concentration; EF, Nash–Sutcliffe efficiency; PBIAS, percent bias; RMSE, root mean square error; RSR, ratio of the RMSE to the standard deviation of measured data RZWQM, Root Zone Water Quality Model; OBS, average observed.

‡ drainflow, cm; FWNC, mg N L^{-1}; N loss, kg N ha^{-1}.

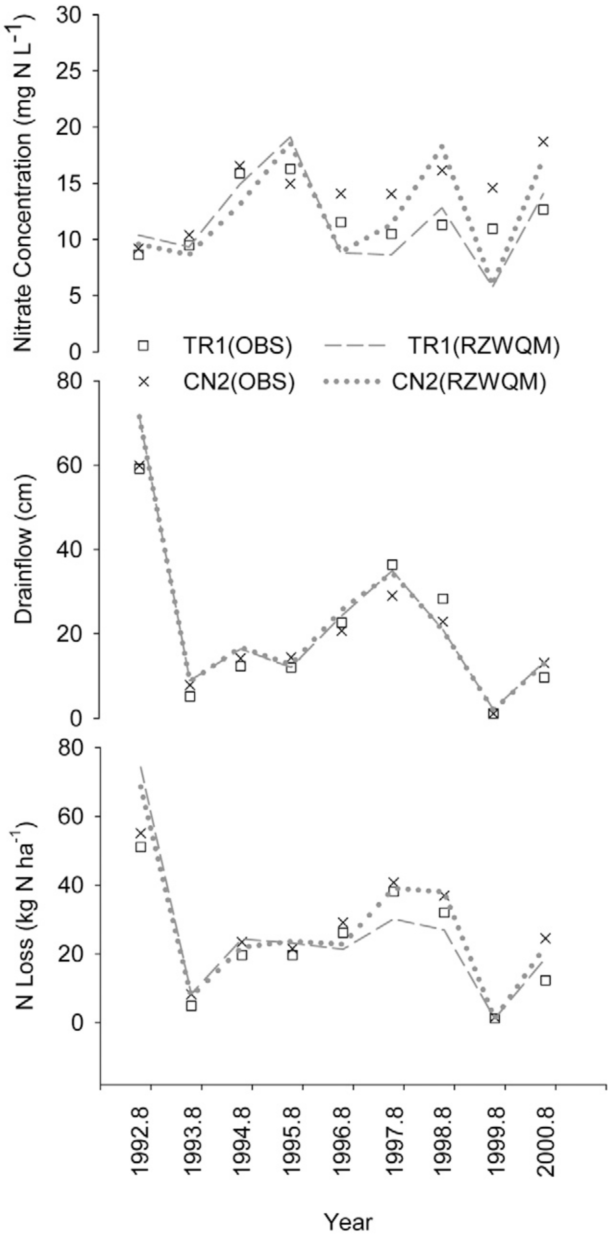

Fig. 5. Annual observed (OBS) and Root Zone Water Quality Model (RZWQM) predicted nitrate concentration, drain flow, and nitrate loss from the two watersheds. The annual values are presented from mid-October to mid-October. For example, 2000.8 include 16 October 2000 to 16 October 2001. TR1 and CN2 are the subbasin with the LSNT treatment and the southernmost control subbasin.

