

COMPARISON OF PESTICIDE ROOT ZONE MODEL 3.12: RUNOFF PREDICTIONS WITH FIELD DATA

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Abstract—As part of a process to improve confidence in the results of regulatory modeling, predictions of pesticide root zone model (PRZM) 3.12 were compared with measured data collected in nine different runoff field studies. This comparison shows that PRZM 3.12 provides a reasonable estimate of chemical runoff at the edge of a field. Simulations based on the best choices for input parameters (no conservatism built into input parameters) are generally within an order of magnitude of measured data, with better agreement observed both for larger events and for cumulative values over the study period. When the model input parameters are calibrated to improve the hydrology, the fit between predicted and observed data improves (results are usually within a factor of three). When conservatism is deliberately introduced into the input pesticide parameters, substantial overprediction of runoff losses occur. Recommendations for future work to improve regulatory models include implementation of more sophisticated evapotranspiration routines, allowing for seasonal variation of various model parameters (such as curve numbers, crop cover, and Manning's surface roughness coefficients), better procedures for estimating site-specific degradation rates in surface and subsoils, and improved sorption routines.

Keywords—Runoff Modeling Pesticides Pesticide root zone model

INTRODUCTION

The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) Environmental Model Validation Task Force, a collaborative effort of scientists from the crop protection industry and the U.S. Environmental Protection Agency (U.S. EPA), was established to improve confidence in regulatory modeling. This task force compared the results of PRZM 3.12 predictions with measured data collected in 18 different leaching and runoff field studies. This paper describes the results of the runoff comparisons. Other papers in this series provide an introduction to the work of this task force, describe the results of the leaching comparison, and present the statistics used in making these comparisons.

METHODOLOGY

Types of comparisons

Three different types of comparisons of model predictions with field data were considered.

Cold. This refers to model runs in which no site-specific data (other than weather data) were employed in the model run. Model input parameters were estimated using the typical U.S. EPA procedure. This type of assessment provided an estimate of how well current practices work to generate regulatory exposure estimates.

Site-specific. This refers to model runs in which all available site-specific measured data were employed to define the input parameters. This would include the use of measured on-site soil, hydrologic, and pesticide properties, such as partition coefficients and observed field dissipation half-lives for the site. This provided an estimate of how well the model can be used to describe movement at a specific site.

Calibration. In these model runs, the experimental results were used to refine the values of selected model inputs to provide closer agreement between model predictions and observed field data. These runs determined which parameters require adjustment, evaluated the improvement in fit, and identified model components that may require improvement.

In the first two types of comparisons, the task force developed procedures to prevent the modeler from having access to the field results. In the third type, the modeler had full access to all relevant data.

Model version

All results presented in this paper were generated with PRZM 3.12. Although earlier versions were used for some of the work of the task force, simulations were rerun for consistency.

Water movement is modeled in PRZM 3.12 using a capacity-based water flow (tipping bucket approach) and a daily time step for all hydrological processes. Runoff is based on the soil conservation service curve number technique, and soil erosion is based on the universal soil loss equation. The runoff routines in PRZM have changed significantly since PRZM 2 was issued as part of risk of unsaturated/saturated transport and transformation of chemical concentrations (RUSTIC) in the late 1980s.

Selection of experimental data sets

Data sets were selected using criteria for determining ideal and acceptable data sets, based on the data requirements as identified in the guidance documents for selection input parameters for groundwater loading effects of agricultural management systems (GLEAMS) and PRZM as well as the consensus opinion of the task force scientists and advisers.

