Metamodels and Nonpoint Pollution Policy in Agriculture

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Abstract

Informed debate on agricultural nonpoint pollution requires evaluation of regional water quality in relation to management practices. It is prohibitive, in terms of cost and time, to run the site-specific process models for regional policy analysis. Therefore, a simplified and robust technique—metamodeling—is suggested to evaluate regional water quality. Data from an experimentally designed simulation of complex surface water and groundwater process models, PRZM and STREAM, are used to develop statistically validated metamodels. The estimated metamodels were integrated with a regional agricultural economic decision making model to evaluate the surface water and groundwater loadings of 16 major corn and sorghum herbicides. Spatial probability distributions are derived for herbicide concentrations exceeding the toxicity-weighted benchmark from the EPA. We estimate that 1.2 percent of the regional soils will lead to groundwater detection of atrazine exceeding 0.12 μg/L, which compares well with the findings of the EPA's groundwater monitoring survey. We find no-till practices to significantly reduce the surface water concentration of atrazine and other herbicides with less impact on groundwater contamination suggesting indirect gains to soil conservation policies. But we also note that an atrazine ban could lead to increased soil erosion, even with the conservation compliance provisions fully incorporated.

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1. Introduction

Control of nonpoint pollution from agricultural practices and source reduction of agricultural pollutants for water quality protection are increasingly debated policy goals. These debates must be based on informed evaluations of groundwater leaching and surface runoff of agricultural chemicals from soils in relation to policies under consideration, agri-management practices, and hydro-geological factors. Although complex simulation models have been used by government and industry to evaluate fate and transport of chemicals, such evaluations are economical and practical for site- and target-specific problems only. Use of these simulation models for regional analysis, however, is time consuming and generally prohibitive. Therefore, a simplified tool to assess regional nonpoint pollution is useful and necessary, especially given declining natural resource research budgets and time constraints (Day and Ruttan 1991). Metamodels and response surface methods offer a natural option.

Metamodeling is a statistical method used to abstract away from unneeded detail for regional analysis by approximating outcomes of a complex simulation model through statistically validated parametric forms. The simplification provided by metamodels allows us to evaluate the consequences of alternative regional or site-specific policies without the need for additional simulations. If the complex simulation model is a tool to approximate the underlying real-life system, the analytic metamodel attempts to approximate and aid in the interpretation of the simulation model and ultimately the real-life system. Blanning (1975) and Kleijnen (1979) recommend analytic metamodels for simulation experiments; Lawless et al. (1971) propose their use for sensitivity analysis. Empirical application of metamodels in industrial, computer, and management fields is documented in Kleijnen

(1987). To our knowledge, use of metamodels in agri-ecological systems simulation and, particularly, the simulation of real processes describing the fate and transport of agricultural chemicals, is fairly new (see Bouzaher 1991).

This paper discusses metamodeling in an agri-ecological economic system with specific reference to evaluating nonpoint pollution from agricultural chemicals. Our focus is to identify, estimate, and validate regression metamodels of multimedia simulation responses—surface water and groundwater concentrations. We generated these concentrations from process model simulations calibrated on a sample of soils in a study area comprising the Corn Belt and Lake States in the United States. We find simple nonlinear exponential functions to adequately explain and predict the simulation model responses. We validated the estimated metamodels using standard validation tests and procedures. We used the estimated metamodels to predict the surface water and groundwater chemical concentrations by interpolating to the population of soils in each county in the study area for the baseline regime of herbicide application. The baseline is determined by the agricultural decision model (RAMS—see Bouzaher et al. 1990) in the Comprehensive Environmental Economic Policy Evaluation System (CEEPES).[1] We compared our estimate for the spatial distribution of groundwater concentration of atrazine with that of the EPA's actual groundwater monitoring survey of community water systems and rural domestic wells (EPA 1990). Our estimate of 1.2 percent of the soils in the region contributing to an atrazine detection level exceeding the survey's minimum reporting limit of 0.12 μg/L (ppb) is bounded by the monitoring estimate of 0.7 percent in rural wells and 1.7 percent in community water systems.

We derived cumulative spatial probability distributions for surface water and groundwater concentrations of atrazine under conventional- and no-till practices. Some of our results are:

1. The probability of exceeding the toxicity-weighted benchmark for human exposure from atrazine, as suggested by the EPA, is relatively larger for surface runoff than groundwater. For instance, the probability of exceedance for atrazine was as high as 50 percent in surface water compared with less than 1 percent in groundwater.

2. No-till agricultural practices significantly reduce the surface-water loadings of atrazine and other herbicides relative to conventional tillage. For instance, the concentration of atrazine dropped from about 144 ppb under conventional tillage to about 18 ppb under no-till.

We also examined the implications of an atrazine ban[2] on soil erosion and loadings of substitute herbicides. We find that this policy will lead to more soil erosion, even with the conservation compliance provisions fully incorporated.

2. Metamodeling in an Agri-Ecological Economic System

Major advances in computer technology have made it possible to develop and simulate complex real processes using mathematical models. A variety of mathematical models are available to simulate pesticide movement in the saturated and unsaturated soil zones. See Wagenet and Hutson (1991) for a description and review of pesticide transport and transformation modeling systems. Although simulation models are analogs of real processes, their direct application to analysis of regional nonpoint pollution policy is limited by the expense and time required to conduct additional simulations for each new policy scenario. A policy scenario with an integrated system of models requires a mutually consistent combination of policy, environmental, agri-chemical, management, and technological parameters and behavioral equations. Therefore, it is impractical to simulate each and every possible combination of these factors, especially in a system requiring both timely integration of diverse process models and integration of outcomes over a distribution of diverse input sets. A simplified tool will ease the computational burden while capturing the key process characteristics. Statistically validated metamodels are analytical tools capable of addressing both of these difficulties.

A metamodel is a regression model explaining the input-output relationship of the complex simulation model, which is a computer model structure to mimic the underlying

real-life process. Let g be the unknown function which characterizes the underlying real phenomena relating the response y to the input vector v:

$$y = g(v) \tag{1}$$

Most simulation models mimic outcomes for a variety of possible response variables, and specification of the response of interest may not be a trivial matter.

A simulation experiment is a set of executions of the simulation model intended to approximate the values of y associated with a specified set of input vectors. The output of a simulation experiment is a dataset consisting of specified input vectors and their associated responses, as determined by the simulation model. Choice of the number and values of input vectors for which the simulation model will be executed is the subject of experimental design. For statistical purposes, it would be preferable to experiment with the real life system rather than a simulation model of the system. In that case we would have a statistical model of the system rather than a metamodel. This approach is not adopted because it would mean incurring the cost and delay of waiting, in this case for 30 years of weather to present itself to the real life system. It would also mean tolerating the real environmental damage associated with some experimental input vectors.

