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PLUS: A Regional Groundwater Assessment and Ranking Tool

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There has been interest within the pesticide regulatory community in developing a tool that can provide estimates of potential pesticide exposure in shallow groundwater across an intended use area. Therefore, industry initiated an investigative project based on the PRZM 3.12 model, which uses regional soils and weather in an easy to use interface. The goal of this proof-of-concept is to facilitate the refinement of groundwater exposure estimates. The focus of this paper is to report the effectiveness of the tool as a regional estimator of potential groundwater contamination.

KEYWORDS: PRZM 3.12; groundwater; vulnerability; leaching; modeling; pesticides

INTRODUCTION

There is a recognized need to protect groundwater resources from contamination resulting from agricultural practices. Some geographic settings have a greater potential to contribute to groundwater contamination than others. The relative potential has been defined in various ways, but is generally referred to as groundwater vulnerability. Potential groundwater vulnerability is known to generally be a local phenomenon and has been defined as the relative tendency for mobile contaminants to reach groundwater after introduction at some location above the uppermost aquifer. Approaches to characterize potential groundwater vulnerability have been the focus of lengthy debate; however, some aspects of groundwater resource protection are generally agreed upon. As an example, many shallow groundwater resources have, to some degree, the potential for vulnerability, and that uncertainty is inherent in all vulnerability assessments.

Various approaches are currently used by the regulatory community to predict the potential for pesticide transport to groundwater. These approaches fall into two distinct approaches. The first approach is to use a set of standard soil scenarios as is currently done by the California Department of Agriculture (CDPR), the New York Department of Environmental Conservation (NYSDEC), and the Canadian Pest Management Resource Agency (PMRA). The second approach is to use a single high-exposure upper bound exposure scenario as is currently done by the U.S. Environmental Protection Agency (U.S. EPA). Both of these approaches have their merits. However, other techniques have become available because of increasing computing power that allows for the large-scale modeling of many soils from a single easy-to-use interface. The opportunity to model many soils rapidly can provide decision makers with a greater level of detail than is possible on the basis of approaches currently used by regulators. As a proof of concept, we developed a tool that allows both a spatial and probabilistic vulnerability ranking of over 8000 soil and weather combinations. PLUS, *P*esticide *L*eaching *U.S*., is a publicly available (*1*) tool built around the Pesticide Root Zone Model (PRZM 3.12.12) leaching model. The PLUS tool has a simple interface that allows selection of state soils and crops and the application of water through irrigation or rainfall events across a period of weather years. The user interface (shell) also allows entry of compound-specific data such as application method and rate, number of applications, application interval, and date of initial application. Output from the tool is easily linked to a Geographic Information System (GIS) for visualization of model predictions. We present an approach that is effective and efficient for providing a relative quantification of soil/site vulnerability. Soil vulnerability potential may or may not relate to groundwater vulnerability because it is often not possible to know either the depth to the uppermost aquifer, the underlying lithology, or whether impermeable strata exist between the soil surface and the aquifer. The focus of this work is to present PLUS as a proof-of-concept tool.

METHODS AND MATERIALS

One of the principal challenges of conducting regional model predictions is getting data into the model in a seamless fashion. The PLUS shell takes soil data by soil series and weather data by region and constructs PRZM 3.12 input files for use during model simulations. There are about 8400 soils in the PLUS database, which were derived from the U.S. Department of Agriculture NRCS (Natural Resource Conservation Service) STATSGO and DBAPE (EPA Data Base Analyzer and Parameter Estimator) databases. During the FIFRA Model Validation Taskforce project, soil selection criterion from databases was developed that allowed the best possible match to the predicted and observed data modeled (*2*). As an example, if selecting the minimum organic matter content consistently provided better matches to actual field results as opposed to using the maximum soil organic

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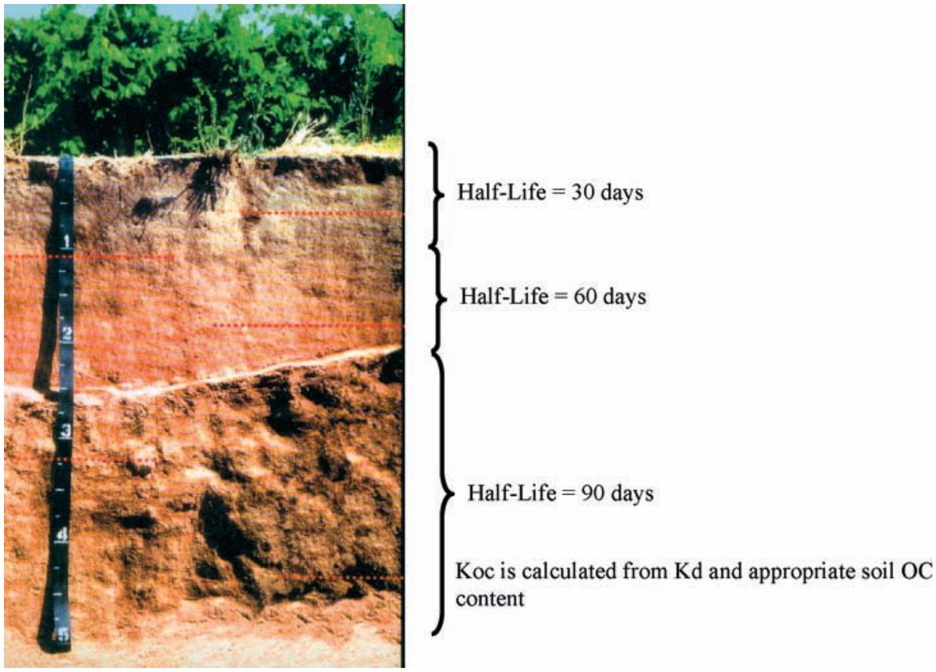

Figure 1. Diagram of soil profile parametrization of half-life by depth.