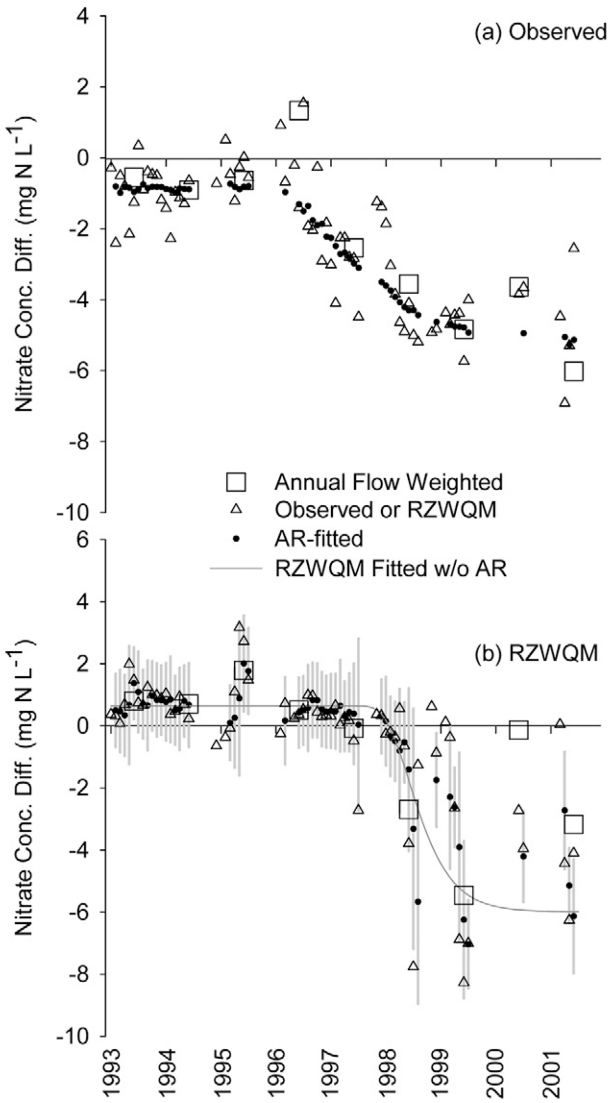

Fig. 6. Monthly nitrate concentration differences (conc. diff.) between late spring nitrate test (LSNT) and control subbasin. The gray error bars are the 95% confidence limits. Data omitted from analysis if observed or RZWQM simulated drainflow <1 mm for month for CN1, TR1, or CN2. TR1, CN1, CN2, and AR are the subbasin with the LSNT treatment, the northernmost control subbasin, the southernmost control subbasin, and autoregressive.

FWNC difference is not shown on Fig. 6 because the observed drain flow for CN2 was <1 mm for this month. The criteria for an observation to be included in the monthly analysis were that all three simulated and observed subbasins produce more than 1mm/month of drain flow.

One notable item for the period before implementation of the LSNT is that RZWQM overpredicted the FWNC difference in TR1-CN2 (Fig. 6, 7). From our knowledge of the watershed management, TR1 should have a somewhat higher annual FWNC than both CN2 and CN1 because it averages 58% of area in corn from 1992 through 1996, whereas CN1 and CN2 averaged <52% (Fig. 2). This suggests that soil and/or N application rate and/or timing are different between TR1 and CN2.

After 1998.3, the 95% confidence bands for the Gompertz function did not include the null hypothesis that the RZWQM simulated concentration differences were equal to the averages before LSNT implementation, which indicates a significant decrease in TR1 nitrate concentration due to the LSNT treatment (0.64 mg N L^{-1} for TR1-CN2; Fig. 6b). Jaynes et al. (2004) reported similar timing for observed differences. Our observed 95% confidence bands did not go above −2.0 (TR1-CN2) after 1998.25 (results not shown). Thus, as Jaynes et al. (2004) reported for the observed data, for the most part the RZWQM simulated nitrate concentration coming from LSNT-treated watershed can be considered significantly lower than nitrate concentration coming from the control watershed after the latter half of 1998. Therefore,

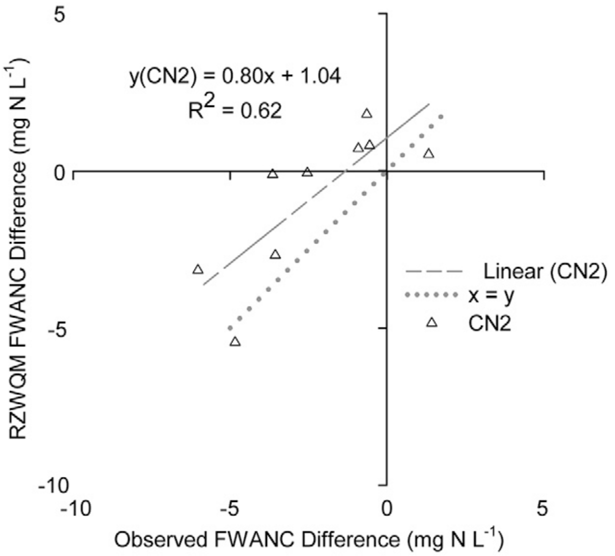

Fig. 7. Annual flow-weighted nitrate concentration (FWANC) differences between the late spring nitrate test treatment (LSNT; TR1) and southernmost control subbasin (CN2).

RZWQM is a promising tool for predicting the water quality effects of LSNT implementation in watersheds.

The 95% confidence bands from the simulated differences approach zero after 1998.5 partly because of runoff or snowmelt (e.g., 2001.25) the preceding month. High simulated runoff or snowmelt results in a high residual value between the RZWQM value and the Gompertz function (e.g., 2001.17; Fig. 6). This in turn results in a high upper confidence band the following month due to the high lag1 autoregressive residual component. For simplicity, we did not include simulated baseflow in our drainflow computations and RZWQM predicts nearly no N loss under runoff. The observed watershed measurements on the other hand included baseflow, which would tend to show differences between treatments.