Given the output of a simulation experiment, we can specify an analytic metamodel with relatively few inputs, x_1 through x_k. Let the metamodel explaining the simulated outcome be represented as:

$$y = f(x_1, x_2, \ldots, x_k, u), \tag{2}$$

where u is the stochastic disturbance term. We can use standard statistical and econometric procedures to identify and estimate the function f describing the metamodel. Because of their simple and precise representation of the complex system, simulation practitioners are favoring metamodels for purposes such as validation, sensitivity analysis, estimation of

interactions among inputs, control, and optimization, without the need for additional simulation runs (Kleijnen 1987).

The multimedia system we use was configured to simulate the fate and transport of herbicides in the major corn and sorghum growing regions of the United States. This regional application is part of an overall CEEPES configuration to evaluate the set of herbicide strategies applicable to corn and sorghum production. Figure 1 illustrates that the core of the multimedia fate and transport component is the Risk of Unsaturated/ Saturated Transport and Transformation of Chemical Concentrations (RUSTIC) system developed by Dean et al. (1989). RUSTIC links the Vadose Zone Flow and Transport (VADOFT) model with the Pesticide Root Zone Model (PRZM) to trace the pesticide movement in the saturated and unsaturated zones. These two models can also be linked to an aquifer model called Saturated Zone Flow and Transport Model (SAFTMOD) in RUSTIC. PRZM is a one-dimensional, dynamic, compartmental model that can simulate chemical movement in the unsaturated root zone. Chemical, soil, and plant characteristics, tillage and management practices, and local hydro-meteorological conditions are this model's major parameters. VADOFT performs one-dimensional transient or steady-state simulations of water flow and solute transport in the saturated zone. See Dean et al. (1989) for a detailed description of these models.

Soil parameters for PRZM and VADOFT were automatically generated with the Data Base Analyzer and Estimator (DBAPE) soil database (Imhoff et al. 1990). Given RUSTIC runoff loadings, the Surface Transport and Agricultural Runoff of Pesticides for Exposure Assessment (STREAM) model (Donigian et al. 1986) is used to simulate surface water concentrations. Because they are edge-of-field loadings, STREAM estimates are considered to be accurate within an order of magnitude and typically overestimate actual concentrations (Donigian et al. 1992). The basic RUSTIC and STREAM configurations for

this simulation experiment are described in Gassman et al. (1991). Note that direct linkage of RUSTIC and STREAM could not have been accomplished without metamodels.

3. Experimental Design and Procedure

Soils selected for the RUSTIC simulations were chosen from a total of 2076 P1 (prime agricultural land) and P4 (irrigated agricultural land) soils. A stratified, self-weighted random sample of soils was drawn where soils were randomly chosen within each stratum with sampling probability proportional to the percentage used. The soil selection was also based on ability to support corn and sorghum. In all, 180 soils from 16 states (strata) were chosen for the RUSTIC simulations. Sixteen herbicides used in corn and sorghum production were selected. Assuming that chemical use is independent of soil type, each of the 16 chemicals was applied to the 180 soils. The simulations were performed separately for conventional-, reduced-, and no-till cultivation practices. Herbicide application timings were simulated for early preplant, preplant incorporated, preemerge, and postemerge.

Many groundwater studies have indicated a relationship between well depth and pesticide loadings. The groundwater table up to 15 meters below the soil surface is the most vulnerable to chemical contamination (Detroy et al. 1988). Therefore, the pesticide concentrations in the solute phase were estimated for 1.2 and 15 meters for each RUSTIC simulation.[3] The simulation was performed dynamically for each day over a 30-year period. Weather data (real 1950-79 data) were used for one weather station in each state from the RUSTIC weather database (Imhoff et al. 1990). A total of 7518 simulation runs were performed and the average (chronic) groundwater concentrations at 1.2 and 15 meters were recorded for each. The runoff loadings from these ysimulations were used as STREAM input to estimate the peak (acute) surface water concentration of herbicides.

4. Regression Metamodeling

In the metamodeling literature the most commonly used models are the general linear and nonlinear ones often referred to as "regression metamodels." A regression metamodel based on simulated data in place of real-life observations will have "better information" for the econometric analysis because of the controls imparted by the experimental design and simulation. In this section, we present the results of a rigorous search to identify a regression model that best explains the data from the complex process models.

4.1 The Data

Multimedia responses from 7518 simulation runs comprise the sample data for the dependent variables in the regression metamodels. Table 1 presents the descriptive statistics, moments, and distributional characteristics of the simulation responses. Preliminary analysis of the data showed large variability in concentrations from one soil to another, which highlights the need for a spatial dimension, and from one management practice to another within a soil. In 90 percent of the observations, herbicide concentrations in groundwater were less than 1 ppb. Twenty percent of the concentrations at 1.2 meters and nearly 50 percent the concentrations at 15 meters were zero. The distributions, in general, were nonnormal and positively skewed (to the right). The sample mean of surface water concentrations was 242 ppb with a standard deviation of 269. The data for the regressors were mostly represented by the simulation inputs. Soil characteristics—organic matter, water retention capacity, bulk density, sand and clay proportions, and soil depth—were obtained from DBAPE, and pesticide characteristics—decay rate, Henry's law constant, and soil sorption coefficient (K_{oc})—were obtained from Wauchop and Goss (1990). See Carsel and Jones (1990) for a description of these databases and their applicability to regional studies.

4.2 The Models

We first fitted a simple linear model using an ordinary least squares (OLS) procedure. Let Y be an n x 1 vector of observations of the simulated response, X be a known, full-rank n x p matrix of observations on the explanatory variables, and ß be a p x 1 vector of unknown, fixed parameters. The simple linear regression model is

$$Y = X\beta + u, \quad E(u_i) = 0, \; E(u_i)^2 = \sigma_i^2, \text{ and } \operatorname{cov}(u_i, u_j) = 0. \tag{3}$$

Given that the response variable is nonnormal with heterogenous (nonconstant) variance, the parameter vector $\hat{\beta} = (X^T X)^{-1} X^T Y$ and the corresponding predictions $\hat{Y} = X\hat{\beta}$ are inefficient (in the minimum variance sense). We examined the studentized residual[4] plots for any patterns indicating heterogeneity of variance. These plots for the linear model (3) exhibited a clear wedge-shaped pattern, violating the classical assumption of homogeneity of variance. Therefore, we used a standard variance-stabilizing transformation on the data, and fitted the linear model in the transformed space. A variance-stabilizing transformation for y_i (i^{th} element of Y) can be found by either using the general form for a power transformation, y_i^{λ}, proposed by Box and Cox (1964),[5] or by using a procedure similar to the one proposed by Lin and Vonesh (1989). The latter consists of estimating the power coefficient λ by fitting an OLS model to each element in the sequence $\{Y^{\lambda}; \lambda = \frac{1}{2}, \frac{1}{4}, \ldots, \}$, and examining the residuals from the regression. We restricted λ to be less than one because the original data had a wide range (i.e. $Y_{min} / Y_{max} \approx 0$) and their variance increased with the magnitude of the observation. Transformations with $\lambda < 1$, called contracting transformations, reduce the gap between the smallest and the largest observation, thus making the data more homogenous. Estimated regression for the transformed data should have an error structure that is normally distributed with constant variance.

