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A REVIEW AND POTENTIAL APPLICATIONS OF MODELS THAT SIMULATE THE FATE OF PESTICIDES IN THE UNSATURATED ZONE

by

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ABSTRACT

The recognition that groundwater supplies are susceptible to contamination by pesticides has led to the development of a number of pesticide transport and transformation models capable of assessing the potential for the contamination of groundwater. The computer codes are categorized into two main groups, screening models or mathematical models, based on the approach taken in the assessment. Mathematical models are further sub-divided into educational, management and research models, according to the level of complexity incorporated in the models. A literature review identified 15 existing pesticide models. These models are briefly discussed, under their appropriate classification. Selection criteria and typical applications for the different model classifications are discussed and typical output from two of the models is presented.

RÉSUMÉ

La reconnaissance du fait que les approvisionnements en eaux souterraines peuvent être contaminés par les pesticides a entraîné l'élaboration de plusieurs modèles de transport et de transformation des pesticides capables d'évaluer le potentiel de contamination des eaux souterraines. Les codes machine sont classés en deux groupes principaux, les modèles de dépistage et les modèles mathématiques, basés sur l'approche adoptée au cours de l'évaluation. Les modèles mathématiques sont subdivisés en modèles éducatifs, modèles de gestion et modèles de recherche selon le degré de complexité incorporé. Une étude de la documentation a identifié 15 modèles des pesticides existants. Ce rapport contient une brève analyse de chacun de ces modèles qui se retrouvent dans la classification appropriée. Le rapport analyse les critères de sélection et les applications types des différentes classifications de modèles et présentent une sortie machine type de deux de ces modèles.

MANAGEMENT PRESPECTIVE

In recent years, a considerable amount of effort has spent in the study of the fate of pesticides in the subsurface environment. Growing from, and also aiding in this work, has been the development of a number of numerical models designed to assess the potential for pesticide contamination of groundwater. Although all the pesticide models attempt to assess the potential for ground water contamination, the models vary widely in the approach taken to the simulation, the level of detail incorporated in the model descriptions, and in their intended use. The models are divided into two main categories, screening models and mathematical models. Screening models simply assess the potential for groundwater contamination based on physical and chemical properties of the pesticide and site. Mathematical models attempt to simulate the processes that actually occur in nature with mathematical relationships. The later group of models is further subdivided into educational, management and research models based on the level of detail incorporated in the model descriptions. The selection of the most appropriate model for a given simulation depends on a number of factors. To select the most appropriate model consideration should be given to (1) the specific objectives of the study, (2) the knowledge and experience of modeller, (3) the assumptions and limitations inherent in the model, (4) the ease of use, and (5) the availability of accurate input characterization data. The selection of the most appropriate model is essential in accurately identifying where the potential exists for groundwater contamination by agricultural pesticides and identification of agricultural development which may or may not be sustainable.

PERSPECTIVE DE GESTION

Au cours des dernières années, de nombreuses études ont été faites sur l'évolution des pesticides dans le sol. Ces travaux et les travaux connexes ont permis de mettre au point plusieurs modèles numériques conçus pour évaluer la possibilité de contamination des eaux souterraines par les pesticides. Bien que tous les modèles de pesticides cherchent à évaluer la possibilité de contamination des eaux souterraines, les modèles varient considérablement selon d'approche adoptée lors de la simulation, le degré de détail incorporé dans les descriptions du modèle, et leur utilisation prévue. Ces modèles sont divisés en deux catégories principales, les modèles de dépistage et les modèles mathématiques. Les modèles de dépistage évaluent simplement la possibilité de contamination des eaux souterraines basée sur les propriétés physiques et chimiques des pesticides et du site. Les modèles mathématiques cherchent à simuler à l'aide d'équations mathématiques les processus qui opèrent dans le milieu observé. Ce dernier groupe de modèles est de plus subdivisé en modèles éducatifs, modèles de gestion et modèles de recherche, en fonction du degré de détail incorporé dans les descriptions du modèle. Le choix du modèle le plus approprié pour une simulation donnée dépend d'un certain nombre de facteurs. Pour choisir le modèle le plus approprié, il faut tenir compte (1) des objectifs particuliers de l'étude, (2) des connaissances et de l'expérience de l'auteur du modèle, (3) des hypothèses et des limites inhérentes au modèle, (4) de la facilité d'utilisation et (5) de la disponibilité de données d'entrée précises. Le choix du modèle le plus approprié est essentiel afin d'identifier avec précision où il peut y avoir contamination des eaux souterraines par les pesticides agricoles et de déterminer le développement agricole durable.

INTRODUCTION

The widespread detection of aldicarb and its transformation products in the groundwater on Long Island, New York in 1979 (Zaki et al., 1982) led to an increased awareness that groundwater supplies are susceptible to contamination by pesticides. Following the work of Zaki et al. (1982), others studies have shown that pesticide contamination of groundwater is widespread (Jones, 1985;1986; Harkin et al. 1986; Priddle et al., 1987;1988;1989; Moye and Miles, 1988; Mutch, 1989 and Bouwer, 1989). During this time, considerable effort has been spent studying the processes that control the fate of pesticides in the subsurface environment. Growing from, and also aiding in this work, has been the development of a number of numerical models designed to assess the potential for pesticide contamination of groundwater. Although the models all assess the potential for ground water contamination, the models vary widely in the approach taken for the simulation, the level of detail incorporated in the model descriptions, and also in their intended use.

Pesticide models may be applied to a number of different situations including the investigation of the fate of pesticides in cases where the contamination has already occurred or where predictions of the consequences of a future pesticide application program are desired. Pesticide models may also be used to aid in the understanding of the processes that are involved in the transport and transformation of pesticides in the subsurface. Sensitivity studies performed with the models may provide a better understanding of the processes that are most influential in fate of the pesticide in the subsurface.