Ideal runoff data sets. Complete site-specific weather data

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Table 1. The main features of the nine data sets used in the runoff simulations

Data set ^a	Area (ha)	Slope (%)	Soil type	Crop	Application method ^b	Half-life ^c (d)	K_d^c (ml/g)
GA1R	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
IA2R	7.0	4.3	Silt loam	Corn	T-band, foliar, and broadcast (G, L)	30	121
IA3R	0.065	5.6	Silt loam	Corn	T-band, foliar, and broadcast (G, L)	30	121
IA4R	1.21	2.9	Silt clay loam	Corn	T-band (G)	52	4,200
IA5R	0.065	2.8	Silt clay loam	Corn	T-band (G)	121	12
KY2R	0.605	4.2–5.2	Silt loam	Corn	T-band (G)	52	3,200
					T-band (G)	121	10
					T-band (G) ^d	52	2,200
MD1R	0.50	2.0	Silt loam	Corn	T-band (G) ^e	121	6
MS1R	2.1	0.25	Very fine sandy loam	Cotton	Ground spray (L)	165	0.6
					Foliar (L)	5.7	4.1

^a Studies are identified by the state name, number of study, and the letter R, indicating a runoff study.

^b Formulation type given in parentheses (G = granular, L = liquid).

^c Site-specific half-life and K_d values for surface horizons reflect the values provided by the registrants.

^d Applied to plots 1 and 2.

^e Applied to plot 3.

covered the period of the study and included daily precipitation, daily temperature, and pan evaporation; site dimensions, slope, and characterization of the occurrence of nonsheet flow; calculation of curve numbers possible for each quantified runoff event; site-specific soil physicochemical properties and profile description; information on time, rate, and method of pesticide application; site-specific laboratory measurements of soil half-life and K_d ; foliar decay rates for foliarly applied materials; daily runoff volume and sediment yield data; water- and sediment-phase pesticide concentrations measured with verifiable methodology and sensitivity; and studies conducted and documented by a verifiable standard for quality assurance/quality control.

Acceptable runoff data sets. These data included spatially and temporally contemporaneous weather data available from a National Oceanic and Atmospheric Administration site; natural field drainage channels known and described from a soil survey map; representative curve numbers obtained from a database using soil hydrologic group, soil texture, management practice, and crop; measured soil texture and organic carbon for the surface horizon; number and thickness of soil horizons obtained from a database; a measured soil half-life and sorption coefficient; documented management practices and timings of critical events, daily runoff volume, and sediment yield data; total pesticide concentration via an acceptable method; and peer-reviewed data and interpretations.

Nine runoff data sets (summarized in Table 1) were chosen for comparisons of measured and predicted values. Data sets fitting the ideal criteria were used when available to the task force, but other data sets were also used to cover a wide range of geography and pesticide properties. The criteria resulted in heavy emphasis on industry data sets developed within the United States to fulfill registration needs, although data sets were also obtained from the literature and from nonindustry researchers. Studies conducted outside the United States were excluded from consideration because of the limitations of the standard operating procedures for selection of input parameters.

The nine runoff studies represented a wide range of hydrological, agronomic, and physiochemical scenarios. The field area for the runoff study sites varied from 0.06 to about

7.0 ha. The slope range was 0.25% to approximately 5%. Soil texture varied from silty clay loam to loamy sand. All the runoff study sites were under corn or cotton production except one site, which was under sweet corn production. Eight of these runoff sites were treated with insecticides, and one site was treated with a herbicide. The half-lives of the chemical applied varied from 6 to 165 d, and K_d value varied from 0.26 to 3,200 ml/g for surface horizons.

Selection of input parameters

To ensure that the validation focused on the model and the associated procedures rather than the ability of the specific modeler, detailed standard operating procedures were developed for preparing input sequences for both cold and site-specific comparisons to minimize the influence of the modeler.

Experimental results were not available to those performing the predictive simulations. One contractor had the job of reviewing the specific data sets and abstracting the relevant input variables as well as the experimental results. The input parameters were then passed on to another contractor who performed the modeling simulations. This two-step process minimized bias due to the judgment of the modeler and helped maintain the confidentiality of the chemical(s) used in each study. All test chemicals were identified by a code number rather than a common name. As a final measure to ensure confidentiality, task force members were not given access to the raw data submitted for each field study.