Another reason for the high upper confidence bands after 1998.5 was that RZWQM-simulated nitrate concentration differences tend to be lower than observed in the spring and summer and higher than observed in the fall and winter. These simulated differences also result in a high residual error with Eq. [7] (r_x). For example, RZWQM simulated concentration differences between 1998.75 through 1999.17 are much higher than observed (and Eq. [7] predicted), whereas differences from 1999.3 through 1999.5 are much lower than observed and much lower than Eq. [7] predicted (Fig. 6). A high r_x component of Eq. [7] for a specific observation results in a wide confidence interval for that observation. Overpredicted winter nitrification by RZWQM was previously reported (Ma et al., 2007b; 1998). This causes RZWQM to simulate deeper peak soil nitrate than field observations for the spring–summer when N fertilizer is fall applied (Malone et al., 2007). Therefore, RZWQM simulates acceptable annual differences between LSNT N applications and fall N applications except when runoff and snowmelt are driving annual FWNC (e.g., 1999.8; Fig. 6, 7); however, the timing of monthly simulated differences are less accurate than desired.

Application of the Tested Model: Long-Term LSNT Treatment Effect

We used the calibrated model to simulate the average 1970 to 2005 plant available nitrogen (NH_4 and NO_3) budget for three treatments: LSNT, average LSNT rate applied at planting, and average LSNT rate applied in the fall after harvest (Table 3). We used the specific LSNT determined rate each year for the LSNT simulations; the average of these variable RZWQM simulated LSNT determined rates from 1970 to 2005 was 150.7 kg N ha^{-1}. These simulations indicate that LSNT lost 1.8 kg ha^{-1} less N (~8%) in tile drainage than the single spring application with <1% corn-yield difference (Table 3). The simulated tile drainage N difference between LSNT and single fall application was much larger at 6.9 kg N ha^{-1} with about 1% corn yield difference. The N budget suggests that LSNT has slightly greater N uptake by crops than fall or single spring applications (1.4–5.4%). This contributes to substantially less percentage N loss in tile drainage (8.8 to 33.8%) due to more N remaining in the root zone for crop N uptake during the growing season under LSNT. Similarly, Malone and Ma (2009) reported that 4% greater crop N uptake results in 30% less N in subsurface drainage in northeastern Iowa. In contrast to these modeling results, the analysis on the field data from this study did not quantify the water quality benefit of soil testing compared to single spring N applications (e.g., Jaynes et al., 2004).

We used the same long-term average N rate for the three treatments. The average annual rate may differ, however, between corn fields with soil testing and fields with no soil test. If average annual N rates were lower for LSNT, N loss would be less. In the Corn Belt, for example, about 17% of corn acres were tested for soil nitrogen during 1996 to 2001. About 4% less nitrogen was applied on those fields than the average for corn fields not tested (Kim and Quinby, 2004). In Iowa, about 6% less nitrogen was applied to fields with soil N tests during 1996 to 2005 (USDA Agricultural Resource

Table 3. Root Zone Water Quality Model (RZWQM) simulated average annual plant available N budget (NO_3 and NH_4) for three treatments (Trt) from 1970 to 2005 (kg N ha^{-1}).†

Trt	Nbal‡§	immob‡	mineral‡	Ntile‡	Nlat‡	fix‡	runoff‡	denit‡	upt‡	appli‡	begin‡	end‡
LSNT	0.4	32.0	116.3	20.4	6.3	79.2	0.3	0.9	223.6	75.4	161.0	89.8
Fall	0.2	31.9	113.3	27.3	8.2	80.0	0.4	1.3	211.5	75.4	246.4	200.1
Spring	0.3	32.0	115.5	22.2	7.0	79.5	0.4	0.4	220.3	75.4	149.0	106.9

† Each treatment is the average of two rotations (corn in odd years and corn in even years). Average rain N was 10.9 kg N ha^{-1} yr^{-1} (National Atmospheric Deposition Program website, http://nadp.sws.uiuc.edu/).

‡ Nbal, N balance; immob, immobilization; mineral, mineralization; Ntile, N in subsurface tile line; Nlat, N in lateral flow below tile line; fix, fixation; runoff, N in runoff; denit, denitrification; upt, N uptake by crops; appli, N application rate; begin, soil nitrate at beginning of RZWQM simulation (31 Dec. 1969); end, soil nitrate at end of RZWQM simulation (31 Dec. 2005).

