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Environmental Toxicology and Chemistry, Vol. 21, No. 8, pp. 1558–1565, 2002
Printed in the USA
0730-7268/02 $9.00 + .00

SENSITIVITY ANALYSIS FOR VALIDATING EXPERT OPINION AS TO IDEAL DATA SET CRITERIA FOR TRANSPORT MODELING

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(*Received* 19 *March* 2001; *Accepted* 21 *January* 2002)

Abstract—Environmental fate modeling results are often used in risk assessment without adequately considering uncertainty in exposure predictions. Sensitivity analysis is fundamental to model validation and error prediction since sensitive model input parameters account for the largest variance in model prediction. Once identified, sensitive model input parameters can be used to propagate parametric uncertainty in numerical predictions. Output sensitivity to variation in input code sequences was investigated for the pesticide root zone model (PRZM 3) using Plackett–Burman analysis for six runoff and leaching data sets. The analysis utilized an incomplete block factorial design with even parameter weighting and uniform proportional input perturbation. Timing and duration of key period rainfall were assumed a priori to be dominant sensitive inputs. Thus, meteorological data were fixed, allowing identification of additional input components contributing to model sensitivity. Results validated expert modeler assumptions concerning parameters most critical for model validation. For leaching data sets, the application rate, soil bulk density (an indicator of available water-holding capacity), chemical partition coefficient, and pesticide degradation rates were commonly the most sensitive inputs. For runoff data sets, the in-crop runoff curve number was the most significant input governing pesticide loss in runoff and erosion flux. The chemical partition coefficient, soil and foliar decay rates, and soil bulk density were also common sensitive components for runoff predictions. These commonly observed sensitive components for runoff and leaching prediction need to be carefully considered in the design and conduct of relevant field studies, modeling assessment of such studies, and future improvements in algorithms for environmental transport modeling.

Keywords—Plackett–Burman Transport modeling Leaching Runoff Sensitivity analysis

INTRODUCTION

The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) Environmental Model Validation Task Force (FEMVTF), a collaborative effort of scientists from the crop protection industry and the U.S. Environmental Protection Agency, was established to improve confidence in regulatory modeling [1]. The work of this task force has compared the results of PRZM 3 predictions with measured data collected in 18 different leaching and runoff field studies [2,3].

One of the goals of FEMVTF is to provide uncertainty bounds for numerical modeling based on comparison of model predictions with data sets for field dissipation, prospective groundwater, and runoff studies. Validation within this context provides a measure of how well current environmental fate models can predict real-world behavior. An integral part of these tasks is determining the quality of data sets that span a wide range of philosophy for design and conduct of field research. Model sensitivity analysis can be instrumental in deducing the quality of the various data sets by indicating those input parameters needed for accurate model predictions. Such information aids in interpretation of modeling results and may be a necessary precursor to any subsequent statistical comparison of model-predicted results to field observations [4]. Sensitivity analysis can also prove useful for future field study design by identifying those parameters requiring the greatest accuracy in measurement.

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Input data sensitivity for transport modeling

Multiparametric transport models may be sufficiently nonlinear in their output response surface to confound simple procedures for validation. Sensitivity to input parameter variance can be used to identify important input parameters and, additionally, allows for evaluation of model efficacy (ability to produce a desired effect [5]). Sensitivity analysis should be conducted across the full range of likely parameter values [6] and for other input assumptions that are not parameters per se (e.g., selection of soil layer thickness for a leaching model [7]).

The intuitive sense developed by transport modelers for sensitive input parameters is restricted to the universe of data sets modelers may have evaluated. Statistical approaches to sensitivity analysis can be used to validate modeler intuition and to extend knowledge of model robustness and efficacy across a wider range of input data sets. Unfortunately, limited documentation of input data sensitivity (either intuitive or statistical) exists for most transport models.

Empirical description of transport model sensitivity

Walker et al. [8] reported the effect of single-parameter variance on output (total pesticide residues with time, residue distribution with depth, and fraction leached) for a standard set of input data for PRZM 2 (as well as LEACHP [9] and VARLEACH [10]). Pesticide degradation half-life in soil and the equilibrium soil–water partition coefficient (K_d) significantly influenced total soil residues and fraction of residues leached, respectively. A 1.5-fold increase in half-life (133–200 d) resulted in a 43% increase in total soil residues. Variance in K_d from 1.7 to 8 resulted in about 10% greater soil residues.

When a Freundlich coefficient (K_f) and 1/n were used instead of K_d for describing the soil–water partition, variance in the Freundlich 1/n was not judged to be particularly sensitive but was more important for a lower associated K_f value. The effect of variance in either half-life or K_f on output was nonlinear.

In this study, soil parameters were varied under fixed inputs for weather and chemical properties [8]. Decreased bulk density (1.5–1.0) resulted in 30% greater mean leaching depth. Initial soil moisture content and field capacity were insensitive soil parameters. In contrast, Monte Carlo analyses with PRZM showed field capacity to be the most sensitive parameter for prediction of leaching for a short-lived (half-life of 30–60 d), weakly sorbed (K_{oc} = 20–40 L/kg) pesticide [11,12].