Guidance for performing calibration simulations

Performing calibration simulations can provide valuable information about selection of input parameters and model performance, but only if calibration simulations do not just consist of a simplistic regression of input parameters to minimize differences between observed and predicted values since most water quality models have enough adjustable parameters to fit a limited set of field observations. Therefore, a guidance document was prepared for performing these types of simulations. Unlike the other comparisons (cold and site specific), the judgment and expertise of the modeler can impact the results of calibration simulations. Therefore, the guidelines

Table 2. The ranges of ratios (predicted value \div observed value) based on individual events and cumulative values for cold simulations performed with GA1R (pesticide concentrations in sediment were not measured in this data set)

Comparison	Runoff	Sediment loss	Pesticide in runoff	
			Mass	Concentration
Individual events	0.5–2.8	0.05–0.3	0.4–120.0	0.4–42.0
Cumulative values	1.0	0.1	3.3	1.6

provide a recommended procedure to make the calibrations as reproducible as possible.

The guidelines emphasize two principles. The first is that both the observed field results and the predicted modeling results contain error and that neither value should be regarded as absolutely correct. The second is that model input parameters should not be adjusted outside the ranges that are reasonable. If parameter adjustment beyond a reasonable range is required to achieve a satisfactory fit, then a potential problem exists with either the model or the experimental data.

The general procedure for calibrating modeling to experimental results was to first calibrate the hydrology of the model to provide a reasonable representation of water movement at the specific study site. Once the hydrology has been calibrated, the simulation of the transport and dissipation of the chemical can be evaluated and calibrated as necessary.

Statistical analysis

The initial evaluation of model performance consisted of comparisons of measured field data and model predictions paired in time. Ratios of predicted and observed values (predicted value/observed value) were calculated for each output parameter for individual events as well as for the cumulative values. Variables considered were runoff volume, sediment loss, pesticide losses with runoff and sediment, and pesticide concentrations in runoff and sediment. Scatter plots were also prepared for all the runoff data grouped together to evaluate the overall variability between the observed and the predicted data. Although the model response data sets were large, a critical issue encountered was the typically small size of the field data set for the runoff studies. For example, calculating the concordance statistic [1,2] with three paired values provided little statistical power.

Therefore, to evaluate the impact of uncertainty, additional statistical analyses were performed on selected data sets. As an initial step to evaluate the impact of uncertainty, a sensitivity analysis was performed using an approach based on that of Plackett and Burman [3] to identify key model input parameters for runoff and leaching simulations. Monte Carlo analyses were then performed to evaluate the effect of uncertainty in the sensitive input parameters on the model predictions. The tools and results of the sensitivity and uncertainty analyses are presented in other papers in this series.

RESULTS

Cold simulations

Cold modeling of the runoff transport was performed for only one data set (GA1R; Georgia, USA) using the guidelines prepared for cold simulations (R. Parker, PRZM Inputs—Level One FEMVTF Validation, unpublished data). The predicted versus observed ratios for cold simulations based on individual events and cumulative values (for runoff volume, sediment

loss, pesticide mass in runoff, and pesticide concentrations in runoff) are presented in Table 2.

Based on the single data set, comparisons of cold simulation results and observed values for runoff volume indicated that predicted results were within one order of magnitude of observed values. However, the sediment yield was consistently underpredicted, indicating a need for refined/modified erosion parameters. The pesticide mass and concentrations in runoff were substantially overpredicted (e.g., 3–120 times). The overestimations in the cold simulations were likely caused by the highly conservative estimates of foliar and soil degradation rates for the simulated chemical. Thus, the general observations from the cold simulations are as follows: The cold simulations provide reasonable estimates of the runoff volume, and the results for sediment yield and chemical mass and concentration in runoff indicate a need for improved parameterization of erosion and chemical environmental fate parameters.

Site-specific simulations

The predicted versus observed ratios based on individual events and cumulative values are presented in Tables 3 and 4, respectively, for site-specific simulations. The range of ratios given in Table 3 demonstrates that the site-specific runoff predictions were generally within one order of magnitude of observed values for all the data sets except for MD1R (Maryland, USA). The runoff volumes were consistently overpredicted for the MD1R site. The predicted sediment losses were within one order of magnitude of observed sediment losses for GA1R, IA3R (Iowa, USA), KY2R (Kentucky, USA), and MS1R (Mississippi, USA) data sets. However, sediment losses were underpredicted significantly (mainly because of underprediction of runoff) for IA2R, IA4R, and IA5R. The values for pesticide mass in runoff were also roughly within one order of magnitude of observed values, except for the IA4R and IA5R data sets. The pesticide mass in runoff was usually underpredicted for the IA4R and IA5R sites. The measured pesticide mass in the sediment was available only for two runoff sites (IA2R and IA3R), and predicted values for pesticide mass in sediment were within one order of magnitude of observed data except for two events (IA2R day 181 and IA3R day 196). The predicted pesticide concentrations in runoff and sediment were also within one order of magnitude of measured data except for a few events.