The optimum λ obtained for the groundwater data was ⅛ and for the surface water data was zero implying a logarithmic transformation.[6] Using the optimum power transformation we estimated the linear model (3) for the transformed data. The regression with the transformed data gave a higher R-square and well-behaved residuals compared to the regression with the untransformed data. But the predictions from the regression model for the transformed data were poor, with only 54 percent correlation between the actual and the predicted data, and the standard errors of individual and mean predictions were very large. Also, in the groundwater model 25 percent of the predictions were negative because the actual groundwater concentrations were close to zero (75 percent of the observations were less than 0.1).

Due to the poor predictability of the regression model for the transformed data, we tried a class of generalized least squares models, namely, the weighted least squares (WLS) model using appropriately derived weights. Given the variance-stabilizing transformation Y^{λ}, we can use Bartlett's (1947) procedure to relate the variance of the response variable in the original and transformed spaces and get an approximate weight w_i for WLS analysis. Suppose the variances in the original and transformed spaces are related as,

$$\mathrm{Var}(Y) \approx \mathrm{Var}(^{\lambda})\,[dY/dY^{\lambda}]^2\,\big|_{X\beta} = \sigma^2\,(X\beta)^{2(1-\lambda)}, \quad \because \mathrm{Var}(Y^{\lambda}) = \sigma^2 I \tag{4}$$

where I is the identity matrix. Since $\mathrm{Var}(y_i) = k_i\sigma^2$ is assumed, we have $k_i \approx (X\beta)^{2(1-\lambda)}$. Therefore, the weight $w_i = 1/\sqrt{k_i}$ is equal to $(X\beta)^{\lambda-1}$ such that the variance of the weighted observation $(w_i y_i)$ is finite and constant. Using the weights w_i we fitted a WLS model to the data, resulting in a best linear unbiased estimator $\hat{\beta} = (X^T W X)^{-1} X^T W Y$. Intuitively, in WLS analysis, responses with a high standard error are assigned a lower weight. While residual diagnostics were greatly improved by using WLS, predictions were still poor, with only 50 percent correlation between the actual and predicted data. The failure of these

linear models to adequately predict the response variable naturally led us to fit a nonlinear model using nonlinear least squares (NLS).

Sometimes, variance heterogeneity may be introduced by specifying a linear model where the actual underlying structure is a nonlinear one. Such instances are common in models for chemical, biological, and kinetic processes (Box and Hill 1974). Therefore, we fitted a nonlinear model of the form

$$z_i = f(x_i;\theta) + \epsilon_i, \qquad E(\epsilon_i) = 0,\ E(\epsilon_i)^2 = \sigma^2,\ \text{and } \operatorname{cov}(\epsilon_i,\epsilon_j) = 0, \tag{5}$$

where f is the nonlinear expectation function, ϵ is the random disturbance term and θ is the unknown parameter vector to be estimated. A desirable estimate of $\hat{\theta}$, denoted by , has optimal large sample properties; i.e., $\hat{\theta}$ is asymptotically normally distributed with mean θ, and variance $\sigma^2[\Sigma(\partial f(x_i;\theta)/\partial\theta)(\partial f(x_i;\theta)/\partial\theta)^T]^{-1}$. Because our objective is to find a model with theoretical as well as empirical justification and better predictive ability we chose the simple exponential model

$$f(x_i;\ \theta) = \exp(X\theta), \tag{6}$$

and used SAS's Gauss-Newton algorithm to solve for the optimal parameter vector. The exponential model is a satisfactory representation for several reasons: (1) the optimal power transformation parameter λ^* was small for both surface water and groundwater; (2) the original (untransformed) data have a positively skewed distribution; and (3) other studies that evaluated the groundwater pollution potential of pesticides (Jury et al. 1987 and Khan and Liang 1989) used an exponential model.

5. The Results

Table 2 summarizes the results from the nonlinear fit and gives the parameter estimates of the nonlinear model for (transformed) average groundwater concentration at 1.2 and 15 meters and peak concentration in surface runoff. We relied mainly on theory in

identifying a parsimonious specification. Care was taken to avoid significant multicollinearity among the regressors. Collinearity between linear and quadratic regressors was reduced by centering the variables.[7] The adjusted R^2 was more than 80 percent in all three fitted equations. The correlations between the actual and the predicted concentrations in surface water and groundwater were roughly between 70 and 95 percent. Figure 2 shows the distribution of actual and predicted concentrations for both surface water and groundwater.

The coefficients of the continuous regressors (other than the 0,1 type dummy variables) were all different from zero at the 5 percent level of significance and their signs were consistent with theory. The interaction term between bulk density and sorption coefficient (BD * K_{oc}), generally referred to as the retardation factor (Khan and Liang 1989), is expected to have a negative impact on chemical concentration. The estimated coefficient of this regressor (BD * K_{oc}) is negative and significant. The estimated coefficient for decay is significant with a negative sign for groundwater and a positive sign for surface water because fast decay implies less leaching and more runoff potential. The higher the sand percentage the greater the seepage, implying positive impact on groundwater, which is what our results show.

Qualitative variables were represented in the nonlinear model by 0-1 dummy variables. The dummy variables for tillage practice were all different from zero at the 5 percent level of significance. These coefficients measure the difference in leaching/ runoff potential of reduced- and no-till practices relative to conventional tillage. Intuitively, no-till, which causes less soil erosion, should allow more leaching and hence less runoff than conventional till. The coefficient on no-till, which shows a positive impact on groundwater and a negative impact on surface water, clearly support the theory. The estimated equation also captures the differences between hydrologic groups and timing of application through 0,1 regressors. Fifteen dummy variables were included to

represent the 16 different weather stations in the simulation of the study area. Most of these coefficients were significantly different from zero, highlighting the importance of climate in determining chemical concentration levels. A dummy variable was included to capture the difference in the leaching/runoff potential of sorghum. This coefficient was significant with a positive sign for groundwater, implying that herbicide leaching is more severe in sorghum than in corn.

