



# Department of Pesticide Regulation

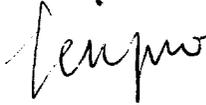


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## MEMORANDUM

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SUBJECT: EVALUATION OF ENVIRONMENTAL MODELS FOR ASSESSING  
SURFACE WATER CONTAMINATION BY PESTICIDES

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### Introduction

The contamination of surface water has received increased attention due to the recent adoption of total maximum daily load (TMDL) regulations. The fundamental difference of the TMDL approach from previous water quality management concepts is its requirement to address nonpoint source pollutions. In California, off-site movement of pesticides with runoff from nonpoint sources such as agricultural land and urban areas has been identified as a major transport pathway that caused the widespread contamination of surface water in the state's major rivers and tributaries (Foe and Sheipline, 1993; Kratzer, 1998; Panshin et al., 1998; Domagalski et al., 2000). As the lead state agency for pesticide regulation, the Department of Pesticide Regulation (DPR) is responsible for protecting surface water resources from pesticides, and thus fulfilling the goals of TMDLs.

The environmental fate and transport of contaminants, whether from point or nonpoint sources, are affected by many factors related to soil properties, land use, management strategies, contaminant properties, and climate. Field investigations exploring these relationships are limited in space and time; yet the interplay of soil-water-vegetation-climate in determining contaminant transport sometimes may be obscure and difficult to observe over short spatial and time scales. This is particularly true for nonpoint source pollutions because they are highly dispersed in the environment. In addition, the lack of the capability to manipulate liberally the environmental parameters regulating contaminant transport also restricts the transport scenarios that a field study can explore.

The limitations of conventional field methods in investigating the environmental fate and transport of contaminants have led to the development and use of simulation models. Due to the rapid advance and availability of high-speed computers in recent years, modeling has become a popular approach for investigating environmental problems. Although abstract in nature, simulation models are built upon the fundamental principles and empirical relations that are well established or tested. As a result, modeling, when exercised properly, provides a cost-effective, yet scientifically rigorous framework to assess contaminant transport in a prompt manner.



The purpose of this paper is to describe the concepts and methods of major environmental models that are formulated to simulate pesticide movement, in particular, runoff potential from the field, and to highlight the features and limitations of these models and thus to ascertain their proper application to field transport problems. This document is intended to be used as a practical guidance for potential model users, and discussion on algorithms is minimized. Our focus is on major process-based simulation models that are suitable for addressing pesticide transport under agricultural settings.

### **Overview of Models**

There is a wide selection of model options for predicting off-site movement of pesticides into surface water. In general, two major modeling approaches can be recognized. They are regression analysis and process simulation. The regression approach predicts concentrations or loads based on the statistical relationship of contaminant transport and a set of known predictor variables. The most simplistic form of regression analysis probably is the popular rating-curve technique, which relates loads directly to flow rate or volume (U.S. EPA, 1973; Huber, 1980; Tasker and Driver, 1988). Recently the U.S. Geological Survey (USGS) developed a more complex statistical model called SPARROW (Spatially Referenced Regressions on Watershed Attributes) to quantify stream loads based on characteristics of contaminant sources and watershed attributes (Smith et al., 1997). Regardless of its sophistication, however, the regression approach can only predict means, and thus is incapable of providing time-series information. The reliability of this approach is dependent on a large degree on the representativeness and quality of the original source data that enter into the regression. In general, regression analysis is only suitable for contaminants that are widely monitored and have a large data set of historical results.

Process simulation using conceptually based mathematical models represents the mainstream approach in environmental modeling. These conceptual models are developed to simulate physically transport processes occurring in the environment. With respect to pesticide contamination, most such models were developed to address pesticide movement in agricultural watersheds. Table 1 (attached) is a summary and overview of major watershed models that are widely used for water quality assessment. For easy reference, the features and capabilities of each model were presented based on several key simulation functions: in-stream flow, overland flow, groundwater flow, mixed land uses, management practices, chemical movement, and vegetation dynamics. It should be noted that others incorporate some of the simpler models. For example, ARM (Agriculture Runoff Model) is incorporated by HSPF (the Hydrological Simulation Program-Fortran), and the latter is incorporated by BASINS (Better Assessment Science Integrating Point and Nonpoint Sources).

Among the models listed in Table 1, GLEAMS (Groundwater Loading Effects of Agricultural Management Systems) and PRZM (Pesticide Root Zone Model) are probably the most widely used simulation models designed for simulating pesticide transport at the field scale.

GLEAMS is particularly suitable for studying pesticide transport with runoff and erosion. It employs a sophisticated algorithm in the estimation of sediment yield during runoff, accounting for detailed land surface characteristics such as the presence or absence of ridges, furrows, channels, etc. For mixed land uses, SWAT (Soil and Water Assessment Tool) is probably the most versatile among these models, allowing simulation of runoff and percolation in both urban and agricultural areas. SWAT also has a comprehensive management operation package dealing with agricultural activities such as tillage, irrigation, graze/harvest, etc.

HSPF is also a comprehensive model capable of simulating hydrological and transport processes for both urban and non-urban land uses. HSPF is highly recommended and widely used by hydrologists and hydraulic engineers. It has superior water quality routines for sediment erosion and pollutant interactions. But unfortunately the program lacks the feasibility of describing vegetation dynamics and management operations, and therefore is only of limited use in evaluating runoff quality for agricultural settings.

The major advantage of conceptual over regression models is their capability of simulating routing processes on a continuous time basis and their flexibility in describing management options. These features are important for evaluating specific pathways of pesticide transport and impacts of site-specific agricultural activities. However, no single model can adequately represent all possible agricultural management systems and activities. Limitations and uncertainty are an inherent part of modeling techniques. Following is an elaborated evaluation of several selected conceptual models that are of particular relevance to DPR goals. To help understanding these models, case studies were presented where possible to illustrate the type of scenarios that the model may apply to.

## **GLEAMS**

Model description and applicability: The GLEAMS model was developed to simulate pesticide or nutrient movement under different climate, soil, crop, and management conditions.

The model was evolved from an earlier version of the field model CREAMS (Chemicals, Runoff and Erosion from Agricultural Management Systems) to allow simulation of pesticide transport within and through the plant root zone in addition to transport in surface runoff from a field.