§ appli + fix + mineral + rain + begin/36 – upt – denit – runoff – Nlat – Ntile – immob – end/36 = Nbal

Management Survey, http://www.ers.usda.gov/Data/ARMS/app/Crop.aspx). Small changes in nitrogen-containing fertilizer use (e.g., adjusted according to annual soil testing) may substantially reduce nitrate delivery to the Gulf of Mexico (McIsaac et al., 2001).

Although lower N fertilizer rates are often recommended with the LSNT, implementing the program within the Walnut Creek watershed costs about \$5 ha^{-1} yr^{-1} (Saleh et al., 2007). This additional cost partly explains why only about 12% of corn fields in Iowa were tested for soil nitrogen in 2005 (USDA Agricultural Resource Management Survey, http://www.ers.usda.gov/Data/ARMS/app/Crop.aspx). Part of the higher LSNT cost is due to soil sampling (Saleh et al., 2007). An improved understanding of the year-to-year variability of soil mineral N could lead to a reduced need for soil testing and help increase adoption of side dressing.

To explore the relationship between LSNT rate and weather variables before soil testing, we developed the following cross-validated equation that accounts for 90% of the variation in 1970 to 2005 RZWQM-simulated annual LSNT rate (Nrate; Fig. 8):

$$\text{Nrate} = 1992.7 + 0.3704 \times \text{etemp} \times \text{eprecip} - 1406.36 \times \text{etemp}^{0.1} - 0.005418 \times \text{eprecip}^{3} \qquad [8]$$

where etemp is early season average maximum temperature for (date –10) > doy > (date – 64), doy is day of year, date is LSNT sample date (doy), and eprecip is the total early season precipitation for (date + 1) > doy > (date – 28). The equation was developed as discussed above in "Long-Term RZWQM Simulations" and by systematically adjusting the timing of eprecip and etemp for weather variable calculation similar to Malone et al. (2009), which minimized the variance between annual RZWQM simulated rate and Eq. [8] predicted Nrate.

In addition to the excellent correlation between Eq. [8] and RZWQM simulated LSNT rates, Eq. [8] also accounts for 76% of the variation in 1997 to 2000 observed LSNT rates determined by field soil testing (Fig. 8). The lowest LSNT rates for observed and Eq. [8] were in 2000 and the highest rates were in 1999. The least-accurate Eq. [8] determined N rate compared to field observations was in 1998 when the difference between the two values was 28 kg N ha^{-1}. The large 1998 difference between Eq. [8] using observed versus RZWQM estimated sampling dates (Fig. 8) was because of the high early June rainfall (16.4 cm for 1–14 June); the observed RZWQM-simulated sampling dates were 27–28 May and 14 June, respectively. This all suggests potential for development of simple tools to estimate side-dressing rates, which could reduce the need for soil testing.

Figure 9a illustrates the relationship among early-season precipitation and temperature (eprecip, etemp), and LSNT rate estimated using Eq. [8]. For example, Nrate increases as etemp decreases and eprecip increases. Although interpreting the dependence of rate on the interaction between etemp and eprecip is possible with Fig. 9a, Fig. 9b helps clarify this interaction. The variable eprecip affected Nrate positively at high etemp but slightly less so at low etemp, and Nrate remained higher throughout the range of eprecip when etemp was low (Fig. 9b). This is supported by the slightly smaller slope of

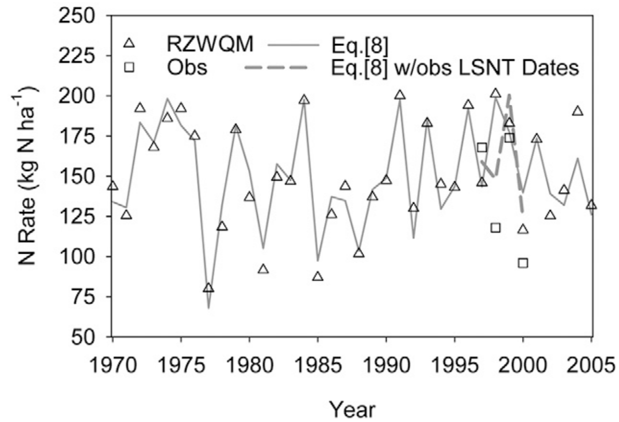

Fig. 8. N fertilizer rate (N rate) determined from the late spring nitrate test (LSNT) as a function of year. N fertilizer rate determined from Root Zone Water Quality Model (RZWQM) or Eq. [8] according to observed (obs) annual weather variables etemp and eprecip: early-season temperature and precipitation described in text. Observed LSNT rates and Eq. [8] rates with observed LSNT dates are also presented (Jaynes et al., 2004). The Eq. [8] soil testing dates were according to RZWQM and Eq. [8] with observed soil testing dates are according to field notes.

the linear trend through the Eq. [8] computed values under low etemp compared with high etemp (Fig. 9b). Under the condition of high eprecip compared with low eprecip, Nrate remained higher and less affected by etemp (Fig. 9b) due to more leaching of crop available N.