6. Validation

Validating the simulation metamodels is important because they are two steps away from the underlying real processes. We have greater confidence in the empirical metamodels, their estimated parameters, and predictions if they are statistically validated before being integrated into the unified modeling system. The standard validation methods (Snee 1977) include (1) validation of the estimated metamodel with new data; (2) cross-validation (split-half validation) in which the original data set is randomly split into two halves, a model is fit for each half separately, and the fit models are used to predict the other half of the data; and (3) comparison of empirical results with those from other simulations and monitoring surveys. Validation with new data and cross-validation are the two widely accepted methods in the literature (Marquardt and Snee 1975; McCarthy 1976; Berk 1984; Friedman and Friedman 1985). We briefly outline these three methods and present the results from the validation tests.

6.1 Validation with New Data

In the absence of any limitations to obtaining new data the best approach to validate the predictive power of a regression metamodel is to evaluate its ability to predict the new data. Models explaining time-series data can use natural time split to get the validation sample (new data), and those explaining cross-sectional data can use the data on new respondents or sample points as a validation sample. In our case, we utilized the structural

make-up of the data set, namely the hydrologic conditions and management practices, to split the data into original and validation samples. Specifically, we used 3264 observations of conventional tillage, hydrologic groups A, B, and D, and timing of application (EPP, PPI, and POST) as our original sample. The validation data consisted of four different samples representing reduced-till (640 observations), no-till (1218), hydrologic group C (1539), and preemergent application timing (1637).

Table 3 shows the validation results of the estimated metamodel with the new data. The two important validation statistics shown in this table are the mean squared error (MSE) and the R^2. The ratio of original MSE to validation MSE is less than 2 and the validation R^2 is close to the original (model) R^2 for all validation samples, except for the no-till sample in the surface-water model and the hydrologic group C sample in the groundwater model. These results suggest good predictive ability of the estimated metamodels.

The small validation R^2 for the no-till sample (0.22) may be explained by the fact that no-till practice has a strong negative impact on surface water concentrations, suggesting the possibility of a significant difference in the distance between these two samples. Berk (1984) examines this issue of the relationship between the validation error and the distance between the validation sample and the original sample and suggests performing a hypothetical test, the Chow (1960) test, comparing the residual sums of squares from the two submodels with that of the full model. We performed this classical Chow test for the null hypothesis and found that the mean distance between these two samples is not significant. The test gave an F value of 41.6, rejecting the null hypothesis, which explains the low validation R^2. As long as we recognize the structural shift between conventional- and no-till cultivation practices in our empirical metamodel, we can be fully assured of the model's predictive validity.

6.2 Cross-Validation

Validation with new data seems most appealing, but in those instances where obtaining new data is either expensive or impossible, cross-validation offers a natural alternative. Stone (1974) and Snee (1977) provide a good review and discussion of cross-validation and alternative data splitting methods. According to Snee, cross-validation by data splitting is a method to test the in-use prediction accuracy of the model and simulate the complete or partial replication of the study. For purposes of cross-validation or split-half validation, we split the data randomly into two approximately equal halves. The first subset, ss1, was used to estimate the model, while the second subset, ss2, was used to measure the predictive ability of the model, and vice-versa. The cross-validation results, which are shown in Table 4, demonstrate good predictive accuracy of the estimated metamodels. We also compared the sign and magnitude of the estimated coefficients from the two split-half models. In the groundwater metamodel the signs of all the coefficients were the same in both samples, and the estimated coefficients were comparable in their magnitude. In the surface water metamodel, only 2 out of 31 coefficients had unmatching signs. These two coefficients, however, were not significantly different from zero in both models.

6.3 Validation with Monitoring Surveys

This would be the ideal method of validation provided we had adequate monitoring data and the process models are adequately validated. Given the limited information on surface water and groundwater monitoring in a wide geographical area, we elected to perform approximate validation tests with the EPA's groundwater monitoring Survey estimates. Some of these results are shown in Table 5. Atrazine and simazine are the two herbicides that were detected at reasonably high percentage rates in the EPA's survey. The estimates predicted using the metamodels, shown in Table 5, indicate the same trend. The EPA estimates that atrazine is present, at or above 0.12 μg/L (survey minimum

reporting limit), in about 1.7 percent of community water systems and 0.7 percent of rural domestic wells. Our estimation indicates that 1.2 percent of the soils in the region contribute to the groundwater detection limit of atrazine at or above 0.12 μg/L, which is clearly bounded by the EPA's estimates. At a minimum, we can state that the trends from our results are consistent with actual monitoring data.

7. Herbicide Policy Application

Statistically validated metamodels for predicting regional agricultural nonpoint pollution enhance the scope of evaluating alternative agricultural chemical policies. By integrating the metamodels with the agricultural economic decision making model, which allows for substitution between herbicides and between weed control management strategies, chemical and nonchemical, we can evaluate the consequences of water quality policies regulating or restricting the use of herbicides. In this section we briefly discuss the optimization model, the integration of the fate and transport models with the agricultural decision making model, and the results from a herbicide policy of banning atrazine in corn and sorghum production in the study area. Atrazine is the second most commonly detected herbicide in surface water and groundwater, forcing the EPA to reevaluate its ecological-economic tradeoffs. To illustrate the application of metamodels, we present results pertaining to the consequences of an atrazine ban policy on surface water and groundwater loadings.

Assume the agricultural production is represented by a joint production process where the two outputs, crop and pollution, are separable. The agricultural production and the nonpoint pollution process can be represented by the following expressions:

$$q = f(x), \text{ and} \tag{7}$$

$$z = g(\Omega_x, \Phi, \delta). \tag{8}$$

Expression (7) represents farm outputs (q) as a function of inputs (x). The production technology f is assumed to follow the standard regularity conditions, including strict concavity. The damage function g translates the level of polluting inputs and practices employed in the production process into the amount of chemical concentrations in surface water and groundwater (z), via the physical and chemical characteristics (Ω_z) of the polluting inputs, the soil characteristics (Φ), and the meteorologic conditions (δ).

For the empirical analysis we used an optimization model specified for a representative farm defined at the watershed level [producing area (PA)] and the nonpoint damage functions (metamodels). We used the basic agricultural economic decision making model (RAMS) of the integrated CEEPES system. RAMS is a regional, short-run profit-maximizing model that assumes a risk-neutral and competitive producer managing a multioutput-farm firm defined at the producing area level. A major feature of RAMS is that it has a weed control subsector, which defines the weed control and herbicide application activities, and provides the important linkage with the chemical policy space (Bouzaher et al. 1990).