GLEAMS uses a conceptual representation of watershed hydrologic and transport processes by assuming homogeneous conditions of land use, soils, and precipitation. Surface water runoff and sediment erosion are estimated based on the U.S. Department of Agriculture (USDA)-Soil Conservation Service (SCS) curve number method and a modified Universal Soil Loss Equation, respectively. The model tracks movement of pesticides with percolated water, runoff, and

sediment. The simulation results provide daily, monthly, annual or storm event-based water and chemical loadings at the bottom of the root zone and the edge of the field. Runoff and sediment can be directly routed into a farm pond or impoundment if needed.

GLEAMS permits the investigation of effects of varying chemical and watershed properties and management options on transport, and thus is best suited to assess consequences of farm level management decisions on water quality. GLEAMS can provide estimates of the impact of management systems, such as planting dates, cropping systems, irrigation scheduling, and tillage operations, on the potential for chemical movement. Irrigation and chemical application rates, methods, and timing can be altered to test whether it is possible to reduce root zone leaching or surface runoff. Multiple applications of up to 10 different pesticides can be simulated simultaneously for periods of up to 50 years. The model also considers pesticide metabolites produced by sequential first-order reactions and plant uptake of pesticides. Pesticide application methods simulated include soil surface application, soil incorporation, soil injection, foliar application, or chemigation. Compared to other similar models that predict leaching and runoff, a major strength of GLEAMS is its flexibility to account for detailed local soil and land conditions in the runoff and leaching processes. The detailed description of channel and overland flow in the erosion/sedimentation subroutine is considerably advantageous for incorporation of field-specific ridges and furrows into the accounting algorithm.

Parameter requirements: The formulation of GLEAMS consists of four major components: hydrology, erosion, pesticide transport, and nutrient transport. Besides climatic data, the parameters required to drive GLEAMS are listed in Table 2 (attached). The hydrology component accepts input data related to the description of soil layers and properties, runoff curve number, and vegetation growth. This information is used to calculate water balance and redistribution with infiltration, percolation, evapotranspiration (ET), and runoff. The erosion component provides estimation of sediment yield, thus, requires parameters describing surface water flow profile and those parameterizing the universal soil loss equations. The input parameters contained in the hydrology and erosion components are the minimal input requirements of the GLEAMS model. The other two components, the pesticide and nutrients transport components, are used to computer the mass balance of pesticides or nutrients based on the results of the hydrology and erosion components. For pesticide simulation, the required information includes pesticide properties and specifics of application. In general, the input parameters of GLEAMS are readily available, so its simulation is also relatively easy to implement.

Limitations and uncertainty: The GLEAMS model is most suited for comparisons among management options over extended periods. The model is not intended to provide specific predictions on single storm events, although such uses have been widely reported in the literature. As with all other modeling formulations, GLEAMS involves significant simplifications and averaging for computational purpose. Therefore, a good understanding and

representation of the physical system that the model is simulating is essential for any meaningful results.

From a practical sense, the major limitation of applying GLEAMS to simulate pesticide movement is related to its accounting algorithms for hydrologic calculations. GLEAMS uses the "tipping bucket" technique to simulate percolation and the SCS curve number approach to simulate runoff. These methods, although computationally efficient, are unable to consider sub-daily temporal changes of precipitation and irrigation intensity. As a result, without calibration, the model's prediction on leaching and runoff may deviate substantially from observations for extremely events. Nevertheless, the runoff model based on the SCS curve number technique has been tested extensively for various basins with the drainage area ranging from 0.25 to 38.8 hectare. The test results showed that the model generally approximated long-term water yield well (Smith and Williams, 1980). In addition, average evapotranspiration and percolation predictions of the model seem also realistic (Smith and Williams, 1980).

The sensitivity analyses indicated that the runoff curve number is a very sensitive parameter exerting a significant influence on the final outcome of runoff and thus the overall water balance (Williams and LaSeur, 1976; Cryer and Havens, 1993; Jones and Russell, 2001). Therefore, if calibration is required for the model, it is very important that great care and objectivity be observed when selecting values of this parameter for alternative management systems. Other sensitive model parameters include field capacity, soil organic carbon content, pesticide degradation rate, and pesticide adsorption constant (Wauchope et al., 1995; Jones and Russell, 2001). Inaccurate representation of these parameters would incur a great uncertainty in the model predictions.

Case Studies: The case study presented here for GLEAMS was developed for comparing the runoff potential of the two pesticides, diazinon and esfenvalerate, from a hypothetical peach orchard. The primary chemical and physical properties of these two pesticides are shown in Table 3 (attached). Due to its low water solubility, esfenvalerate is believed to have a low potential for off-site movement and is being considered as a candidate for replacing diazinon in orchard sprays.

Application for two irrigation schedules and two soil conditions were developed in this case study to demonstrate the type of application that the GLEAMS model may have in evaluating soil and management practices on pesticide transport. The orchard was assumed to be located in the west of Marysville in Yuba County, next to the Feather River. Soil profile data were taken from the description of the Valdez series (Va) in the soil survey of the county (Herbert and Begg, 1969). The pesticides were applied three times each year, one as dormant spray in January and two in May, at the rates specified by labels. The two irrigation schedules considered were a one-day application of 1.25 cumulative crop evapotranspiration (1.25 ETc) vs. a two-day application of 0.63 ETc (2 x 0.63 ETc). Eight or 16 irrigations were made between the months

of April and October determined by the water budget method based on the typical cumulative ETc curve for deciduous orchards (University of California, 1989). The two soil conditions simulated included the presence and absence of a restrictive drainage layer at the depth of 20 to 40 cm below the soil surface. The primary model inputs defining the physical and hydraulic properties of the soil and field characteristics are provided in Table 4 (attached). The precipitation data was taken from the National Oceanographic and Atmospheric Administration (NOAA), first order meteorologic station data for Sacramento, California (Station #W23232), and the irrigation was superimposed on the precipitation. For the two irrigation schedules, no restrictive soil layer was assumed in the simulation. Likewise for the two soil conditions, only the one-day irrigation of 1.25 ETc was considered.

