Incorporating Spatial Variability into GIS to Estimate Nitrate Leaching at the Aquifer Scale

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ABSTRACT

We evaluated the effect of spatial variability of selected intrinsic soil properties and extrinsic management practices on the groundwater quality in the 330-ha recharge area of a high yield well site in Rhode Island. The analyses were performed at different support scales, ranging from point level to a support level equal to the entire recharge area. We used a mass balance model that relates leaching from the vadose zone to long-term estimates of NO₃-N concentration at the well. We used a GIS database and stratified sampling for both soil characterization and assessment of spatial variability of NO₃ leaching. The LEACHA/N rootzone model was used in conjunction with Monte Carlo simulation to generate cumulative distribution functions (CDFs) for leaching from different land strata (given by combinations of soil type and land use). To simulate the spatial variability of properties that served as inputs to the root zone model, we used CDFs of spatial distributions of soil properties and CDFs of the spatial variability of fertilizer application rates within a field. These strata scale CDFs were then combined to generate CDFs of the NO₃-N concentrations at the well, i.e., at a recharge area support scale. Although considerable variability was found at a point support scale, the analyses generated a markedly lower variability at the recharge area support scale. The results suggest that GIS data bases generated at scales available to resource managers (i.e., 1:12 000 and 1:24 000) may be well suited to manage the water quality of large production scale wells.

Nitrate (NO₃-N) leaching from many types of land use activities has been found to exceed the U.S. drinking water standard of 10 mg L⁻¹ NO₃-N (USEPA, 1976; Keeney, 1986; Gold et al., 1990). Because NO₃-N is relatively easy to measure and widely studied, it has been used by resource managers as a generalized indicator of groundwater degradation. To assist with wellhead protection efforts, a number of water resource agencies use a mass balance model that is predicated on the assumption that a long-term estimate of the groundwater NO₃-N concentrations of a production-scale well can be obtained based on the land use activities within the recharge area of the well (Nelson et al., 1988; Frimpter et al., 1990; Hantzsche and Finnemore, 1992).

The model stratifies a recharge area into distinct land uses and computes an area-weighted mean concentration at the well from the annual recharge and NO₃-N loading expected from the vadose zone of each strata.

\[ <x> = \frac{\sum_{i=1}^{N} A_i L_i}{\sum_{i=1}^{N} A_i R_i} \]  

where

\[ <x> \] = long-term concentration of NO₃-N at the well (g m⁻³)
\[ A_i \] = area of land stratum i (m²)
\[ L_i \] = loading of NO₃-N per stratum (g m⁻² yr⁻¹)
\[ R_i \] = recharge per stratum (m yr⁻¹)

Additional assumptions are that NO₃-N is conservative below the rootzone and that the well fully penetrates the saturated zone, thereby intercepting and mixing all the water from the recharge area.

This simple model is well-suited to the GIS data bases of many resource protection agencies, in which features are identified by a single value that is representative of the entire polygon, line, or point. Rarely are features encoded with an estimate of variability (Burrough, 1986; Chrisman, 1991). Therefore, the model typically is used in a deterministic fashion with loading and recharge factors fixed for several types of land uses. Generally, the model generates a single estimate of NO₃-N concentration at a well for a particular land use scenario within the recharge area of the well. The model is intended to be used as a functional screening tool, i.e., a simplified representation of the system to generate practical results (Addiscott, 1994). However, the lack of variance or uncertainty that is associated with the estimate relating land use to water quality at the well could mislead the resource manager. Land-use scenarios that generate different estimates of mean NO₃-N concentration at the well could be associated with different tradeoffs or costs to the community (i.e., suburban development vs. preservation of agricultural lands), yet the practical differences in well water quality may be minor if the variance of the estimates was considered.

Nitrate-N leaching from the vadose zone has been found to be highly variable, both spatially and temporally (Böttcher and Strebel, 1988; McBratney and Webster, 1981). The variability is a result of both intrinsic variation due to natural features of the site as well as extrinsic factors such as those generated by management activities (Rao and Wagener, 1985). A major challenge when estimating watershed or aquifer scale NO₃-N leaching is to incorporate this heterogeneity in our analyses and our results.