The information on yield loss and cost trade-off from alternative weed control strategies and the relative herbicide substitution is inputted into RAMS through the WISH (weather impact simulation of herbicide) simulator (Bouzaher et al. 1992). A weed control strategy captures both the management and the technological aspects of weed control. A weed contral strategy is made up of a primary herbicide treatment and a secondary herbicide treatment that will be applied only if the primary treatment fails due to weather-related reasons. The choice of alternative weed control strategies determines the rate of substitution between herbicides and also the substitution between chemical and mechanical weed control. The estimated fate and transport metamodels, which are proxies for social damage functions, and the RAMS model were exogenously[8] linked to determine

the concentration of atrazine and other herbicides used in corn and sorghum production under different tillage practices.

Given the baseline estimates of RAMS, we determined the chemical concentrations for the complete distribution of soils in each of the counties in the study area. Figure 3 illustrates the cumulative spatial probability distribution of atrazine under conventional- and no-till practices. Comparing our estimates with the toxicity weighted benchmarks [Maximum Contaminant Level (MCL)] for chronic and acute exposure levels of atrazine in drinking water, 3 ppb and 100 ppb, we estimate that the probability of exceeding the benchmark is higher for surface runoff than for groundwater. The probability that the concentration in surface runoff will exceed the benchmark is reduced from 51 percent under conventional-till to 10 percent under no-till practice. In general, a similar result holds for other herbicides (see Figure 4). Figure 4 shows the differential impacts of tillage on actual herbicide loadings in surface water in the Corn Belt region. As for groundwater, the probability of exceedance is only 0.2 percent, regardless of tillage.

A major implication of these results is that groundwater quality is unimpaired by the conservation compliance policy. This result suggests that implementing of conservation policy will not lead to any unfavorable trade-offs between soil conservation and groundwater quality goals. But this is not the case for the water quality policy of banning atrazine. Our preliminary investigation suggests an increase in soil erosion in the Corn Belt (an increase of 3.6 percent from the baseline) due to shifts in cultivation practices from conservation tillage to conventional tillage (see Table 6). These results are interesting in light of a recent debate on compatibility of conservation and water quality policies. Table 6 shows the changes in the total soil erosion due to the atrazine ban policy relative to the baseline for conventional and conservation tillage in the Corn Belt. Overall, soil erosion increased by 3.6 percent despite the conservation compliance provisions. By relaxing the provisions, we expect a more significant increase in soil erosion.

Another useful set of information generated from this analysis is the area-wide probability that the surface water and groundwater concentrations will exceed the benchmark. Table 7 shows the spatial probability that the herbicide concentration in surface water will exceed the MCL. Atrazine, cynazine, bentazon, and simazine have probabilities of exceedance greater than 25 percent in the baseline. The probabilities of exceedance of all herbicides, except propachlor, are higher when atrazine is banned. Propachlor is a preemergent herbicide mostly used in weed control strategies that includes atrazine, which explains the decrease in surface water concentration of propachlor when atrazine is banned. For groundwater, at a 15-meter depth, only atrazine exceeded the EPA's benchmark with the probability of exceedance equal to less than 1 percent in the baseline.

8. Conclusion

Informed debate on nonpoint pollution policy requires evaluation of surface water and groundwater quality at the regional level in relation to agri-management practices and hydro-geological conditions. It is prohibitive, in terms of cost and time, to run and rerun site-specific process models for regional policy analysis. Therefore, a simplified and robust tool to evaluate regional water quality using data from process model simulation is suggested—metamodels. Metamodeling has enormous potential in integrated agri-ecological economic systems designed for policy evaluation. The estimated metamodels were used to evaluate the concentration of atrazine in surface water and groundwater. Results compare well with a recent EPA groundwater monitoring survey. The overall implication of this study is that the metamodeling strategy can support integrated multimedia policy analysis in an environment of existing policy interventions with agents who respond to policy changes. The present illustration incorporates groundwater and surface water media, models relevant to existing policy interventions such as conservation compliance, and allows agents to respond to policy changes by altering weed control strategies. Without the

method of metamodels, policy analysis would necessarily be less comprehensive, and consequently, less adequate to the difficult but important task at hand.

Endnotes

1. CEEPES is an integrated agri-ecological economic system configured to evaluate the tradeoffs of alternative policies restricting the use of herbicides, particularly atrazine, in corn and sorghum production (Cabe et al. 1991).

2. Atrazine is a widely used herbicide to control many annual broadleaf weeds and certain grasses on cropped and noncropped lands and is also the second most commonly detected herbicide in surface water and groundwater (EPA 1990).

3. Adsorptive properties of the chemicals under study are such that the sediment phase is negligible, and was therefore not simulated.

4. The studentized residuals are the residuals weighted by the respective standard errors, $u_i/s\sqrt{(1-h_{ii})}$, where h_{ii} is the n^{th} diagonal element of the "hat" matrix $\mathbf{H}=\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$.

5. Suppose there exists an unknown power transformation, y_i^λ, such that $\mathrm{Var}(y_i^\lambda) = \sigma^2$, d fine:

$$y_i^\lambda = \begin{cases} (y_i^\lambda - 1) / \lambda & \lambda \neq 0 \\ \ln y_i & \lambda = 0 \end{cases}$$

where we can estimate the optimum λ using maximum likelihood estimation.

6. If $\lambda = 0$, we obtain $(y_i^\lambda - 1)/\lambda = 0/0$, which is indeterminate. We can, however, use L'Hopital's rule to show that in the limit $\lambda \to 0$, $y_i^\lambda = \ln y_i$ (see Johnston 1984, pp. 62-64).

7. This transformation does not change the meaning or fit of the model, but by reducing collinearity it tends to stabilize the sampling variance of the estimates.

8. Using an exogenous social damage function is consistent with the nonpoint pollution theory where the firm has no incentive to internalize the negative externalities (surface water and groundwater pollution).

