A COMPARATIVE STUDY OF MATHEMATICAL MODELS FOR MIGRATION OF PESTICIDES IN SURFACE AND SUBSURFACE WATERS

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INTRODUCTION

Development, validation, and application of mathematical models for evaluating fate and transport of pesticide in the environment have received considerable attention during recent years. Mathematical modeling provides a conceptually valid and meaningful approach to integrate environmental properties and chemical processes affecting ecological and/or human health. Additionally, modeling results can be used by Federal and State Regulatory Agencies to support registration decisions or generally planning decision-making efforts.

A part of this comprehensive management-oriented modeling process is the simulation of transport and transformation of pesticides in agricultural watersheds. A number of models have been developed during the last decade and are used widely as predictive tools for assessing the impact of pesticides on surface and groundwater quality. Usually these models are used as screening tools to evaluate a new pesticide or an existing one used in a specific agricultural area which may pose an environmental problem. The models are also useful as management tools for assessing the effects of agricultural management practices on non-point source pollution control.

In this study, comparisons between two well known pesticide loading models are performed. Model predictions are compared for a number of parameters, including surface runoff, soil erosion, and mass transport of two herbicides in surface runoff and in the soil profile. Given the ability of both models for potential use for environmental risk assessment problems, historical data were used in order to estimate frequency distributions of the pesticide mass reaching the edge of the field and leaching from the crop root zone.

MODEL DESCRIPTIONS

The Pesticide Root Zone Model (PRZM) was developed by the U.S. Environmental Protection Agency (Carsel et al., 1984) for pesticide registration decisions and is based on the compartmental representation of the soil profile. The Groundwater Loading Effects of Agricultural Management Systems Model (GLEAMS) (Leonard et al., 1987; Davis et al., 1990) is an extension of the U.S. Department of Agriculture CREAMS model (Knisel, 1990) and is designed to evaluate various management scenarios and practices that affect potential pesticide transport in the surface runoff and through the plant root zone. PRZM and GLEAMS can simulate the transport of pesticides from agricultural areas in surface runoff (in water and on eroded sediment) and also in percolating water. However, it should be noted that the models were developed for field scale or small agricultural watershed problems and should not be used for stream or lake basin scale modeling.

Both PRZM and GLEAMS include runoff, leaching and erosion mechanisms that move the pesticide from the application point to the boundaries of the field. The dynamic processes in both models can be categorized in three cycles: a. the hydrologic cycle which includes rainfall, surface runoff, infiltration, soil moisture, evapotranspiration and percolation to the groundwater, b. the sediment cycle which includes sediment washload as a result of rainfall, c. the pesticide cycle which includes transport through vertical zones in the soil column, partitioning between water and particulate phases, and degradation/ decay processes.

Although the general conceptual basis for both models is similar, there exist differences in their components. For more detail and complete description of each model, the reader is referred to the given references.

MODELING PROCEDURE

The processes simulated by the models include runoff, erosion, and pesticide transport. The first step in assessing soil loss and pesticide transport is to establish a water budget. In regard to this, the model abilities to simulate observed monthly surface runoff water were tested. The site chosen in this study is a small single watershed located in the Southern Piedmont Conservation Research Center near Watkinsville, Georgia. The area of the watershed is 1.29 hectares with drainage patterns converging to a central draw. The soil types range from a sandy clay loam to loam, with the major soil being Cecil sandy loam. The average depth to the groundwater table is 12 m. Detailed hydrological and chemical transport monitoring was conducted over three planting periods. The field monitoring program was a joint effort of the U.S. Environmental Protection Agency and the U.S. Department of Agriculture and was designed to provide a database for the conceptual development of operational models describing pesticide and nutrient transport from agricultural lands. Measured data include runoff, evaporation, soil water content, precipitation, and concentration in surface runoff and at seven depths in the soil profile for four widely used herbicides: atrazine, paraquat, cyanazine and 2,4 D. In this study data for only two of the above pesticides (atrazine and paraquat) were used as input to the models. These data were obtained from Smith et al. (1978) who also discuss the experimental design and sampling procedures in detail. Additional weather information is obtained from NOAA data base stored at the Athens EPA Research Laboratory.

