5194 *J. Agric. Food Chem.* **2007,** *55,* 5194–5198

JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY

Comparison of Leaching Predictions Based on PRZM3.12, LEACHP, and RZWQM98 Using Standard Scenario Modeling

SCOTT H. JACKSON*,† AND TAMMARA L. ESTES§

BASF Corporation, 26 Davis Drive, Research Triangle Park, North Carolina 27709, and Stone Environmental Inc., Stone Cutters Way, Montpelier, Vermont 05602

Regulatory agencies in the NAFTA region use ground water leaching models to help determine risks to ground water resources. The results of three models for leaching predictions are compared using a standard soil and weather scenario currently used by the New York Department of Environmental Conservation (NYDEC) to simulate the Riverhead soil found on Long Island, New York. The three models, PRZM3.12, LEACHP, and RZWQM98, were configured to simulate the behavior of two example molecules in corn, turfgrass, and bare soil. For the bare soil simulations, LEACHP and RZWQM98 predicted similar peak concentrations and timing of peak concentration. Depending on the dissipation rate of the molecule, PRZM3.12 predicted similar to reduced peak concentrations due to the delayed timing to reach the peak concentration. For the corn and turfgrass simulations, peak concentrations and timing to reach peak concentrations varied between the models due to differences in how each simulates plant growth and evapotranspiration.

KEYWORDS: Leaching; PRZM3.12; LEACHP; RZWQM98; ground water

INTRODUCTION

Groundwater in North America is a valuable natural resource that must be protected from deleterious human activities. To help assess the risk to these resources from crop protection products, exposure models have been developed to help predict and extrapolate compound behavior. However, even with the use of complex ground water modeling tools, assessing true ground water vulnerability can be difficult. Approaches to characterize ground water vulnerability have been the focus of a great deal of scientific discussion. There are aspects of ground water resource protection that are easily agreed upon, for example, that many shallow ground water resources have the potential for vulnerability. Researchers also agree that uncertainty is inherent in all vulnerability assessments. To determine if there is potential for ground water exposure, various approaches have been developed to assess vulnerability. Currently the regulatory community has focused on using either deterministic or regression models to predict shallow ground water vulnerability. Agencies using deterministic ground water models include the California Department of Agriculture (CDPR), the New York Department of Environmental Conservation (NYDEC), and the Canadian Pest Management Resource Agency (CDPR). All three of these agencies have chosen to use the leaching estimation and chemistry model (LEACHM) or LEACHP (1/03 release), which is the pesticide version of the model. LEACHP has been in use as a regulatory model for many years, but has not continued to be actively developed. LEACHP has various solute transport modes, but is run by the agencies using the Green-Ampt/Richards's equation mode. For further information about LEACHP, the user's guide can be consulted (*1*). The North American agencies implementing this model for regulatory evaluations use standard scenarios. This work will examine the NYDEC Riverhead soil series standard scenario in LEACHP (version) and compare those results to two other commonly used ground water models, the U.S. Environmental Protection Agency's (EPA) Pesticide Root Zone Model, version 3.12 (PRZM3.12) (*2*), and the U.S. Department of Agriculture's (USDA) Root Zone Water Quality Model, version 98 (RZWQM98) (*3*). The goal of this examination is to evaluate the usefulness of these other models in running the standard scenario. The PRZM3.12 model uses a capacity-based approach to handle soil profile flux. Like LEACHP, the RZWQM98 model uses a Green-Ampt/Richards's equation approach to handle soil profile flux, but offers many features compared to LEACHP to help more accurately determine flux. The focus of this research was to evaluate RZWQM98 as a surrogate for the currently implemented LEACHP model for regulatory purposes. PRZM3.12 has been included in the evaluation because it is the most widely evaluated model of its type.

EXPERIMENTAL METHODS

Two example molecules were used in the comparisons. The first example molecule was simulated in all three models running both a bare ground and a corn crop scenario, and a second molecule was simulated in all three models for both a bare ground and a turf crop scenario. A standard ground water vulnerability scenario has been developed and historically used by NYDEC. This standard scenario is based on the physical chemical properties of the Riverhead soil series,

* Corresponding author (e-mail scott.jackson@basf.com).
† BASF Corp.
§ Stone Environmental Inc.

