Modeling Pesticide Transport Under Field Conditions

51.8001 (95-18)

.

# MODELING PESTICIDE TRANSPORT UNDER FIELD CONDITIONS

R. Zhang, A. J. Krzyszowska, G. F. Vance and R. D. Allen<sup>1</sup>

## ABSTRACT

The impact of pesticides on groundwater quality was studied in a two-year field experiment to determine the movement and fate of two pesticides, picloram and dicamba, in a rangeland soil. Computer models were used to simulate pesticide transport under field conditions. Soil water content and pesticide concentrations were utilized to validate the mathematical models and to describe field-scale transport processes. The computer models were applied to simulate various physico-chemical processes in layered soils, including infiltration due to rainfall and irrigation, evaporation, root uptake, convection, dispersion, adsorption, and degradation. The computer models provided reasonable predictions of average water flow and solute transport under field conditions. However, it was very challenging to simulate the three-dimensional transport processes due to the soil heterogeneity and spatial variability. Keywords: Numerical models, Pesticide transport, Soil heterogeneity

## INTRODUCTION

Pesticides used extensively in agricultural and rangeland soils have the potential for leaching into the soil/substrata environment resulting in the possible contamination of groundwater. Many pesticides have been detected in water supplies throughout the United States; pesticide contamination of water supplies has become a national issue (Moody, 1990). Some pesticides, such as dicamba and picloram, have been listed by the EPA for restricted use due to their high potential for leaching in soils and for their persistence in groundwater (U.S. EPA, 1987). Very few studies have had direct applications in semi-arid and arid states, where a combination of persistent or mobile pesticides and their use on extensive areas of rangeland and irrigated crops may potentially lead to groundwater contamination.

Modeling is increasingly being used as a tool for evaluating the transport and fate of pesticides in soil-water systems. An extensive review of pesticide simulation models was performed by Wagenet and Rao (1990). These models were evaluated and categorized according to their purpose and complexity as research, screening, management and instructional models.

The focus of this study was to use computer models to simulate pesticide transport and fate in semi-arid and arid agricultural and rangeland soils. Data from a field experiment were used to validate various computer models. Predictions of solute transport based on computer models were compared with the experimental data.

<sup>&</sup>lt;sup>1</sup>Department of Plant, Soil and Insect Sciences University of Wyoming, Laramie, WY 82071-3354.

# MATERIALS AND METHODS

A two-year field experiment was conducted during 1993 and 1994, at the Agriculture Experimental Farm, University of Wyoming. Two pesticides, picloram and dicamba, were applied at different application rates. Soil solutions were collected by applying soil water collectors. Neutron probe access tubes were installed to estimate water flux and moisture profiles. The hydrological conditions of the experimental site were checked by measuring soil water using a neutron probe before and after irrigations. Soil and water samples were analyzed to determine the concentrations of picloram and dicamba. Soil samples collected from the study site were used for standard batch adsorption studies. Adsorption isotherm parameters for the pesticides were calculated from the Freundlich equation. Soil hydraulic properties, such as soil water retention and hydraulic conductivity, were also determined from the soil samples. Saturated conductivity in the field was measured using the auger-hole method and ring infiltration test.

Two numerical models, LEACHP (Hutson and Wagenet, 1992) and SWMS\_2D (Simunek et al., 1992), were used to simulate water flow and pesticide transport under field conditions. LEACHP is a one-dimensional finite difference model, while SWMS\_2D is a twodimensional finite element model. Both can be used to simulate water flow, root uptake, and solute transport in variably saturated soils. The chemical processes simulated by the models include convection, dispersion, diffusion, adsorption, and first- and/or zero-order decay. Physical and chemical parameters required by the models were obtained from the field and laboratory experiments, and batch studies (Krzyszowska et al., 1994). Meteorological data, such as rainfall and evaporation data, were obtained from a weather station nearby the experiment site.