Figure 1 (attached) shows the simulated annual losses of runoff for both pesticides. The irrigation management had a profound effect on pesticide runoff. The two-day 0.63 ETc schedule reduced the runoff loss by 39% for diazinon and 44% for esfenvalerate. However, the effect of the restrictive drainage was minimum for both pesticides. In any event, diazinon showed a larger tendency for runoff than esfenvalerate, with the runoff loss ranged from 1.68 to 2.83% of the total application amount, compared to 1.02 to 1.76% for esfenvalerate.

## **PRZM**

Model description and applicability: PRZM is a one-dimensional conceptual model that can be used to simulate chemical movement within and through the crop root zone. As GLEAMS, PRZM assumes homogenous soil, crop and weather conditions, and is best fitted for field scale evaluations. PRZM also uses the empirical run-off curve number approach and Universal Soil Loss Equation concepts to calculate runoff and sediment erosion. Despite the minor differences of these two models in accounting water routing, pesticide degradation, vapor transport, and in the flexibility of handling vegetation dynamics and pesticide application, PRZM and GLEAMS have very similar capabilities for evaluating pesticide movement at the field scale. The PRZM approach to pesticide degradation is more comprehensive, allowing simulation of microbial reactions and bi-phasic kinetics. PRZM is also more advantageous for pesticides with a high vapor pressure, due to its explicit inclusion of vapor phase diffusion in the transport equation.

In the most recent release of the PRZM model (PRZM-3), the simulation of pesticide transport through the vadose zone was enhanced greatly by enabling a coupled vadose zone model. VADOFT (Vadose Zone Flow and Transportation Model) can simulate detailed water flow and solute transport in the unsaturated zone by solving the Richard's equation using the constitutive relationships between pressure, water content, and hydraulic conductivity. In addition, in order to perform probability-based exposure assessments, PRZM3 is also equipped with a Monte Carlo processor. This addition allows the user to evaluate transport stochastically and obtain the distribution and statistical summaries for output variables.

Parameter requirements: The input parameters of PRZM for simulating pesticide transport are presented in Table 5 (attached). Besides the climatic data for precipitation, pan evaporation, temperature, wind speed, and solar radiation, the parameters can be divided roughly into three categories: hydrological, chemical, management. The hydrological parameters such as soil properties, runoff curve number, and erosion factors, are needed for calculating water distribution and soil erosion. The chemical parameters include pesticide half-lives in soil, water, gas phase, on foliage, Henry's constant, sorption coefficient, and the washoff fraction. The management related parameters include crop data, irrigation data, pesticide application date, method, and rate. The parameter requirement for PRZM is not intensive and the input data file can be prepared normally within a few hours or days.

Limitations and uncertainty: PRZM uses similar approaches as GLEAMS for its hydrological calculations. Therefore, the entire limitations and uncertainties summarized for GLEAMS also apply to PRZM. The most sensitive parameters are the runoff curve number, soil organic carbon content, field capacity, pesticide decay rates, and adsorption coefficient.

Many of the limitations of the previous PRZM releases were overcome in the most recent version of PRZM-3. In general, PRZM is less sophisticated in its algorithm of calculating sediment erosion compared to GLEAMS. Detailed structure and properties of the channel network and the area for overland flow are not considered in computing the detachment and subsequent transport of soil particles.

Case studies: The case studies for PRZM are parallel examples to those of GLEAMS. Descriptions for the simulation scenarios are not repeated here. The purpose was to compare the difference in the prediction of pesticide runoff loss of the two models that are most widely used in industry and by the U.S. Environmental Protection Agency (U.S. EPA). Table 6 (attached) presents the major model inputs for the simulation. Except for those parameters that are unique to PRZM, the basic soil and field characteristics were kept unchanged as much as possible.

For both pesticides, the runoff losses predicted by PRZM were consistently lower than those predicted by GLEAMS. Runoff losses for diazinon from the orchard were 1.06% and 0.71% for the two irrigation schedules, respectively; and the two-day 0.63 ETc schedule reduced diazinon loss by approximately 33% (Figure 2, attached). The presence of the restrictive drainage layer increased the runoff loss of diazinon significantly (approximately 30%), which disagreed from the GLEAMS results (Figure 1). For esfenvalerate, the runoff loss ranged from 0.61 to 0.91%. The two-day irrigation schedule also reduced esfenvalerate loss by 33%. The presence of the restrictive layer, however, did not affect this pesticide; and the runoff loss was about 0.9% for both soil conditions (Figure 2).

## **EXAMS**

Model description and application: EXAMS (The Exposure Analysis Modeling System) is a mechanistic model designed to simulate chemical processes in aquatic ecosystems. EXAMS's core is a set of process modules that link fundamental properties of chemicals to the limnological parameters that control the kinetics of chemical fate and transport. The system of stream networks or water bodies may be represented by up to 100 segments, which can be further divided into several compartments depending on the physical properties or boundaries. For each segment, the balance of up to 28 different species or substances may be simulated simultaneously. The model takes into consideration the processes of accumulation, chemical transformation, biological transformation, and transport. The simulation results of EXAMS provide predictions of environmental concentrations and mass balance broken down for each compartment and by dissipation pathways. This information is useful for the evaluation of potential exposure of aquatic species and fate of the chemicals in aquatic ecosystems.

Parameter requirements: The input parameters of EXAMS include those related to (1) description of the aquatic ecosystem under evaluation; (2) chemical properties and kinetics of the contaminant; and (3) contaminant loadings. A detailed list is provided in Table 7 (attached). Although EXAMS allows for the entry of extensive environmental data, the program can be run with a reduced data set if the chemistry of the contaminant precludes some of the transformation processes.

Limitations and uncertainty: EXAMS is designed to evaluate only the routing of chemicals in receiving water bodies under steady-state water flow and constant water-volume/physical size conditions. Therefore, the program does not address the loading or the land-phase transport of contaminants before they enter into the surface water network. This limitation, however, can be easily overcome by linking the output of a land-phase transport model such as PRZM to EXAMS. The linked PRZM-EXAMS model, in fact, is a recommended procedure by U.S. EPA to evaluate pesticide concentrations in surface water for drinking water and aquatic exposure assessments.