10.1021/jf070276r CCC: $37.00
Published on Web 06/05/2007

Table 1. Summary of Soil Profile Physical Properties Used in the Standard Scenario

layer	% clay	% silt	% organic carbon	bulk density (kg/dm^3)	thickness (cm)
1	12.9	38.3	2.7	1.5	10
2	12.9	38.3	2.7	1.5	10
3	11.4	22.4	0.7	1.5	10
4	11.4	22.4	0.7	1.5	10
5	10.2	16.4	0.5	1.5	10
6	10.2	16.4	0.5	1.5	10
7	10.2	16.4	0.5	1.5	10
8	8.2	20.8	0.6	1.5	10
9	8.2	20.8	0.6	1.5	10
10	8.2	20.8	0.6	1.5	10
11	8.2	20.8	0.6	1.5	10

Table 2. Summary of the Meterological Data Used in the Standard Scenario

	rain[a] (cm)	ETo (cm)	air temp (°C)	wind (cm/s)	solar (Ly)
min	0	0.02	−21.15	0	32.05
max	11.4	1.75	39.5	1959.20	804.19
avg	0.26	0.36	13.21	450.49	318.43

[a] Recorded single-day events.

which can be commonly found in the Long Island region of the state. The soil has been described by the USDA Natural Resource Conservation Service (NRCS) as a "coarse-loamy, mixed, active, mesic Typic Dystrudepts". The Riverhead series consists of very deep, well-drained soils formed in glacial outwash deposits derived primarily from granitic materials. The series can be found on outwash plains, valley trains, beaches, and water-sorted moraines. The soil was first described in Suffolk County, New York, where the mean annual temperature is 10.5 °C and the mean annual precipitation is 120 cm. The thickness of the solum ranges from 50 to 100 cm. Depth to bedrock is typically >150 cm. The first horizon is described as an Ap horizon, indicating the presence of a weak plow layer. The soils can be found on a range of slopes, but typically are found on nearly level sites (about 2%). A summary of the physical chemical properties of the soil as implemented in the scenario can be found in **Table 1**. The weather data used in the scenario is a compilation of 10 years of varying weather conditions from the state of New York. The meteorological conditions used in the scenario are summarized in **Table 2**. Originally, the standard scenario was obtained from NYDEC. However, the file had to be modified to work with the currently available release of LEACHP (1/10/03 compile date). The required changes to the input file were structural rather than changes to the scenario itself.

The basis for parametrizing the other two models, PRZM3.12 and RZWQM98, is the LEACHP Riverhead scenario. Therefore, we transferred the data from the scenario as directly as possible into the other models based on the Riverhead scenario. Because both the LEACHP and RZQWM98 models use a Green-Ampt/Richards equation approach for calculating infiltration and solute movement, the input data transferred directly. PRZM3.12 uses a capacity-based approach for handling solute transport, and therefore field capacity (FC) and permanent wilting point (PWP) values were calculated by depth for each soil layer. To calculate the field capacity (FC) and permanent wilt point (PWP) values, a pedo transfer function method was used (*4*).

Two example molecules were simulated in each of the models. Each molecule's adsorption/desorption property was entered into LEACHP and RZWQM98 as a K_{oc} value. In PRZM3.12, adsorption/desorption was entered as a K_d value. To accurately use both K_d and K_{oc} values, the K_d value used in PRZM3.12 was calculated from the K_{oc} used in the other two models. The physical/chemical properties as well as application rates used for the simulation are summarized in **Tables 3** and **4**. An additional parametrization difference between LEACHP, PRZM3.12, and RZWQM98 is how the soil profile is discretized. Layers designated in a model may or may not directly correspond to the soil horizons. In practice, the layers in a model should correspond to the pedogenic horizons, but may not. LEACHP takes the total profile depth and divides it equally between the number of layers specified. Therefore, it is not possible to directly replicate exactly how a soil profile is described. In PRZM3.12 and RZWQM98, a soil profile may be discretized as the horizons are taxonomically described. Because we are making a comparison between models, the soil layering followed the method used in LEACHP rather than how the profile was described. In the case of PRZM3.12, the discretization method used was based on the recommendations of the FIFRA model validate taskforce (*5*). Degradation is also handled differently between the models. To account for degradation differences between RZWQM98, PRZM3.12, and LEACHP, we used a lumped half-life for the soil layer. In RZWQM we set degradation equal to the same half-life used in both the soil and water phases of LEACHP and PRZM. Mathematically, this degradation parametrization should allow the models to behave identically.