#### RESULTS

<u>Modeling Results of LEACHP</u>: LEACHP was used to simulate the average pesticide movement in the soil profile. The modeled profiles were assumed one-dimensional two-layer soil columns. LEACHP simulated water flow processes of infiltration, redistribution, and drainage of soil water, incorporating information of irrigation, rainfall, and evapotranspiration. Solute transport processes simulated with LEACHP included convection, dispersion, molecular diffusion, decay, non-linear adsorption, and reaction. As shown in Fig. 1, the concentration distributions simulated by LEACHP had a relatively close agreement with the measured mean concentration profiles in both the general shapes and in the magnitude of concentration peaks. However, the modeling results became less comparable with the measured data as the depth increased.

<u>Modeling Results of SWMS\_2D:</u> A two-dimensional model, SWMS\_2D, was also used to simulate the average pesticide concentration and transport in the soil profiles. Again, the three-dimensional field was simplified as a one-dimensional problem. Figure 2 compared the simulated breakthrough curves with measured picloram concentrations vs. time at the depths of 15 and 60 cm. The simulated results were comparable with the measured data at the 15 and 30 cm depths, while the simulated results became less satisfactory as the depth increased.



Figure 1. Measured and LEACHP-simulated picloram concentration distributions at the depths of 15 and 60 cm.



Figure 2. Measured and SWMS\_2D-simulated picloram concentration distributions at the depths of 15 and 60 cm.

Because of soil heterogeneity, it is expected that the dispersivity may be a scale-dependent variable with travel time and travel distance. We used two approaches to model the scale-dependent problem. First, we used different dispersion values at different depths. At a shallow soil depth, the travel time of solute should be longer than that at deeper soil; therefore, a larger dispersivity value was used. Second, we treated the dispersivity as a function of simulation time and a decreasing function with depth. Such numerical strategies resulted in a significant improvement in the simulation results.

## DISCUSSION AND SUMMARY

LEACHP is a relatively simple model which can be used to simulate one-dimensionalproblems. The model is comprehensive enough to describe most of transport processes of water flow and solute movement in soils. Simulation results using LEACHP were in a general agreement with the field measured data. Nevertheless, the one-dimensional model may oversimplify multidimensional physical problems.

SWMS\_2D can be used to simulate two-dimensional problems. Therefore, spatial variability of hydraulic properties are readily incorporated into the simulation processes. Simulated results can be significantly improved if spatial information on hydraulic properties are available. Unfortunately, detail hydraulic data are usually rare. Thus, SWMS\_2D does not necessarily provide better results than LEACHP.

Modeling strategies were utilized to take into account the scale-dependent hydrodynamic dispersion. Preliminary modeling results illustrate a high degree of spatial variability in pesticide movement. Hydraulic conductivity was found to have the greatest effect on modeling pesticide transport.

#### REFERENCES

τ

Hutson, J.L. and R.J. Wagenet. 1992. LEACHM. version 3. New York State College of Agriculture and Life Science. Cornell University, New York. pp.8-13.

Krzyszowska, A.J., R.D. Allen, and G.F. Vance. 1994. Assessment of the fate of two herbicides in a Wyoming rangelands soil: column studies. J. Environ. Qual. 23:1051-1058.

Moody, D.W. 1990. Groundwater contamination in the United States. J. Soil Water Cons. 45:170-179.

Simunek, J., T. Vogel, and M. Th. van Genuchten. 1992. The SWMS\_2D code for simulating water flow and solute transport in two-dimensional variably saturated media. U.S. Salinity Lab. Research Report No. 126.

U.S. Environmental Protection Agency. 1987. Health Advisory, Office of Drinking Water.

Wagenet, R.J. and P.S.C. Rao. 1990. Modeling pesticide fate in soils. In Pesticides in the soil environment - SSSA Book Series, no.2. F. Cheng (ed.). SSSA, Madison, WI. pp:351-399.