Of equal importance is selecting the appropriate support scale to ensure that the spatial and temporal variability is weighted correctly (Isaaks and Srivastava, 1989; Webster and Oliver, 1990). The support scale represents the area or volume for which data and estimates are derived (Isaaks and Srivastava, 1989). Often, the support scale of the sample data may differ from the support scale at which estimates are desired.

A large production-scale well integrates leaching from the entire recharge area, often in excess of 2 km². In

Abbreviations: CDF, cumulative distribution function; CV, coefficient of variation; IMC, Inverse Monte Carlo.
this situation, the entire recharge area constitutes the support scale for well water quality estimates. Estimating concentrations at the well therefore requires calculation of a regional mean that results from the aggregation of many smaller units, i.e., leaching points. Point locations generating high losses of NO$_3$-N are expected to be balanced by point locations generating low losses, thus the variance of predictions at the well is expected to be smaller than the variance associated with individual points in the recharge zone (Isaaks and Srivastava, 1989; Webster, 1993).

Most sampling and modeling of NO$_3$-N leaching is performed at the point scale and intensive sampling and estimates of variability are often required to characterize the variation at the point scale. This sampling intensity may require a high commitment of time and resources and often is unattainable for most GIS data bases (1:12 000-1:24 000 scale) that are used for resource management. In contrast, the estimate of recharge scale phenomena may be well-suited to the level of detail in existing GIS data bases, due to the inherent dampening of variability that results from the large support area. The objective of our study is to explore and quantify the uncertainty of estimates of NO$_3$-N concentrations at a production scale well that result from the intrinsic variability of the soils in conjunction with various land management activities. We used Monte Carlo analyses with the rootzone N fate model LEACHA/N (Hutson and Wagenet, 1992) together with a stratified field sampling scheme to create cumulative distribution functions (CDFs) of NO$_3$-N leaching for different soil/land management strata. These stratum scale CDFs were then combined to generate CDFs of the NO$_3$-N concentrations at the well. Additional analyses were performed on a point support scale and at hypothetical sampling intensities to elucidate the variance associated with estimates derived at different support scales.

**METHODS**

**Watershed Description**

The Beaver River watershed, a subwatershed of the Pawcatuck River located in Southern Rhode Island, served as a physical setting for this study. The USDA-SCS has mapped 63 soil series in the watershed (Rector, 1981). Seventy percent of the watershed is covered by forest and wetlands. The northern part of the watershed is dominated by till deposits. The southern part contains a high transmissivity stratified drift aquifer. The Beaver River watershed, a subwatershed of the Pawcatuck River located in Southern Rhode Island, served as a physical setting for this study. The USDA-SCS has mapped 63 soil series in the watershed (Rector, 1981). Seventy percent of the watershed is covered by forest and wetlands. The northern part of the watershed is dominated by till deposits. The southern part contains a high transmissivity stratified drift aquifer. The Beaver River as baseflow. In contrast, the USGS assumes that all the recharge from the vadose zone of the stratified drift deposits reaches the well. We used these recharge ratios throughout our study to weight the effects of leaching from till vs. stratified drift locations.

**Characterization of Soil Strata**

Using the Rhode Island Geographic Information System soils data base and the GIS software ARCMINFO Version 6.1 (Environ. Syst. Res. Inst., Redland, CA), the 63 soil series in the watershed were stratified into six broad soil strata. These were sandy, silty, and organic soils on till and on stratified drift deposits. The distribution of the sandy, silty, and organic soils is shown in Fig. 1B. The soils GIS data base was created from 1:15 840 scale maps, whereas the superficial geology, topography, and surface water GIS coverages were derived from 1:24 000 scale sources. We sampled sandy and silty soils in the field using stratified random designs in several locations where land owners permitted us to sample. The organic soils are primarily found in saturated, forested wetlands that border streams and are not expected to generate recharge to the groundwater. Our analyses focused entirely on the silty and sandy soil textural classes.