Table 3. Summary of Input Variables Used for Model Parametrization in the Turf Scenario

variable	value used	model used
soil adsorption/desorption	13 mL/g	all
soil dissipation time ($t_{1/2}$)	42 days	all
application rate	0.017 lb of ai/ac	all
foliar dissipation rate	35 days	PRZM/RZWQM
mowing cycle interval	7 days	RZWQM

Table 4. Summary of Input Variables Used for Model Parametrization in the Corn Scenario

variable	value used	model used
soil adsorption/desorption	18 mL/g	all
soil dissipation time ($t_{1/2}$)	10.1 days	all
application 1 rate	0.08 lb of ai/ac	all
application 2 rate	0.05 lb of ai/ac	all
foliar dissipation rate	35 days	PRZM/RZWQM

All three of the models allow a crop to be simulated. The difference between models is how much control the modeler has over the plant model and the complexity in plant simulation routine. PRZM3.12 and LEACHP have simple crop models. In this comparison, both bare soil and soil supporting turf grass or corn were modeled. Both models allow for the depth of rooting to be described, but the distribution of roots by depth may not be described. The extraction of soil solution via the evapotranspiration routine is weakly parametrizable (*6*−*8*). RZWQM98, in contrast, has the most developed crop modeling algorithm of the three models. RZWQM98 allows crops and roots to be parametrized using a standard, detailed method or by using the model's built-in QUICKPlant routine. For the corn parametrization in RZWQM98, the built-in corn scenario from QUICKPlant module was used. For the turf simulations in RZWQM98, the built-in QUICKTurf module was used to parametrize the grass simulation. The species modeled in QUICKTurf is Kentucky bluegrass. Because the original LEACHP scenario had root growth limited to a 30 cm depth, this was also used in both RZWQM98 and PRZM3.12. The turf was modeled to start growth on April 15th of each simulation year and to go dormant on November 1st. PRZM3.12 and RZWQM98 allow for simulation of mowing cycles primarily by changing plant height. When the models were run simulating turf, the plant height was adjusted every 2 weeks to mimic mowing cycles. Adjusting plant height to mimic mowing cycles in LEACHP was not possible. All three models were parametrized so that the soil profile was free draining.

For the corn the built-in QUICKPlant module was used in RZWQM98 to parametrize the corn simulation. In PRZM3.12 and LEACHP, parametrization was the same as for turf, because the plant parametrization is relatively insensitive in both models.

For bare soil simulation in all three models, plant parameters were turned off.

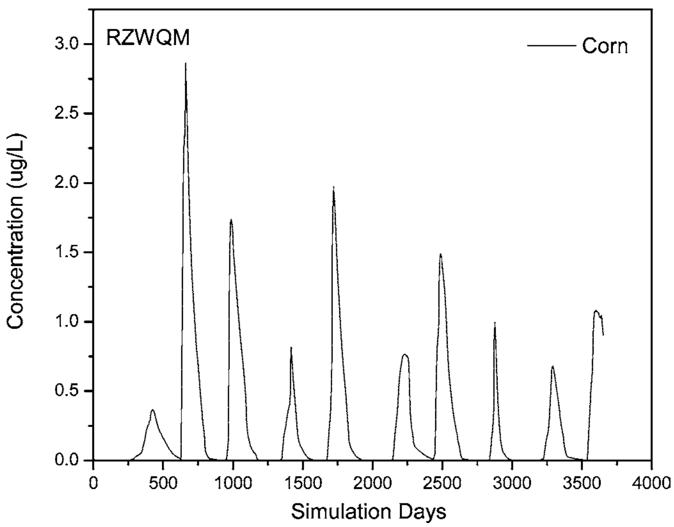

Figure 1. RZWQM98 exposure predictions for a corn crop. The plot is of pore water concentration flux at the bottom of the soil profile.