Finally, the sensitivity of PRZM 2 to the treatment of dispersion was an important modeling consideration [6]. PRZM 2 proved particularly sensitive to thickness of layer segments, especially in the surface few centimeters, as this influenced the effect of numerical dispersion. This can be minimized by careful initial evaluation of the effect of segment thickness or through use of an analytical dispersion value if appropriate site hydrological information is available. Although results are not reported for PRZM 2, with LEACHP set to a 3-cm layer thickness, a change in numerical dispersion from 0 to 20 mm caused an approximate 10% decrease in peak pesticide concentration without an increase in leaching loss. A further increase to 50 mm resulted in significantly increased leaching loss and a flatter pattern of pesticide residue concentration in the soil profile. Dispersion assumptions have additionally been cited as a critical aspect of PRZM model performance by Carsel et al. [11,12] and have been addressed in PRZM 2 and PRZM 3 with the inclusion of the method of characteristics option that solves the chemical transport equation with minimization of numerical dispersion [13].

Leonard and Knisel [14] observed that for groundwater loading effects of agricultural management systems (GLEAMS [15]) leaching predictions, much of the variance in model outcomes for probabilistic modeling with 50 years' weather was attributable to rainfall distribution relative to timing of pesticide application. A given large rainfall event on the day of application is sufficient to initiate leaching even for a short-lived molecule. Worst-case rainfall scenarios were suggested as a means to reduce variances. When K_{oc} (K_d/soil organic fraction) varied from 100 to 10 L/kg for a pesticide with a 60-d half-life, the predicted 50th-percentile leaching losses were increased by about threefold on a sandy clay loam soil (pesticide leached increased from 5–15%). A similar sensitivity analysis on a sand-textured soil showed the same relative magnitude of effect, but the absolute amount leached was considerably more significant (pesticide leached increased from 12–35%). Leonard et al. [16] presented similar conclusions regarding annual runoff losses for pesticides as predicted by GLEAMS (rainfall, especially in a short postapplication interval, has an overriding importance on runoff predictions). These authors simulated moderately to strongly sorbed pesticides (K_{oc} of 100–1,000) with short soil half-lives (15 d) and also stressed that as half-life increased, sensitivities to inputs such as rainfall might decrease and/or variables related to sediment transport might increase in importance.

Truman and Leonard [17] investigated GLEAMS predictions of pesticide leaching losses as influenced by environmental fate parameters (surface and subsurface half-lives as well as K_{oc}) for two soil scenarios subjected to the same 50-year pattern of rainfall. As would be expected, increased surface and subsurface half-lives (5–30 and 2.5–360 d, respectively) and decreased K_{oc} (10–100 L/kg) increased the amount of predicted leaching loss. Rainfall timing immediately after application was especially important when pesticide half-lives were short. For selected scenarios, potential leaching losses from the root zone increased two- to sevenfold as subsurface half-life increased sixfold.

Sensitivity analysis for pesticide runoff and sediment transport for the chemicals, runoff and erosion from agricultural management systems (CREAMS) model was performed for weakly and strongly sorbed pesticides by Lane and Ferreira [18]. Rainfall was highly significant for a weakly sorbed molecule but not for a strongly sorbed molecule. Application rate and runoff yield, as well as application and incorporation efficiency, was always significant.

Documentation for GLEAMS similarly indicates sensitive input parameters [19]. Runoff curve numbers are particularly sensitive parameters that increase in sensitivity as values of the curve number increase. The runoff curve number for the soil while in crop is especially sensitive in this regard. Porosity and field capacity are additional sensitive parameters governing water flow (leaching vs runoff). When overland flow is segmented to reflect complex slopes, the soil loss ratio (C-factor in the universal soil loss equation) becomes a sensitive parameter. The K_{oc} is the most sensitive pesticide input parameter. For K_{oc} less than 500, surface runoff decreases as K_{oc} decreases because of mobilization below the 0- to 1-cm surface layer. For K_{oc} greater than 1,000, increased K_{oc} shifts pesticide loss from runoff to sediment transport. Soil half-life is sensitive as well. Application rate may be sensitive depending on the effect of soil half-life and foliar interception to reduce the amount of pesticide available for transport.

Zacharias and Heatwole [20] used comparisons of bromide and pesticide leaching from uncalibrated and calibrated runs of PRZM and GLEAMS to gain insight as to sensitive components of these transport models. Curve number, field capacity, and wilt point were considered sensitive parameters for both models, as were leaf area index for GLEAMS and depth of soil water extraction for PRZM. Ma et al. [21,22] concluded that GLEAMS, PRZM 2, and PRZM 3 were all highly sensitive to runoff curve number, soil water contents at field capacity, and wilt point in their evaluation of surface water and atrazine runoff. Additionally, the effective mixing depth for chemical transfer to surface runoff and the kinetic sorption rate coefficient were found to be highly sensitive components for PRZM 3 atrazine runoff prediction [22].