The assumption of the steady-state water flow and constant water volume made by EXAMS also grossly deviates from natural aquatic ecosystems. This assumption poses a major limitation on the utility of the model. In California, water flow in surface water bodies and volumes of surface water respond rapidly to the precipitation and irrigation management, both change greatly from day to day. The fluctuations in the hydrological conditions of the surface water bodies would surely cause changes in concentration which would not be reflected by the model. In addition, EXAMS uses the mass conservation law as an accounting principle in representing inputs/outputs from the loadings, transport and transformation processes. The chemical itself is assumed not to change the environmental variables that drive its transformations. For example,

an organic acid or base is assumed not to change the pH of the system; and bacterial populations do not significantly increase or decline in response to the presence of the chemical. The assumptions of linear and equilibrium sorption, and second order biotransformation kinetics likewise would also introduce errors for some chemicals.

Case Studies: The case studies presented for EXAMS simulated routing of diazinon and esfenvalerate in the Sacramento River, from the Butte City to Freeport, a flow path of approximately 33 river miles. The streamflow and physical dimension data, as shown in Table 8 (attached), were so chosen that they represent as closely as possible this part of the river. The daily mean flow based on at least ten years of records as reported at the following three USGS gaging stations was taken as the average flow conditions at various sections of the river: Station #11389000 at Butte City for the Sacramento River before Feather River; Station #11425000 at Nicolaus for Feather River; and Station #11446500 at Fair Oaks for American River. The length and width of the river at various sections were determined from the USGS 7.5 Minute Series topographic map and the depth of the river was then estimated from the daily mean flow and the width. The depth of the active benthic layer of the riverbed was defaulted to 2.0 cm for the entire river of all sections. The 2.0 cm was a median value based on those used by other modelers for rivers, ponds, and lakes (from 0.4 to 5 cm).

A simulation of ten years' routing of these pesticides was performed to predict their disposition and fate in the river system. The basic physicochemical properties and kinetic constants of the pesticides are presented in Table 3. Each pesticide was introduced into the river as discrete pulses by individual winter storm runoff events. The total mass of input, entered by 36 storm pulses, was set equal to 1% of that applied for both pesticides, which was in the rough order of magnitude simulated by PRZM (Figure 2). The difference in the runoff potential of the two pesticides was not considered in the simulation, because the focus was on the in-stream processes. For diazinon, all the input mass was assumed in the dissolved form, and the partition of the mass between the water column and river sediment was initiated by the program. For esfenvalerate, due to its extremely low solubility (0.2  $\mu\text{g/L}$ ), which may provoke a violation to the assumption of linear sorption, the input mass was allocated artificially between the dissolved and sediment-associated phases by the ratio of 30 to 70%. This scenario represents a case involving the rapid settlement of river sediment.

The simulation results of EXAMS are shown in Figures 3 and 4 (attached) for diazinon and Figures 5 and 6 (attached) for esfenvalerate. Less than 90 kg of diazinon and 250 kg of esfenvalerate was stored in the simulated segment of the Sacramento River over the ten-year period of input. The highest surface water concentration simulated for diazinon was 0.875  $\mu\text{g/L}$  (Figure 5) which agrees well with the 95<sup>th</sup> percentile concentration (0.82  $\mu\text{g/L}$ ) reported for Sacramento River for the pesticide in the DPR's surface water monitoring database, SURF. The dissipation of diazinon seemed to have reached an equilibrium for both the water column and

sediment in the first year, and the maximum concentration of the pesticide showed no noticeable increase or decrease in either phase during the remaining years of simulation. The distribution of diazinon was primarily in the water phase, and its cumulative mass in the water column accounted for nearly 100% of the total residue in the river (Figure 3).

The simulated concentration of esfenvalerate in the water column was below 0.055  $\mu\text{g/L}$  at any time, which is slightly above its current detection limit (0.05  $\mu\text{g/L}$ ). The simulated concentration of esfenvalerate for sediment, however, reached a peak value of 480  $\mu\text{g/kg}$  (0.48  $\text{mg/kg}$ ) during the first year of pulses, and the concentration did not drop to zero before pulses of the following year started (Figure 6). The maximum amount of the pesticide in the sediment showed an initial increase during the first three years, but remained as quasi-equilibrium thereafter. In contrast to diazinon, the primary compartment for esfenvalerate accumulation was the sediment; its total mass in the sediment accounted for at least 93.5% of that in the whole river system (Figure 5).

## SWAT

Model description and application: SWAT is a process-based, basin scale model that was developed to simulate point and nonpoint source loadings from watersheds containing mixed subbasins of different characteristics of climate, land use, soil, hydrology, and management strategy. SWAT was a direct outgrowth of the SWRRB model (Simulator for Water Resources in Rural Basins). The program incorporates many simulation algorithms of GLEAMS, such as the SCS curve number method and Modified Universal Soil Loss Equation, for hydrologic cycle and transport. Likewise, it is intended for predicting the impact of land management practices on water, sediment and agricultural chemical yields in large complex watersheds over long periods of time.

The formulation of SWAT consists of three levels of divisions: watershed, subbasins, and hydrological response units (HRUs). The HRUs with uniform land use and similar hydrological characteristics are the basic elements of a watershed. Runoff is predicted separately for each HRU and routed to obtain the total quantity for the watershed. The simulation of hydrologic cycle and transport in SWAT is divided into two phases: the land phase and the water or routing phase. The land phase of the hydrologic cycle controls the amount of water, sediment, and pesticide (or nutrient) loadings to the main channel of each subbasin. The routing phase directs the movement of water, sediments, and chemicals through the channel network to the outlet of the watershed. SWAT uses a command structure for routing runoff and chemicals through a watershed. Commands are included for routing flows thorough streams and reservoirs, adding flows from different subbasins, and incorporating upstream loadings and point sources. Output results from other simulation models can also be routed using the commands through the drainage network of the watershed. SWAT also has linkages to geological information systems, enabling access to soil type, crops, streams, lakes and climate databases.