This paper gives a brief review of 15 available pesticide assessment models, and discusses the type and classification of the pesticide models and their most appropriate applications. Simulations were performed with two of the mathematical models to demonstrate the results that might be expected from the models.

PESTICIDE MODELS

In general, pesticide models can be grouped into two broad categories of models: screening models and mathematical models. Screening models simply assess the potential for a pesticide to leach to the water table on a relative basis and do not attempt to quantify the amount, or rate, of pesticide leaching to the water table. Mathematical models however, attempt to simulate the physical, chemical, and biological processes that are occurring in nature with simplified mathematical representations. The mathematical models attempt to quantify both the amount, and rate, of pesticide leaching to the water table.

A literature review was conducted and 15 existing pesticide assessment models were identified. The categorization of the 15 pesticide transport models into groupings based on their complexity and intended use is shown in Figure 1. The models are briefly reviewed in the following sections.

SCREENING MODELS

Screening models are simple models that assess the potential for groundwater contamination by a pesticide on a relative basis. The screening models do not use a complex mathematical representation of the processes that are occurring in the subsurface. Rather, they make use of the physical and chemical characteristics of the pesticide to provide a quick and

general assessment of the potential for groundwater contamination by a pesticide. The models provide a relative index of the potential for a pesticide to leach to the water table in comparison to other pesticides that have been known to contaminate groundwater supplies. In general, the models operate by comparing two or more chemical characteristics of the pesticide, and/or hydrogeological properties of the application site, to similar pesticides and situations where contamination of the groundwater is known to have occurred. Because the models do not directly simulate the processes involved, they do not attempt to quantify the amount or rate of pesticide leaching to the water table. The main advantage of screening models is the speed and ease with which they can be used.

Five of the 15 models identified are classified as screening models and are:
(1) DRASTIC (Aller et al., 1985);
(2) CDFA screening model (Wilkerson and Kim, 1986);
(3) Cohen et al. (1984) screening model;
(4) Jury et al. (1987) screening model;
(5) GUS (Gustafson, 1989).

DRASTIC (Aller et al., 1985) - is a screening model available for use in evaluating the potential for groundwater contamination in different hydrogeological settings. Two versions of the model are available, one for general use, and one for agricultural applications of pesticides. The model evaluation is based on seven physical parameters from which the name DRASTIC is derived (Depth to water, net Recharge, Aquifer media type, Soil media type, Topography, Impact of the vadose zone media, and the hydraulic Conductivity) of the site. Each parameter at a particular site is ranked in a range from 1 to 10 (1 to 9 in the case of net recharge) and this ranking is then multiplied by a weighting factor, indicating the importance of each parameter in determining if groundwater contamination is likely to occur. The resultant product for each of the seven parameters is then summed to arrive at the DRASTIC index for the particular site. The value of the index can then be used to assess the potential for groundwater contamination at the site. The weighting factors and rating ranges for the two versions of the DRASTIC model are shown in Table 1.

Table 1. Weighting factors and rating ranges for the two versions of DRASTIC.

		Weighting Factors	
Feature	Rating Range	General Use	Pesticide Applications
Depth to water	1-10	5	5
Net recharge	1-9	4	4
Aquifer media type	1-10	3	3
Soil media type	1-10	2	5
Topography	1-10	1	3
Impact of vadose zone	1-10	5	4
Hydraulic conductivity	1-10	3	2
Index range		23-226	26-256

The four remaining screening models are all similar. Rather than assigning mathematical representations to describe physical, chemical and biological processes, screening models make use of the physical and chemical characteristics of the pesticide and site to provide a quick and general assessment of the potential for groundwater contamination by a pesticide. Often two pesticide properties (the organic carbon partition coefficient, K_{oc}, and the half-life of the pesticide in the soil, $t_{1/2}$) are used to screen pesticides for their potential to leach to the water table. Based on the value of the parameters, the pesticides are divided into one of three groups; "leachers", "non-leachers", or "transition pesticides" (where conflicting evidence exists as to whether these pesticides leach to the water table or not). The four screening models that follow, all make use of these two parameters.

CDFA screening model (Wilkerson and Kim, 1986) - the California Department of Food and Agriculture screening model is based on a list of chemical properties for 22 different pesticides compiled by the CDFA. From this list, they determined the average K_{oc} and soil half-life values for the 22 pesticides and, by plotting the soil half-life ($t_{1/2}$) of the pesticide against the K_{oc} values for the pesticide on a log-log scale, were able to determined that the known pesticide "leachers" occupied one portion of the plot (see Figure 2). The CDFA established a classification system whereby any pesticide with a K_{oc} less than 512 cc/g and a soil half-life ($t_{1/2}$) in excess of 11 days would be classified as a "leacher", with a high potential for groundwater contamination. Pesticides with one or both of these properties outside the specified range would be classified as a "non-leacher" and thus exhibit little potential to contaminate groundwater supplies. Pesticides being classified as "leachers" may be restricted from use in certain areas or may be subject to additional application constraints. The CDFA chose a distinct separation criteria between "leachers" and "non-leachers" and did not provide for a transition zone between the two groups.

Cohen et al. (1984) screening model - is very similar to the CDFA model in that it uses K_{oc} and half-life values of the pesticide to classify the leachability of a pesticide. However, it provides for a transition zone between the "leachers" and "non-leachers" (see Figure 2). Pesticides with both K_{oc} values less than 300 cc/g and soil half-lives ($t_{1/2}$) in excess 3 weeks are classified as "leachers", while those with K_{oc} values greater than 500 cc/g or soil half-lives less than two weeks are classified as "non-leachers". "Transition pesticides" have K_{oc} values between 300 and 500 cc/g and soil half-lives between 2 and 3 weeks.

