SIMULATION OF ATRAZINE RUNOFF AND LEACHING FOR SOUTHWESTERN NEBRASKA FOR THE PERIOD 1986 TO 1999

D.D. Adelman

Adelman Associates, 4535 Y Street, Lincoln, Nebraska 68503-2344, U.S.A. (Emai: dadelma1@bigred.unl.edu)

ABSTRACT

Atrazine runoff and leaching will be simulated for cropland conditions in Nebraska based on the pesticide component of the model AGNPS and the soil moisture model developed at the University of Minnesota. This computer program will simulate an atrazine concentration occurring at the outlet of a hypothetical watershed and at three possible water table depths below the watershed. The objective of this project will be to determine the risk of excessive atrazine levels at the outlet and three water table depths for different farm management practices, soil moisture conditions, six topographic regions of Nebraska and at least two atrazine threshold concentrations that, if exceeded, a risk to the environment will be hypothesized to exist. Three pesticide fate and transport processes will be modeled with the program. Degradation will be simulated using first order kinetics. Absorption/desorption will be modeled assuming a linear soil-water partitioning coefficient. Advection will be based in part on the USDA-NRCS curve number method. The fate and transport processes for atrazine will be simulated using inputs that include degradation half-life, soil-water partitioning coefficient, and daily storm event rainfall depth. Daily rainfall data from the Automatic Weather Data Network (AWDN) of the University of Nebraska-Lincoln High Plains Climate Center will be used to, in part, compute the soil moisture conditions on a continuous basis from 1986 to 1999. After each rainfall event, the pesticide runoff and three subsurface pesticide concentrations will be compared to at least two different atrazine threshold concentrations. The concentrations that exceed these threshold values will be converted to a risk percentage.

Keywords: Adsorption, Advection, Atrazine, Degradation, Leaching, Monte Carlo Simulation.

INTRODUCTION.

The National Institute of Health recently published a report on the toxicological effects of atrazine on freshwater amphibians. One finding reported in the April 16, 2002, issue of the Los Angeles Times was that atrazine is an endocrine disrupter in frogs. Female tadpoles were put in a solution of water and atrazine. Atrazine was found to stop the production of estrogen in them. The male sex hormone testesterone predominated in these tadpoles and they started growing testes.

In Nebraska, there has not been a great deal of concern about atrazine contamination of water resources because atrazine has a moderate solubility and half-life. It is not very mobile in the environment and has a fast enough rate of degradation to not cause a great deal of alarm. However, from the author's recent attendance at a European pesticide conference, it was learned that one of atrazine's daughter products is much more soluble and refractory. Conversations with pesticide researchers from several European countries revealed that atrazine has been restricted to use only on such things as railroad right-of-ways and is not used in any agricultural pursuits in Europe. The Europeans have also learned that the daughter product is a carcinogen. This author is not aware of any restriction on atrazine use in Nebraska.

These concerns have prompted this proposed simulation of the risk of excessive atrazine levels in surface and ground water resources in Nebraska. The objective of this work will be to determine this risk of excessive atrazine levels at the outlet of a hypothetical watershed and at different water table depths in the watershed for different farm management practices; time series of daily rainfall at different weather stations; two threshold atrazine concentrations that, if exceeded, it is hypothesized that a risk to the environment exists; and six Nebraska topographic regions that will have at least one of the preceding weather stations located in them. This risk analysis will be based on, at a minimum, the USEPA maximum contaminant level (MCL) of three parts per billion for atrazine in drinking water, and a proposed modified atrazine maximum contaminant level that is being proposed for regulation of atrazine in light of the fact that atrazine may no longer be found to be carcinogenic to the drinking water consumer (Nebraska Department of Agriculture, written communication, 2002).

MODEL THEORETICAL BASIS.

Surface Runoff Component.

The pesticide runoff component of AGNPS models the transport processes advection, degradation, and dissolution/adsorption. The concentration of pesticide in the soil is computed with the equation (Young, et al., 1987):

$$C_i = AR_{eff}^* 1.12^* d/rho_b \tag{1}$$

Where,

 C_i =Initial concentration, AR_{eff}=Amount of pesticide that reaches soil surface,

D = Soil interaction layer depth, =10 mm, and

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 rho_b =Bulk density, =1.4 g/cm³.