Parameter requirements: The data input for SWAT is quite intensive. The input data files can be separated into four groups: data files that apply to the entire watershed, data files that are required for each subbasin, data files that are required for each HRU, and data files containing miscellaneous databases. The first group of input files (i.e., the watershed data files) provides parameters that define the configuration of the watershed and specify the operation and relationship of the subbasin divisions. The subbasin input files include those related to climate, HRUs divisions, ponds/reservoirs characteristics, and the description of the main and tributary channels draining the subbasins. The input files for HRUs (the third group) include data, for each HRU, of soil profile and properties, hydrological characteristics, crop and management practices, and chemical application. In addition, there are five databases that come with the program, including the pesticide property database, land cover/plant growth database, tillage database, fertilizer database, and urban area database. For a watershed consisting of a single subbasin and HRU, a minimum of 28 input files are need for simulation.

Model limitations and uncertainties: As a simulation model for large complex watersheds, the input data requirement for SWAT is intensive. The preparation of input data for parameterizing a watershed, including its subbains and HRUs, requires extensive and profound knowledge on all aspects regarding the weather, land use, topography, geology, hydrology, soil, characteristics of growth for specific vegetations, and the cultivation and management practices of specific crops in the watershed. Even for simple watersheds, an initial compilation of such data set may easily take weeks. For complex watersheds with multiple subbasins, a team effort of collaboration would be necessary.

In addition, SWAT have all the shortcomings inherited from GLEAMS simulation algorithms: the daily time step, sensitivity of the runoff curve number, simplified assumptions regarding kinetics of adsorption and decay, lack of accounting algorithms for spray drift, foliar interception and washoff, etc. SWAT has an option for using Green & Ampt infiltration equation with smaller time steps to determine surface water runoff, but it is not operational at this time.

Case Studies: Due to the time constraint in preparing the input data files, case studies for SWAT are not presented in this report.

## **Conclusions**

A review of the surface water models identified the following models as being most relevant and appropriate for addressing pesticide runoff in agricultural settings:

Field scale models: GLEAMS, PRZM, or coupled PRZM-EXAMS (if instream routing is desired)

Watershed models: SWAT

These models are chosen because technically they were developed specifically for addressing impacts of agricultural practices on transport of pesticides in the field which suits the DPR needs. In addition, these models are mostly recommended by U.S. EPA for exposure assessments, and as such have been widely used and validated under a variety of real-world field conditions. The prediction quality for runoff of GLEAMS and PRZM in general are acceptable and in many cases satisfactory based on the extensive testing data published in the literature. Although there are many limitations with these models, there are no better alternatives at present, based on the limited effort of this review, for simulating field runoff processes. RZWQM (Root Zone Water Quality Model) may be a promising alternative in the future because of its more rigorous physical basis for calculating percolation and runoff, but currently its crop model is very limited and its erosion component is not functioning. RZWQM has a large and active developing group consisting of USDA scientists, and it is hoped that these problems would be solved in the near future.

In order to use these models to facilitate DPR decisions, additional validation studies are recommended using both DPR's own data and those published in the literature. Upon such validation, simulation scenarios can then be developed to address areas of concern that might be regulated so that pesticide loading can be reduced at the edge of field and in streams.

Attachments

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Kean S. Goh, Ph.D.  
April 18, 2002  
Page 14

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Table 1. Comparison of environmental models capable of simulating surface water runoff and quality.

Feature	Model*									
	BASINS	AGNPS	HSPF	RZWQM	SWAT	SWIM	GLEAMS	PRZM	QUAL2E	EXAMS
Developer	USEPA	USDA	USEPA	USDA	USDA	Germany	USDA	USEPA	USEPA	USEPA
Scale	Basin	Basin	Basin	Field	Basin	Basin	Field	Field	In-stream	In-stream
Submodels Incorporated	HSPF	CONCEPTS	ARM		SWRRB	SWAT	CREAMS			
	QUAL2E	SNTEMP	NPS		ROTO					
	TOXIRoute	SIDO								
Instream Flow	Yes	Yes	Yes	Yes	Yes	Yes	No	No	Yes	Yes
Overland Flow	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	No
Groundwater Flow	Yes	No	Yes	Yes	Yes	Yes	No	No	No	No
Chemical Movement	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Mixed Land Uses	Yes	Yes	Yes	No	Yes	Yes	No	No	No	No
Vegetation Dynamics	No	No	No	Yes	Yes	Yes	Yes	Yes	No	No
Management Practices	No	Yes	No	Yes	Yes	Yes	Yes	Yes	No	No

Abbreviation:

- AGNPS - Agricultural Non-point Source Pollution Model
- ARM - Agriculture Runoff Model
- BASINS - Better Assessment Science Integrating Point and Nonpoint Sources
- CONCEPTS - Instream Hydrodynamic Processes
- CREAMS - Chemicals, Runoff, and Erosion from Agricultural Management Systems
- EXAMS - Exposure Analysis Modeling System
- GLEAMS - Groundwater Loading Effects of Agricultural Management Systems

Table 1. (Continued)

HSPF -	Hydrological Simulation Program - FORTRAN
NPS -	Non-Point Source
PRZM -	Pesticide Root Zone Model
QUAL2E -	Two Dimensional Sediment Transport Model
ROTO -	Routing outputs to Outlet
RZWQM -	Root Zone Water Quality Model
SIDO -	Sediment Intrusion and Dissolved Oxygen
SNTMP -	Stream Network Water Temperature
SWAT -	Soil and Water Assessment Tool
SWIM -	Soil and Water Integrated Model
SWRRB -	Simulation for Water Resources in Rural Basins
TOXIRoute -	Routing of Toxic Pollutant in Streams and Rivers

Table 2. Major parameters required to drive the GLEAMS model (pesticide model)