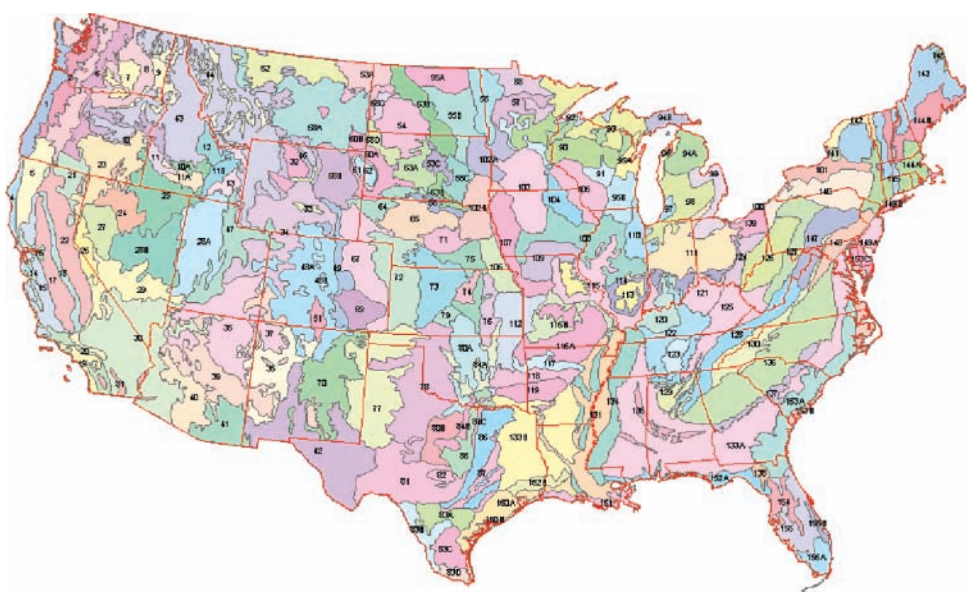

Figure 2. Continental United States divided by Major Land Resource Area (MLRA). PLUS provides results by MLRA.

matter content, then that same database selection criterion was used by the PLUS shell to parametrize the PRZM 3.12 input files. In PLUS, soils are selected by state, but the shell allows the user to select soils within the state by percent area (e.g., top 5%, top 25% acreage soils). Additionally, the tool allows the execution of the FIFRA Exposure Model Validation Task Force (FEMVTF) prospective groundwater scenarios, which serve to benchmark state soil model results. The FEMVTF scenarios are calibrated datasets to prospective groundwater study results (*2*−*5*). The PLUS shell generates soil profile parametrization for PRZM 3.12 to a depth of 4.6 m for all soils. The depth below the NRCS defined horizons can be designated sand or a continuance of the last horizon to the bottom of the 4.6 m depth. Soil pesticide degradation is parametrized by dividing the soil profile into thirds, with the possibility to use multipliers for increasing the pesticide degradation rate by depth. **Figure 1** is an example diagram of how PLUS divides the soil profile by depth for parametrization of degradation rate.

There are 184 weather stations used in PLUS, which are divided regionally by Major Land Resource Area (MLRA). **Figure 2** is a presentation of the continental United States divided by MLRA. When PLUS is run, 30−36 years of weather data from the most appropriate weather station are utilized. The weather data used in PLUS was prepared by the U.S. EPA Center for Exposure Assessment Modeling (CEAM) in Athens, GA (*6*). These are the same meteorological files used by the EPA for their tier II surface water models. **Figure 3** is a presentation of the location of meteorological stations throughout the United States used in PLUS. The groundwater model selected for use in PLUS is PRZM 3.12 (FOCUS version compile date January 20, 2006). PRZM 3.12 was chosen as the leaching model for this project because it is the most widely evaluated model of its type (*7*). Additionally, in recent comparisons by government agencies such as EPA-EFED and CDPR (*8*, *9*), PRZM 3.12 was shown to be a conservative groundwater model from an overprediction perspective, making it a good regulatory tool choice.

PLUS is configured so that approximately 30 years of weather data are run for each soil, and the irrigation feature in PRZM 3.12 is turned on. Crops are also selected such as cotton, corn, and pasture (etc.). For

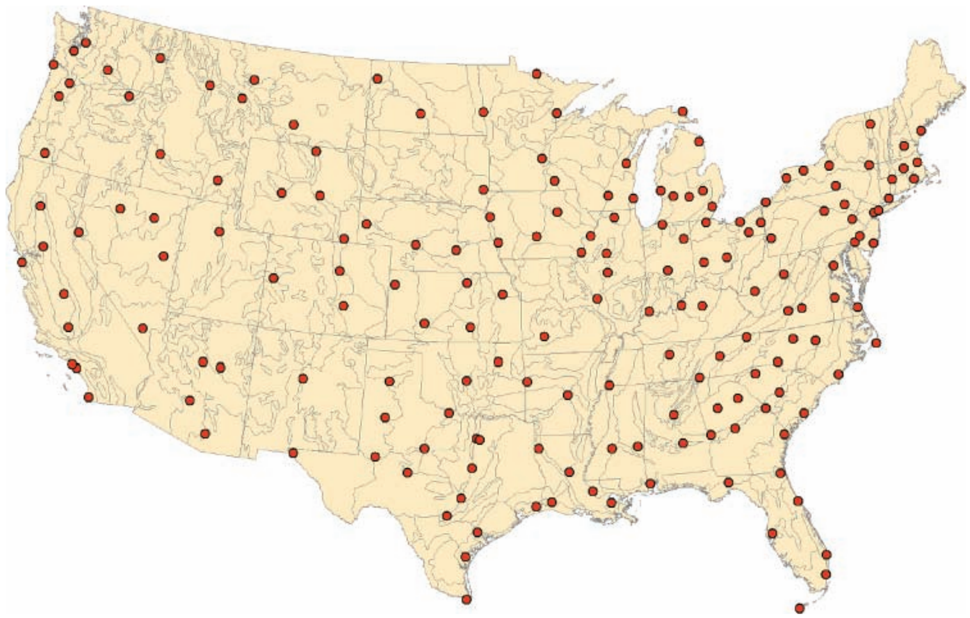

Figure 3. Locations of meteorological stations throughout the continental United States.