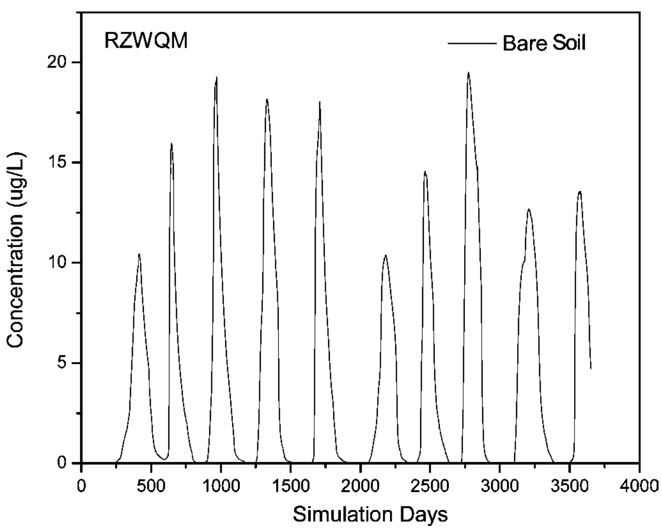

Figure 2. RZWQM98 exposure predictions for a bare soil. The plot is of pore water concentration flux at the bottom of the soil profile.

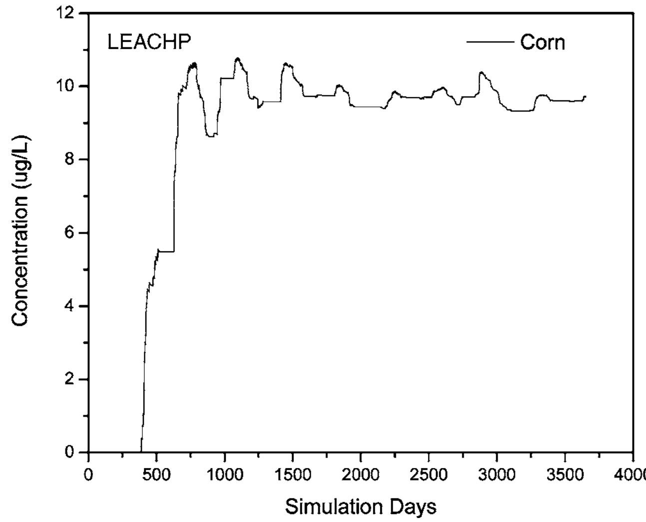

Figure 3. LEACHP exposure predictions for a corn crop. The plot is of pore water concentration flux at the bottom of the soil profile.

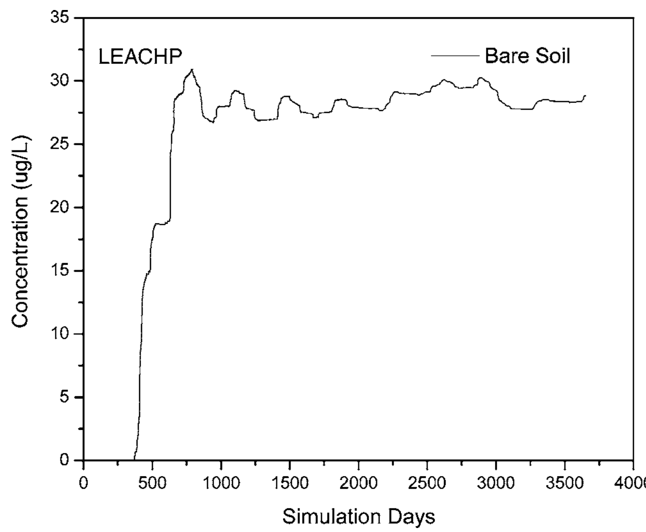

Figure 4. LEACHP exposure predictions for a bare soil. The plot is of pore water concentration flux at the bottom of the soil profile.

RESULTS AND DISCUSSION

Results from model runs are presented as graphs, which display compound concentration at the bottom of the root zone. Because the typical regulatory endpoint examined is the flux from the bottom of a predetermined rootzone depth, we have created graphs that reflect this result from each model simulation for bare soil, corn, and turf grass simulations.

The first set of comparisons used the first example molecule and both bare soil and corn crop. **Figures 1** and **2** display results from RZWQM98 configured for corn and bare soil, respectively. On the basis of this comparison it is evident that the inclusion of a crop reduced peak concentrations from about 20 μg/L to about 2.7 μg/L. **Figures 3** and **4** display results from LEACHP configured for the first example molecule with both corn crop and bare soil. On the basis of this comparison it is evident that the inclusion of a crop reduced peak concentrations from about 30 μg/L to about 11 μg/L. **Figures 5** and **6** display results from PRZM3.12 configured for a corn crop and bare soil. On the basis of this comparison, it is evident that the inclusion of a crop reduced peak concentrations from about 20 μg/L to about 5.5 μg/L. Principal reasons for the above peak concentration reductions between the bare ground and corn crop simulations are attributed to the increased removal of available soil water from the profile due to crop transpiration.