Jury et al. (1987) screening model - is based on simulations performed with a simple mathematical pesticide transport and transformation model. The mathematical model assumes, steady-state water flow, linear equilibrium sorption, and depth-dependent, first-order degradation. The model is reduced to a simple inequality given by:

$$K_{oc} < a(t_{1/2}) - b \qquad (1)$$

where a and b are constants determined by environmental conditions. The inequality is used to assess two possible environmental scenarios; one in which the parameters are chosen to correspond to a low contamination potential (ie. high organic carbon content, high average water content, slow drainage and a thick zone of maximum biological activity), and the other, representing a high contamination potential (low organic carbon content, low average water content, relatively fast drainage, and a shallow zone of maximum biological activity). The results of the simulations are plotted on a log soil half-life ($t_{1/2}$) versus log K_{oc} plot (see

Figure 2) and act to separate pesticides into three groups; "leachers" even in low pollution potential areas, "leachers" only in high pollution potential areas and probable "non-leachers".

GUS - Groundwater Ubiquity Score (Gustafson, 1989) - is based on the CDFA data described earlier and makes use of a hyperbolic function to separate the "leachers" from the "non-leachers". Gustafson observed that a curved line provided better distinction between the known "leachers" and "non-leachers" in the CDFA data (see Figure 2). The function derived for the GUS model is given below:

$$GUS = \log_{10}(t_{1/2}) \cdot (4 - \log_{10}(K_{OC})) \quad (2)$$

Sensitivity studies were performed (Gustafson, 1989) and GUS values of 2.8 and 1.8 were found to most accurately define the transition zone from "non-leachers" to the "leachers". These studies were also performed to determine if the inclusion of additional physical parameters (solubility, octanol-water partition coefficient, and volatility) into the GUS equation would improve the ability of the model to classify pesticides according to their potential to contaminate groundwater supplies. The sensitivity studies revealed that the additional physical parameters did not provide GUS with any additional power in separating "leachers" from "non-leachers".

Summary of screening models

The major weakness of the DRASTIC model is that it consider only one aspect (i.e. the hydrogeologic properties of the site) of the potential for contamination. DRASTIC, when used for pesticide leaching assessments, does not take into consideration any of the specific properties related to the pesticide in question. In effect, the vulnerability assessment is performed assuming that the pesticide is a non-degrading, non-adsorbing chemical. In reality, however, the adsorption and degradation of a pesticide generally have a significant effect on the amount and rate of pesticide leaching to the water table. Processes such as adsorption and degradation, in turn are affected by a number of site specific parameters (e.g. pH and temperature) that are not considered in the DRASTIC model. In essence, DRASTIC assesses only the presence, or lack there of, of the physical characteristics that would make a site susceptible to groundwater contamination. It is, therefore, most applicable for use in preliminary groundwater contamination susceptibility mapping, where no specific chemical, or chemical family, has yet been identified for investigation. The model may be useful in prioritizing a proposed groundwater quality sampling program.

The remaining screening models, while considering certain chemical and physical parameters of the pesticide and site, do not simulate the processes involved in the transport and transformation of a pesticide in the unsaturated zone and cannot predict pesticide concentrations or leaching rates at the water table. They are, therefore, applicable only in very general assessment of the vulnerability of groundwater to pesticide contamination. The speed and ease with which screening models are used, however, makes these model most useful in mapping large areas that may be susceptible to groundwater contamination. Screening models can be useful for quickly narrowing the scope of a large investigation, identifying and directing attention to areas that warrant additional study with a more sophisticated model and/or field studies.

MATHEMATICAL MODELS

In assessing the potential for groundwater contamination by pesticides, mathematical models attempt to simulate the processes that are involved in the transport and transformation of the pesticides in the unsaturated zone of a soil. The models describe these processes with mathematical representations that quantify both the amount and rate of pesticide leaching through the soil profile. Mathematical models account for the major physical, chemical and biological processes affecting the transport and transformation of pesticides in the unsaturated zone. They generally simulate pesticide transport in the unsaturated zone in one dimension, based on an advective-dispersive equation for transient conditions.

The majority of the mathematical models use a simplified water flow representation for the unsaturated zone and, to varying degrees, represent the subsurface as a series of soil compartments. This gives the models the capability of simulating pesticide transport in layered soils, characterized by different physical, chemical, and biological properties.

The models account for first-order pesticide degradation, equilibrium sorption (linear, reversible) and plant uptake (as function of the transpiration rate). A few models also simulate the fate of daughter products generated from the transformation of a parent pesticide.

The models are all designed for relatively nonvolatile pesticides and generally do not account for volatilization losses and volatile transport in the soil profile. Surface runoff and erosional losses are account for in only a few of the mathematical models.

Classification of mathematical models

Mathematical pesticide transport models are subdivided into one of three categories: educational, management, or research models (see Figure 1). The categories (Wagenet, 1986) are based upon;

(1) the extent to which they describe the basic processes involved;
(2) the sensitivity and accuracy of the simulations;
(3) the amount of input characterization data required.

Educational models are the simplest of the mathematical models, and are applicable to only a limited number of near ideal situations (e.g. homogeneous soil profile, steady state conditions). The amount of input characterization data required is restricted to a few parameters. Results from the model provide only qualitative information.