Component	Parameters
Hydrology	<p>Drainage area</p> <p>Saturated conductivity below root zone</p> <p>Evaporation constant</p> <p>Curve number</p> <p>Field hydraulic slope</p> <p>Watershed length width ratio</p> <p>Effective rooting depth</p> <p>Elevation and Latitude</p> <p>Soil horizon description: number and depths</p> <p>Soil physical properties: porosity, field capacity, wilting point, saturated conductivity, organic matter, clay, and silt content</p> <p>Soil chemical properties: pH, base saturation, calcium carbonate content</p> <p>Crop data: crop ID and leaf area index profile, plant date, harvest date, truncation date, rooting depth, maximum height</p> <p>Irrigation data: method, beginning and ending date, depth</p>
Erosion	<p>Overland flow profile: points, distances, slopes</p> <p>Soil erodibility profile: points, distance, erodibility factors</p> <p>Channel flow profile: points, outlet conditions, subdrainage areas, slopes</p> <p>Pond (impoundment) data: drainage area, saturated conductivity, embankment slope, inflow channel slope, side slope, outlet control</p> <p>Soil loss parameters: p-factor, c-factor, Manning's n for channel, Manning's n for overland flow, Manning's n for outlet, erodible depth</p>
Pesticide	<p>Pesticide properties: adsorption coefficient, name, metabolites and kinetics of transformation, solubility, foliar half-life, soil half-life, washoff fraction, coefficient of plant uptake</p> <p>Application: method, date, rate, depth of incorporation, foliage/soil partition</p>

Table 3. Major chemical and physical properties of diazinon and esfenvalerate used in modeling

Parameter	Diazinon	Esfenvalerate
Molecular weight	304.35	420
Solubility, mg/L	60	2.00E-04
Koc, mg/L	1520	5273
Kow, mg/L	2000	1.58E+05
Foliar residue half-life, day	7	21
Soil half-life, day	39	74
Vapor pressure, torr	1.06E-04	2.80E-07
Henry's constant	0.072	0.042
Melting point, °C	120	60
2nd order rate constant for base-catalyzed hydrolysis, 1/(mole [OH-].hr)		11.5
1st order rate constant for neutral hydrolysis, 1/hr	3.75E-03	4.51
Arrhenius activation energy for base-catalysed hydrolysis, kcal/mol		12
Arrhenius activation energy for neutral hydrolysis, kcal/mol	-	12
Photolysis constant, hr <sup>-1</sup>	5.67E-03	9.58E-04

Table 4. Major soil and field characteristics simulated in GLEAMS model

GLEAMS parameter	Value
Catchment area, hec	1.0
SCS runoff curve number	78
Hydraulic slope, m/m	0.05
Soil porosity, cm <sup>3</sup> /cm <sup>3</sup>	0.43
Field capacity, cm/cm	0.32
Wilting point, cm/cm	0.12
Clay content, %	
without pan	20.0
with pan (20-40 cm)	35.0
Silt content, %	
without pan	60.0
with pan (20-40 cm)	30.0
Sand content, %	20.0
Organic matter %	
0-20 cm	1.25
40-120 cm	0.625
Effective saturated conductivity, cm/hr	
without pan	0.36
with pan (20-40 cm)	0.25
Root depth, cm	120
Crop height, m	3.0
Maximum leaf area index, m <sup>2</sup> /m <sup>2</sup>	3.0
Soil erodibility factor	0.2
Crop factor	0.1
Contouring factor	1.0
Manning's N factor	0.033

Table 5. Major parameters required to drive the PRZM model (pesticide model)

Category	Parameters
Hydrology	<p>Soil depth and horizen, bulk density, field capacity, wilting point, drainage rate, organic carbon content, clay content, sand content, soil temperature and thermal conductivity.</p> <p>Pan factor</p> <p>Snowmelt factor</p> <p>Evaporation depth</p> <p>Erosion parameters: soil erodibility, topographic factor, p-factor, c-factor, field area, slope, hydraulic length, Manning's n</p> <p>Runoff curve number</p>
Management	<p>Crop data: number of crops for rotation, crop ID, interception storage, rooting depth, canopy coverage, maximum weigth, maximum height, emergence date, maturate date, harvest date</p> <p>Irrigation data: method, leaching factor, application rate, furrow irrigation parameters</p> <p>Pesticide application data: method, date, rate, depth of incorporation, spray drift fraction</p>
Chemical	<p>Pesticide properties: solubility? kinetics of transformation, plant uptake factor, volatilization rate, decay rate contants for dissolvd, sorbed and vapor phases, washoff coefficient, adsorption coefficient, Henry's constant, hydrodynamic dispersion coefficient, air dispersion coefferient</p> <p>Microbial data for decay: population density, carbon source concentration, saturation constant, inhibition constant, growth rate, death rate, dissociate constant of enzyme-chemical complex,</p>

Table 6. Major soil and field characteristics simulated in PRZM-3

PRZM parameter	Value
Catchment area, hec	1.0
SCS runoff curve number	78
Hydraulic slope, m/m	0.05
Field capacity, cm/cm	0.32
Wilting point, cm/cm	0.12
Bulk density, g/cm <sup>3</sup>	1.4
Soil drainage parameter, 1/day	
0-20 cm	1.8
20-40 cm (pan)	1.55
40-120 cm	2.4
Organic carbon %	
0-40 cm	0.725
40-120 cm	0.362
Root depth, cm	120.0
Crop height, cm	300.0
Maximum areal coverage of the canopy, %	80.0
Maximum interception storage, cm	0.25
Universal Soil Loss Equation C-factor	0.1
Pan factor	0.75
Universal Soil Loss Equation of soil erodibility	0.2
Universal Soil Loss Equation topographic factor	0.54
Manning's N factor	0.03

Table 7. Typical input requirements for EXAMS model

Category	Input
Chemical	Molecular weight Henry's constant Vapor pressure Melting point Partition coefficient or octanol-water partition coefficient Solubility Hydrolysis rate constant Photolysis rate constant Biolysis rate constant Oxidation rate constant Reduction rate constant Volatilization rate constant Loading data: mode of input, time, location, mass
Aquatic system	Type and structure Physical geometry: area, depth, length, width Advective flow field: advective flow rate, flow path, stream sediment input, sediment concentration Dispersive flow field: flow cross section, characteristic length, dispersion coefficient
Environmental	Elevation and latitude Monthly rainfall Monthly temperature Monthly relative humidity Wind speed Dissolved organic carbon content Dissolved oxygen content Sediment properties: bulk density, suspended density, water content, organic carbon content, cation exchange capacity, anion exchange capacity Bacterial density pH

Table 8: EXAMS model inputs representing the physical geometry and flow characteristics of Sacramento River

Segment number	Segment type*	Length, m	Width, m	Depth, m	Streamflow, m3/hr
1	L	3.22E+04	2.41E+02	2.60E+00	1.09E+06
2	B	3.22E+04	2.41E+02	2.00E-02	
3	L	2.09E+04	2.41E+02	5.00E+00	8.24E+05
4	B	2.09E+04	2.41E+02	2.00E-02	
5	L	3.54E+04	2.41E+02	6.30E+00	3.98E+05
6	B	3.54E+04	2.41E+02	2.00E-02	

\* Segment type: L - Littoral; B - Benthic zone.