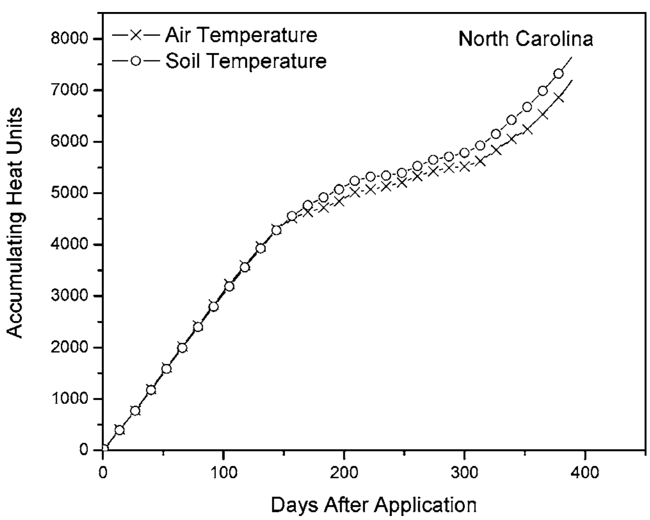

Figure 4. Comparison of soil and air temperature based heat unit accumulation at a North Carolina site.

the runs presented in this work, the pasture/grassland crop option was used. PLUS includes a groundwater receiving model ADAM, which was developed by Waterborne Environmental Inc. (WEI). ADAM allows the inclusion of groundwater degradation as well as other factors including water organic carbon partitioning, Darcy's parameter, and a well screening depth. PLUS also allows the user to obtain groundwater concentration by dividing total mass leached by the total leachate quantity based on the bottom of the profile flux (at 4.6 m). We present concentrations based on the flux mass/water volume method rather than using concentrations calculated in the groundwater receiving model ADAM. The PLUS shell provides the option for the user to run the FEMVTF soils using either the actual meteorological data from the in-life portion of the studies or the regional (MLRA) meteorological data from the state selected.

One of the major limitations of regional modeling methods is the limitation that comes inherently from using a single soil pesticide degradation rate to represent an entire region (*10*). Therefore, we implemented a previously published method into PRZM 3.12 that adjusts soil half-life based on soil temperature and available water content (*11*).

Adjusting Half-Life in the Model by Region and by Soil. To calculate site-specific soil half-life values, a method needed to be implemented into PRZM. In a previously published work, the use of an accumulating heat unit model was explored to predict compound degradation times. Accumulating heat unit models have been used successfully to predict plant and insect life cycles. The concept behind accumulating heat units, or degree-days, is that plants, insects, and pathogens require an amount of heat to develop from one point in their life cycle to another. Similarly, to obtain a half-life, a certain number of accumulating heat units should be required. The measure of accumulated heat is known as physiological time. Physiological time is often expressed and approximated in units called degree-days (°D) or heat units.

Heat unit (HU) calculations have almost exclusively been developed and used for plant and insect life cycle predictions. Accordingly, the basis for the accumulation of heat units has been air temperature. However, because the organisms and processes being modeled here are soil based, it seems to be more appropriate to use soil temperature. One difficulty in using soil temperature is the differences observed by changing the depth at which measurements are taken. Because the goal of the technique is to normalize and predict degradation at different sites, differences in heat unit accumulation due to sensor depth are problematic. It is apparent that unless the soil temperature sensors used at each site are at precisely the same depth, a prediction or normalization will not be possible. Air temperature might appear to be a better alternative because sensor placement is generally not an issue. A relationship between air temperature and soil temperature was developed in the original paper defining the HU approach (*11*). Results from the developed relationship are presented in **Figure 4**. The use of air temperature corrected to soil temperature was the technique implemented into the PLUS version of PRZM 3.12.

It was also clear that changes in soil water content affect pesticide degradation. However, the HU concept was not designed with soil xenobiotic degradation in mind. It is known that compound degradation occurs at an optimum soil water content, and a decrease or increase in water content from this would be expected to retard degradation. To account for daily changes in volumetric water content and the effect they would have on degradation, an adjustment to accumulating heat units needed to be made. Several approaches were attempted, including the use of a convex polynomial. In the original paper on the HU approach, a slope intercept concept was presented for moisture correction. Although the slope intercept concept worked well, the polynomial method proved to be less complex. A graphical representation of the two approaches can be found in **Figure 5**. For implementation of the PLUS version of PRZM3.12, the convex polynomial method was used.