Statistical description of transport model sensitivity

Fontaine et al. [23] statistically evaluated the effect of input parameter variance for prediction of leaching depth at a fixed total residue concentration when modeled by PRZM within a Monte Carlo shell. Sensitivity analysis was performed for 35 PRZM input parameters when simultaneously varied over a range appropriate for preemergence soybean herbicide use in the midwestern United States. The results were evaluated by both Plackett–Burman (PB) [24] and Fourier amplitude (FAST [25]) sensitivity analysis. Both statistical tools produced comparable relative sensitivity rankings. The PB analysis proved preferable to FAST because of the much-reduced computational intensity of this approach. (PB utilizes a partial factorial design, whereas FAST generates a sequence of scenarios by oscillating inputs at different frequencies between lower and upper bounds.)

The most critical input parameter in the work of Fontaine et al. [23] was key period rainfall, which refers to the postapplication timing of a rainfall event sufficient to initiate leaching and indicates the overriding importance of rainfall/irrigation distribution as a critical PRZM input. Other parameters that were sensitive in most ranges were pesticide half-life, detection limit, K_{oc}, soil organic carbon, and available water in the surface horizon. Variables that were important for many ranges included runoff curve numbers 3 and 2, the bulk density in the surface horizon, and the total pesticide applied. In some cases the bulk density and available water content in the second horizon were also important. The PRZM 3 will not be markedly different from PRZM in the relative importance of these key input parameters as long as the aforementioned sensitivity to surface layer thickness/dispersion is addressed.

Cryer et. al. [26] have utilized PB designs to evaluate sensitive parameters affecting pesticide runoff predictions from GLEAMS and the erosion-productivity impact calculator, water quality (EPICWQ) model as well as leaching predictions from PRZM 2. Analysis of 20 input parameters for EPICWQ used a fixed single year of weather (weather was assumed a priori to be the most significant input class) with a significant effect judged any variance significant at $p < 0.01$ to 0.02. For chlorpyrifos application to corn in the Midwest (USA), sensitive parameters (ranked) were runoff curve number after planting, timing of the third application date, timing of the second application date, and the planting date. Similar sensitivity analysis for GLEAMS indicated the sensitive inputs (ranked) were the runoff curve number, pesticide water solubility, and pesticide soil half-life. (The variance ranges for the analyses were 70–95 for the Soil Conservation Service curve number, water solubility of 1–6 μg/L, and soil half-life of 4–70 d; output variables considered were daily maximum and annual fractional runoff and leaching of pesticide, daily maximum and annual water flow rates, and erosion mass.) The experience of these modelers is that for fixed pesticide properties, ranked sensitivity for runoff inputs is

$$\text{weather} \gg \text{runoff curve number} \gg \text{all other inputs}$$

and for leaching, the dominant sensitive parameters are porosity, field capacity, and hydraulic conductivity (S. Cryer, Dow AgroSciences, personal communication).

Cryer and Havens [27] have performed global sensitivity analysis for GLEAMS using Plackett–Burman techniques. Characteristic runoff and leaching results for seven geographically diverse scenarios were investigated for both a hydrophilic and a hydrophobic pesticide. Weather patterns characteristic of 50th-, 90th-, and 99th-percentile return frequencies for each region were used. It was found that geographic conditions such as weather, soil crop and management practices, and the physicochemical pesticide properties define both the number and the sensitivity ranking for GLEAMS-sensitive input parameters. Several water hydrology parameters were consistently found as sensitive. These include runoff curve number, soil porosity, and the soil evaporation parameter. Important pesticide properties were K_{oc} and half-life. The sensitivities of the GLEAMS inputs were largely dependent on the nominal values initially chosen and the geographic region simulated.

METHODOLOGY FOR CONDUCTING SENSITIVITY ANALYSIS

Plackett–Burman fractional factorial design [24] was chosen as the procedure for conducting FEMVTF sensitivity analyses because of its simplicity and suitability for the identification and ranking of variance components in multiparametric models. The PB analysis isolates variable main effects through a contrast of outcomes at two different levels. This is accomplished by investigating equal numbers of combinations of each variable at predetermined *high* and *low* levels that in this exercise are dictated by the selection of a perturbation factor. The average difference in outcomes over the various combinations of variable input parameters allows for determining the effect for each input parameter. The average effect is described as

$$E_i = x_h - x_l = \frac{2}{n}\sum_{j=1}^{n/2} Y_{(+1)} - \frac{2}{n}\sum_{j=1}^{n/2} Y_{(-1)} \quad (1)$$

where

E_i = average effect on model output for parameter "*i*"

n = number of model simulations

x_h = effect at a high level of the parameter given by $\frac{2}{n}\sum_{j=1}^{n/2} Y_{(+1)}$

x_l = effect to be contrasted at a low level of the parameter given by $\frac{2}{n}\sum_{j=1}^{n/2} Y_{(-1)}$

$Y_{(+1)}$ = model output result when input parameter "*I*" was high (+1)

$Y_{(-1)}$ = model output result when input parameter "*I*" was low (−1)

The PB design uses an incomplete block factorial design where each input parameter is evenly weighted. This reduces the number of unique model simulations required at the expense of assuming that interactions between more than two variables are insignificant, as this variance is grouped with the model error. Plackett and Burman [24] present designs for contrasts at two levels.