Degradation of a pesticide is modeled with first order kinetics, or the equation:

$$C_t = C_i \exp(-0.693 t/t_{1/2})$$
 (2)

where: C_t =Soil pesticide concentration at time of runoff event, t =Time after pesticide application, and $t_{1/2}$ =Pesticide half life, (=25 days for atrazine (U.S. EPA web site)).

To compute pesticide adsorption/dissolution, the soil/runoff partitioning coefficient is calculated first with the equation:

$$K_d = K_{oc} * OM / 100 / 1.67$$
 (3)

 where:
 K_d
 =Soil/water partitioning coefficient,

 K_{oc}
 =Organic carbon/water partitioning coefficient, (=100 L/kg for atrazine (U.S.EPA web site)), and

 OM
 =Soil organic matter percent, (=2.0 percent.)

Solving Eq. 3 reveals that K_d is computed to be 1.20 for atrazine.

To compute the pesticide available for runoff, the following relation is used (Young, et al., 1987):

$$C_{av} = C_t \exp(I_{eff}^* d_s / (n + K_d^* rho_b))$$
(4)

 $\begin{array}{lll} \mbox{where:} & C_{av} & =& \mbox{Soil pesticide concentration available for runoff,} \\ & I_{eff} & =& \mbox{Effective infiltration,} \\ & d_s & =& \mbox{Assumed surface soil depth, (=0.1 mm (Sauer, 1998)), and} \\ & n & =& \mbox{Porosity.} \end{array}$

Normally, there is a linear relation between the pesticide concentration in runoff and the pesticide adsorbed in soil (Novotny and Olem, 1994), or the following linear relation can be used:

$$C_{\rm w} = C_{\rm av}/K_{\rm d} \tag{5}$$

where: C_w =Pesticide concentration in soil moisture.

To compute I_{eff} in Eq. 4, the potential retention is first computed with the curve number method (Young, et al., 1987) using the relation:

$$S = (1000/CN) - 10$$
(6)

where: S =Potential retention, and CN =Curve number.

CN is a function of four variables. Three of these can be identified from a table of curve number values for average antecedent moisture conditions. These three consist of land use, hydrologic condition of the soil surface and the percentage breakdown of four hydrologic soil groups. The SSURGO Soils data base (Nebraska Department of Natural Resources web site) has one of the four possible hydrologic soil groups assigned to each of the soil series polygons in most of Nebraska's ninty-three counties. This will allow computing a composite curve number for most counties for average antecedent moisture conditions where the composite value will be a weighted average based on area.

Antecedent moisture condition is the fourth factor in determining CN. CN(II) is for average conditions and will be initially computed as described above. CN(I) signifies dry conditions.

$$CN(I) = ((4.2CN(II)) / (10 - 0.58CN(II)))$$
(7)

If the previous five-day antecedent rainfall during the growing season is less than 1.4 inches, dry conditions will be considered to prevail. CN(III) signifies wet conditions.

$$CN(III) = ((23CN(II)) / (10 + 0.13CN(II)))$$
(8)

If the previous five-day antecedent rainfall during the growing season is greater than 2.1 inches, wet conditions will be considered to prevail. Daily rainfall data will be used to compute antecedent rainfall.

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Runoff for a storm can be computed with the equation:

$$Q = (P - .2*S)^2 / (P + .8*S)$$
(9)

where: Q =Runoff depth, and P =Rainfall depth.

 I_{eff} can then be computed with the relation:

$$I_{\rm eff} = P-Q \tag{10}$$

AGNPS does not directly model volatilization of pesticides in its pesticide runoff component. Rather than follow this approximate approach, this model will assume volatilization of atrazine in Nebraska cropland conditions is generally negligible.