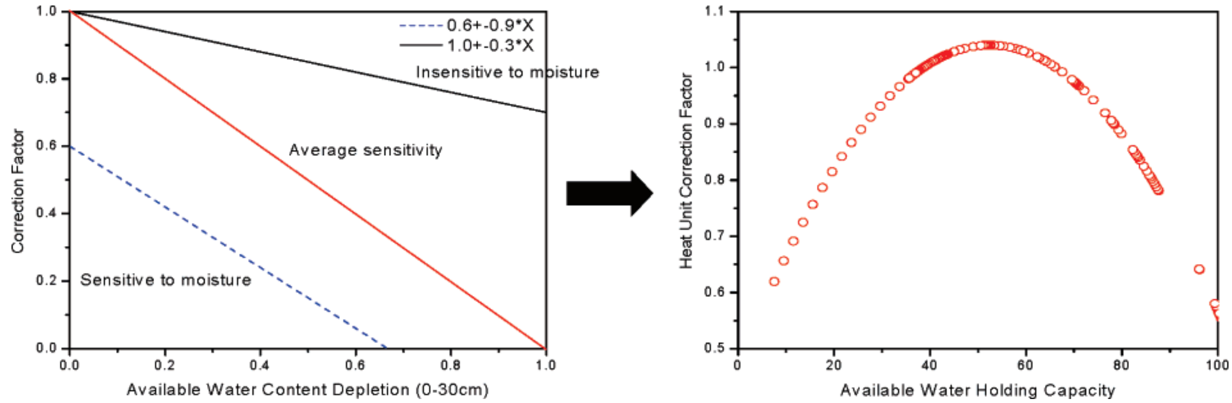

Figure 5. Comparison of the original heat unit moisture correction method to the method implemented into PRZM 3.12.

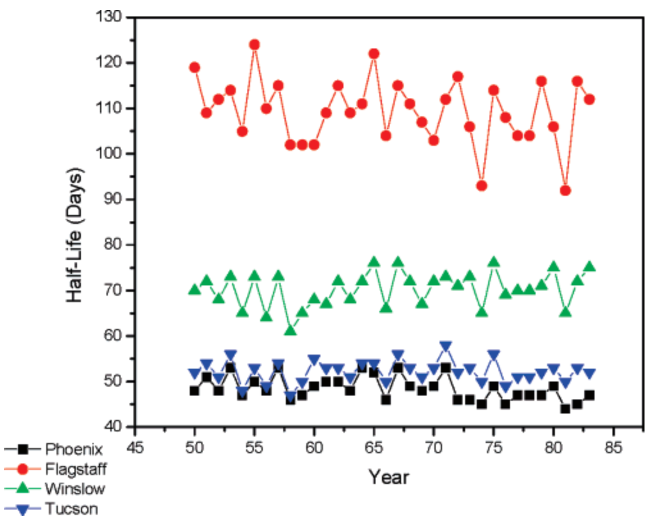

Figure 6. PRZM 3.12 calculated half-life values for each year of the model runs for the state of Arizona MLRAs.

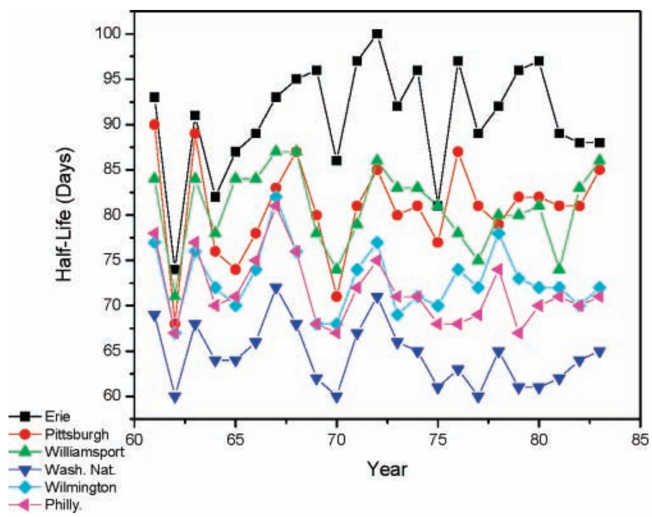

Figure 7. PRZM 3.12 calculated half-life values for each year of the model runs for the state of Pennsylvania MLRAs.

The final version of the accumulating HU method is presented in equations as

$$C_{1a} = 0.31313 - 0.0113 \times AT + 6.0379E{-}4 \times AT^2 + 2.67596E{-}6 \times AT^3 - 1.60536E{-}7 \times AT^4 + 8.7408E{-}10 \times AT^5 \quad (1)$$

$$C_2 = \left(\frac{\theta_{fc}\theta_v}{\theta_{fc}\theta_{wp}}\right) \quad (2)$$

$$C_3 = 0.46622 + 0.02188 \times C_2 + -0.000208638 \times C_2^2 \quad (3)$$

$$HU = C_{1a} \times C_3 \text{ using AT} \quad (4)$$

where AT is air temperature in °F, θ_{fc} is water content at field capacity, θ_v is actual water content, θ_{wp} is water content at wilt point, and HU is the daily heat unit amount.

Implementation of the HU Approach into PRZM 3.12. First, a representative field dissipation site must be selected (mid latitude) as well as the heat units required to obtain the field pesticide half-life. As an example, 1500 heat units might accumulate within the 60 days required to obtain one soil half-life at the site. Next, 1500 heat units would be entered into PLUS rather than the 60 day half-life. The actual half-life entered for each soil is then calculated by PRZM 3.12 on the basis of daily adjusting soil water content and meteorological conditions. Before PRZM 3.12 can start leaching scenario simulations, it must first calculate the soil specific half-lives and then enter the resulting half-life values back into the input files before starting the simulation model runs. For this analysis, soils from the states of North Dakota,