Inclusion of a subset of dummy variables is used to characterize the variance (V) and standard error (s). These dummy variables have no physical significance, and thus any effect on model output resulting from changes is purely random. The average difference in the sum of *high* and *low* inputs for the test and dummy parameters is determined. The standard error variance of an effect is the variance due to dummy variables (E_{Di}, where $i = 1,n$ with n being the total number of dummy variables; typically, $n = 5$ degrees of freedom for the PB program):

$$V = \frac{\sum_{i=1}^{n} (E_{D_i})^2}{n} \quad (2)$$

The standard deviation of the effect is thus

$$s = V^{1/2} \quad (3)$$

A simple t test allows for testing of the significance of the effects found for the mean difference between two real variables (x):

$$t = (x_h - x_l)/s_x \quad (4)$$

where

$$s_x = \frac{s}{\sqrt{n}} \quad (5)$$

The result of PB analysis is, therefore, a ranked listing of variables in order of their relative effect on model outcomes, along with a determination of relative significance of the effect. The PB analysis has been used to evaluate input parameter sensitivity for transport modeling of pesticides at the regional scale [23,26,27].

Soil correlations to eliminate potential nonsense parameter combinations

In addition to the experimental design considerations, several physically based correlations for soil properties are employed to avoid possible nonsense parameter combinations that can be obtained from the PB analysis. The following simple equality must be obeyed for all soils:

$$\text{wilting point} \leq \text{field capacity} \leq \text{porosity} \quad (6)$$

If wilting point (WP), field capacity (FC), and porosity (POR) are treated as independent parameters with certain magnitudes, then the PB design could result in violation of Equation 6 since inputs are perturbed around a nominal value. This typically causes a soil transport model to generate erroneous results or not run at all. The following soil correlations are implemented for both the GLEAMS and the PRZM model to avoid potential nonsense soil parameter combinations [28]:

$$\text{FC}(i) = 0.3486 - 0.0018\text{sand}(i) + 0.0039\text{clay}(i) + 0.0228\text{OM}(i) - 0.0738\text{BD}(i) \quad (7)$$

$$\text{WP}(i) = 0.0854 - 0.0004\text{sand}(i) + 0.0044\text{clay}(i) + 0.0122\text{OM}(i) - 0.0182\text{BD}(i) \quad (8)$$

$$\text{BD}(i) = 2.65[1 - \text{POR}(i)] \quad (9)$$

The array subscripts (i) in Equations 2 and 3 represent layers i, from $i = 1$ to n, where n = total number of soil layers that are being modeled.

In these correlations, both WP and FC are treated as dependent variables and are functions of soil texture (%clay and %sand), bulk density (BD), and soil organic matter (OM). Thus, %sand, %clay, OM, and BD can be investigated in the sensitivity analysis. The inputs FC and WP are calculated from these independent variables. Certain parameter combinations substituted into Equations 7 through 9 may not satisfy Equation 1. In cases where WP > FC, WP is set equal to FC minus a small amount. In cases where FC > POR, FC is set to a value slightly less than POR. This guarantees that Equation 6 will always be true for all independent variable combinations regardless of whether the parameter combinations were real or imaginary.

Soil properties that vary with depth

Several soil properties can vary with depth throughout the soil horizon. Examples include porosity/bulk density, field capacity, wilting point, organic matter, and pH. The user specifies as input the soil depth increments where property values differ, along with the magnitudes of the properties at each specified depth. The number of PB simulations required if all soil intervals were modeled as being independent would dramatically increase if each soil layer were treated as a separate entity. Therefore, parameters that can change with depth are grouped together and changed according to the original user-defined magnitude (via the nominal file) at each depth. For example, if soil organic matter is chosen as an input parameter to investigate, the PB program changes all soil organic matter by the same perturbation factor specified by the user. If the user specifies a 10% perturbation around the nominal value and the PB design specifies a −1, then all the soil organic matter values for each soil layer and for this simulation are decreased by approximately 10%. Thus, the same value for organic matter is not simulated for all soil depth intervals (unless the user specifies that the organic matter does not vary with depth in the nominal file), but rather a consistent and constant percentage change occurs for each depth value.