Our long-term modeling results confirm other modeling and field research. Using the LEACHMN model, Sogbedji et al. (2001) reported that lower economic optimum N application rates were associated with low early-season precipitation due to less denitrification and leaching. This agrees with Kay et al. (2006), where field measurements were used to report that increasing early-season rainfall result in less plant available nitrogen. Increasing soil temperature is usually associated with increasing soil organic matter decomposition (e.g., Kirschbaum, 1995; Eq. [1], Fig. 3), and thus higher plant available nitrogen during years with higher early-season temperature. Of course, higher early-season temperature also contributes to increased soil evaporation and reduced tile flow, and thus higher temperature contributes to reduced N leaching below the root zone.

Conclusions

Our results suggest that N fertilizer rates determined from the LSNT protocol are strongly correlated with early-season air temperature and precipitation. This conclusion should be treated as an impetus for further research. However, we have demonstrated that a cross-validated statistical model based on early season weather variables could be developed that predicts year-to-year variation in central Iowa LSNT-determined N fertilizer rates. Further refinement of this model may lead to simple tools that will enhance implementation of the LSNT by farmers, which could be of economic and environmental significance.

Development of the statistical model used long-term simulations from the agricultural system model RZWQM, which was thoroughly tested using observed data from the Walnut Creek watershed in central Iowa. The long-term simulations