Unsaturated Zone Component

Four processes are involved in contaminant transport in porus media: adsorption, advection, degradation, and dispersion. The process of dispersion is generally found to be negligible in the unsaturated zone due to low soil moisture conditions. Advection for the unsaturated zone is the rate at which soil moisture moves through it. Adsorption of pesticides to soil is incorporated into the unsaturated zone component by applying a retardation factor. Combining these relationships, the travel time for pesticides to be transported from the surface through the unsaturated zone to the water table will be calculated using the following relation (Lokke, 1992; and Stephens, 1996):

$$\mathbf{t}_{\rm wt} = (2 * z * \dot{\mathbf{E}}_{\rm v} * \mathbf{R} * \mathbf{D}) / (\mathbf{D}\mathbf{P}^*\mathbf{I}_{\rm eff})$$
(11)

where: t_{wt} =Travel time of pesticides through the unsaturated zone to the water table, t;

z =Midpoint depth of the unsaturated zone, L;

 \dot{E}_v =Volumetric soil moisture content of the unsaturated zone, 1;

DP =Decimal fraction of "I_{eff}" that becomes deep percolation (Dutcher, written communication, 2000), 1;

- D =Storm event duration, days; and
- R =Retardation factor, 1.

The volumetric moisture content, \dot{E}_v , will be calculated with the relations Gardner, 1958; Lopez-Bakovic and Nieber, 1989; and Warrick, 1974):

$$\dot{\mathbf{E}}_{\mathbf{v}} = \mathbf{n} * \mathbf{C}_{1} \tag{12}$$

where: \dot{E}_v =Volumetric soil moisture content, 1;

n =Unsaturated zone porosity, 0.425;

 C_1 =A dimensionless coefficient, 1; and

$$C_1 = ((alpha/K)*(((-DP*I_{eff}/D)/alpha)+c*exp(-alpha*z)))^{-N}$$
(13)

where: alpha=An empirical constant that varies from $0.000787-0.315 \text{ in}^{-1} (0.002-0.8 \text{ cm}^{-1})$; the

higher values are normally for coarse textured soils (Warrick, 1974), L^{-1} ;

K =Saturated hydraulic conductivity, 31.5 m/yr;

N =An empirical constant that varies from 1.5 to 4, (Lopez-Bakovic and Nieber, 1989);

- z =Midpoint of depth to the water table, L;
- c =A coefficient, L^2/t ; and

$$=((I_{eff}/D)+K)/alpha.$$
(14)

Table 1 shows values for saturated conductivity, alpha and porosity for six topographic regions of Nebraska.

Pesticide degradation in the unsaturated zone will be modeled assuming first order kinetics using the relation:

$$C_{wt} = C_w exp(-0.693 * t_{wt}/t_{1/2})$$
(15)

where: C_{wt} =Pesticide concentration at the water table, micrograms/liter.

Diffuse Pollution Conference Dublin 2003 **SIMULATION PROCEDURE.**

The time series of daily rainfall data allowed simulating runoff and leaching of atrazine each time a rainfall event occurred. After each simulation the pesticide runoff concentration will be compared to an atrazine threshold value or concentration. If it exceeds the value, a counter will be incremented by one. After the simulations have been completed, the counter will be divided by the total number of rainfall events for the year being simulated with this quotient being multiplied by 100 to give the risk of excessive atrazine levels in percent (Bogardi, et al., 1986).

For each rainfall event, the model will compute the concentration of atrazine in the soil using Eq. 1. Based on how much time has elapsed by the time the rainfall occurs, the model will compute the remaining atrazine concentration in the soil using Eq. 2. The model will use Eq. 4 to compute how much atrazine is sorbed to the soil particles. Using the soil water partitioning coefficient computed in Eq. 3, the model will calculate the atrazine concentration dissolved in the soil moisture using Eq. 5. This soil moisture concentration is the concentration in the runoff and also in the leachate. Eq. 11 will compute the time it takes for the atrazine to leach to selected depths below the surface where the water table could exist. This time period will then be substituted into Eq. 15 to compute the atrazine concentration left after degradation has occurred. This concentration will be compared to the atrazine MCL to compute the risk of excessive atrazine levels for different water table depths and time periods between atrazine application and the occurrence of a rainfall event.

RESULTS AND CONCLUSION.

The risk of atrazine levels exceeding the atrazine U.S. EPA MCL in runoff reaching surface water was computed for the AWDN, Champion weather station as shown in Figure 1. Note that the risk is trending upward through 1999. For the same location, risk results are also shown for atrazine risk to groundwater in Figure 2 for three water table depths of 5, 10 and 15 m. The champin location was picked, because the author has been involved in some work (Adelman and Dutcher, 2001) at this site in terms of the division of rainfall infiltration between plant uptake and deep percolation. The value for the variable "DP" in Eq. 11 was taken from this work.



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