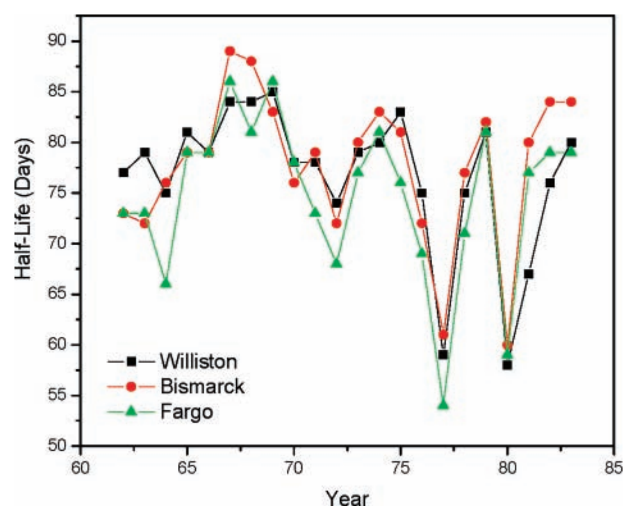

Figure 8. PRZM 3.12 calculated half-life values for each year of the model runs for the state of North Dakota MLRAs.

Pennsylvania, Georgia, and Arizona were run using the tool. The crop selected was grass/pasture, and the compound application rate was 0.56 kg of ai/ha. The soil partition coefficient (K_d) selected for the example compound used in this analysis was 0.3 L kg^{-1}. The accumulated HU value of 1500 (HUs) was used for the calculations, which is the basis for calculating and adjusting half-lives across MLRAs. All applications were made on April 15th of each model run year.

Table 1. Summary of MLRA Half-Life Values (Days) Calculated by PRZM 3.12

state	station	mean	minimum	maximum	range	median
Pennsylvania	Erie	90.8	74	100	26	92.0
Pennsylvania	Pittsburgh	80.8	68	90	22	81.0
Pennsylvania	Williamsport	80.9	71	87	16	81.0
Pennsylvania	Washington National Airport, Washington, DC	64.5	60	72	12	64.0
Pennsylvania	Wilmington, DE	72.8	67	82	15	72.0
Pennsylvania	Philadelphia	71.6	67	81	14	71.0
Arizona	Phoenix	48.5	44	53	9	48.0
Arizona	Flagstaff	109.4	92	124	32	109.5
Arizona	Winslow	70.1	61	76	15	71.0
Arizona	Tucson	52.3	47	58	11	52.5
North Dakota	Williston	76.7	58	85	27	78.5
North Dakota	Bismark	77.7	60	89	29	79.0
North Dakota	Fargo	74.8	54	86	32	77.0
Georgia	Chattanooga, TN	63.2	57	71	14	63.0
Georgia	Knoxville, TN	64.2	56	75	19	64.5
Georgia	Macon	54.7	50	59	9	54.0
Georgia	Athens	64.2	56	75	19	64.5
Georgia	Jacksonville, FL	51.8	48	59	11	51.5

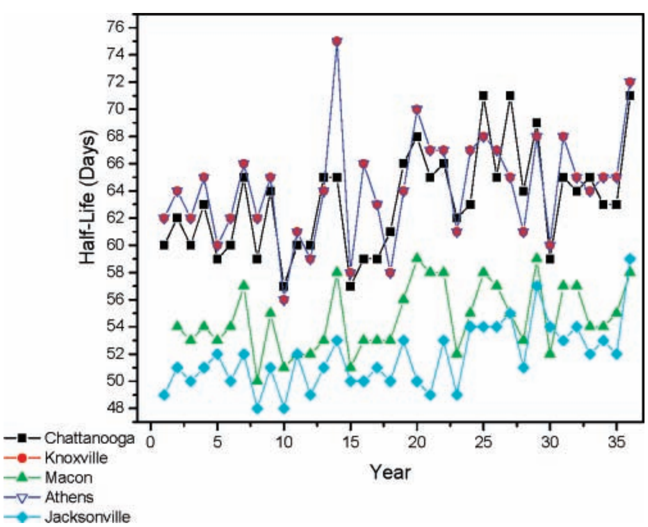

Figure 9. PRZM 3.12 calculated half-life values for each year of the model runs for the state of Georgia MLRAs.

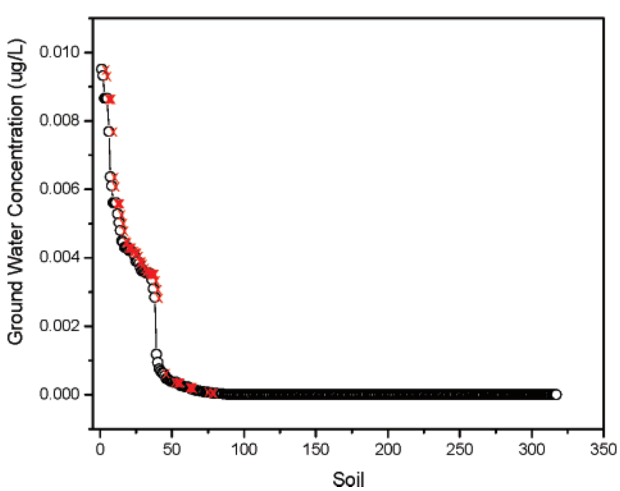

Figure 10. Groundwater concentration cumulative frequency distribution for the state of Arizona. The × markers are the MVTF soils.