Management models move a step beyond educational models and describe the processes involved in more detail. For example, management models may allow for a layered soil profile simulation with transient conditions. They require larger (yet still not restrictive) amounts of input characterization data and provide semi-quantitative results. They are intended to provide managerial guidance and are designed to present results in a manner that allows for quick interpretation.

Research models attempt to simulate the natural processes in as much detail as possible. As an example, research models may describe the flow of water in the unsaturated zone using a direct solution to Richards equation, as opposed to management and educational models which generally employ a simplified water balance. As a result of the more detailed

description, research models often require large amounts of input characterization data, some of which may not be readily available. The results provided by research models are more quantitatively informative than are the results from a management or educational model. However, the use of research models is often more cumbersome (i.e. input data sets are more difficult to formulate, and they require considerably longer execution times).

Mathematical models are also categorized as either deterministic or stochastic models. Given a set of input data, a deterministic model provides a single, unique and repeatable output data set. The models often assume field-averaged values for parameters that describe the natural system. They do not account for the spatial variations that may occur in the natural system.

Stochastic models use statistical representations to describe the spatial and temporal variations found in the natural system. The spatial and temporal variations are described in the model by parameter distribution functions. A number of simulations (enough to provide a statistical measure on the predicted results) are performed, by randomly selecting values for these parameters from their distribution functions in each new simulation (Monte Carlo approach). The resulting model predictions are analyzed with a statistical probability of occurrence.

Ten of the models identified in the literature search are classified as mathematical models (see Figure 1). A list of the models is given below.

Educational models:

(1) MOUSE - Method Of Underground Solute Evaluation (Steenhuis et al., 1987);

(2) PESTAN - PESTicide ANalytical model (Enfield et al., 1982);

(3) CMLS - Chemical Movement in Layered Soils (Nofziger and Hornsby, 1986).

Management models:

(4) PRZM - Pesticide Root Zone Model (Carsel et al., 1984);

(5) GLEAMS - Groundwater Loading Effects of Agricultural Management Systems (Leonard et al., 1987);

(6) VULPEST - VULnerability to PESTicides (Villeneuve et al., 1987);

(7) SESOIL - SEasonal SOIL model (Bonazountas and Wagner, 1984);

(8) MELEF-3v (Padilla et al., 1988).

Research models:

(9) LEACHM - Leaching Estimation And CHemistry Model (Wagenet and Hutson, 1987);

(10) SUTRA - Saturated-Unsaturated TRAnsport model (Voss, 1984).

A brief description of each model follows.

EDUCATIONAL MODELS

MOUSE (Steenhuis et al., 1987) - is a transient, one-dimensional, advective-dispersive model based upon a simplified water flow representation. MOUSE tracks the position of a single solute peak by adjusting its position according to the amount of water moving past the position of the peak. Dispersion around the peak is calculated according to an error function representation. The model assumes only four soil layers or compartments and allows separate degradation rates to be entered into each soil compartment. However, its ability to vary other soil, chemical and hydraulic parameters with depth is limited to two layers, the root zone and below root zone layers. The model calculates surface runoff and will generate the required climatic data when this information is not available.

MOUSE was developed primarily as an educational tool and the simulation procedure is not as rigorous as in the other models considered. The model presents its results using clear graphical representations, however, no tabular output data files are generated. Hornsby et al. (1988) state that MOUSE tends to over predict evapotranspiration in comparison to other model results and that because of the less rigorous approach, it is not recommended for use as a management or research tool. The interactive approach of the model and the graphical output make this model most applicable to providing instructional guidance.

PESTAN (Enfield et al., 1982) - is a one-dimensional, solute transport model based on an analytical solution to the advective-dispersive equation. The model assumes steady state, one-dimensional flow within a homogeneous soil profile and tracks the movement and degradation of a single pesticide species. The model makes use of a solid-phase degradation in its simulations and degradation rates obtained from field experiments may be 3 to 5 times too high (Jones, 1989).

PESTAN was one of the first pesticide models to be developed and is relatively simple to use (requires only a few input parameters). However, with the development of more sophisticated models, it now receives little use. The model is limited in its applicability because it cannot accurately simulate situations were there are large variations in the seasonal rainfall or where the solute transport is occurring through a layered soil.

CMLS (Nofziger and Hornsby, 1986) - is an updated version of an earlier model called PISTON (Rao et al., 1976). The model calculates the movement and position of a single solute front, as well as the fractional amount of the pesticide remaining in the profile, using a simplified water balance. The model includes processes such as degradation and adsorption, and allows parameters describing these processes to vary with depth, but the water flow and solute equations describe advective flow with no dispersion of the solute. CMLS is easy to use and provides both graphical and tabular output, however, it does not calculate the chemical concentration profile, or leaching rate, of the pesticide and is therefore most applicable in an educational setting.

MANAGEMENT MODELS

PRZM (Carsel et al., 1984) - is the most widely used of all the mathematical pesticide transport and transformation models. PRZM simulates one-dimensional water flow and solute transport through the unsaturated zone under transient conditions. Although PRZM simulations are based on the advective-dispersive equation, water flow is represented as a lumped parameter model by representing the unsaturated zone as a series of soil compartments. At each time step, the flux of water and solute is calculated and cycled through the soil compartments with a simplified lumped parameter representation for the water balance (eg. flux is simulated with a "tipping bucket" concept) (Figure 3). The unsaturated zone is divided into three soil regions where runoff, evaporation, precipitation and snowmelt affects only the surface layer, and transpiration occurs only within the root zone layer. No additional sources or sinks occur in the below root zone layer. For example, the change in water storage in the PRZM model can be expressed for the three soil regions as:
Surface zone compartments:

$$\Delta SW_i = SW_{i,t-1} + P + SM - I_i - Q - E_i \quad (3)$$

Root zone compartments:

$$\Delta SW_i = SW_{i,t-1} + I_{i-1} - U_i - I_i \quad (4)$$

Below root zone compartments:

$$\Delta SW_i = SW_{i,t-1} + I_{i-1} - I_i \quad (5)$$

where:

ΔSW_i	=	net change in soil water content in layer i during present time step (cm),
$SW_{i,t-1}$	=	soil water content in layer i from the previous time step (cm),
P	=	precipitation minus crop interception (cm/day),
SM	=	snow melt (cm/day),
Q	=	runoff loss (cm/day),
E_i	=	evaporational losses (cm/day),
U_i	=	transpirational losses (cm/day), and
I_i	=	percolation out of soil compartment i, (cm/day).
I_{i-1}	=	percolation out of soil compartment i-1, (cm/day).