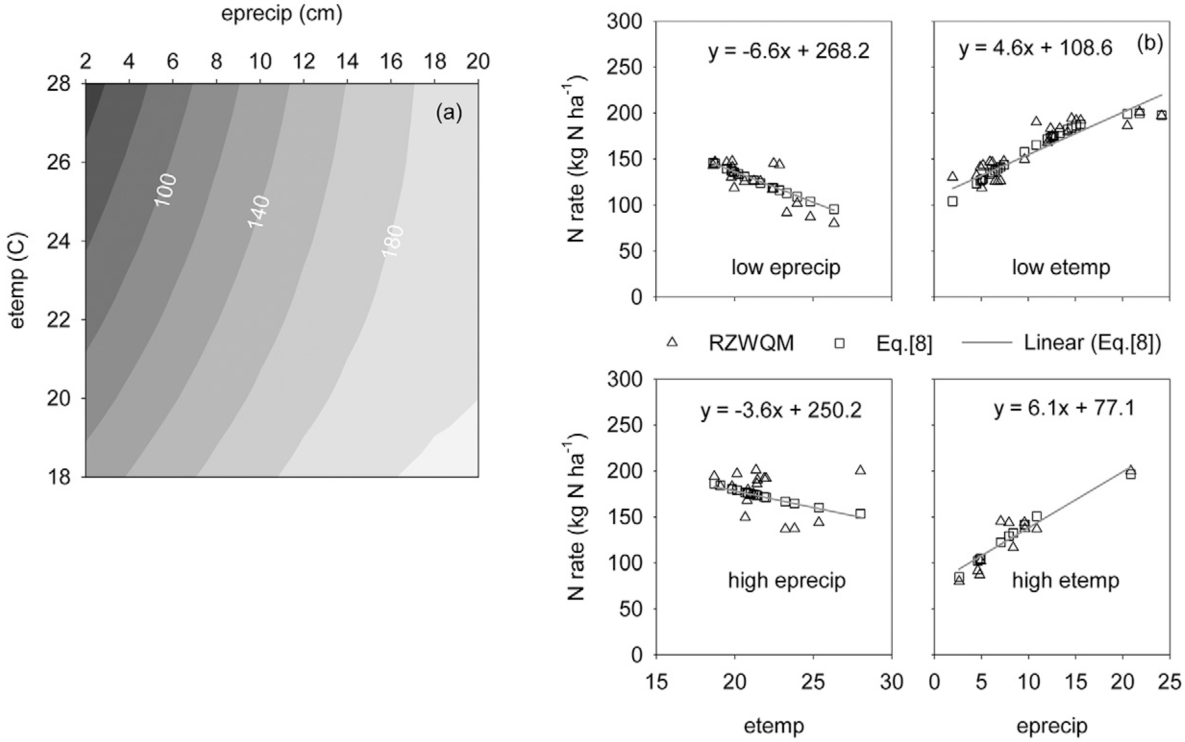

Fig. 9. N fertilizer rate as a function of early-season temperature (etemp) and early-season precipitation (eprecip). (a) is estimated using Eq. [8] (contour intervals of 20 kg N ha^{-1}). (b) N fertilizer rate (N rate) from long-term annual Root Zone Water Quality Model (RZWQM) predicted (1970–2005) and Eq. [8] estimated. For (b), the Eq. [8] estimated N rate was calculated with median weather variables for the given figure except where adjusted according to the *x* axis variable. Also for (b), the linear trend through the Eq. [8] predicted N rate is presented along with the associated equation of the linear trend.

suggest that the N loss difference between LSNT, single spring, and single fall applications is mainly from more N remaining in the root zone for crop uptake. The model testing suggests that RZWQM is a promising tool for predicting the water quality effects of LSNT implementation in watersheds.

References

Allen, R.G. 1996. Assessing integrity of weather data for reference evapotranspiration estimation. J. Irrig. Drain. Eng. 122:97–106.

Bakhsh, A., J.L. Hatfield, R.S. Kanwar, L. Ma, and L.R. Ahuja. 2004a. Simulating nitrate drainage losses from a Walnut Creek watershed field. J. Environ. Qual. 33:114–123.

Bakhsh, A., L. Ma, L.R. Ahuja, J. L. Hatfield, and R. S. Kanwar. 2004b. Using RZWQM to predict herbicide leaching losses in subsurface drainage water. Trans. ASAE 47:1415–1426.

Blackmer, A.M., R.D. Voss, and A.P. Mallarino. 1997. Nitrogen fertilizer recommendations for corn in Iowa. PM-1714. Iowa State Coop. Ext., Iowa State Univ., Ames.

Bundy, L.G., and T.W. Andraski. 1995. Soil yield potential effects on performance of soil nitrate tests. J. Prod. Agric. 8:561–568.

Doherty, J., and J.M. Johnston. 2003. Methodologies for calibration and predictive analysis of a watershed model. J. Am. Water Resour. Assoc. 39:251–265.

Doherty, J. 2004. PEST: Model independent parameter estimation user manual. 5th ed. Watermark Numerical Computing, Brisbane, Australia.

Du, B., J.G. Arnold, A. Saleh, et al. 2005. Development and application of SWAT to landscapes with tiles and potholes. Trans. ASAE 48:1121–1133.

Gowda, P.H., D.J. Mulla, and D.B. Jaynes. 2008. Simulated long-term nitrogen losses for a midwestern agricultural watershed in the United States. Agric. Water Manage. 95:616–624.

Hanson, J.D., K.W. Rojas, and M.J. Shaffer. 1999. Calibrating the root zone water quality model. Agron. J. 91:171–177.

Hatfield, J.L., D.B. Jaynes, M.R. Burkart, C.A. Cambardella, T.B. Moorman, J.H. Prueger, and M.A. Smith. 1999a. Water quality in Walnut Creek watershed: Setting and farming practices. J. Environ. Qual. 28:11–24.

Hatfield, J.L., J.H. Prueger, and D.W. Meek. 1999b. Spatial variation of rainfall over a large watershed in central Iowa. Theor. Appl. Climatol. 64:49–60.

Heiberger, R.M., and R.A. Becker. 1992. Design of an S function for robust regression using iteratively reweighted least squares. J. Comput. Graph. Statist. 1:181–196.

Jaynes, D.B., T.S. Colvin, D.L. Karlen, C.A. Cambardella, and D.W. Meek. 2001. Nitrate loss in subsurface drainage as affected by nitrogen fertilizer rate. J. Environ. Qual. 30:1305–1314.

Jaynes, D.B., D.L. Dinnes, D.W. Meek, D.L. Karlen, C.A. Cambardella, and T.S. Colvin. 2004. Using the late spring nitrate test to reduce nitrate loss within a watershed. J. Environ. Qual. 33:669–677.

Karlen, D.L., D.L. Dinnes, D.B. Jaynes, C.R. Hurburgh, C.A. Cambardella, T.S. Colvin, and G.R. Rippke. 2005. Corn response to late-spring nitrogen management in the Walnut Creek watershed. Agron. J. 97:1054–1061.

Kay, B.D., A.A. Mahboubi, E.G. Beauchamp, and R.S. Dharmakeerthi. 2006. Integrating soil and weather data to describe variability in plant available nitrogen. Soil Sci. Soc. Am. J. 70:1210–1221.