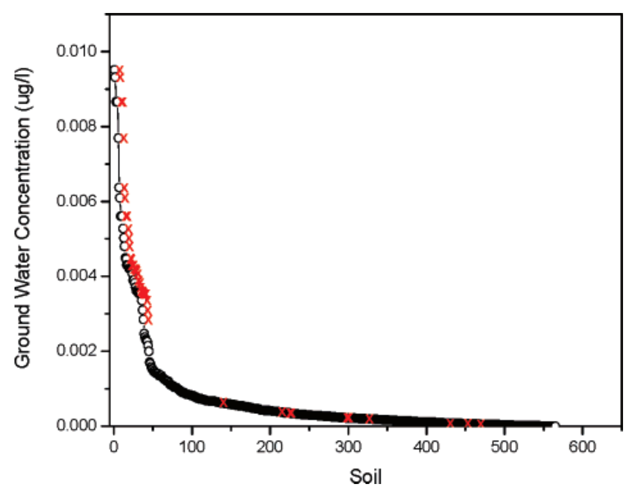

Figure 11. Groundwater concentration cumulative frequency distribution for the state of Pennsylvania. The × markers are the MVTF soils.

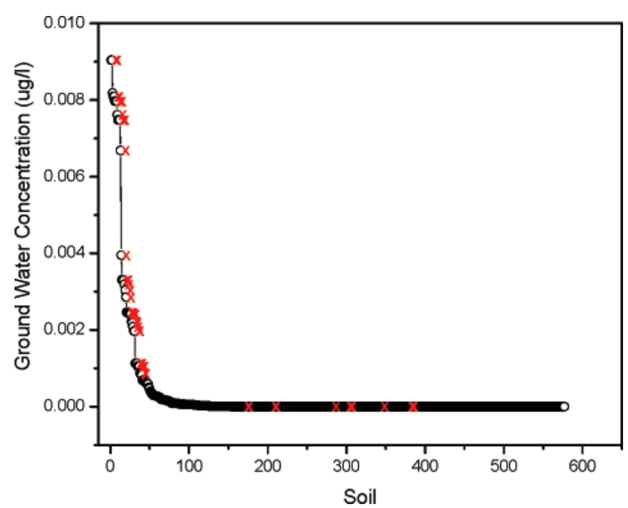

Figure 12. Groundwater concentration cumulative frequency distribution for the state of North Dakota. The × markers are the MVTF soils.

RESULTS AND DISCUSSION

The PLUS PRZM 3.12 output has been designed so that it allows the knowledgeable user maximum flexibility in deciding how final calculations can be done while providing full documentation of the input values. Standard PRZM3.12 output is generated (*12*), but additional output is also produced to facilitate further data analysis. For a detailed description of the output possible from the tool, the user's guide posted on the WEI Website should be consulted (*13*). Of specific interest are the ranges of pesticide half-life PRZM3.12 estimates using the

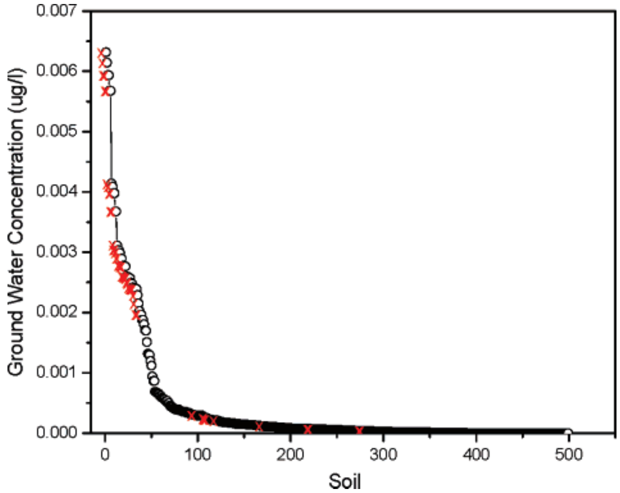

Figure 13. Groundwater concentration cumulative frequency distribution for the state of Georgia. The × markers are the MVTF soils.

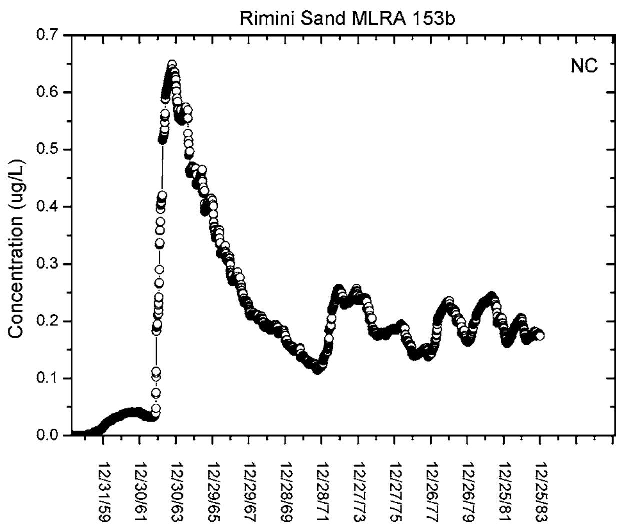

Figure 14. PRZM 3.12 output from the model for a single soil on a daily basis.

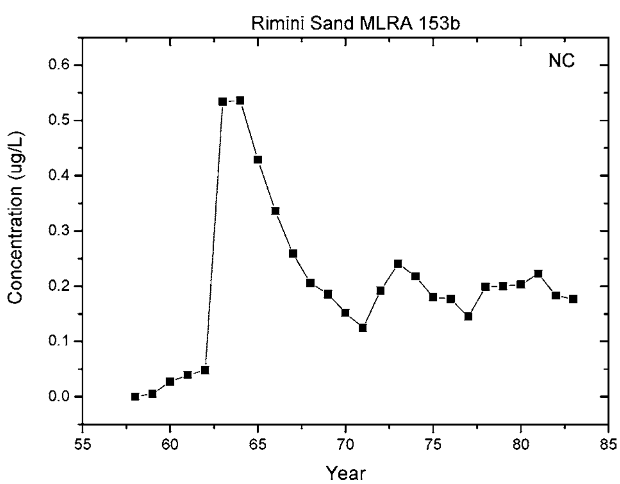

Figure 15. PRZM 3.12 output from the model for a single soil on an annual basis.