The second set of comparisons used the second example molecule and both bare soil and turf as the vegetative "crop". **Figures 7** and **8** display results from RZWQM98 configured for turf and bare soil, respectively. On the basis of this comparison, it is evident that the inclusion of a turf crop reduced peak concentrations from about 10 μg/L to about 6 μg/L. **Figures 9** and **10** display results from LEACHP configured for a turf crop and bare soil. On the basis of this comparison it is evident that the inclusion of a crop reduced peak concentrations from about 10 μg/L to about 8 μg/L. **Figures 11** and **12** display results from PRZM3.12 configured for a turf crop and bare soil. On the basis of this comparison, it is also evident that the inclusion of a crop reduced peak concentrations from about 4.5 μg/L to about 1.5 μg/L. As with the first set of comparisons, the principal reason for the above peak concentration reductions between the bare ground and turf simulations is attributed to the increased removal of available soil water from the profile due to crop transpiration.

In general, larger difference rootzone fluxex were observed in the corn scenario compared to the bare soil simulations for all three models than were observed in the turf and bare soil

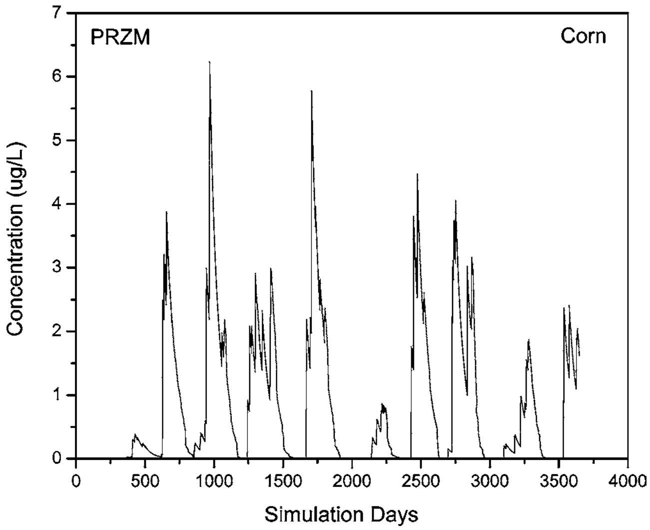

Figure 5. PRZM3.12 exposure predictions for a corn crop. The plot is of pore water concentration flux at the bottom of the soil profile.

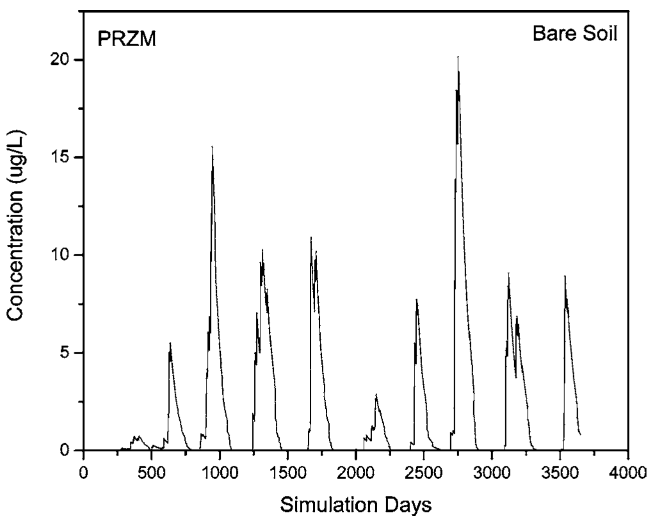

Figure 6. PRZM3.12 exposure predictions for a bare soil. The plot is of pore water concentration flux at the bottom of the soil profile.