Implementation of sensitivity analysis within FEMVTF

Plackett–Burman sensitivity analysis has been an integral part of numerical modeling risk assessment within the Dow AgroSciences GRASP and DEGAS systems where it has been used to discern sensitive inputs to chemical transport models [23,26,27]. The sensitivity analysis in DEGAS has been automated and consists of FORTRAN and UNIX shell scripts. The system is robust and usable and fits well with the goals of FEMVTF; therefore, the original code for PB analysis has been repartitioned and altered by FEMVTF to be hosted in a DOS-based environment. These executables have been linked such that they run in the DOS window on Windows 3.1, 1995, or NT as well as from the standard DOS prompt. The sensitivity analysis program has three components: (1) a FORTRAN program for the sensitivity analysis using a PB design that generates model input files, (2) a shell script (batch file) that executes the PRZM 3 model, and (3) a routine for summarization of statistical results for input and output parameters investigated.

Interim releases of the PB software (PB 1.0b, PB 1.0, and PB 1.01) compatible with interim releases of PRZM 3 were used for sensitivity analysis of two leaching and two runoff data sets in the FEMVTF Phase II pilot exercise. Two additional data sets (one runoff and one leaching) were analyzed using PB 1.2b3, a version coded for compatibility with the beta release of PRZM 3 (Ver 3.12 beta; http://www.epa.gov/ceampubl/softwdos.htm).

This PB numerical tool additionally supports GLEAMS simulations. This aspect of PB is well documented [23] and, therefore, was not considered within FEMVTF.

The FEMVT evaluations

Sensitivity analyses were conducted with three leaching and three runoff data input sets. Each data set represents physical properties from large-scale field studies involving commercial pesticides. The main features of these data sets are summarized in Tables 1 and 2 and are comprehensively described by Singh and Jones [2] and Russell and Jones [3]. The approach for conduct of the sensitivity analysis within the FEMVTF project is described here.

The PRZM 3 input data sets [2,3] were subjected to individual sensitivity analyses conducted for each model output parameter of interest. For runoff data sets, total runoff flux (mg/ha/year) and total erosion flux (mg/ha/year) were the output quantities evaluated. For leaching data sets, the maximum total pesticide in compartment X (mg/kg, where X is the layer

Table 1. The main features of the leaching data sets analyzed by the Plackett–Burman technique

Data set	Soil association	Soil type	Hydrologic group	Crop	Application rate (kg a.i./ha)	Half-life (d)	K_d (ml/g)
NC1L	Kenansville	Loamy sand	A	Soybean	0.56	100	0.361
NC2L	Tarboro	Loamy sand	A	Soybean	0.14	47	0.425
NC3L	Tarboro	Loamy sand	A	Cotton	0.14	14	0.091

[a] NC = North Carolina, USA.

of interest and may represent the lowest computational layer at which a detect occurs or the computational layer where the pesticide center of mass occurs), maximum pesticide dissolved in compartment *X* (mg/L), and total dispersion flux at soil core depth (mg/ha/year) were the output quantities monitored.

General rules for preparing the source data (a PRZM 3 input file) for analysis were followed. First, identification of those inputs that, when adjusted by the perturbation factor (PF), would exceed acceptable input limits for PRZM was sought. These inputs were adjusted such that perturbed bounding limits were not exceeded (preferred approach) or alternatively were eliminated from consideration (not perturbed). The source meteorological file was truncated to include only one year of data, under the a priori assumption that meteorology is the dominant contributor to modeling sensitivity. The output data file created by PB was monitored to determine if PB-generated PRZM runs are properly executing. In particular, if total dispersion flux showed that fluxes were well below the method sensitivity for the pesticide considered, the soil core depth was adjusted upward through modification of the source input file (selection of a soil core depth within the described root zone at less than 100 cm was preferred).

Two analyses, denoted as quasi global and constrained, were conducted for each data set–model combination. A quasi-global analysis considered all input parameters implemented within the PB program for a given model (a maximum of 64 possible inputs for PRZM). This portion of the sensitivity analysis served as a check on data set quality used as the basis for data set inclusion into the FEMVTF exercise. Sequential runs were performed where the PF was lowered from an initial value of 0.10 (10% perturbation of inputs) in steps of 0.02 to the point where the range in output probability of a greater $|t|$ ranged from zero (0.0000) to approximately 1 for the output correlation of interest. This represented the optimized PF. Next, constrained analysis excluded those parameters identified as not sensitive ($p\ |t| \geq 0.05$) from the quasi-global analysis at the optimized PF and the PB routine was rerun at the optimized PF for this reduced set of inputs. Relative sensitivities for a given PB model run were calculated as E/E_{max}, where E is the effect for an input parameter and E_{max} is the maximum effect observed for the parameters input into the PB run. Results of the quasi-global analysis were plotted as E/E_{max} versus parameter number. Results of the constrained analysis, expressed as $|E/E_{max}|$ as a percentage, were used to describe the relative importance of significant model inputs on output sensitivity.