HU algorithm, and the resulting predicted variation in predicted concentrations in groundwater. The resulting groundwater concentration estimates are presented as a Cumulative Frequency Distribution and include the Model Validation Task Force

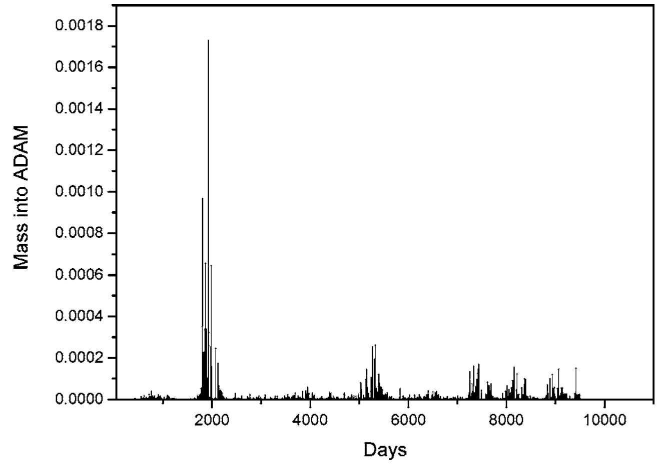

Figure 16. Mass generated by PRZM 3.12 passed to the ADAM groundwater model.

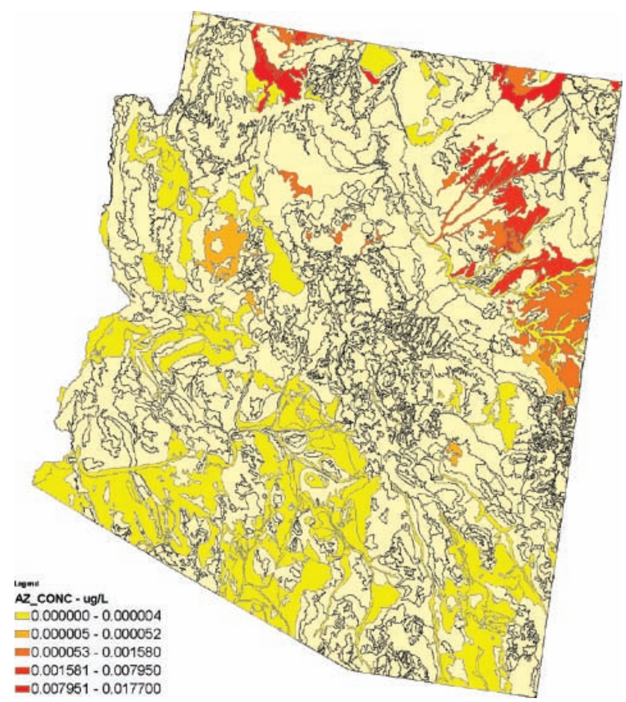

Figure 17. Spatial distribution of soil vulnerability for the state of Arizona.

benchmark soils. The predicted concentrations are also presented as GIS coverages so that the estimated spatial distribution of potential leaching can be evaluated.

Figures 6−9 display the pesticide degradation estimated for the MLRAs represented in each state. **Table 1** presents a summary of results from the data presented in **Figures 6−9** for the example compound. The modeled pesticide degradation rate ranged from a minimum of 44 days in Phoenix to a maximum of 124 days in Flagstaff. The largest range in half-lives was observed in both the Fargo and Flagstaff MLRAs at 32 days. The minimum range in half-lives was observed in both the Phoenix and Macon MLRAs at 9 days. The model provides results by soil series within each MLRA. The FEMVTF benchmark soils are also run alongside the state/MLRA soils. The FEMVTF soils represent sites selected following U.S. EPA prospective groundwater study guidance to be worst-case leaching areas. The inclusion of the FEMVTF soils as benchmarks allows the evaluation of how soils in a given state compare to soils with acknowledged high leaching potential.

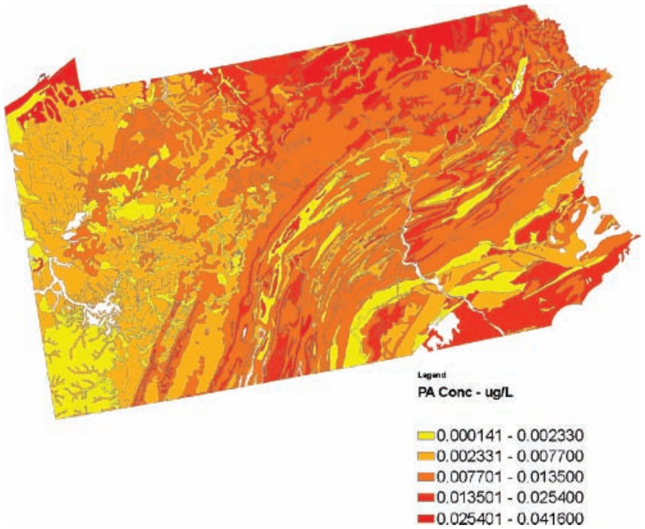

Figure 18. Spatial distribution of soil vulnerability for the state of Pennsylvania.