Each of the three layers shown in Figure 3 may actually consist of several individual cells, with each described by different physical and chemical parameters.

The percolation of water is dependent on two soil parameters, field capacity and wilting point. Field capacity is defined as the moisture content that soils attain after all excess water is drained from the system under the influence of gravity, while the wilting point of soil is defined as the soil moisture content below which plants are unable to extract water from the soil (Carsel et al., 1984). The flow of water is simulated according to the following simple drainage rules:

(1) any water which infiltrates into a soil compartment in excess of the field capacity will be drained to the compartment immediately below within one day;

$$\text{If} \quad SW_i > FC_i \quad \text{then} \quad I_i = (SW_i - FC_i) \cdot \Delta z, \quad \text{else} \quad I_i = 0$$

where:

FC_i = the water content of soil compartment i at field capacity (cm^3/cm^3),
Δz = the thickness of the soil layer (cm).

(2) moisture between the field capacity and the wilting point in the root zone compartments is available for evapotranspiration;

$$AWETi = (FC_i - WP_i) \cdot \Delta z$$

where:

$AWET_i$ = available water for evapotranspiration in soil compartment i (cm),
WP_i = water content of soil compartment i at the wilting point (cm^3/cm^3).

(3) the moisture content of a soil compartment cannot fall below the wilting point.

SW_i is always $\geq WP_i$

Compartments below the root zone quickly reach, and are maintained at field capacity. Water in the compartment in excess of the field capacity is simply flushed to the next lowest compartment and eventually to the water table.

The transport of pesticides in the subsurface is calculated with a finite difference approximation to the solute transport equation:

$$\frac{\partial c\Theta}{\partial t} = \left(\frac{\partial D}{\partial z} \cdot \frac{\partial c\Theta}{\partial z}\right) - \frac{\partial (vc\Theta)}{\partial z} - S \qquad (6)$$

where:

c = the dissolved solute concentration (mg/L),
Θ = the soil water content, ($\Theta = SW/\Delta z$) (cm^3/cm^3),
D = the liquid diffusion/dispersion coefficient (mm^2/day),
v = the soil water velocity, ($v = I \cdot \Delta z/\Delta t$) (cm/day),
S = pesticide source/sink terms, (mg/L·day)
t = time (day), and
z = depth (cm).

The soil water velocity term (v) and the water content term (Θ) are obtained from the lumped parameter description of the water balance given above.

PRZM accounts for many of the processes affecting solute transport in the unsaturated zone. Surface runoff and soil erosion are simulated with a Soil Conservation Service (SCS) curve number approach (Haith and Loehr, 1979; McCuen 1982) and a modified Universal Soil

Loss Equation (Williams and Berndt, 1977), respectively. A degree-day technique is used to calculate snowmelt and snowpack storage. The model accounts for simplified plant root and crop cover growth, and evapotranspiration is calculated using either daily pan evaporation data, or is empirically estimated from the daily temperature. Plant uptake of pesticide is related to the transpiration rate in the model and equilibrium adsorption (linear and reversible) and first-order degradation are included but are restricted to a single pesticide species.

PRZM does not actually attempt to simulate dispersion, but makes use of the numerical dispersion created in the solution of the finite difference equations to account for hydrodynamic dispersion of the pesticide in the unsaturated zone. If additional dispersion is desired, PRZM also accepts a hydrodynamic dispersion factor input parameter and dispersion created with this factor is superimposed on the numerical dispersion.

The time step in PRZM is constant and is set to one day. The solution to the set of equations representing flow through each compartment is undertaken by a tridiagonal finite difference technique. Execution times (on a 286-based machine, with a math co-processor) for a one year simulation are less than ten minutes.

Output from the model may include total, dissolved and adsorbed pesticide concentrations in each soil compartment, soil moisture contents and various pesticide and water flux parameters. However, these output parameters are limited to daily, monthly or yearly summaries.

Although PRZM is a dramatic improvement over the educational models, the main disadvantage of the PRZM model is its simplified approach to the flow of water (and thus the transport of solute) through the unsaturated zone. The processes are not described in as much detail as in a research model, however, execution times are relatively short and the amount of input data required by the model is not excessive and is generally available from existing data bases. PRZM is also limited to the simulation of one pesticide species. The model cannot simulate the fate of any metabolites generated from the transformation of the parent pesticide. In addition, PRZM does not account for surface volatilization losses of the pesticide.