Hydraulic conductivity was measured in the field using the inverse auger hole method (Landon, 1991). Samples for bulk density were extracted using a 100 cm$^3$ root corer and dried for 24 h at 105°C. Organic matter was determined by the loss on ignition method. We used tensiometers to obtain estimates of the spatial variability of the field capacity parameter used in the LEACHA/N model. In each soil textural class, we installed tensiometers at a depth of 15 cm. The soil was wetted with 10 cm/d of irrigation water for 3 consecutive days, then soil–water potential was observed over a period of drainage. We covered the soil around the tensiometers with black plastic to eliminate evapotranspiration. The soil–water potential registered by all the tensiometers stabilized within 24 h and we defined field capacity as the stable soil–water potential at 48 h following the cessation of wetting.

Summary statistics of these soil property analyses are given in Table 1. For each soil textural class, the number of replicate measurements for the properties listed above varied between 15 and 117. Since the coefficient of variation was highest for the saturated hydraulic conductivity, we sampled this parameter most intensively. Texture was determined for each textural class by the methods of Day (1965).

Rather than assume a recognized distribution for these data, we calculated a CDF for each of these properties by soil textural class and then parameterized the CDF by the two parameter sigmoid equation

$$P(x_i < X) = 1 - e^{-a(X-x_i)}$$

where $x_i$ = value of soil property

$X$ = value of the (100*P)th percentile

$a, b =$ the sigmoid parameters obtained by curve fitting

**Evaluation of the Land Strata within the Well Recharge Area**

The exact site and recharge area of the hypothetical well is not identified in Fig. 1 because of the volatile public reactions that may be caused by local groundwater extraction decisions. However, a separate outline of the recharge area (Fig. 2)
displays the six soil strata. The area of each soil type within the recharge area was computed through the GIS.

For our analyses, we assumed that the silt and sand strata in the recharge area were completely covered by three different agricultural land uses. Within each of the soil strata we assumed that 70% of the area was silage corn managed in a conventional fashion, 20% was silage corn managed following best management practices to minimize water quality degradation (hereafter known as the water quality system), and 10% was modeled as commercial turf production practice. Hereafter, we will refer to the combination of a soil stratum with a land-use practice as a land stratum. To incorporate some of the effects of extrinsic spatial variability inherent in agricultural practices, we used CDFs for fertilizer application rates within a field. For manure-based fertilizer we used a normal distribution with a coefficient of variation (CV) of 50% (Wilhoit et al., 1992) and for inorganic fertilizer formulations we used a normal distribution with a CV of 30% (Ndiaye and Yost, 1989). Fertilizer and irrigation inputs to these systems are summarized in Table 2.

**Modeling**

Because we were interested in exploring the variation in NO₃-N leaching that could result from the effect of intrinsic soil variability in combination with several agricultural management practices, we needed to use a model that could rapidly assess hundreds of different scenarios. We selected the LEACHA/N simulation model for our study, since it combines a sophisticated N cycling algorithm with a fast, capacity-based hydrology model (Hutson and Wagenet, 1991, 1992, 1993). During extended periods, the capacity-based and Richards

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**Table 1. Mean and coefficient of variation of selected A horizon soil properties based on field sampling.†**

<table>
<thead>
<tr>
<th>Property</th>
<th>Sand textural class</th>
<th>Silt textural class</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean</td>
<td>CV (%)</td>
</tr>
<tr>
<td>Organic matter (%)</td>
<td>3.3</td>
<td>12%</td>
</tr>
<tr>
<td></td>
<td>((n = 15))</td>
<td>((n = 23))</td>
</tr>
<tr>
<td>Sat. hydraulic conduct., mm d⁻¹</td>
<td>1200</td>
<td>62%</td>
</tr>
<tr>
<td></td>
<td>((n = 97))</td>
<td>((n = 117))</td>
</tr>
<tr>
<td>Bulk density, g cm⁻³</td>
<td>1.06</td>
<td>11%</td>
</tr>
<tr>
<td></td>
<td>((n = 47))</td>
<td>((n = 47))</td>
</tr>
<tr>
<td>Field capacity, kPa</td>
<td>−10.6</td>
<td>24%</td>
</tr>
<tr>
<td></td>
<td>((n = 20))</td>
<td>((n = 20))</td>
</tr>
</tbody>
</table>

† In practice, we did not assume a normal distribution for these parameters. The Monte Carlo simulation used values from cumulative distribution functions derived directly from the field data.
equation–based versions of this model have been found to yield reasonably close results, yet the capacity-based version ran approximately 10 times faster than the Richards equation version.