Although no attempt for model calibration, in the sense of a typical model calibration process, has been undertaken, models were partially calibrated using soil water content and monthly surface runoff.

RESULTS AND DISCUSSION

The measured and simulated monthly runoff at the edge of the watershed in terms of water depth versus time are given in Figure 1. As shown in that figure, the results compare well. However, for some months, there are differences between the measured and calculated data and also between the calculated results. This may be attributed to the hydrologic water budget formulations used by the models. For instance, rainfall intensity, duration and distribution influence runoff values, but these effects are not incorporated in the hydrologic approaches used by the models.

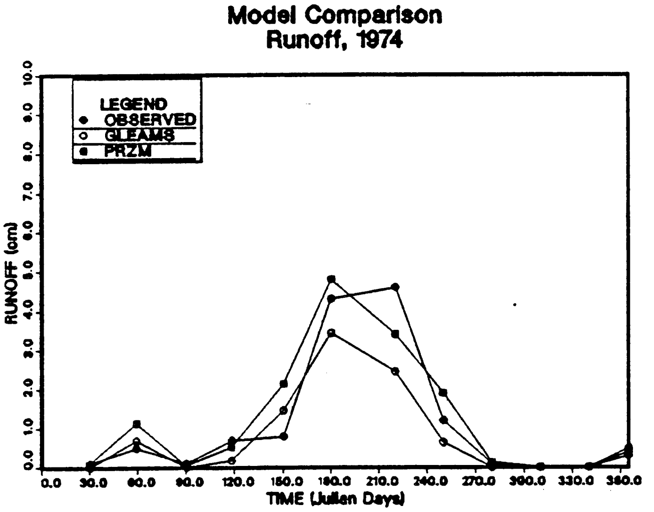

FIGURE 1. Model Comparison for Runoff Calculation.

Figure 2 shows the sediment results as amount of eroded soil in kg/ha versus time. For evaluating sediment results, the standard error (SE) and the coefficient of variation (CV) have been calculated. Values for SE and CV for GLEAMS and PRZM are 11.55 and 0.074 and 27.72 and 0.18 respectively. This indicates that the GLEAMS results are closer to the observed data than PRZM. This is due to the fact that PRZM does not have a channel component in the erosion cycle. Therefore, channel processes such as deposition and transport are not considered. On the other hand, GLEAMS results indicate channel deposition and therefore sediment yield at the edge of the field is less than overland sediment yield.

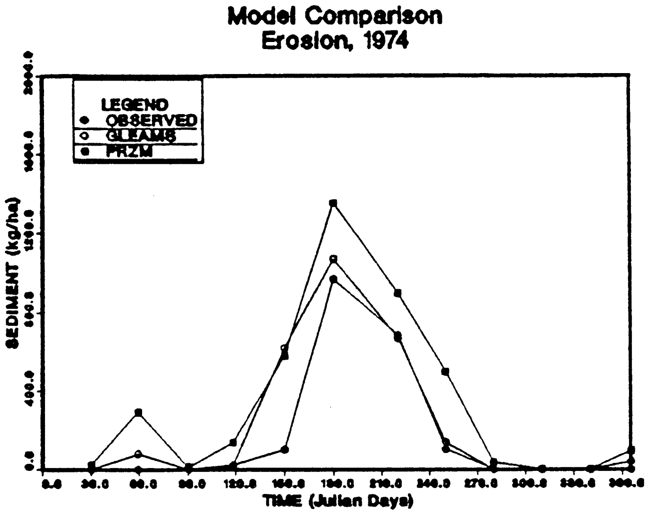

FIGURE 2. Model Comparison for Sediment Calculation.