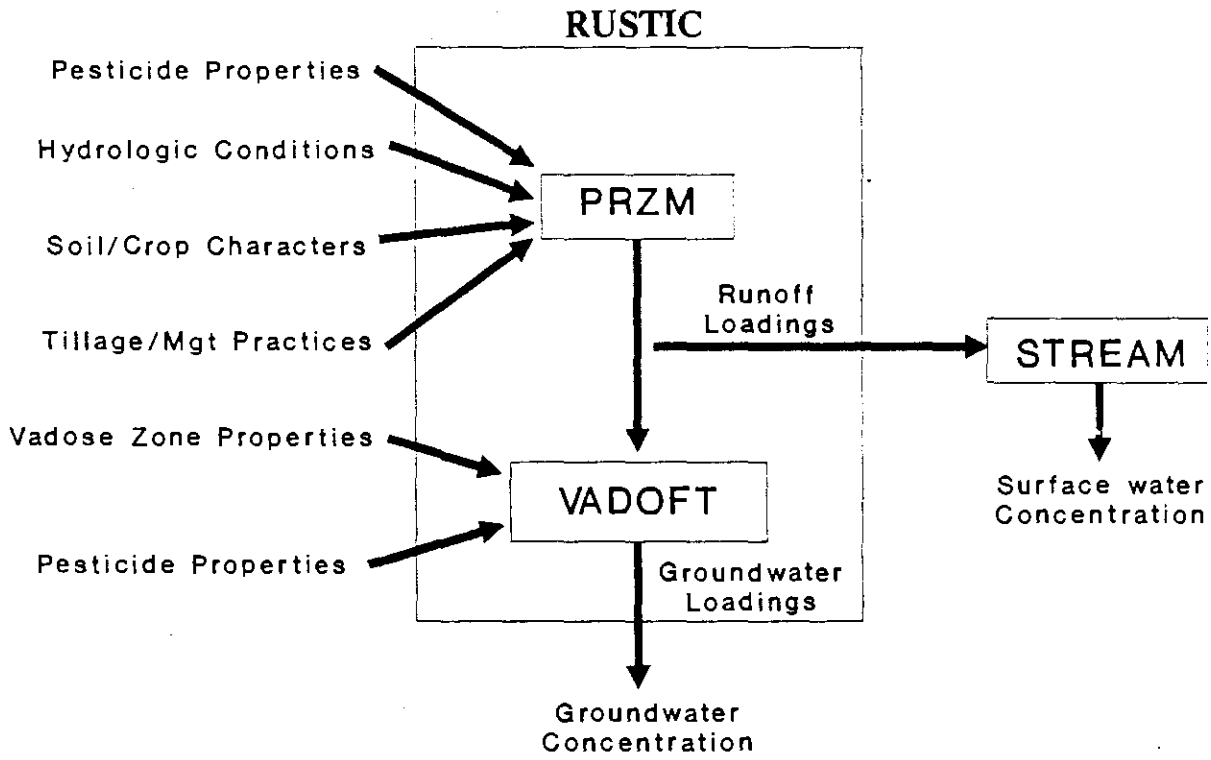
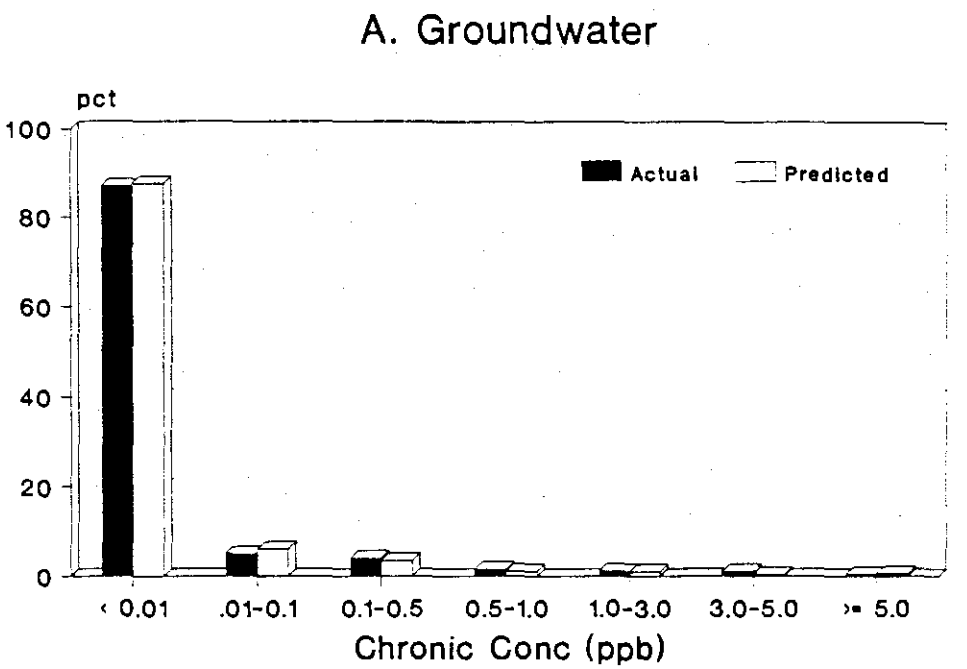