All of our scenarios used 3 yr of daily weather records (1987–1989) from the University of Rhode Island Weather Station in Kingston, RI, located 12 km from the study area. We calibrated selected N transformation rate constants (mineralization, nitrification, denitrification, and urea hydrolysis rate) used by the model with field monitoring data on NO₃-N leaching that were obtained from replicated silage corn and turf plots located in Kingston, RI. Constants relating to the partitioning of C were taken from Hansen et al. (1991). We assumed a microbial biomass and humus C:N ratio of 10, representing the center of the range reported in the literature (e.g., Van Veen et al., 1984). The NO₃-N leaching data used to calibrate the rate constants were obtained from 22 suction plate lysimeters (28 cm diam.) distributed among several corn and turf treatments that were sampled during every leaching event in 1987 and 1988 (Gold et al., 1990). During the 3 yr of simulation the capacity-based LEACHA and the Richards equation-based version of LEACHW models generated almost identical estimated annual recharge from the rootzone of a silt loam under corn, 67 and 70 cm yr⁻¹, respectively.

To model the spatial variability of NO₃-N leaching to groundwater, we incorporated an Inverse Monte Carlo (IMC) algorithm (Ross, 1990) into the LEACHA/N model. The IMC algorithm was run 100 times for each land stratum. For each soil stratum and fertilizer regime, it randomly selected model input values from the appropriate CDFs of fertilizer application rate, saturated hydraulic conductivity, organic matter, bulk density, and the soil–water potential at field capacity. The model then calculated unsaturated soil hydraulic properties from pedotransfer functions. For all simulations we used a soil water potential of −200 kPa as the division between mobile and immobile water (Addiscott, 1977). To use IMC we inverted the function in Eq. [2] giving the expression:

\[ x_i = b \left( \frac{-\log(1 - P(x_i < X))}{a} \right) \]

where
- \( x_i \) is the random selection of an intrinsic or extrinsic property
- \( X \) = the value of the (100*P)th percentile
- \( P(x_i < X) \) = a random number between 0 and 1
- \( a, b \) = parameters describing the CDF of the property within a soil stratum

For each land stratum the Monte Carlo simulations generated annual CDFs of NO₃-N flux (g m⁻² yr⁻¹), water flux (mm yr⁻¹) and flow weighted annual mean NO₃-N leaching concentrations (g m⁻³) from the root zone (Fig. 3A).

Because our goal was to portray the variability of the NO₃-N concentration at the well, i.e., the variability of the regional mean of NO₃-N leaching at a support scale equal to the entire recharge area, we had to modify the variability that existed at a point scale. As explained by Webster (1993), in classical statistics the variance of a regional or global mean \( s^2(B) \) differs from the variance of the sample mean, \( s^2 \). The variance of the sample (or point samples) mean is computed...
Soil Property CDF

for Soil 1

Leaching CDF for
Land Stratum 1,J

LEACHA/N
with Monte Carlo
selection of soil
and management
parameters

100 simulations per
land stratum

CDFs for Land Management J

Fig. 3. Use of Monte Carlo simulation and the LEACHA/N model to generate estimates of leaching CDFs at the (A) land stratum support scale and at the (B) recharge area support scale. The CDF at the recharge support scale (B), represents a CDF of well water quality, and was obtained from 100 weighted means computed with Eq. [6]. The following abbreviations are used in (A): OM, organic matter; p, bulk density; K, saturated conductivity; FC, field capacity.

by the well-recognized equation:

$$s^2 = \frac{\sum_{i=1}^{n} (x_i - m)^2}{N - 1}$$  \[4\]

where

- $x_i$ = the value of each individual point sample
- $N$ = the total number of point samples
- $m$ = the mean of the point samples

In contrast, the variance of the regional (or global mean) is:

$$s^2 (B) = \frac{s^2}{N}$$  \[5\]

The variance of the regional mean, which in our case is the variance of our well water quality predictions, is the quotient of the overall point sample variance, divided by the total number of observations. Therefore, regional variance can drop dramatically in response to sampling intensity.