Kim, C.S., and W. Quinby. 2004. ARMS data offer new perspectives on cropping practices. Amber Waves. 2:12–13.

Kirschbaum, M.U.F. 1995. The temperature-dependence of soil organic-matter decomposition, and the effect of global warming on soil organic-C storage. Soil Biol. Biochem. 27:753–760.

Klapwyk, J.H., and Q.M. Ketterings. 2006. Soil tests for predicting corn response to nitrogen fertilizer in New York. Agron. J. 98:675–681.

Kutilek, M., and D.R. Nielsen. 1994. Soil hydrology. Catena, Cremlingen-Destedt, Germany.

Li, L., R.W. Malone, L. Ma, T.C. Kaspar, D.B. Jaynes, S.A. Saseendran, K.R. Thorp, Q. Yu, L.R. Ahuja. 2008. Winter cover crop effects on nitrate leaching in subsurface drainage as simulated by RZWQM-DSSAT. Trans. ASABE 51:1575–1583.

Linn, D.M., and J.W. Doran. 1984. Effect of water-filled pore-space on carbon-dioxide and nitrous-oxide production in tilled and nontilled soils. Soil Sci. Soc. Am. J. 48:1267–1272.

Luo, W., G.R. Sands, M. Youssef, J.S. Strock, I. Song, and D. Canelon. 2010. Modeling the impact of alternative drainage practices in the northern Corn-belt with DRAINMOD-NII. Agric. Water Manage. 97:389–398.

Ma, L., L.R. Ahuja, S.A. Saseendran, R.W. Malone, T.R. Green, B.T. Nolan, P.N.S. Bartling, G.N. Flerchinger, K.J. Boote, and G. Hoogenboom. 2010. Step-by-step parameterization and calibration of RZWQM2 in field research. *In* L.R. Ahuja and L. Ma (ed.) Methods of introducing system models into agricultural research. ASA, CSA, and SSSA, Madison, WI (in press).

Ma, L., R.W. Malone, P. Heilman, L.R. Ahuja, T. Meade, S.A. Saseendran, J.C. Ascough II, R.S. Kanwar. 2007a. Sensitivity of tile drainage flow and crop yield on measured and calibrated soil hydraulic properties. Geoderma 140:284–296.

Ma, L., R.W. Malone, P. Heilman, D.L. Karlen, R.S. Kanwar, C.A. Cambardella, S.A. Saseendran, and L.R. Ahuja. 2007b. RZWQM simulation of long-term crop production, water and nitrogen balances in northeast Iowa. Geoderma 140:247–259.

Ma, L., R.W. Malone, D.B. Jaynes, K.R. Thorp, and L.R. Ahuja. 2008. Simulated effects of nitrogen management and soil microbes on soil nitrogen balance and crop production. Soil Sci. Soc. Am. J. 72:1594–1603.

Ma, L., M.J. Shaffer, and L.R. Ahuja. 2001. Application of RZWQM for soil nitrogen management. p. 265–301. *In* M.J. Shaffer et al. (ed.) Modeling carbon and nitrogen dynamics for soil management. CRC Press, Boca Raton, FL.

Ma, L., M.J. Shaffer, J.K. Boyd, R. Waskom, L.R. Ahuja, K.W. Rojas, and C. Xu. 1998. Manure management in an irrigated silage corn field: Experiment and modeling. Soil Sci. Soc. Am. J. 62:1006–1017.

Magdoff, F.R., D. Ross, and J. Amadon. 1984. A soil test for nitrogen availability to corn. Soil Sci. Soc. Am. J. 48:1301–1304.

Magdoff, F. 1991. Understanding the Magdoff pre-sidedress nitrate test for corn. J. Prod. Agric. 4:297–305.

Malone, R.W., S. Logsdon, M.J. Shipitalo, J. Weatherington Rice, L. Ahuja, and L. Ma. 2003. Tillage effect on macroporosity and herbicide transport in percolate. Geoderma 116:191–215.

Malone, R.W., and L. Ma. 2009. N uptake affects corn yield and N loss in tile drains as simulated by the Root Zone Water Quality Model (RZWQM). p. 259–275. *In* L. Ma, T. Bruulsema, and L. Ahuja, (ed.) New advances in understanding and quantification of plant N uptake. CRC Press, Boca Raton, FL.

Malone, R.W., L. Ma, P. Heilman, et al. 2007. Simulated N management effects on corn yield and tile-drainage nitrate loss. Geoderma 140:272–283.