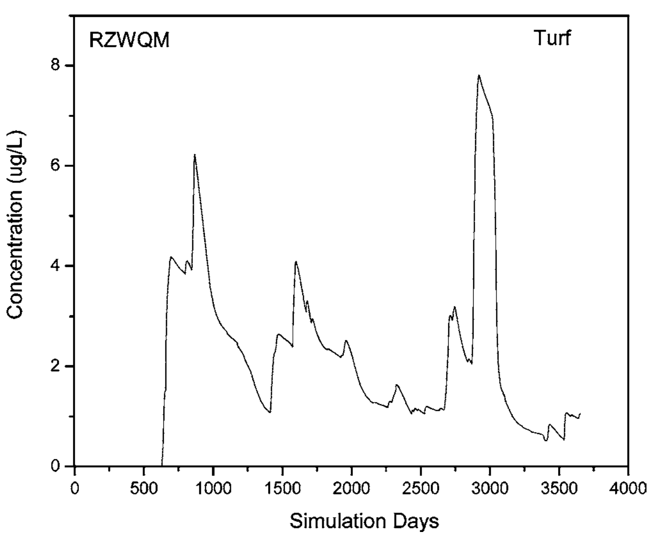

Figure 7. RZWQM98 exposure predictions for turf. The plot is of pore water concentration flux at the bottom of the soil profile.

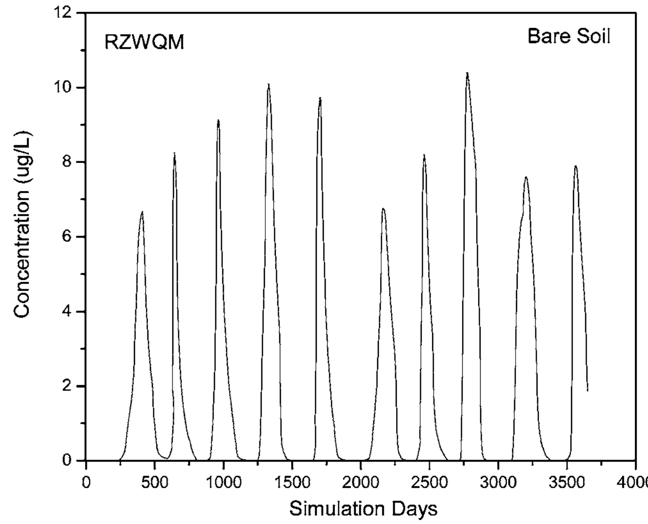

Figure 8. RZWQM98 exposure predictions for bare soil. The plot is of pore water concentration flux at the bottom of the soil profile.

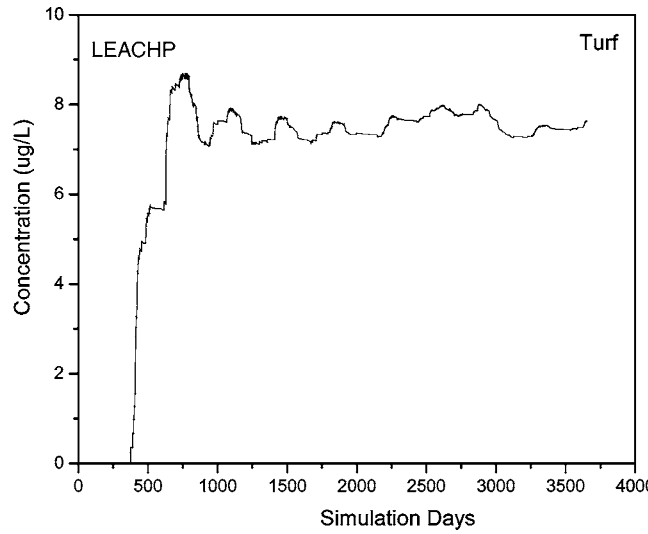

Figure 9. LEACHP exposure predictions for turf. The plot is of pore water concentration flux at the bottom of the soil profile.

comparisons. The example molecules used in the scenarios influence the difference found between corn and turf to some degree. One significant difference between all three models was the sophistication of the crop development component of each model. The RZWQM98 model has an advanced crop module (*3*), which in principle should lead to estimations that are more predictive when one is looking at the differences between cropped soil and soil without growing plants. Both PRZM3.12 and LEACHP have simple crop routines compared to RZWQM98 (*9*−*11*). Because the focus of this work was to evaluate standard scenario modeling, the parametrization difference between the bare soil and the cropped scenario involved turning the existing plant parametrization off or on.