RESULTS OF LEACHING ASSESSMENTS

Data set NC1L

Quasi-global analysis. A total of 33 PRZM 3 input parameters for the NC1L data set were initially varied to optimize the PF for ranking of input parameter sensitivity by quasi-global analysis. The output parameters monitored were the maximum total and dissolved pesticide residue observed in compartment 139 (~1 m depth in the soil profile). Figure 1 compares the relative sensitivity (E/E_{max}) when an initial quasi-global analysis was conducted with a PF of 10 and 8% for total and dissolved pesticide, respectively. Both results show similar parameters as the most sensitive inputs: chemical application rate (TAPP), BD indicative of available water-holding capacity, the adsorbed phase decay rate (DSRATE), the maximum rooting depth of the crop (AMXDR), and the chemical partition coefficient (KD). Parameter nomenclature refers to the input parameter selected for perturbation and is fully described in Havens et al. [29].

Constrained analysis. The quasi-global analysis identified sensitive inputs for further analysis. The outputs monitored by constrained analysis (optimized PF of 8%) were maximum total pesticide concentration at 1 m depth and maximum dissolved pesticide concentration at 1 m depth. Twenty-seven input parameters were shown to have statistically significant ($p < 0.05$) effects on leaching predictions. Six of these parameters were shown to account for >80% of the relative model sensitivity ($|E/E_{max}|$). Results (Table 3) show the same six parameters as having the greatest sensitivity for predictions of maximum total and dissolved pesticide occurring at the bottom of the nominal root zone. These parameters include total applied mass, bulk density (an indicator of available water-holding capacity in PB), adsorbed phase decay rate, max-

Table 2. The main features of the runoff data sets analyzed by the Plackett–Burman technique

Data set	Area (ha)	Slope (%)	Soil type	Crop	Application method[a]	Half-life (d)	K_d (ml/g)
GA1R[b]	3.64	3.5	Loamy sand	Cotton	Aerial (L)	6	4
GA2R	3.04	3–5.5	Sandy loam	Sweet corn	Foliar (L)	8	0.43
IA2[c]	7.0	4.3	Silt loam	Corn	T-band, foliar, and broadcast (G, L)	30	121

[a] Formulation type given in parentheses (G = granular, L = liquid).
[b] GA = Georgia, USA.
[c] IA = Iowa, USA.

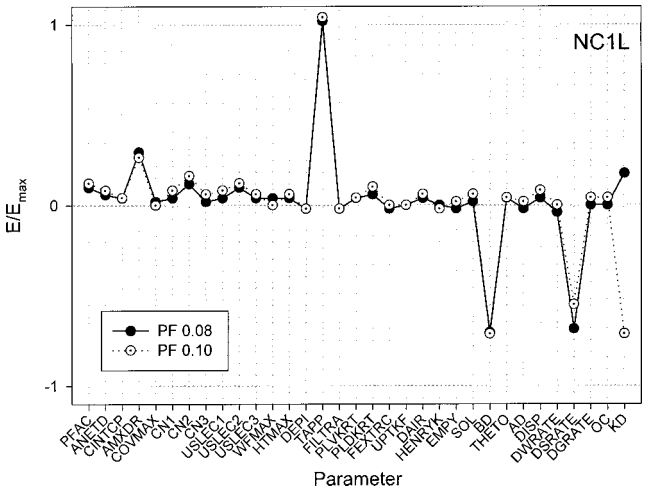

Fig. 1. Influence of the perturbation factor (PF) on E/E_{max} for sensitivity of predictions of maximum total pesticide at a 1-m depth in the soil profile as influenced by the pesticide root zone model (PRZM) 3 input parameters, data set NC1L (NC, USA).

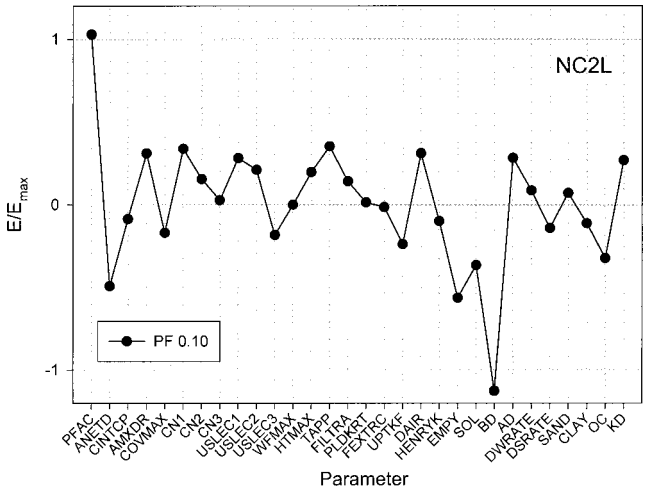

Fig. 2. Calculated E/E_{max} for sensitivity of predictions of maximum total pesticide at a 1-m depth in the soil profile as influenced by the pesticide root zone model (PRZM) 3 input parameters, data set NC2L (NC, USA).

imum rooting depth of the crop, pesticide K_d, and runoff curve number 2.