Figure 1. Multimedia Fate and Transport Simulation



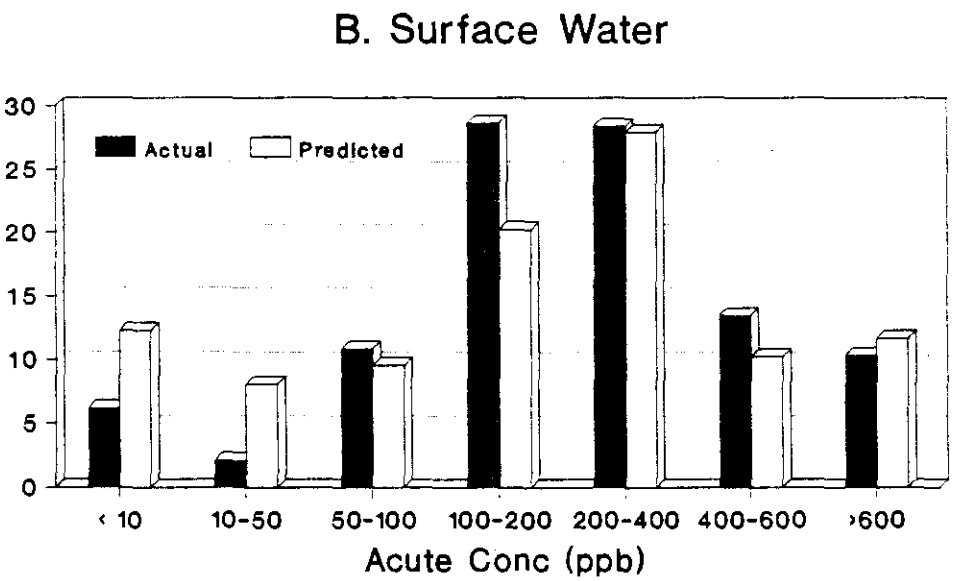
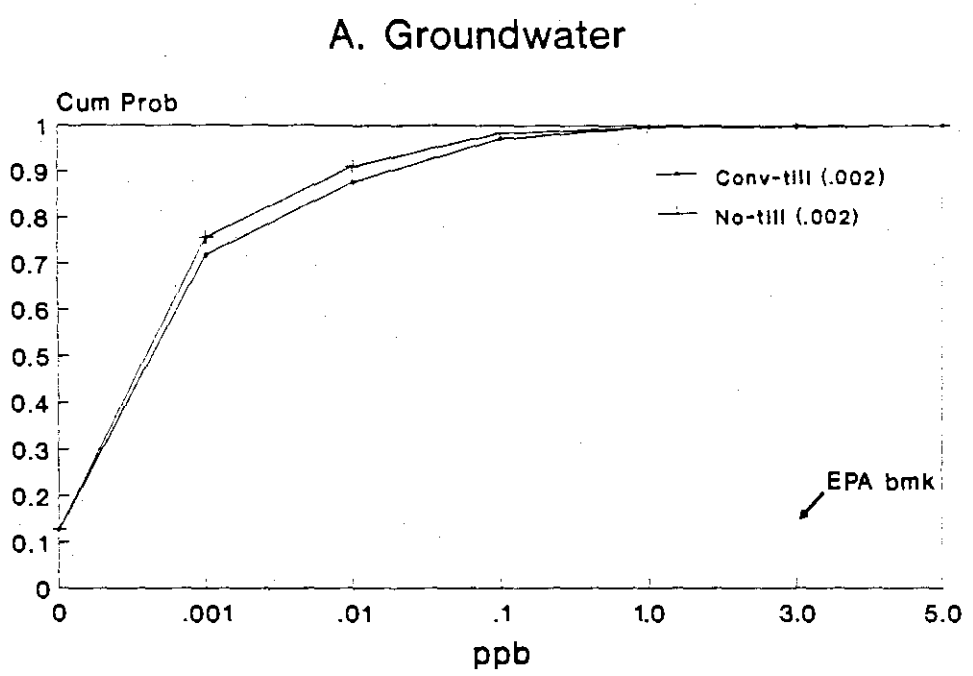


Figure 2. Freq. Distribution of Actual and Predicted Responses for A. Groundwater and B. Surface Water



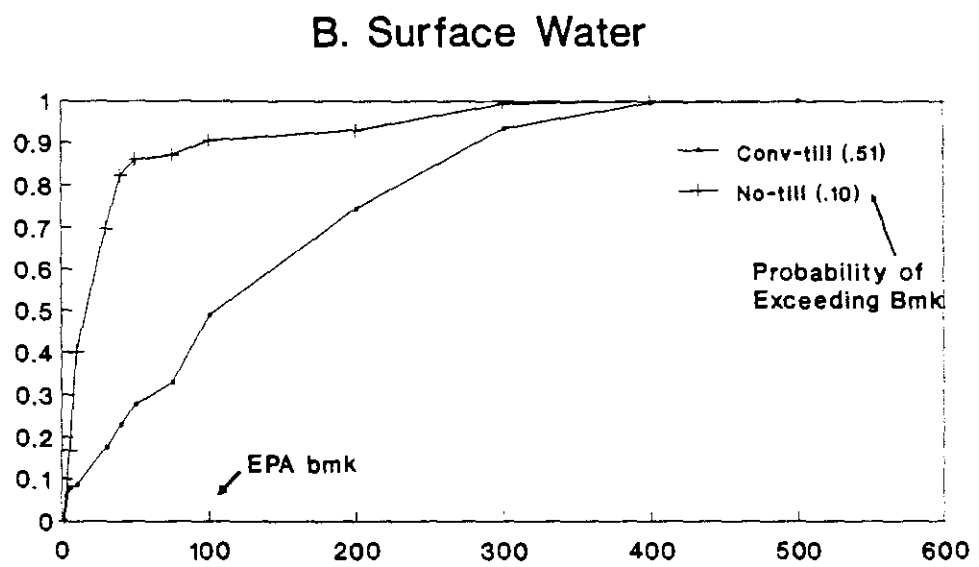


Figure 3. Cum. Probability Distribution of Atrazine Conc. by Tillage for A. Groundwater and B. Surface Water