The predicted versus observed ratios derived for cumulative values represented a much narrower band around the ideal value of 1.0 in comparison with those derived for individual events. In general, the ranges for predicted versus observed ratios were 0.3 to 5.0 for runoff volume, 0.2 to 8.0 for sediment loss, 0.2 to 4.0 for pesticide mass in runoff, 0.3 to 4.0 for pesticide mass in sediment, 0.5 to 2.7 for total pesticide mass in runoff and sediment, 0.2 to 3.0 for pesticide concentration in runoff, and 1.0 to 4.0 for pesticide concentration in sedi-

Table 3. The ranges of ratios (predicted value/observed value) for individual events for site-specific simulations (no entry indicates no measured data were available for comparison)

Data set ^a	Runoff	Sediment loss	Pesticide mass		Total pesticide mass	Pesticide concentration	
			Runoff	Sediment		Runoff	Sediment
GA1R	0.6–6.4	0.02–1.3	0.7–1.2			0.3–1.3	
GA2R	0.4–4.4					0.9–9.0	
IA2R	0.8–3.8	0.001–3.5	0.4–29.0	0.007–7.2	0.02–8.5		
IA3R	0.28–1.5	0.08–13	0.04–3.3	0.04–43	0.04–7.8	0.14–2.6	0.5–6.8
IA4R ^b	0.01–0.8	0.003–0.7	0.0–2.1			0.0–2.7	
			0.07–1.8			2.3–5.8	
IA5R ^b	0.01–0.8	0.0001–11.8	0.0–0.89			0.0–1.4	
			0.0–0.7			0.0–8.7	
KY2R ^{b,c}	0.8–2.4	0.4–2.3	0.6–5.8			0.6–2.6	
			2.4–6.0			2.8–3.1	
MD1R	0.9–32		2.3–7.4			0.0–4.4	
MS1R	1	2.3	0.3			0.3	

^a Data set abbreviations defined in Table 1.^b The multiple rows represent the results for multiple pesticides in the same order as in Table 1.^c Data pooled from the three plots.

ment. Thus, model predictions based on cumulative values (over the entire study period) were in better agreement with measured data than those based on individual events.

A more detailed analysis of the data also shows that the variability between the observed and predicted values of an output variable usually decreased with the increasing magnitude for runoff volume, pesticide mass in runoff (excluding bromide data), and pesticide concentrations in runoff. In other

words, the values for predicted versus observed ratios (Table 3) beyond one order of magnitude are usually associated with very small events. However, this trend was not very clear for sediment loss, pesticide mass in sediment, and pesticide concentration in sediment. The better agreement between measured and predicted values in larger rainfall events can be attributed largely to the inherent limitations of the Soil Conservation Service curve number method, which is based on a rainfall–runoff relation with no consideration for time as a variable for soil water dynamics and/or rainfall intensity.

The site-specific simulations also show that more accurate predictions of runoff and erosion generally lead to more accurate predictions of chemical losses with runoff or sediment, indicating reasonable representations of environmental fate and transport processes in the model.

Runoff predictions are generally in better agreement with measurements than sediment predictions. The more scattered sediment predictions indicate greater uncertainty involved in the parameterization of the soil erosion module. For example, the regional rainfall distribution, a non-site-specific parameter used in the erosion submodel for calculating the peak runoff, likely does not accurately represent the rainfall intensity for the specific event. Another source of potential uncertainty associated with erosion prediction is that the seasonal variations in the crop cover (C) and Manning's roughness (N) factors were not taken into account.