Data set NC2L

Quasi-global analysis. A total of 30 PRZM 3 input parameters for the NC2L data set were initially varied for quasi-global analysis to optimize the PF for the ranking of input parameter sensitivity. The output parameter monitored was the maximum total pesticide residue observed in compartment 150 (1 m depth in the soil profile). Figure 2 compares the relative sensitivity (E/E_{max}) when an initial quasi-global analysis was conducted with a PF of 10%. Subsequent runs were conducted at smaller PF.

Constrained analysis. The normalized results from the quasi-global runs identified 22 sensitive inputs for further analysis, and an optimized PF of 1% was selected. For constrained analysis, three outputs were monitored that include the maximum total pesticide concentration at 1 m depth, maximum dissolved pesticide concentration at 1 m depth, and total dispersive flux of pesticide at the soil core depth (2 m). Ten (11 in the case of dispersive flux) of the 22 input parameters were shown to have statistically significant effects on leaching predictions. The results (Table 3) show very similar rankings in the relative importance of significant parameters. Soil bulk density (BD, an indicator of available water-holding capacity in PB) and the KD were shown to be approximately twofold more sensitive than the next group of sensitive inputs. These findings confirmed the opinion of expert modelers as shown in calibrated model runs where stepwise changes in selection of available water-holding capacity and K_d were used to optimize the fit of modeled results to field observations.

Data set NC3L

Quasi-global analysis. A total of 39 PRZM 3 input parameters for the NC3L data set were initially varied for quasi-global analysis in order to optimize the PF for the ranking of input parameter sensitivity. The output parameters monitored were the maximum total and dissolved pesticide residue at the 20-cm core depth as well as total dispersive flux at the 90-cm core depth. Comparison of the relative sensitivity (E/E_{max}) when an initial quasi-global analysis was conducted with an optimized PF of 10% (Fig. 3) shows similar parameters as the most sensitive inputs—TAPP, BD indicative of available water-holding capacity, the DSRATE1 and DSRATE2, the

Table 3. Results of Plackett–Berman analyses for leaching expressed as relative importance of sensitive components (where relative sensitivities do not sum to 100, additional parameters were significant but minor contributors to the overall model sensitivities observed)

		NC1L[a]		NC2L			NC3L		
Parameter	Parameter description	Total	Dissolved	Total	Dissolved	Flux	Total	Dissolved	Flux
BD	Bulk density	22	16	51	77	15	20	14	13
TAPP	Chemical application rate	26	23				20	19	12
AMXDR	Maximum rooting depth	7	6	3	1	6	8	8	16
DSRATE1	Adsorbed phase chemical	20	16	34			7	7	6
DSRATE2	decay rate (layer 1, 2, 3)						4	4	11
DSRATE3									2
KD1	Chemical partition coefficient	4	17		4	60	5	5	
KD2	(layer 1, 2)						3	9	6
CN1	Runoff curve number	3	2	4	2	5			4
CN2	antecedent moisture condition 2 (cropping stage 1, 2)			5	4	10			
PF	Pan factor		2	4		2	4	3	8

[a] NC = North Carolina, USA.

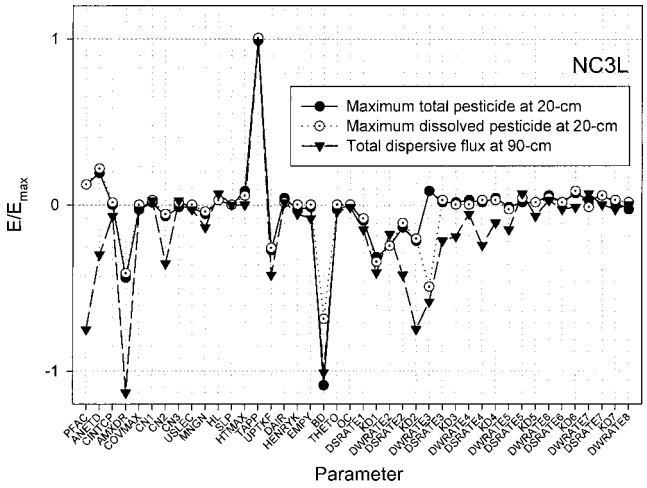

Fig. 3. Comparison of E/E_{max} for sensitivity of predictions of maximum total pesticide in the 20-cm soil depth increment, maximum dissolved pesticide in the 20-cm soil depth increment, and total dispersive flux at a 90-cm depth in the soil profile as influenced by the pesticide root zone model (PRZM) 3 input parameters, data set NC3L (NC, USA).

AMXDR, the PF, and the KD1 and KD2. (Two parameters each are associated with decay rates and chemical partition coefficients to reflect properties for two different soil horizons.)