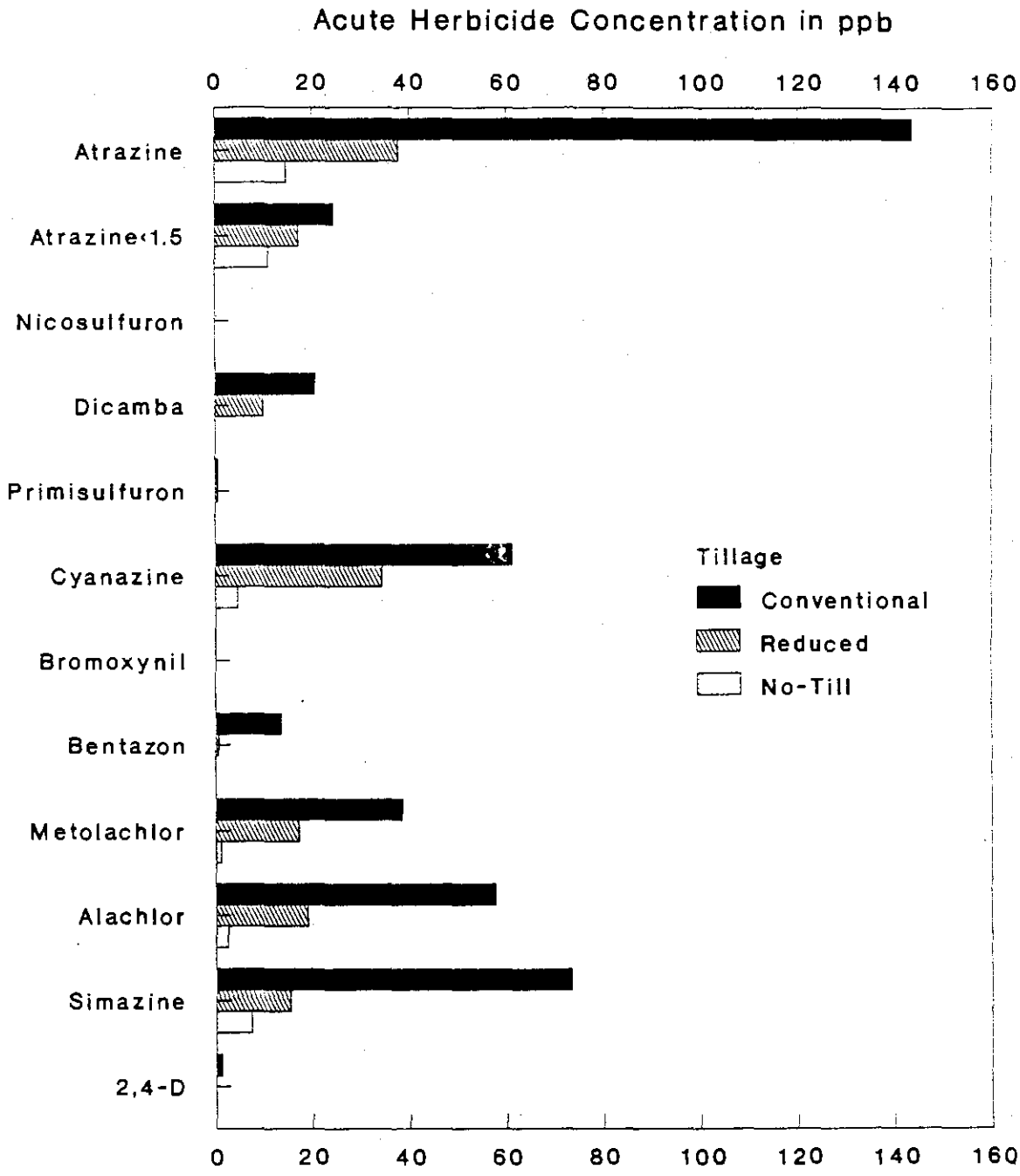


Figure 4. Herbicide Loadings in Surface Water by Tillage

Table 1. Summary Statistics of Simulation Responses

Statistics	Avg 1.2 mts	Avg 15 mts	Peak Stream
Mean (ppb)	3.25	0.087	242
Std Deviation	11.8	0.5	269
Skewness	5.1	8.5	2.9
Range	0-110	0-7.3	2-2114
Percent Zeros	20	48	0

Table 2. Summary of NL Regression Coefficients and Statistics

Dep. Variable	$\sqrt[8]{}$Avg 1.2	$\sqrt[8]{}$Avg 15	Peak Stream
Adj R^2	0.84	0.84	0.83
$\sqrt{}$MSE	0.19	0.11	112
Mean Pred	3.06 [3.25]	0.077 [.087]	225 [242]
ρ(act * Pred)	0.78	0.73	0.91
	NL Regression Coefficients		
Intercept	-0.892	-1.239	7.258
Avg1.2	-	0.374	-
OM*Henry'	123.317	-	-1685.510
BD*K_{oc}	-0.002	-0.001	-0.006
OM*Decay	-8.359	-67.379	-0.859
Decay	-19.051	-20.333	6.484
$(Decay)^2$	142.391	-	-197.149
Org Mat	-1.070	-0.496	-
$(Org\ Mat)^2$	0.222	-	-
Percent Sand	0.003	0.008	-
WRC	0.529	1.458	-
Soil Depth	-0.002	-0.001	-0.0004
D-Sorghum	0.199	0.453	-0.054
D-Red Till	0.071	0.045	-0.005
D-No Till	0.101	0.126	-0.341

Notes: All the coefficients are significant at 5 percent level of CI.
ρ is the correlation coefficent and D indicates a dummy variable.
Figures in [ ] are the actual (sample) means. Sample size, N=7,518.
OM - organic matter, BD - bulk density, and WRC - water retention capacity (available water).

Table 3. Metamodel Validation with New Data

New Data[a] (Validation Sample Size)	Avg 15 meters R^2 .85		Peak Stream R^2 .75	
	MSE^v/MSE^o	R^2	MSE^v/MSE^o	R^2
Reduced Till (640)	1.19	.85	1.12	.75
No Till (1218)	1.75	.79	2.14	.22[b]
Hy.Group C (1539)	2.19	.51	1.91	.75
Preemergent (1637)	0.64	.88	1.49	.81

MSE^v = Validation Mean Squared Error and MSE^o = Original MSE.

[a] Sample size for original model was 3,264, comprising data for corn and sorghum: conv-till, hydrologic groups (A,B,D), and timing of application (EPP, PPI, and Postemergent).

[b] Chow Test (H0: that the mean distance between the conv- and no-till samples is not significant) gave an F value of 41.6, rejecting the null hypothesis at 1 percent CI, which will explain the poor validation R^2.

Table 4. Cross-validation of the Metamodels

Validation Statistics	Avg. 15 meters		Peak Stream	
	ss1 (Pre-ss2)	ss2 (Pre-ss1)	ss1 (Pre-ss2)	ss2 (Pre-ss1)
R Square	.83 (.87)	.85 (.88)	.83 (.82)	.83 (.82)
MSE^v/MSE^o	0.70	0.84	1.02	1.04

ss denotes sub sample (split-half sample). $N_{ss1} = 3,748$ and $N_{ss2} = 3,770$.

Table 5. Metamodel Validation with the Groundwater Monitoring Survey Estimates

Nonpoint Pollutant	% of wells containing NPS pollutants in excess of the survey[a] min reporting limit		Our estimate of spatial-prob. exceeding the min shown in next column	Survey minimum reporting limit
	Rural Wells	CWS[b]		
Atrazine	0.7	1.7	1.2%	0.12 μg/L
Alachlor	<.1	0	0	0.50 μg/L
Bentazon	0.1	0	0	0.25 μg/L
Simazine	0.2	1.1	1.2	0.38 μg/L

[a] National Pesticide Survey: Summary Results (EPA 1990). [b] Community water systems.

Table 6. Shifts in Soil Erosion by Tillage in the Corn Belt

Tillage	Soil Erosion (mil tons)	
	Baseline	Atrazine ban
Conventional	429.1	452.3 (+5.4)
Conservation[a]	131.9	128.9 (-2.3)
All	561.0	581.2 (+3.6)

[a] Conservation tillage includes reduced-till and no-till.

Table 7. Probability of Exceeding the Benchmarks: Surface Water

Chemical[a]	Benchmark[b] (μg/L)	Baseline	Atrazine ban
Atrazine	100	.276	-
Dicamba	300	.163	.281
Cyanazine	100	.253	.621
Bentazon	25	.428	.494
Metolachlor	100	.020	.038
Alachlor	100	.030	.038
Simazine	50	.829	.870
Propachlor	350	.076	0

[a] Of the 16 herbicides, only eight had concentrations exceeding the EPA's benchmark.

[b] These are the EPA's drinking water standards, also referred to as the "Maximum Contaminant Level" (MCL) for acute toxicity.

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