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Modeling of the Leaching Potential of Mobile, Persistent Chemicals

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1. Background

The leaching potential of mobile and persistent chemicals was evaluated using the USEPA Pesticide Root Zone Model (PRZM 3.12b) using soil and weather data representing the conditions along the Ohio River in Washington County, OH.

PRZM is a one-dimensional, dynamic, compartmental model that can be used to simulate chemical movement in unsaturated soil systems within and immediately below the plant root zone. This daily time step model has two major components: hydrology and chemical transport. The hydrologic component for calculating runoff and erosion is based on the USDA Soil Conservation Service curve number technique and the Universal Soil Loss Equation. Infiltration is simulated by the use of generalized soil parameters, including field capacity, wilting point and saturation water content. Chemical transport is represented using a convection-dispersion equation.

The goal of this modeling effort is to estimate potential chemical concentrations in shallow groundwater following continuous application of a mobile and persistent chemical to the land surface. This work will permit estimation of potential groundwater concentrations as a function of chemical application rate (kg/ha/yr) and the rate of chemical degradation in soil.

2. Model inputs and Assumptions

The PRZM model requires four types of inputs in order to perform a leaching simulation:

- Chemical data
- Soil profile data
- Crop / agronomic data
- Climatic data

The following values were used for the various required input data:

2.1 Chemical data

Appl rate: For modeling purposes, it is necessary to specify the chemical application rate to soil (mass/area/time). The base case application assumed in this modeling work is 0.1 kg/ha/yr. Since the model

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cannot handle a continuous application, this loading is simulated as a series of 48 quarterly applications of 0.025 kg/ha, resulting in a semi-continuous application of chemical to the soil. This application frequency was selected because PRZM can only handle 50 applications and it is necessary to apply the chemical over an extended period of time to accurately simulate potential accumulation of chemical residues in the soil profile over time. The 48 quarterly applications result in twelve years of semi-continuous exposure. For estimating groundwater concentrations resulting from other application rates, it is important to note that the simulated concentrations are directly proportional to the application rate.

Sorption: $K_{oc} = 25 \text{ ml/g}$ (an assumed value, representative of a highly mobile chemical)

Half-life in soil: assumed values — 1 yr, 3 yr, 5 yr and 10 yr.

Uniform degradation was assumed throughout the soil profile. Typically, chemicals which are microbially degraded demonstrate slower rates of degradation with depth. For this simulation, since the degradation rates were already relatively slow, the additional effect of the degradation rate decreasing with depth was neglected.

2.2 Soil profile data

Information from geologic boring logs indicates the following basic stratigraphy in the area of interest:

<u>Depth interval (ft)</u>	<u>Textural description</u>
0 — 14	brown clay
14 — 27	brown clayey sand
27 — 34	brown sand
34 — 60	brown sandy gravel

The typical depth to shallow groundwater at the site of interest is 15 feet, indicating that the soil profile should generally be characterized as having a high clay content.

The USEPA soils database (DBAPE, based on Soils 5 soil profile data) was searched for high clay content soils in Washington County OH and the data for a Licking silt loam underlain by a high clay layer was selected for use in simulations. Based on the data in DBAPE and the PRZM manual, the properties of the selected soil profile are as follows:

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Table 1: Soil profile data for Licking silt loam (Hydrologic Group C)

Soil depth (cm)	Soil texture (sand/silt/clay%)	Bulk density (g/cm ³)	Organic matter (%)	1/3 bar (FC) moisture (cm ³ /cm ³)	15 bar (WP) moisture (cm ³ /cm ³)
0-30	silty loam (20 / 55 / 25)	1.40	2.5	0.33	0.17
30-170	clay (20 / 30 / 50)	1.50	1.0	0.42	0.28
170-340	clay (20 / 30 / 50)	1.50	0.7	0.42	0.28
340+	clay (assumed) (20 / 30 / 50)	1.50 (assumed)	0.2 (assumed)	0.42 (assumed)	0.28 (assumed)

In general, mean values were used for the reported soil texture, bulk density, organic matter and water contents. Soil data was not available beyond a depth of 340 cm so the values of the 170-340 cm layer were used for the 340+ layer, adjusting the organic matter from 0.7% to 0.2%.

A Licking silt loam is listed as a hydrologic group C soil which implies that this profile has a relatively low organic matter, is usually high in clay and has a minimum infiltration rate of 0.1-0.4 cm/hr under saturated conditions. This soil has a moderate rate of surface runoff (typically 5-15%) and is likely to temporarily pond water on relatively flat areas.