The amount of sediment eroded from the watershed usually has a characteristic relationship with the value of runoff. Figure 3 shows these relationships for measured and simulated data. Both models work well for runoff values of close to 1 cm runoff and above; below 0.2 cm, both models overestimate erosion; between 0.2 and 0.7 , GLEAMS is better than PRZM.

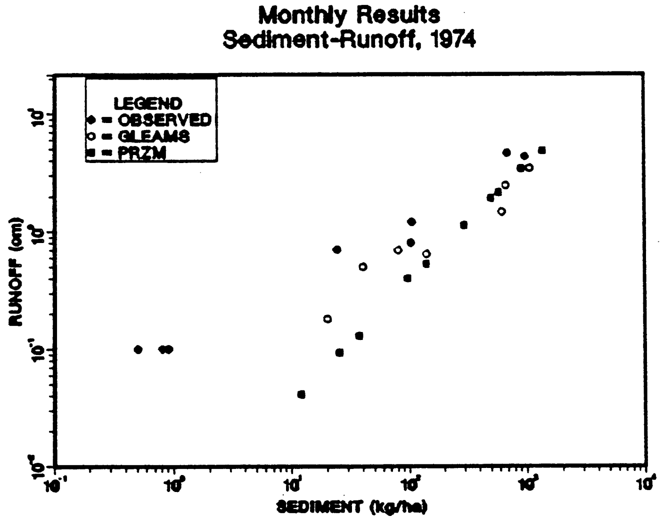

FIGURE 3. Predicted and Measured Sediment–Runoff Relationships.

The calculated and measured values of the vertical distribution of atrazine in the soil for three different dates after its application are given in Figures 4, 5, and 6. Although there are differences between the measured and simulated values, in general, these differences are not considered significant. It is important to note that both models have shown the same behavior concerning the following point: the observed data indicate that atrazine decays rapidly prior to the first rainfall event following its application, and then decays slowly after this first event. This type of degradation cannot be simulated explicitly by the models. The user may run the models for two different periods (before and after the first rainfall event) with different degradation rates.

For atrazine and paraquat simulations in runoff, both models slightly overpredicted pesticide amount during May 1974 and under-predicted during the next months. This is due to that both models have overestimated runoff and erosion for May. Additionally, atrazine shows a tendency to increase its sediment associated phase over time after its application. Again, both models could not predict this behavior, and this underestimated the adsorbed phase. This could be due to the equilibrium single-value linear isotherm assumption, which is used in the adsorption/desorption calculations by both models. However, the sediment associated amount is on the order of 10% or less of the total amount; therefore we can consider that both models can predict well the weakly adsorbed pesticides.

The results for pesticide predictions indicate that the existing models concepts and algorithms concerning pesticide decay and adsorption-desorption mechanisms have a good predictive capability, especially when they are used for typical environmental risk problems. For screening level assessments for which concentrations estimates are required, order of magnitude accuracy is the generally accepted criterion for environmental concentrations for exposure assessments (US EPA, 1982). However, more sophisticated and mechanistic algorithms would increase model capabilities, performance and usefulness, especially when the outputs of these models are used as inputs to aquatic fate models.

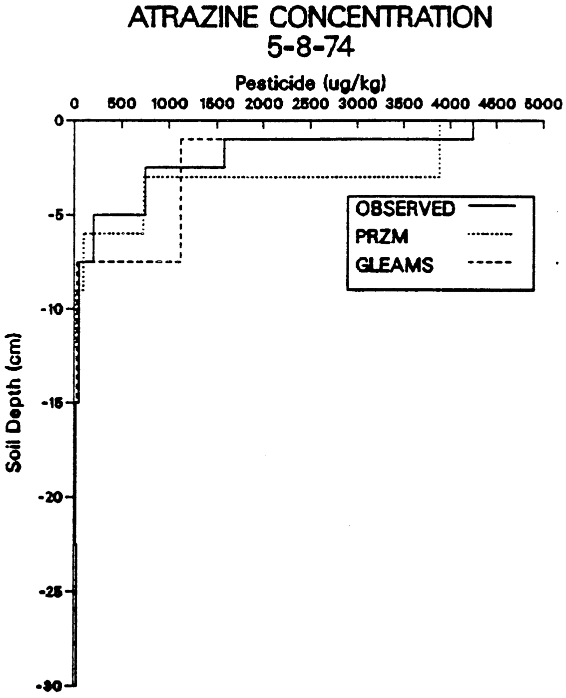

FIGURE 4. Predicted and Measured Pesticide Concentration.