Constrained analysis. The quasi-global analysis identified sensitive inputs for further analysis. The outputs monitored by constrained analysis (optimized PF of 10%) were maximum total pesticide concentration and maximum dissolved pesticide concentration at a 20-cm depth and total pesticide flux at a 90-cm depth. Up to 37 input parameters had statistically significant ($p < 0.5$) effects on leaching predictions. Six of these parameters were shown to account for >80% of the relative model sensitivity ($|E/E_{max}|$). Results (Table 3) show the same six parameters as having the greatest sensitivity for predictions of maximum total and dissolved pesticide occurring at the bottom of the nominal root zone: chemical application rate, bulk density (an indicator of available water holding capacity in PB), adsorbed phase decay rate, maximum rooting depth of the crop, chemical partition coefficient, and in-crop runoff curve number.

RESULTS OF RUNOFF ASSESSMENTS

Data set GA1R

GA1R—Foliar applications only. Quasi-global analysis of data set GA1R resulted in selection of an optimized PF of 0.1% for constrained analysis of GA1R. Predictions of erosion flux were sensitive to a greater number of input parameters than were predictions of runoff flux. Curve number 2 (in crop, CN2) was clearly the most sensitive input parameter accounting for >70% of output variance from significant inputs in output of both runoff and erosion flux (Table 4). This was confirmed with calibrated modeling where in-crop changes in the runoff curve number were shown to have occurred; PRZM cannot use multiple in-crop runoff curve numbers and therefore is limited in its ability to capture both early and late runoff events for the GA1R data set.

Data set IA2R

Data set IA2R involved both foliar and soil applications within the same season of use. These cases were treated individually in separate PB analyses. Quasi-global analysis resulted in selection of an optimized PF of 0.1% for constrained analysis of both foliar and soil applications for IA2R.

IA2R—Foliar applications only. The in-crop runoff curve number (CN2) was the most sensitive input parameter affecting output of both runoff and erosion flux (Table 4). Both KD and BD were important secondary inputs for erosion flux (Table 4).

IA2R—Soil applications only. The CN2 was the most sensitive input parameter affecting runoff and flux predictions. Both BD and KD were important secondary inputs. The KD was the most sensitive parameter affecting pesticide loss in erosion flux (Table 4).

Data set GA2R

Quasi-global analysis of data set GA2R resulted in selection of an optimized PF of 8% for constrained analysis of GA2R. Runoff curve numbers 1 and 2 (fallow and in crop) accounted for about 50% of the model sensitivity to model input parameters.

SUMMARY AND CONCLUSIONS

Evaluation of six data sets using Plackett–Burman sensitivity analysis and FEMVTF guidance documentation allowed

Table 4. Results of Plackett–Berman analyses for runoff expressed as relative importance of sensitive components (where relative sensitivities do not sum to 100, additional parameters were significant but minor contributors to the overall model sensitivities observed)

		GA1R[a] (foliar)		IA2[b] (foliar)		IA2R (soil)		GA2R (foliar)	
Parameter	Parameter description	Runoff	Erosion	Runoff	Erosion	Runoff	Erosion	Runoff	Erosion
CN1	RO[c] curve number 1							25	26
CN2	RO curve number 2	85	71	73	30	37	63	32	21
KD1	K_d (layer 1)		8	5	23	23	14		6
DSRATE1	Adsorbed phase chemical decay rate (layer 1)	9	4	18	6	15			
PLDKRT	Decay rate on foliage		7		12		17	4	4
BD	Bulk density	6		4	14	22			
MNGN	Manning's *N*		5		8				4
UPTKF	Plant uptake factor		5		7	3	6		

[a] GA = Georgia, USA.
[b] IA = Iowa, USA.
[c] RO = runoff.

for quantitative evaluation of sensitive input parameters for leaching and runoff predictions using PRZM 3. The quantitative results of PB analysis validated expert modeler assumptions concerning those parameters most critical for model validation. Results for leaching data sets (Table 3) show that chemical application rate, soil bulk density (an indicator of available water-holding capacity), the chemical soil partition coefficient, and chemical degradation rates were commonly the most sensitive inputs. For runoff data sets (Table 4), the in-crop runoff curve number was the most significant input governing runoff and erosion flux. The chemical partition coefficient, soil and foliar decay rates, and soil bulk density were also commonly shown to be sensitive components for runoff predictions. These commonly observed sensitive components for runoff and leaching prediction need to be carefully considered in the design and conduct of relevant field studies, modeling assessment of such studies, and future improvements in algorithms for environmental transport modeling. In addition, parametric uncertainty in these sensitive input parameters should be propagated through error bounds on model output predictions.

Acknowledgement—The work of the FIFRA Environmental Model Validation Task Force was a collaborative project involving scientists from the crop protection industry and the U.S. Environmental Protection Agency with funding from Aventis CropScience, BASF, Bayer, Dow AgroSciences, DuPont, FMC, ISK Biosciences, Monsanto, Rohm and Haas, Syngenta, Uniroyal, and Valent. Coding of the Plackett–Burman shell for PRZM 3 was performed by Michael Fouch, Sphere Software. Amy Ritter, Waterborne Environmental, provided modeling support for portions of the sensitivity analysis. The editorial assistance of Russell Jones is gratefully acknowledged.

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