When the flux patterns between models were compared, it became evident that the models behaved differently in how they produced flux patterns for the multiple years of model runs. Both RZWQM98 and PRZM3.12 produce a flux pattern that is a typical sawtooth pattern, whereas LEACHP produces a flux pattern atypical of those observed soil mobility experiments where a plume normally moves through the soil followed by leachate with little to no remaining residue [reference]. LEACHP produced a flux pattern that reached a peak concentration and then tended to remain at that concentration with little fluctuation for the duration of the simulation. This model behavior is not consistent with field experiments (*12*−*15*).

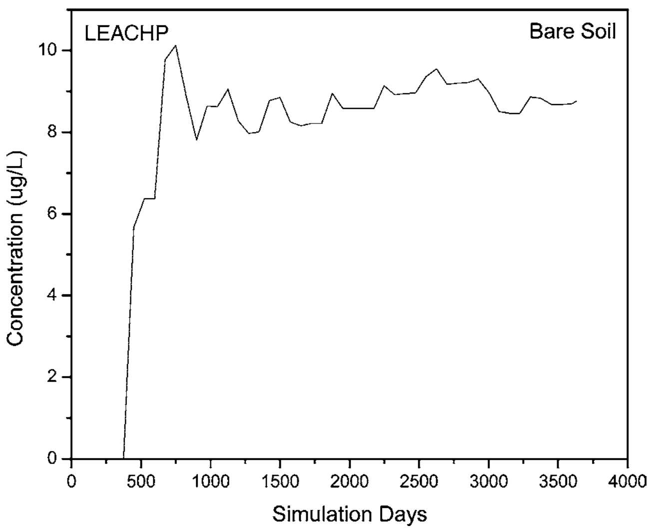

Figure 10. LEACHP exposure predictions for a bare soil. The plot is of pore water concentration flux at the bottom of the soil profile.

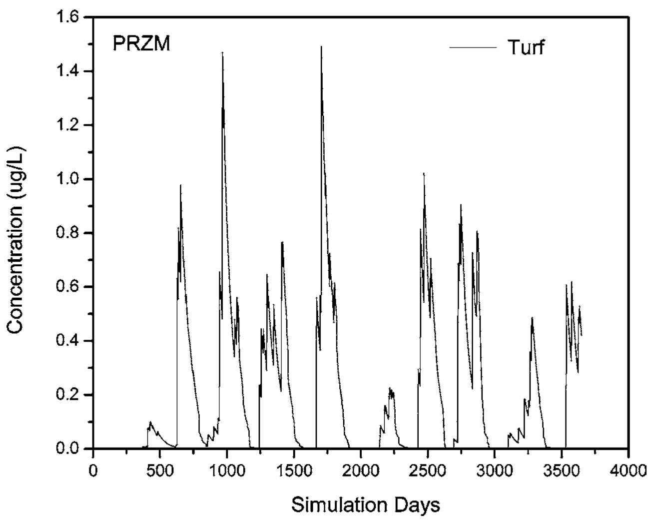

Figure 11. PRZM3.12 exposure predictions for turf. The plot is of pore water concentration flux at the bottom of the soil profile.

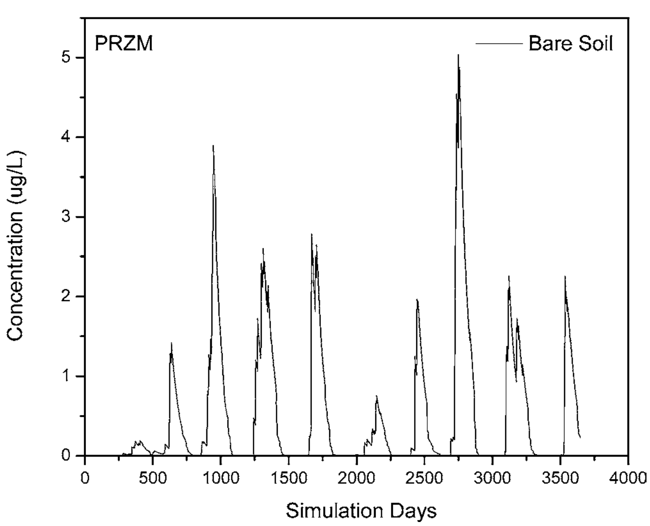

Figure 12. PRZM3.12 exposure predictions for a bare soil. The plot is of pore water concentration flux at the bottom of the soil profile.