Malone, R.W., L. Ma, R.D. Wauchope, L.R. Ahuja, K.W. Rojas, Q. Ma, R. Warner, and M. Byers . 2004. Modeling hydrology, metribuzin degradation, and metribuzin transport in macroporous tilled and no till silt loam soil using RZWQM. Pest Manag. Sci. 60:253–266.

Malone, R.W., D.W. Meek, J.L. Hatfield, et al. 2009. Quasi-biennial corn yield cycles in Iowa. Agric. For. Meteorol. 149:1087–1094.

Malone, R.W., D. Meek, L. Ma, D. Jaynes, B.T. Nolan, and D. Karlen. 2010. Quality control of weather data for agricultural system model input. *In* L. R. Ahuja and L. Ma (ed.) Methods of introducing system models into agricultural research. ASA, SSSA, and CSSA, Madison, WI (in press).

McIsaac, G.F., M.B. David, G.Z. Gertner, and D.A. Goolsby. 2001. Eutrophication–nitrate flux in the Mississippi River. Nature 414:166–167.

Meisinger, J.J., and J.A. Delgado. 2002. Principles for managing nitrogen leaching. J. Soil Water Conserv. 57:485–498.

Miller, C.T., G.A. Williams, C.T. Kelley, and M.D. Tocci. 1998. Robust solution of Richards' equation for nonuniform porous media. Water Resour. Res. 34:2599–2610.

Moriasi, D.N., J.G. Arnold, M.W. Van Liew, R.L. Bingner, R.D. Harmel, and T.L. Veith. 2007. Model evaluation guidelines for systematic quantification of accuracy in watershed simulations. Trans. ASABE 50:885–900.

Nangia, V., R.H. Gowda, D.J. Mulla, and G.R. Sands. 2008. Water quality modeling of fertilizer management impacts on nitrate losses in tile drains at the field scale. J. Environ. Qual. 37:296–307.

Nolan, B.T., R.W. Malone, L. Ma, C.T. Green, and D.B. Jaynes. 2010a. Inverse modeling with RZWQM2 to predict water quality. *In* L.R. Ahuja and L. Ma (ed.) Methods of introducing system models into agricultural research. ASA, CSSA, and SSSA, Madison, WI (in press).

Nolan, B.T., L.J. Puckett, L. Ma, C.T. Green, E.R. Bayless, and R.W. Malone. 2010b. Predicting unsaturated zone nitrogen mass balances in agricultural settings of the United States. J. Environ. Qual. 39:1051–1065.

Rawls, W.J., D.L. Brakensiek, and K.E. Saxton. 1982. Estimation of soil water properties. Trans. ASABE 25:1316–1320, 1328.

Rose, K.A., B.A. Megrey, F.E. Werner, and D.M. Ware. 2007. Calibration of the NEMURO nutrient–phytoplankton–zooplankton food web model to a coastal ecosystem: Evaluation of an automated calibration approach. Ecol. Modell. 202:38–51.

Russo, D., and E. Bresler. 1980. Field determinations of soil hydraulic properties for statistical analysis. Soil Sci. Soc. Am. J. 44:682–687.

Saleh, A., E. Osei, D.B. Jaynes, et al. 2007. Economic and environmental impacts of LSNT and cover crops for nitrate-nitrogen reduction in Walnut Creek watershed, Iowa, using fem and enhanced SWAT models. Trans. ASABE 50:1251–1259.

Schroder, J.J., J.J. Neeteson, O. Oenema, and P.C. Struik. 2000. Does the crop or the soil indicate how to save nitrogen in maize production? Reviewing the state of the art. Field Crops Res. 66:151–164.

Sogbedji, J.M., H.M. van Es, S.D. Klausner, D.R. Bouldin and W.J. Cox. 2001. Spatial and temporal processes affecting nitrogen availability at the landscape scale. Soil Tillage Res. 58:233–244.

Sogbedji, J.M., H.M. van Es, C.L. Yang, L.D. Geohring, and F.R. Magdoff. 2000. Nitrate leaching and nitrogen budget as affected by maize nitrogen rate and soil type. J. Environ. Qual. 29:1813–1820.

Thorp, K.R., R.W. Malone, and D.B. Jaynes. 2007. Simulating long-term effects of nitrogen fertilizer application rates on corn yield and nitrogen dynamics. Trans. ASABE 50:1287–1303.

USDA National Agricultural Statistics Service. 2009. Cropland data layer: Examples. Available at http://www.nass.usda.gov/research/Cropland/sarsexample3.html (verified 25 June 2010). USDA National Agricultural Statistics Service, Washington, DC.