Calibrated simulations

Calibration simulations were performed for all runoff sites except for GA2R and MS1R sites (mainly because of time and budgetary constraints), following the guidelines described earlier, which involved mainly the adjustment of hydrological parameters to better simulate the measured hydrology. The predicted versus observed ratios for calibrated simulations based on individual events and cumulative values are presented in Tables 5 and 6, respectively.

The calibrated simulations generally resulted in improved predictions as evident from a narrower range of predicted versus observed ratios calculated for calibrated simulations (Table 5) than for site-specific simulations. As in the case of site-specific simulations, the predicted versus observed ratios derived for cumulative values also indicated a better agreement between predicted and observed data than that based on in-

Table 4. The ratios of predicted and observed values (predicted value/observed value) for cumulative values (average for concentrations) for site-specific simulations (no entry indicates no measured data were available for comparison)

Data set ^a	Runoff	Sediment loss	Pesticide mass		Total pesticide mass	Pesticide concentration	
			Runoff	Sediment		Runoff	Sediment
GA1R	1.47	0.28	1.00			0.39	
GA2R	2.03					1.43	
IA2R							
1992	1.63	2.56	2.64	1.75	2.03	3.32	3.84
1993	1.19	0.23	3.99	0.32	0.50		
IA3R							
1992	1.45	7.69	1.71	3.78	2.66	1.33	1.98
1993	1.02	0.93	0.66	0.51	0.55	0.31	1.20
IA4R ^b	0.34	0.25	0.38			0.83	
			1.01			2.73	
			0.15 ^c			0.15 ^c	
IA5R ^b	0.57	0.25	0.18			0.27	
			0.40			0.83	
KY2R							
Plot 1	1.41	1.32	1.00			0.63	
Plot 2	1.30	0.78	2.29			1.70	
Plot 3	1.24	0.76	4.11			2.90	
MD1R							
1990	3.82		3.70			0.41	
1991	4.75		3.67			0.83	
MS1R	1.00	2.34	0.30			0.30	

^a Data set abbreviations defined in Table 1.^b The multiple rows represent the results for multiple pesticides in the same order as in Table 1.^c Value for bromide.

Table 5. The range of ratios (predicted value/observed value) based on individual events for calibrated simulations (no entry indicates no measured data were available for comparison)

Data set ^a	Runoff	Sediment loss	Pesticide mass		Total pesticide mass	Pesticide concentration	
			Runoff	Sediment		Runoff	Sediment
GA1R	0.5–4.6	0.4–1.7	0.7–1.4			0.2–1.8	
IA2R	0.08–2.9	0.002–1.7	0.2–23.0	0.04–4.1	0.07–5.4		
IA3R	0.14–1.3	0.05–5.7	0.03–4.1	0.11–23	0.09–5.5	0.23–4	0.4–15
IA4R ^b	0.59–0.99	0.3–2.57	0.2–5.1			0.3–5.2	
			0.4–1.7			0.8–1.7	
IA5R ^b	0.7–0.9	0.2–10.2	0.08–0.89			0.1–1.4	
			0.0–2.36			0.0–3.4	
KY2R ^{b,c}	0.8–1.4	0.5–1.2	0.7–3.6			0.5–2.7	
			1.1–2.4			1.3–1.8	
MD1R	0.17–13		0.3–0.86			0.0–2.6	

^a Data set abbreviations defined in Table 1.^b The multiple rows represent the results for multiple pesticides in the same order as in Table 1.^c Data pooled from the three plots.

dividual events. Also, the predicted versus observed ratios based on cumulative values for calibrated simulations indicated a substantial improvement over site-specific results for all output variables except for average pesticide concentration in runoff and sediment. This was somewhat expected because the calibrated simulations effort focused primarily on improving the predictions for runoff volume, sediment losses, and pesticide masses in runoff and sediment. This procedure did not always result in improved predictions for pesticide concentrations in the runoff and sediment.