2.3 Crop / agronomic data

The presence of perennial grasses and/or brush was assumed, resulting in selection of the following runoff curve numbers:

Table 2: Runoff curve numbers selected for grasses / brush

Crop condition	Runoff curve number
fallow (winter)	86
cropping (spring / summer)	80
residue (autumn)	86

Curve numbers represent the tendency of precipitation to horizontally runoff from a soil surface rather than infiltrate the soil profile. These numbers range from 0 to 100 with higher numbers representing an increasing tendency to runoff. Curve numbers of 80 to 86 are appropriate for a Hydrologic Group C soil that is continuously vegetated with senescence of the grasses and brush over the winter and no spring cultivation.

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2.4 Climatic data

The closest available daily meteorological file is from McConnellsville, OH (~ 30 miles NW of the site of interest in Washington County, OH). This file consists of daily weather parameters for a period of 36 years, extending from January 1, 1957 to December 31, 1992. Daily data in the file include precipitation, pan evaporation and mean air temperature. The 36-year-average precipitation for this site is 1052 mm which agrees reasonably well with other long-term averages for the area (Parkersburg, WV: 976 mm, 1941-1970; Charleston, WV: 1035 mm, 1941-1970).

2.5 Calibration of hydrology

Based on the soil properties, the assumed curve numbers and the climatic data, two simulation cases were considered for the Washington County site: a "normal" recharge case and a "low" recharge case.

Annual average value simulated over a period of 36 years

Input

Precipitation: 1052 mm (~ 41 in)

Output

	<u>"normal" recharge case</u>	<u>"low" recharge case</u>
30% { Runoff:	113 mm (11% of precip)	113 mm (11%)
70% { Recharge:	272 mm (26% of precip)	190 mm (18%)
× Evapotranspiration:	643 mm (61% of precip)	726 mm (69%)
Change in water storage:	24 mm (2% of precip)	23 mm (2%)

3. Simulation results

The continuous application of a mobile, persistent chemical was simulated in PRZM as a series of repetitive quarterly applications extending over a period of twelve years, resulting in a total of 48 discrete application events. This approach was taken because PRZM can only handle a maximum of 50 application events. The simulation of a semi-continuous application of chemical over an extended period of time permits the estimation of long-term average concentrations in shallow groundwater.

The groundwater concentration at a depth of 5 m (equivalent to ~16 ft) was simulated by dividing the mass flux of chemical moving past this depth by the infiltration volume. The simulated concentration represents the concentration in soil pore water at a depth of 5 m and is equivalent to the concentration that is being loaded onto the top of the surficial aquifer at the study site. When a relatively uniform concentration is loaded into the aquifer over an extended period of time, this concentration will correspond reasonably well to concentrations measured in monitoring wells with relatively short screens (i.e. ~2 m) that intersect the top of the local water table.

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Two concentration values have been calculated for groundwater: the highest daily concentration simulated at a depth of 5 m (the peak concentration) and the highest long-term average value (a five-year-average concentration). Both values are directly proportional to the assumed annual application rate of 0.1 kg/ha. Groundwater concentrations resulting from alternative application rates can easily be estimated through linear adjustment of the reported concentrations.

Table 3: Simulated groundwater concentrations for a mobile, persistent chemical in Washington County, OH applied at 0.1 kg/ha/yr for 12 consecutive years ("normal" recharge case)

Degradation half-life (years)	Peak concentration at 5 m depth (ug/L)	Highest 5-yr-average conc at 5 m depth (ug/L)
1	0.11	0.067
3	5.2	4.4
5	11.6	10.4
10	22.0	20.4

The simulated concentration in shallow groundwater (5 m) is a function of the half-life of the chemical in the soil profile. Continuous application of 0.1 kg/ha of a mobile chemical with a relatively slow rate of degradation in soil (i.e. a soil degradation half-life of 5-10 years) can result in groundwater concentrations of approximately 10-20 ug/L. Less persistent chemicals are simulated to have significantly lower groundwater concentrations.

The peak concentration and the five-year-average concentration are reasonably similar indicating that the simulated application for a period of 12 years provided a reasonable estimate of a longer-term, steady-state concentration.

Over a period of five years, the groundwater recharge from an application site would result in approximately $5 * 360\text{mm}$ or 1800 mm of recharge, which would approximately occupy the top 3.6 m of the surficial aquifer (assuming 50% porosity). As a result, the 5-yr-average concentration is likely to correspond to the concentration measured in a monitoring well which provides samples of surficial groundwater.