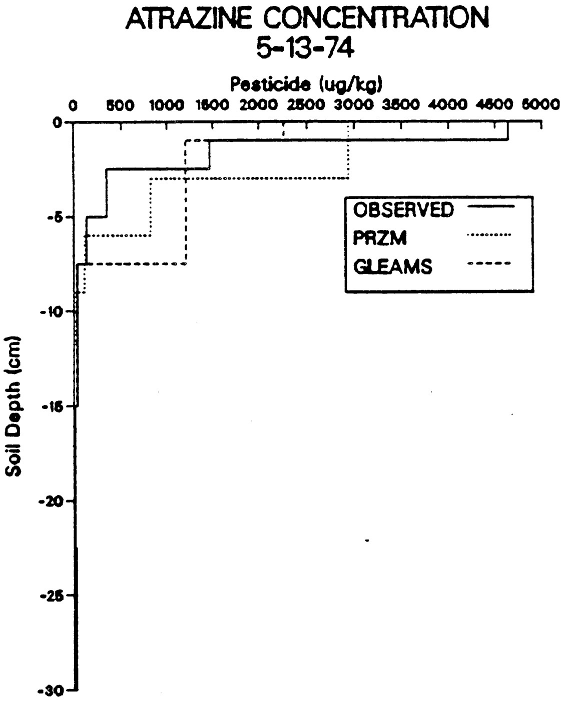

FIGURE 5. Predicted and Measured Pesticide Concentration.

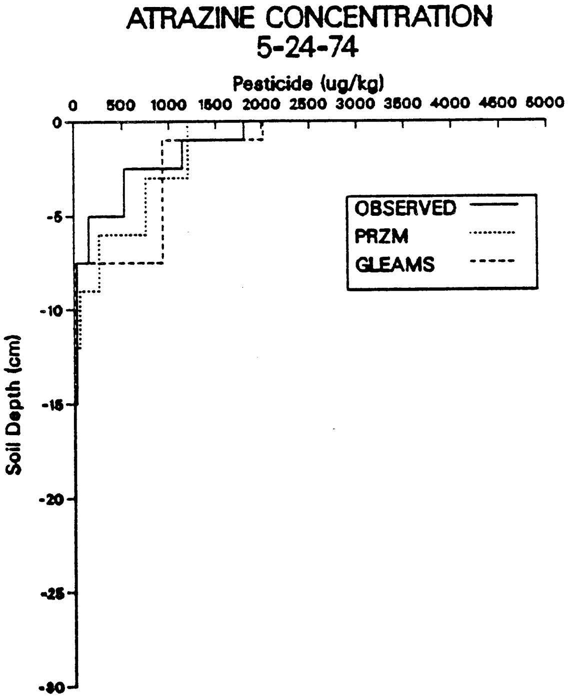

FIGURE 6. Predicted and Measured Pesticide Concentration.

CONCLUSIONS

The comparative study of the models showed that the simulated results are well within the order of magnitude of the measured data, which generally is required in the exposure assessment modeling process. In the same context, field averaged conditions are usually of interest, rather than spatial dynamic concentrations. Given the above, both models have shown predictive capability and utility as screening tools used for pesticide evaluation. However, in the applications of these models, their limitations should be considered. Based on the results of this study, these limitations have been discussed with emphasis in the differences between the predictions of the two models.

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This paper reports the results of research only. Mention of a pesticide does not constitute a recommendation for use by the US EPA. Mention of trade names or commercial products is for information purposes only and does not constitute endorsement or preferential treatment by US EPA.

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