Table 6. The ratios of predicted and observed values (predicted value/observed value) based on cumulative values (average for concentrations) for calibrated simulations (no entry indicates no measured data were available for comparison)

Data set	Runoff	Sediment loss	Pesticide mass		Total pesticide mass	Pesticide concentration	
			Runoff	Sediment		Runoff	Sediment
GA1R	1.21	0.82	1.15			0.54	
IA2R							
1992	1.36	1.50	2.20	1.16	1.49	3.32	7.08
1993	0.90	0.32	3.01	0.30	0.43		
IA3R							
1992	1.21	4.04	1.48	2.47	1.94	1.37	3.76
1993	0.80	0.84	0.79	1.31	1.16	0.43	2.23
IA4R ^b	0.74	0.53	0.62			1.07	
			0.94			1.27	
			0.39 ^c			0.31 ^c	
IA5R ^b	0.75	0.44	0.33			0.42	
			0.38			0.50	
KY2R							
Plot 1	1.16	1.19	0.85			0.72	
Plot 2	1.03	0.60	1.82			1.86	
Plot 3	1.00	0.61	1.71			1.61	
MD1R							
1990	1.19		0.80			0.31	
1991	1.68		0.27				

^a Data set abbreviations defined in Table 1.^b The multiple rows represent the results for multiple pesticides in the same order as in Table 1.^c Value for bromide.

Sensitivity analysis

A detailed sensitivity analysis was also performed for three runoff data sets (GA1R, IA2R, and GA2R) using the Plackett–Burman sensitivity analysis tool. This analysis indicated that runoff curve numbers, bulk density, partitioning coefficient, and degradation rates were among the most sensitive input parameters affecting pesticide losses in runoff and sediment (Table 7).

Uncertainty analysis

Monte Carlo simulations were also performed with IA2R and GA1R to evaluate the effect of uncertainty in the most sensitive input parameters identified using the Plackett–Burman tool on the model predictions (Carbone et al. [4]). The data set IA2R contained a total of seven runoff events. All measured values of runoff volume fell within the interquartile range (between the 25th and the 75th percentile of the prediction distribution) of the model predictions, indicating that the model was very reliable. For sediment yield, measured values fell within the interquartile range for three events, within the bounds of the distribution for two events, and outside the bounds of the distribution for two events. For dissolved pesticide runoff mass, five measured values fell within the interquartile range, and the remaining measurements fell within the bounds of the distribution. For pesticide mass in sediment, three measured values fell within the interquartile range of the predictions, three fell within the bounds of the predictions, and one fell outside the bounds of the model predictions. At GA1R, pesticide runoff mass was the only value measured. For each of the four runoff events for which the measurements were available, the measured value fell within the interquartile range of the model predictions.

CONCLUSIONS

The initial work conducted by different contractors showed the importance of having a standard operating procedure that completely defines the selection of all model input parameters. The most satisfactory way to implement regulatory modeling is through the development of a shell that provides all input parameters related to the scenario, with the user providing only the parameters related to the specific pesticide being assessed.

The overall model predictions for individual events are usually within one order of magnitude of measured data. When

Table 7. Results of Plackett–Burman analyses for runoff expressed as relative importance of sensitive components (percentage model sensitivity attributed to a given parameter)

Variable	GA1R (foliar) ^a		IA2R (foliar) ^a		IA2R (soil) ^a		GA2R (foliar) ^a	
	Runoff	Erosion	Runoff	Erosion	Runoff	Erosion	Runoff	Erosion
RO curve number 1 ^b							25	26
RO curve number 2	85	71	73	30	37		32	21
K _d (layer 1)		8	5	23	23	63		6
Decay rate (layer 1)	9	4	18	6	15	14		
Decay rate on foliage		7		12			4	4
Bulk density (AWHC) ^c	6		4	14	22	17		
Management factor 2		5		8				4
Plant uptake factor		5		7	3	6		

^a Abbreviations are defined in Table 1.^b RO = runoff.^c AWHC = available water-holding capacity.

the cumulative or average values (values summed or averaged over the study period) are compared, the agreement between the simulated and measured values is improved. For example, predicted pesticide concentrations in the runoff (averaged over the study period) are approximately within a factor of 0.3 to 3 of measured values for both site-specific and calibrated simulations.

More accurate predictions of runoff and erosion generally lead to more accurate predictions of chemical losses with runoff and sediment, indicating reasonable representations of environmental fate and transport processes in the model.