For reference, the simulated results reported in Table 3 are also plotted in Figure 1. This figure clearly shows the similarity between the daily peak concentration and the 5-yr-average concentration. To a first approximation, the groundwater concentration is proportional to the chemical half-life.

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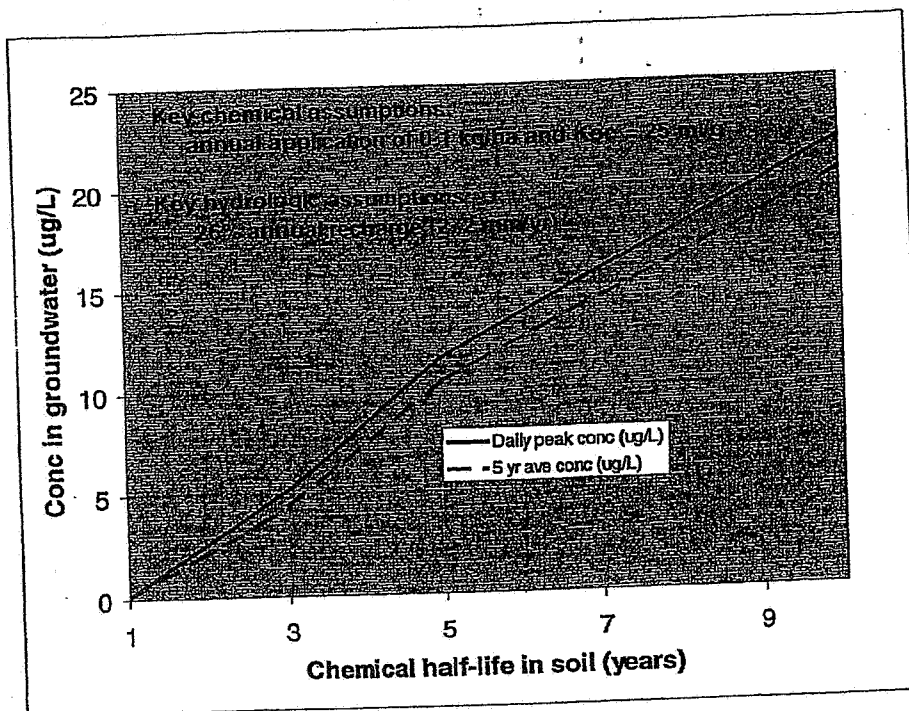


Figure 1: Simulated concentration of a mobile, persistent chemical in shallow groundwater in Washington, OH

Lower rates of recharge can result in lower concentrations for more rapidly degrading chemicals since this situation provides increased residence time in the unsaturated zone and additional time for degradation. However, for chemicals which degrade relatively slowly (i.e. those with half-lives greater than 5 years), the effect of increased residence time is outweighed by the reduced recharge volume. As a result, estimated groundwater concentrations for slowly degrading chemicals are slightly higher under conditions of low recharge, as shown in Table 4.

Table 4: Simulated groundwater concentrations for a mobile, persistent chemical in Washington County, OH using two recharge conditions, "normal" and "low" recharge (same application rate sequence as in Table 3)

Groundwater Recharge	Annual recharge (mm)	Chemical half-life in soil (years)	Peak concentration in groundwater (ug/L)	5-yr-ave conc in groundwater (ug/L)
Typical	272 (26%)	1	0.11	0.067
		10	22.0	20.4
Low	190 (18%)	1	0.023	0.012
		10	25.7	23.6

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4. Conclusions

Continuous application equivalent to 0.1 kg/yr of a mobile, persistent chemical can result in concentrations of 1 to 20 ug/L in shallow groundwater in a setting with a clay soil profile and 300-400 mm of groundwater recharge per year.

The simulated concentration in groundwater is a distinct function of the half-life of the chemical in the soil profile, with longer half-lives resulting in higher concentrations.

Lower rates of recharge will reduce the predicted concentrations for rapidly degrading chemicals but will slightly increase simulated concentrations for chemicals which degrade slowly.

The simulated concentrations are directly proportional to the application rate. All concentrations shown in this report correspond to an annual application rate of 0.1 kg/ha.

5. References

Carsel, R.F., J.C. Imhoff, P.R. Hummel, J.M. Chaplick, and A.S. Donigian, Jr., 1996. "PRZM-3, A Model for Predicting Pesticide and Nitrogen Fate in the Crop Root and Unsaturated Soil Zones: Users Manual for Release 3.0", USEPA, Center for Exposure Assessment Modeling.