In our study we used a stratified sampling scheme and did not assume normal distributions of our land strata CDFs, so that the approach outlined in Eq. [4] and [5] needed modification to obtain the CDF of NO$_3$-N concentration at the well. We again used a Monte Carlo approach to create a series of weighted regional means, i.e., means at the recharge area support scale (Fig. 3B). Each estimate of the mean was intended to represent the aggregated effects of the entire recharge area on the water quality at the well. Each mean resulted from a predetermined number of samples generated randomly from each land stratum NO$_3$-N leaching CDF. Essentially, we used our Monte Carlo technique to mimic field sampling. A single estimate of the regional mean concentration at the recharge area support scale is given by

$$<x> = \frac{\sum_{i=1}^{M} \sum_{j=1}^{N} A_{ij} R_{ij} x_{ij}}{\sum_{j=1}^{M} \sum_{i=1}^{N} A_{ij} R_{ij}}$$  \[6\]

where

- $<x>$ = the regional mean NO$_3$-N concentration at the recharge area support scale
- $j$ = the land stratum
The Monte Carlo simulation was performed with inputs from the six land strata, representing three land uses and two soil types. To illustrate the importance of sampling intensity on the variance of a regional mean we generated two different CDFs. In the first case we generated 100 regional means based on 15 samples per land stratum. Thus, each regional mean combined 180 values. This simulation intensity approximated the sampling intensity for field measurements of saturated hydraulic conductivity within each soil textural class. For comparison, we also generated a CDF of 100 regional means based on 100 samples per land stratum. In this scenario each regional mean combined 1200 values.

In addition to computation of CDFs of the mean NO₃-N concentrations at the well, we also generated a CDF of NO₃-N leaching from the entire recharge area that was computed at the point scale. In this case, we used our Monte Carlo technique to sample each land stratum in the recharge area in proportion to its relative area. We performed a total of 1000 point simulations over the entire recharge area.

RESULTS AND DISCUSSION

At the outset of our study, we chose to exclude the effects of temporal variability in weather patterns from our estimates of NO₃-N variation at the well. Water extracted from a large production well is expected to be the aggregation of recharge that originated over a wide time period, and therefore dampens the effects of short-term weather patterns. Water derived from locations adjacent to the well usually originates from relatively recent leaching events (i.e., within the same season), while water derived from the borders of the recharge zone could have originated from recharge events that occurred more than 10 yr earlier.

Our study focused on the effects of the variability of intrinsic factors and fertilizer applications on the variation of NO₃-N leaching from the rootzone. Our stratified sampling and Monte Carlo simulations produced CDFs for a variety of land use practices and soil types in the recharge zone. The land strata CDFs directly reflect the scale of our sampling scheme. As displayed in Fig. 4 and 5, the level of aggregation or support scale selected for analysis alters the variability of estimates of NO₃-N leaching in the recharge area. At the strata support scale (Fig. 4), the interquartile range of NO₃-N leaching varied from a high of 47.9 mg L⁻¹ for conventionally managed silage corn over sand to a low of 1.5 mg L⁻¹ for turf over sand. In Fig. 5a, we conceptualized the entire recharge zone at a point support-scale and generated a CDF of NO₃-N leaching. This point support-scale CDF was based on individual estimates from a large number of small areas, each located within a specified land use–soil type stratum. In this case the distribution of the NO₃-N leaching concentrations expected from these points had a relatively wide range of values, with an interquartile range of 14.2 mg L⁻¹. This type of analysis can show the proportion of the recharge area that is contributing leaching concentrations above an acceptable threshold concentration. However, it does not specifically identify the location of those hot spots, nor does it reflect the water quality at the well.