The variability between the predicted and measured values decreases with the increase in magnitude or event size. For example, the variability of more than one order of magnitude is usually associated with very small events.

Since cold simulations were performed with only one data set, definitive conclusions cannot be drawn about the appropriateness of the current method of input parameter selection using current regulatory procedures. The exercise indicates that introducing conservatism into input parameters results in a bias toward overestimating pesticide losses and concentrations.

RECOMMENDATIONS

The following recommendations would improve the agreement between the simulations and the measurements. However, some of these recommendations may have little relevance in a standard regulatory scenario in which input parameters are usually fixed and an event-by-event match between simulated and measured results is not the objective.

Although observed and predicted hydrological balances could not be compared (mainly because of a lack of comprehensive measured data), a general concern exists about the model's ability to adequately represent evapotranspiration (ET). This is particularly critical for a tipping-bucket type of model such as PRZM in which soil moisture can move only downward (upward movement of water due to evaporation at the soil surface is ignored). Evapotranspiration can affect soil moisture, which can in turn affect the relative daily CN on a runoff day. To improve the predictions for runoff volumes (and sediment losses), hydrologic balance calculations should be considered. Soil moisture and bulk density may also impact ET, and their significance in ET calculations may need to be investigated. In addition, the model needs to account for upward water movement because of the ET in the upper soil profile. The ET extraction depth in the topsoil is somewhat

arbitrary, and upward water movement is not considered in PRZM 3. Evaluating the effects of the soil water content at field capacity and the soil water content at the wilting point on ET and runoff volume would be useful in better representing the soil water dynamics and overall hydrological balance.

Although some variability is expected between observed and predicted soil loss values due to the empirical nature of the soil loss equation, the predictions may be improved by a better representation of storm intensity in the soil erosion sub-model. Currently, the peak runoff rates in the erosion model are derived from generalized regional rainfall distributions. A better representation of the rainfall distribution may be helpful in improving the soil loss predictions for individual events.

Pesticide root zone model 3.12 allows multiple sets of input values for crop cover (C) and Manning's surface roughness coefficients (N). A more detailed description of C and N factors during the cropping period represents the dynamic nature of crop cover and roughness and improves the sediment loss predictions.

A seasonal variation in runoff curve numbers (similar to C and N factors) may be helpful in representing the effects of changing crop growth stages on predicted runoff. Also, further investigations are warranted for determining the source of discrepancies and improving the model predictions for smaller runoff events.

The actual time and extent of maximum canopy coverage may vary, depending on how well the crop is growing. The extent of maximum canopy and time of maximum canopy in turn affects the interception and therefore pesticide losses with runoff and sediments. The time and extent of maximum canopy cover calculated from measured canopy cover data can improve model predictions for interception and wash-off. The maturation date in PRZM input sequence should represent the time of reaching maximum canopy cover for a given crop.

A large amount of uncertainty is also associated with the physicochemical properties. The selection of these properties by the registrant remains subjective. A standard procedure may need to be developed for determining the physicochemical properties for the modeling purposes. Steps that may help improve the fate and transport predictions are investigating and representing the effects of time and temperature on half-life and K_{oc} on chemical fate and transport and investigating how well the laboratory values can be extrapolated to field situations.

The nonuniform extraction model currently used in PRZM 3.12 does not account for seasonal variations in soil condition

and texture. For example, a freshly tilled porous soil would have different pesticide and extraction characteristics than a compacted soil. A future option in PRZM might be to allow the extraction curve to vary by site or over time.

Site-specific situations (e.g., a runoff event spanning a period of multiple days) need to be carefully represented in the simulation by adjusting the available input/output parameters. Also, the environmental fate parameters (e.g. half-life and K_{oc}) need to be carefully selected for specially formulated chemicals to represent a realistic environmental fate and transport of these chemicals.

The sampling inaccuracies should be carefully noted when analyzing the discrepancies between the measured and predicted results. For example, the study report for the IA2R site indicated termination of sampling due to inundation of a primary sampling flume during the runoff event on JD 185 to 186 in 1993 that would make the observed value suspect for this date.

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