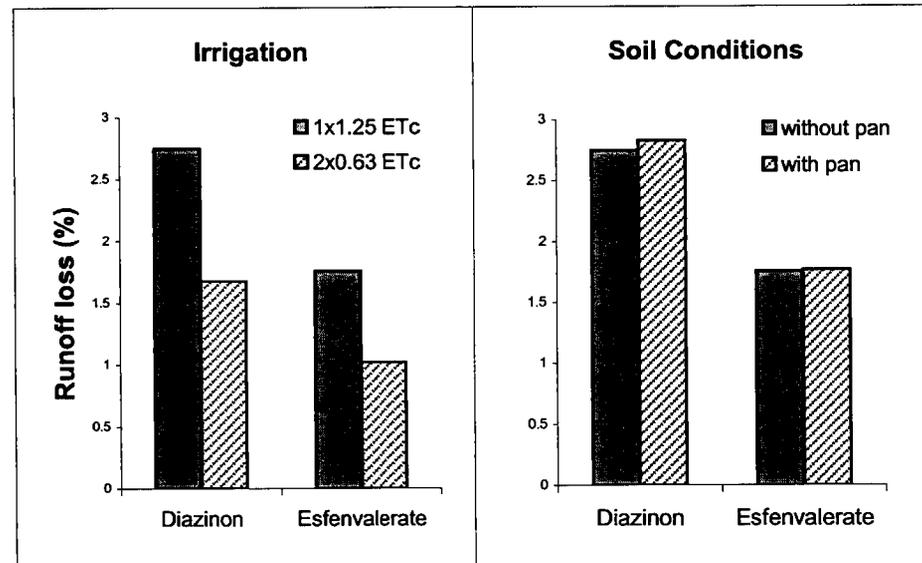


Figure 1. GLEAMS prediction on effects of irrigation management and soil conditions on diazinon and esfenvalerate runoff losses from orchard. Results were two-year means using 1980 and 1981 climatic data.

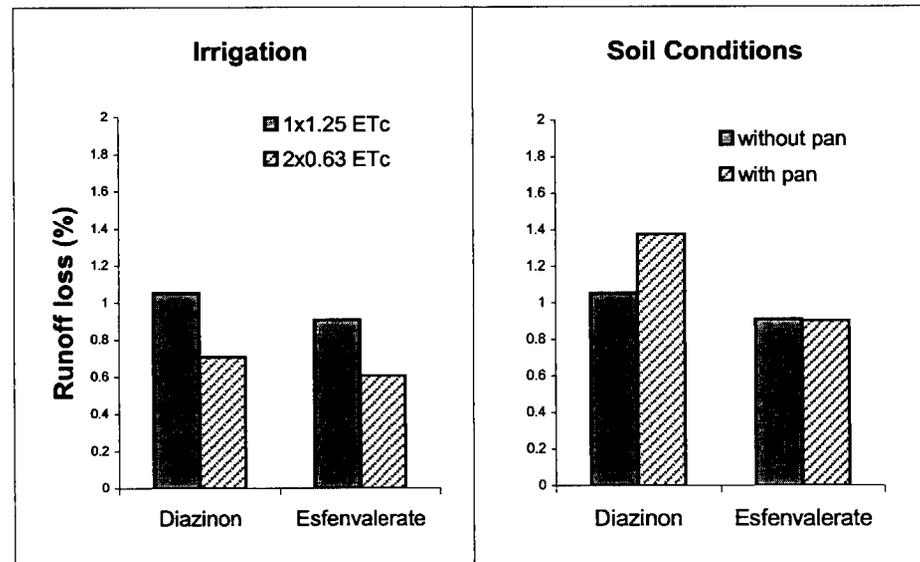


Figure 2. PRZM prediction on effects of irrigation management and soil conditions on diazinon and esfenvalerate runoff losses from orchard. Results were two-year means using 1980 and 1981 climatic data.

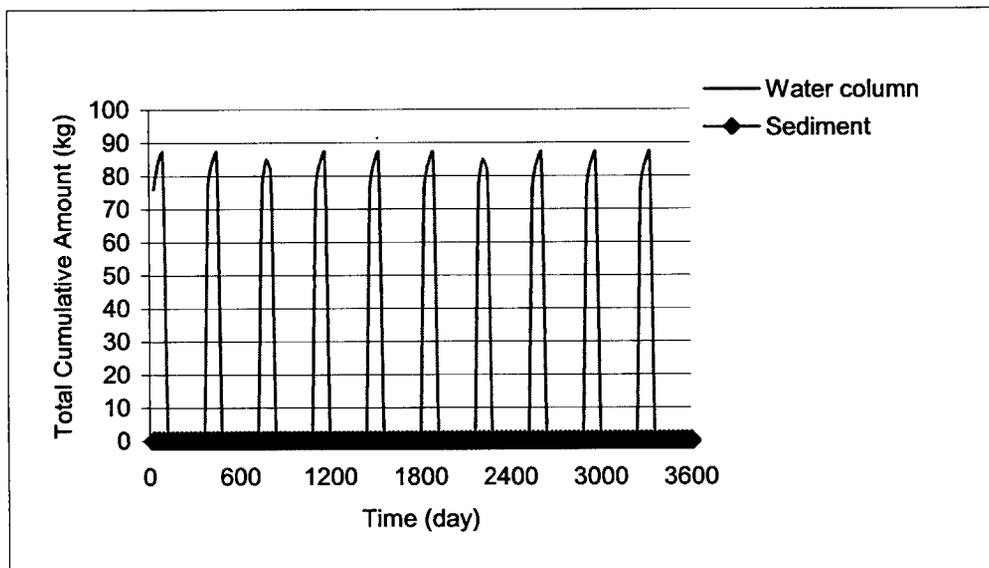


Figure 3. Predicted distribution of diazinon in Sacramento River by EXAMS.