GLEAMS (Leonard et al., 1987) - is a modified version of the surface runoff and erosion model, CREAMS (Knisel, 1980). GLEAMS was created by expanding the CREAMS model to consider the vertical flux of pesticides and to determine the groundwater loadings from a pesticide application. GLEAMS is based on a transient, advective-dispersive equation that makes use of a simplified water balance (similar to PRZM). The model allows for up to seven soil layers or horizons, with the surface layer being automatically set to a depth of 1 cm. All surface effects such as runoff and erosion are limited to this surface layer. The surface runoff component in the model is based on a Soil Conservation Service curve number approach and evapotranspiration and plant uptake are also considered. Upward movement of pesticide towards the surface layer by volatilization is possible in the GLEAMS model, however, volatilization losses from the surface layer are not simulated. The model has the ability to simulate the movement of up to nine metabolites generated from a parent pesticide. Different degradation rate constants may be specified for a pesticide located on the plant foliage, on the soil surface and within the root zone, but within these zones the degradation parameters are constant with respect to depth and time. GLEAMS also includes a weather data generator for simulations where the climatic data set is unavailable.

There are several weaknesses in the GLEAMS model. It is applicable only to simulations within the root zone and is limited to only seven soil compartments. Problems may arise when simulating pesticide transport in highly layered soils. Surface volatilization is not simulated. GLEAMS, being derived from a surface runoff and erosion model, has a very lengthy and detailed description of these two processes and requires a large amount of input characterization data. The amount of input data required may detract from the usefulness of this model when surface runoff and erosional processes are expected to be of little significance.

VULPEST (Villeneuve et al., 1987) - is a deterministic pesticide transport model, employing an analytical solution to a one-dimensional advective equation. However, it is used within a stochastic (Monte Carlo) approach. A simulation within a stochastic framework is undertaken by performing a large number of individual simulations or trials (1000 - 2000) using different values for the input parameters. The model parameters that characterize the site, such as the depth to the water table, the porosities of the soil layers, and the degradation constants, are randomly generated from a statistical distribution of the possible parameter values. Because a large number of trial are undertaken, the results of a simulation are assigned a statistical probability of occurrence. Although the soil column can be separated into distinct layers, all model parameters remain constant in space and time for a given trial. The spatial and temporal variation found in natural systems is accounted for by the probability distributions of the model parameters used during the Monte Carlo approach. The model output provides stochastic breakthrough curves, maximum concentrations and the time of arrival at specified depths, average annual concentrations, and the accumulated mass for each simulation. The results are presented in both tabular data files and as graphical representations.

Several limitations are associated with the use of the VULPEST. The use of an analytical solution in the VULPEST model restricts its application to situations were the soil profile is initially free of pesticide, and after time zero the pesticide concentration at the surface is constant. The model does not simulate dispersion or the fate of metabolites generated from the parent pesticide. VULPEST uses monthly rainfall and evapotranspiration data to produce a simplified water balance where average infiltration values and pore water velocities are generated, from which the solute transport can be calculated. The averaged values for the water balance may act to mask the peak flux of pesticides to the water table.

The stochastic approach provides for a better conceptual representation for the heterogeneities that may exist in the properties characterizing the field site (as opposed to a single-valued, field-averaged, deterministic approach). However, the accuracy of the stochastic simulation is still dependent on an accurate assessment of the distribution of field parameters, which requires an extensive set of field measurements. If the amount of field data available is limited, the stochastic approach, although providing a better conceptual approach to handling the heterogeneities that may exist, may not provide results that are more accurate than that produced using a single-valued, field-averaged approach.

SESOIL (Bonazountas and Wagner, 1984) - is a one-dimensional, advective-dispersive, solute transport model. The model is compartmentalized, however, it can accommodate only four soil layers, which may not provide for enough descretization for simulations in highly layered soils. The representation of water flow is based on a homogeneous soil profile and uses probability density functions for climatic variables, soil properties, and groundwater

elevations to determine long-term, "seasonal", averages for the components of the water balance. Erosional and volatilizational losses are considered in the model, as is the complexation of the solute.

The use of a seasonally averaged components in the water flux may act to mask peak concentrations being leached to the water table that may be of concern. Therefore, as the author of the model notes, the model is most suited to providing long-term, averaged predictions. The limitation of four soil layers also adversely affect the model's ability to simulate solute transport in layered soils.

MELEF-3v (Padilla et al., 1988) - is a one-dimensional, finite element, solute transport model. It is based on an advective-dispersive equation, considering adsorption and degradation. In addition to simulating mass transport in the unsaturated and saturated zones of a soil for transient conditions, the model also simulates heat flow. The degradation rate constants and adsorption equilibrium constants are adjusted to reflect the change in temperature with the Arrhenius and Van't Hoff equations, respectively. The time step in the model is variable and its length is computed at the beginning of each time step to ensure that stable and precise solutions result. The length of the time step depends on a number of factors including the water velocity and the finite element descretization. Several solution methods, such as Crank-Nicolson and the fifth order Runge-Kutta, are available. The execution time of the model depends on both the length of the time step calculated and on the solution method specified.

RESEARCH MODELS

LEACHM (Wagenet and Hutson, 1987) - is actually composed of three solute transport models: LEACHMN (nitrogen), LEACHMS (inorganic salts) and LEACHMP (pesticides). Only the LEACHMP code will be considered in the following discussion, and LEACHMP will henceforth be referred to as LEACHM.

LEACHM is the most detailed and conceptually complex of the models identified and is classified as a research/management model. The objective when formulating LEACHM was to develop a model that would simulate natural processes involved in the transport and transformation of a pesticide in the subsurface in sufficient detail to provide useful and accurate results, while restricting the amount and complexity of the information required to undertake a simulation. It was also intended that the output be organized in such a manner as to allow for quick and simple interpretation.