In summary, three models were used to simulate the behavior of two example molecules in corn, turf grass, and bare soil. All three models produced similar peak concentrations for both vegetated and bare soil conditions. One difference that was evident between models was the flux patterns generated. PRZM3.12 and RZWQM98 produced flux patterns representative of what would be expected based on knowledge of compound behavior in field studies, whereas LEACHP produced a flux pattern that was not. On the basis of the limited modeling combinations and comparisons presented in this work, it would seem that both PRZM3.12 and RZWQM98 provided results more representative of our understanding of compound behavior under actual field conditions.

LITERATURE CITED

(1) Hutson, J. L. *LEACHM Model Description and User's Guide*; Flinders University: Adelaide, Australia, 2001.

(2) Carsel, R. F.; Imhoff, J. C.; Hummel, P. R.; Cheplick, J. M.; Donigian, A. S., Jr. *PRZM-3, Model for Predicting Pesticide and Nitrogen Fate in the Crop Root and Unsaturated Zones: Users Manual for Release 3.0*; U.S. EPA: Athens, GA, 1998.

(3) Rojas, K. W.; Ma, L.; Hanson, J. D.; Ahuja, L. R. RZWQM98 User's Guide. In *The Root Zone Water Quality Model*; Ahuja, L. R., Rojas, K. W., Hanson, J. D., Shaffer, M. J., Ma, L., Eds.; Water Resources Publications: Highlands Ranch, CO, 1999.

(4) Rawls, W. J.; Brakensiek, D. L.; Saxton, K. E. Estimation of soil water properties. *Trans. ASAE* **1982**, 81−2510.

(5) Russell, M. H.; Jones, R. L. Comparison of pesticide root zone model 3.12: leaching predictions with field data. *Environ. Toxicol. Chem.* **2002**, *21* (8), 1552−1557.

(6) Gardner, D. S.; Branham, B. E. Mobility and dissipation of ethofumesate and halofenozide in turfgrass and bare soil. *J. Agric. Food Chem.* **2001**, *49*, 2894−2898.

(7) Raturi, S.; Carroll, M. J.; Hill, R. L. Turfgrass thatch effects on pesticide leaching: a laboratory and modeling study. *J. Environ. Qual.* **2003**, *32*, 215−223.

(8) Roy, J. W.; Hall, J. C.; Parkin, G. W.; Wagner-Riddle, C.; Clegg, B. S. Seasonal leaching and biodegradation of dicamba in turfgrass. *J. Environ. Qual.* **2001**, *30*, 1360−1370.

(9) Ma, Q. L.; Hook, J. E.; Wauchope, R. D. Evapotranspiration predictions: a comparison among GLEAMS, Opus, PRZM-2, and RZWQM models in a humid and thermic climate. *Agric. Syst.* **1999**, *59*, 41−55.

(10) Wauchope, R. D.; Rojas, K. W.; Ahuja, L. R.; Ma, Q.; Malone, R. W.; Ma, L. Documenting the pesticide processes module of the ARS RZWQM agroecosystem model. *Pest. Manag. Sci.* **2004**, *60*, 222−239.

(11) Anapalli, S. S.; Nielsen, D. C.; Ma, L.; Ahuja, L. R.; Vigil, M. F.; Halvorson, A. D. Effectiveness of RZWQM for simulating alternative Great Plains cropping systems. *Agron. J.* **2005**, *97*, 1183−1193.

(12) Caron, J.; Jemia, S. B.; Gallichand, J.; Trepanier, L. Field bromide transport under transient-state: monitoring with time domain reflectometry and porous cup. *Soil Sci. Soc. Am. J.* **1999**, *63*, 1544−1553.

(13) Jackson, S. H. Comparison of calculated and measured volumetric water content at four field sites. *Agric. Water. Manag.* **2003**, *58*, 209−222.

(14) Kohne, J. M.; Gerke, H. H. Spatial and temporal dynamics of preferential bromide movement towards a tile drain. *Vadose Zone J.* **2005**, *4*, 79−88.

(15) Mikata, K.; Schnoder, F.; Braunwarth, C.; Ohta, K.; Tashiro, S. Mobility and degradation of the herbicide imazosulfuron in lysimeters under field conditions. *J. Agric. Food Chem.* **2003**, *51*, 177−182.

Received for review January 31, 2007. Revised manuscript received April 10, 2007. Accepted April 23, 2007.

JF070276R