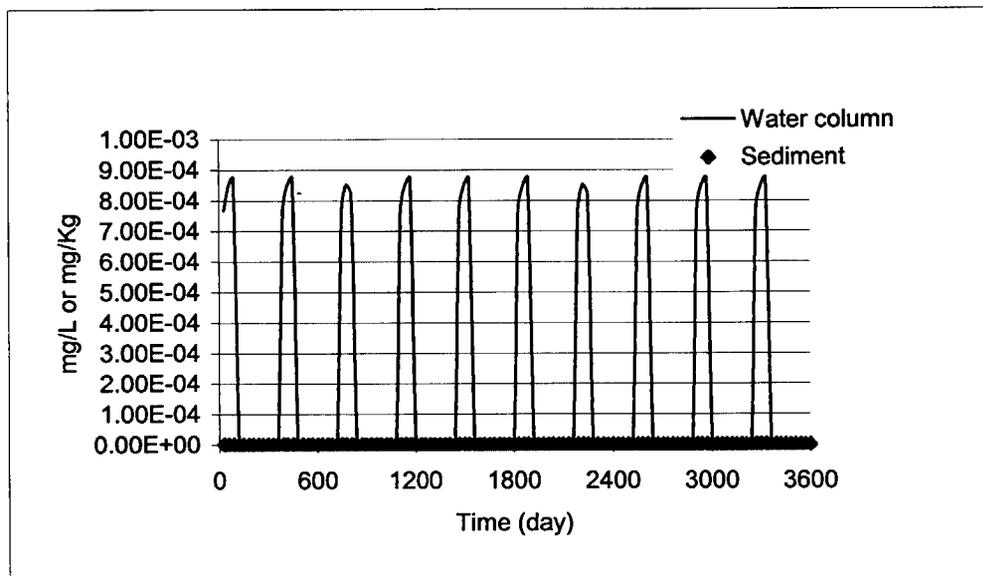


Figure 4. Predicted concentration of diazinon in Sacramento River by EXAMS. Data shown are monthly means.

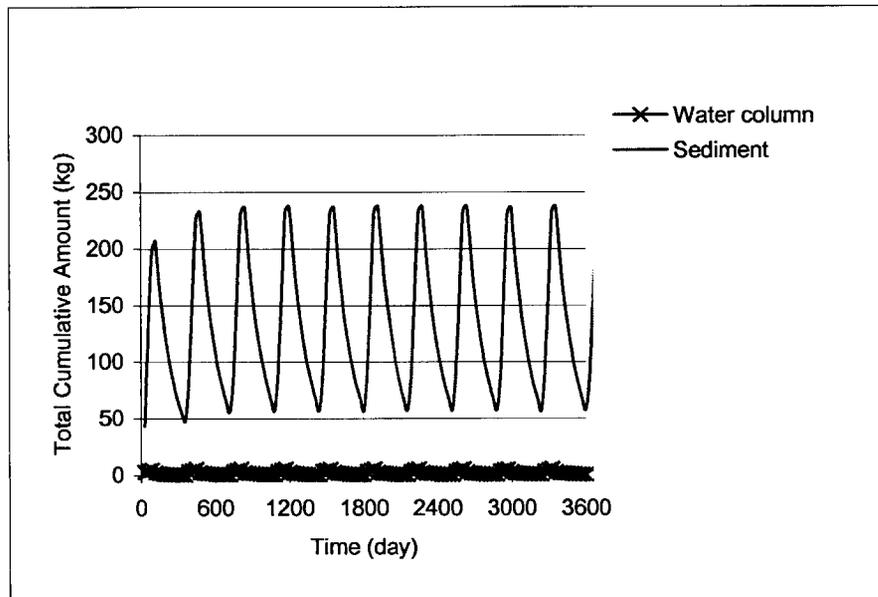


Figure 5. Predicted distribution of esfenvalerate in Sacramento River by EXAMS.

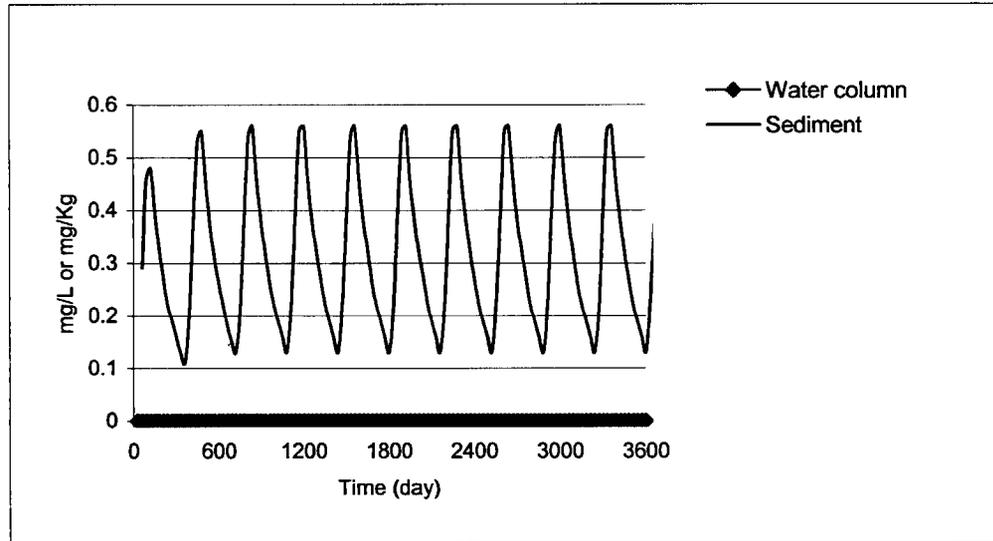


Figure 6. Predicted concentration of esfenvalerate in Sacramento River by EXAMS. Data plotted are monthly means.