LEACHM can be used to simulate pesticide transport in the unsaturated (vadose) zone under transient climatic conditions, with multiple pesticide applications and boundary conditions. The simulation of the flow of water within the model is based on a direct solution to a one-dimensional form of the Richards equation, (Darcy's law and the continuity equation):

$$\frac{\partial \Theta_i}{\partial t} = \frac{\partial}{\partial z}\left(K_i(\Theta) \cdot \frac{\partial H_i}{\partial z}\right) - U_i(\Theta) \qquad (7)$$

where:

Θ = the soil water content (m^3/m^3),
$K(\Theta)$ = the hydraulic conductivity (mm/day),

H = the hydraulic head (mm),
z = the depth of the soil compartment (mm),
t = time (days), and
U(Θ) = represents water loss/gain per unit time (day^{-1}).

LEACHM employs a block-centered, finite difference approach to solving this equation. Basically, the unsaturated zone is divided into a series of nodes in the vertical direction, with the area surrounding each node representing a block or soil compartment (Figure 4). Within LEACHM, the node spacing (Δz) or size of each compartment is assumed constant. In finite difference notation, inflow and outflow from a soil compartment described by Darcy's Law, are:

$$\text{inflow} = \left(\frac{K_{i-1}(\Theta) + K_i(\Theta)}{2}\right) \cdot \left(\frac{H_{i-1} - H_i}{\Delta z}\right) \tag{8}$$

$$\text{outflow} = \left(\frac{K_i(\Theta) + K_{i+1}(\Theta)}{2}\right) \cdot \left(\frac{H_i - H_{i+1}}{\Delta z}\right) \tag{9}$$

Flow through a soil compartment is governed by the continuity equation, which in finite difference notation is given as:

$$\left(\frac{K_{i-1}(\Theta) + K_i(\Theta)}{2} \cdot \frac{H_{i-1} - H_i}{\Delta z^2}\right) - \left(\frac{K_i(\Theta) + K_{i+1}(\Theta)}{2} \cdot \frac{H_i - H_{i+1}}{\Delta z^2}\right) \tag{10}$$

With respect to time, the water content of the soil, in finite difference notation, (with the time derivative approximated by a time step (Δt)) is given as:

$$\frac{\Theta_{i,t} - \Theta_{i,t-1}}{\Delta t} = \left(\frac{K_{i-1}(\Theta) + K_i(\Theta)}{2} \cdot \frac{H_{i-1} - H_i}{\Delta z^2}\right) - \left(\frac{K_i(\Theta) + K_{i+1}(\Theta)}{2} \cdot \frac{H_i - H_{i+1}}{\Delta z^2}\right) - U_i(t) \tag{11}$$

The finite difference form of Richards equation is solved by employing a Crank-Nicolson approach.

After solving Richards equation, LEACHM determines the water flux density (q) across each soil compartment boundary in order to calculate the advective transport of the pesticide with:

$$q_{i+1/2} = K_{i+1/2} - K_{i-1/2} \cdot \left(\frac{H_{i+1} - H_i}{2 \cdot \Delta z}\right) \tag{12}$$

Once the water flux density is known, the model calculates the change in the pesticide concentration with time within each soil compartment. The mathematical expression for this is:

$$\frac{\partial c}{\partial t}(\rho K_D + \Theta + \varepsilon K_H) = \frac{\partial}{\partial z}\left([\Theta D(\Theta,q) + \varepsilon K_H D_{OO}]\frac{\partial c}{\partial z} - qc\right) \pm S \tag{13}$$

where:

c = the dissolved solute concentration (mg/L),

K_D = partition distribution coefficient (dm^3/kg),
ε = gas filled soil porosity (m^3/m^3),
K_H = Henry's Law constant,
q = the flux across a unit area per unit time (mm/day),
$D(\Theta,q)$ = the apparent diffusion coefficient (mm^2/day),
D_{og} = the vapour diffusion coefficient (mm^2/day),
S = a pesticide source/sink term (day^{-1}).

The solute transport equation (13) is solved by the finite difference method within LEACHM in a manner similar to that of the solution to the Richards equation. A detailed description of the theory and finite difference approximations used in the LEACHM model is presented in Wagenet and Hutson (1987).

Dispersion is an important transport process that effects both the concentration and the relative velocity of the pesticide in the unsaturated zone by acting to spread the dissolved mass over an increasingly larger area. The equation for calculating dispersion is given by:

$$D_L = (\alpha_L \cdot v) + D^* \qquad (14)$$

where:
D_L = coefficient of hydrodynamic dispersion (mm^2/day),
α_L = dynamic dispersivity (cm),
v = average linear groundwater velocity (cm/day), and
D^* = coefficient of molecular diffusion (mm^2/day).

LEACHM differs from the PRZM model in that it actually attempts to simulate hydrodynamic dispersion. Longitudinal dispersivity and molecular diffusion parameters are required by the model because LEACHM uses both molecular diffusion (D^*) and dynamic dispersivity (α_L) in its description of hydrodynamic dispersion (D_L). LEACHM also corrects the solution of the finite difference equations for any numerical dispersion that may have been created.

LEACHM may contain as many as 45 soil compartments, each with different values of physical, biological and chemical parameters assigned, thus giving the model the ability to simulate water and solute transport in multi-layered soils. Spatial and temporal variabilities that occurs at a field site are approximated by field averaged values. Flow is controlled by the characteristic curves defined for the soil which relate the retentivity and conductivity of the soil to the existing matric potential.

Pesticide attenuation is represented by equations describing equilibrium sorption (linear, reversible), volatilization, and chemical and/or biological degradation (first-order). Additional processes simulated by LEACHM include:

(1) the formation of two daughter products due to the transformation of the parent pesticide;
(2) the transport of two daughter products, with individual adsorption and degradation parameters assigned to each;
(3) the characteristic curves that define water movement in a particular soil;
(4) plant growth;
(5) daily evaporation and transpiration;

(6) water and pesticide uptake;
(7) the water flux, flux density, water contents and matric potentials for each soil compartment at each time step according to the surface and bottom boundary conditions specified by the modeler;
(8) the amount of chemical and/or biological degradation;
(9) the solute flux and concentration profile;
(10) the flow of heat in the soil profile and temperature distribution in the soil profile;
(11) the degradation rate constants as a function of the temperature profile.