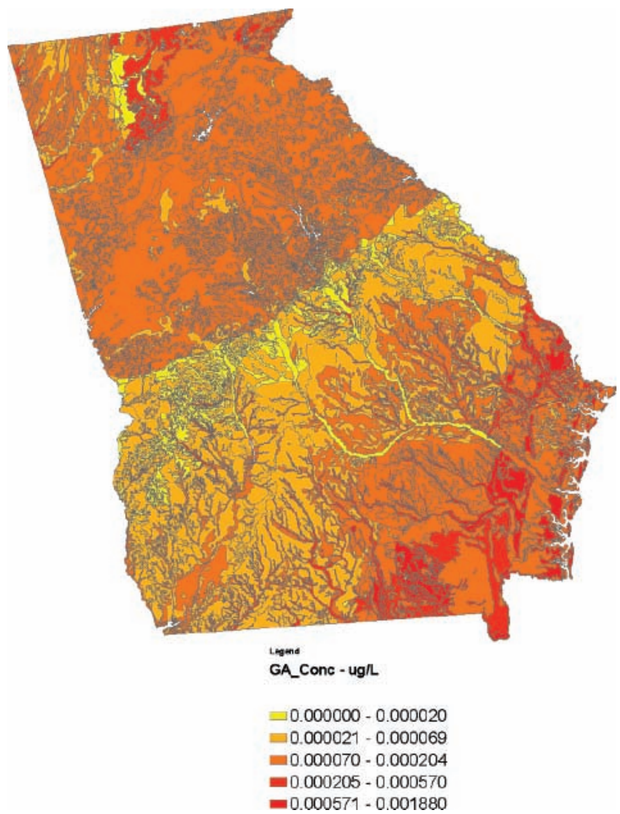

Figure 19. Spatial distribution of soil vulnerability for the state of Georgia.

Figures 10−13 present results from the 30−36 average year model runs presented as cumulative frequency distributions. The results present in these figures are the concentrations estimated at the bottom of the 4.6 m soil profiles and were calculated by taking the total mass leached over the entire model run period (30−36 years) and dividing it by the total volume of leachate. The model also provides estimated concentrations by year or by day. **Figure 14** presents output from the model for a single soil on a daily basis, whereas **Figure 15** represents the output from the model as an annual average for a single soil. In addition to calculating concentrations by the total mass leachate method, PLUS has the groundwater model ADAM coupled to it. ADAM allows the "aquifer" to be parametrized more effectively when compared to simply using the mass leachate method. ADAM

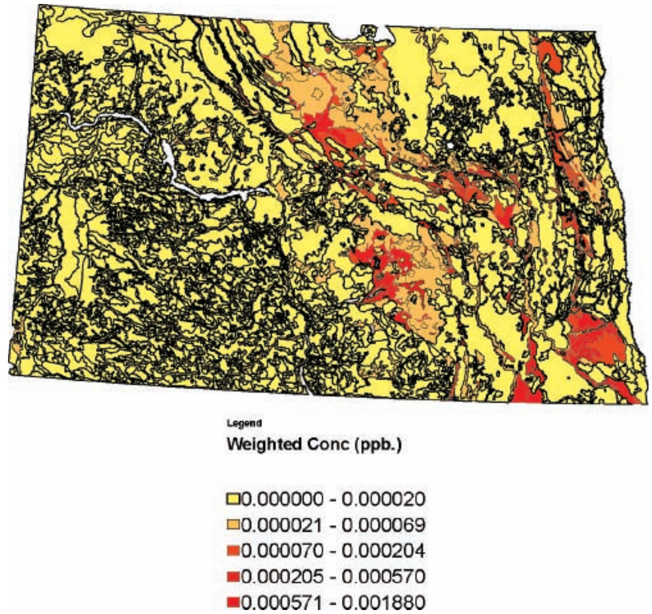

Figure 20. Spatial distribution of soil vulnerability for the state of North Dakota.

concentrations are normally lower than the ones obtained by the mass/leachate method due to dilution and further degradation. ADAM allows the inclusion of more realistic predictions of the concentrations expected from well sampling when compared to the simpler mass-leachate dilution method. **Figure 16** presents an example of mass being passed to the ADAM model by PRZM. The ability to create distributions of exposure concentrations allows the determination of percentile exposure potentials by soil series by region. Whereas the FEMVTF soils were calibrated to actual field study results, PLUS predictions can be sorted high to low to determine relative soil vulnerability.

PLUS output is easily linkable to commonly used GIS software such as ESRI ArcGIS, and therefore groundwater predicted exposure estimates can also be presented spatially. **Figures 17−20** display the spatial distribution of estimated groundwater concentration for North Dakota, Pennsylvania, Georgia, and Arizona and reflect the STATSGO level soil mapping units (polygons). Spatial distributions can be useful as an indication of how possible groundwater vulnerability may vary across the region for a given compound or use pattern. The spatial representation of potentially high exposure settings can be helpful for evaluation of management practices on those soils and for site selection if monitoring should be required.

In summary, the development of the PLUS tool is based on the most widely evaluated leaching model, PRZM 3.12. The tool incorporates widely known and evaluated soil and weather databases. The tool allows for exposure potentials to be estimated across long (30−36 years) historic weather records as well as examining specific annual exposure evaluations. PLUS output also allows exposure evaluation on a daily basis. The software provides convenient graphics displaying the regional scale probability of groundwater exposure potential, and the output may also be investigated spatially. The tool generates predictions based on individual soil series and regionally adjusts degradation rate using a field-based, well-understood method based on temperature and moisture factors. Model run times for states with many soils can take as long as 1 day, but the runs require no user interaction once the simulations are started. We believe that PLUS has proved to be a convenient and user-friendly proof-of-concept example of a tool for regional scale groundwater assessment that can greatly improve regulatory decision-making when compared with single fixed scenario evaluations or simpler national estimates based on regression relationships.

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