Although estimates of the variance of large support areas are expected to have lower variance than estimates associated with smaller support areas, there is not an
exact method for predicting the level of variance reduction (Isaaks and Srivastava, 1989). Although the number of observations obtained with field sampling is constrained by time and resources, with a Monte Carlo simulation huge numbers of observations can be simulated. The effects of these artificially large sample numbers is to dampen the variance of the regional mean compared with the variance associated with sampling intensity that generated the data. For example, we compared CDFs of the NO$_3$-N leaching concentrations expected at the well using 15 vs. 100 simulated observations per land stratum (Fig. 5b). In each case we generated a series of 100 recharge scale estimates of the regional mean (i.e., concentration at the well). The interquartile range of the CDFs decreased from 3.3 mg L$^{-1}$ with 15 simulated sampling observations per land stratum to 1.2 mg L$^{-1}$ when 100 simulated observations per stratum were used. As expected, in both instances, the interquartile range is smaller than the range obtained from our analysis at a point support scale and was lower than the interquartile range of several of the land strata. We recognize that the variance of the large support area should be linked to the actual sampling intensity per stratum that generated the strata based data. Thus, we believe that the CDF representing 15 simulated observations per land stratum more honestly represents the range of variability in well water quality associated with our study.

Our prediction of expected mean NO$_3$-N concentrations at the well has a relatively low variability, suggesting that we can predict the effects of land use on well water quality with a high level of certainty. However, our analysis ignored a number of other sources of spatial and temporal variability. We did not include intrinsic sources of variability such as spatial patchiness in microbial denitrification rates (Parkin, 1987; Christensen et al., 1990). Perhaps the greatest sources of variability left out of this analysis are the effects of changing land use patterns within a recharge area. Our analysis assumes that the well water quality reflects a relatively constant mix of land uses over long periods of time. In reality, land use patterns and rotations are often changed, and the recharge water reaching a well represents a history of different land-use patterns and NO$_3$-N leaching rather than a steady state condition. For this reason, these recharge models need to be viewed as functional models suitable for evaluating various planning and management options.

Regardless of the dampening effect on variability that occurs when recharge area support scale analyses are undertaken, we believe that there is considerable worth in computing variability of NO$_3$-N leaching from the land strata of a recharge area. The CDFs developed at a strata support-scale from the various combinations (strata) of land use and soil type (Fig. 4a-c), are useful for determining the land strata that generate higher probabilities for exceeding threshold leaching concentrations. These CDFs could be of value for targeting best management practices toward selected strata within a recharge area. For example, our results predicted an 80% probability of exceeding the NO$_3$-N drinking water standard for the conventionally managed silage corn over sand (Fig. 4a) vs. a 36% exceedence probability if best management practices are used to produce the same crop on the same soil (Fig. 4b).

The modeling was sensitive to differences in soil strata and generated different CDFs for the same cropping practice. For example, the results of the Monte Carlo simulations for silage corn managed for water quality generated median NO$_3$-N leaching estimates of 4.9 and 5.8 mg L$^{-1}$ and interquartile ranges of 5.4 and 9.6 mg L$^{-1}$ for the silt vs. the sand. This finding may be important for land use planners who attempt to find optimal land use mixes that allow a finite margin of safety.

Our analysis suggests that predictions of water quality for large wells with a steady state land use cover generate considerably less uncertainty than estimates at the point support scale. Even for a relatively low number of samples from each land stratum, the reduction in interquartile range associated with the increase in support scale is quite large, so that relatively precise estimates of mean well water quality may be obtained. GIS coverages generated at scales available to resource managers (i.e., 1:12 000–1:24 000 scale) may be well-suited for estimat-
ing water quality of large production scale wells that are influenced only by nonpoint sources of NO₃-N leaching. However, if NO₃ leaching occurs from nonlinear processes, estimating model parameters using the mean values stored in GIS data bases could still result in erroneous conclusions (Addiscott, 1993).

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