The time step in LEACHM is variable, ranging from $1x10^{-7}$ of a day to $1x10^{1.3}$ of a day. The value for the time step is calculated within the model at the beginning of each time step to meet certain criteria defined by the user (i.e. a specified maximum water flux).

Output from the model includes current and cumulative totals for each pesticide species in each soil compartment, both water and pesticide flux below specified depths, and mass balance checks for the totals to ensure that the simulations are accurate.

The main disadvantage in the use of LEACHM is the lengthy execution times (eg. 7 hours on a 286-based machine with a math co-processor for a one year simulation with 25 soil compartments and 365 water applications). Other problems associated with LEACHM include the lack of a surface runoff and erosion simulator, the amount of input data required to characterize the site is more extensive than for the other models, and some of the parameters are not measured in typical field investigations.

SUTRA (Voss, 1984) - is a two-dimensional, solute or thermal energy transport model. Although the model can simulate transport in both the saturated and unsaturated zones it was primarily intended for the saturated zone. SUTRA allows for either areal or cross-sectional simulations in the saturated zone. It considers equilibrium adsorption and either zero or first order degradation under either steady or transient conditions. Many of the aquifer and fluid properties may be both non-homogeneous and anisotropic. The model uses both finite element and finite difference techniques, combining the geometric flexibility of finite elements with the numerical efficiency of the finite difference approach. Even so, the model is very computationally intensive and the model requires the use of a mainframe computer. Voss (1984) states that SUTRA will only provide accurate answers where the system is well defined and well descretized.

SELECTION AND APPLICATION OF PESTICIDE MODELS

A number of important factors should be considered in the selection and application of pesticide models. The choice of a model must take into account (1) the objectives of the simulations, (2) the knowledge and expertise of the user of the model, and (3) the availability of input data. If the objective of a simulation is to provide a general assessment, or mapping, of large areas of land for their susceptibility to groundwater contamination, then the speed and ease of use of screening models, such as DRASTIC or GUS, make these models most appropriate. Providing general instruction to those unfamiliar with the major processes that control the fate of pesticides in the subsurface is best accomplished with the use of educational models. The ease of use and the graphical representations associated with most educational

models (e.g. MOUSE) make these models suitable for providing insight into the influence of the major processes involved. In addition, the selection of a model may be restricted to these two groups if the amount of field characterization data is limited or the user does not have enough experience in the use of more sophisticated models.

When detailed field characterization data is available, the use of a research model (e.g. LEACHM), will allow for a detailed analysis of fate of a pesticide in the unsaturated zone with respect to both time and depth. Detailed sensitivity analyses to evaluate the influence of each of the processes involved in the transport and transformation of a pesticide are also possible, provided the user has a basic knowledge of the processes involved, and a sufficient level of expertise in the use of research models.

Qualitative assessments of the potential for groundwater contamination by pesticides are appropriate with management models when, in general, there are good data available from either the field or from existing data bases. The user must also have a reasonable knowledge of the processes involved and expertise in the use of pesticide models.

The assumptions and limitations inherent in a model should also be evaluated before a model is chosen. With the exception of the description of adsorption and degradation, the existing models differ from each other in both the number of processes described, the level of detail given in the description, and the limitations imposed by the processes included in the models. Most models assume first-order degradation and linear, equilibrium adsorption. In cases where these assumptions are not appropriate for a particular application, the modeler must make due with the limitations of a model, interpreting the results with these limitations in mind, or choose an alternative model. If, for example, erosional and runoff losses are expected to be of importance, then PRZM or GLEAMS should be considered as they are the only to models that simulate these processes. However, GLEAMS is limited to the root zone only and would be inappropriate if leaching of the pesticide past the root zone is expected. CMLS and MOUSE do not provide pesticide concentrations and would not be appropriate when this type of data is required. LEACHM and GLEAMS are applicable to situations where the transformation of the parent pesticide is of concern, however, the degradation rates for the metabolites generated in the GLEAMS model are depth invariant. PESTAN and VULPEST both make use of analytical solutions and may not be suitable where certain boundary conditions do not exist. The simplified water balance used in the majority of the models is most applicable to sandy soils, where percolation occurs quickly. In heavier soils were percolation is slower, and upward movement of water is possible, the water flow representation in LEACHM is more accurate.

The availability and accuracy of the input data required by the model is also of importance. The selection of a more complex model, because of the additional processes described, will provide no additional insights if the input data necessary to accurately characterize a particular site are not available, or are of questionable accuracy. In fact, errors introduced by incorporating inaccurate input data to describe a complex processes, may in some cases, exceed the error that would be produced had the additional processes not been included in the model, or if a simpler model had been used.

Although not a principle factor, the ease of use and computational requirements of the models should also be considered in the selection process. Research models may appear to be the best choice because of the number of processes included and the detail to which these

processes are described. However, the formulation of the input data set and the execution of the models may be so lengthy that the use of the models on an on going bases is not practical. In some cases, input data required by the research models, LEACHM and SUTRA, may not be collected during a typical field investigation. SUTRA is also a mainframe model which may eliminate it from consideration if such computing facilities are unavailable, and although LEACHM is a PC based model, its executions times are lengthy. Therefore, the use of research model by a trained modeler is appropriate only when detailed simulations are required, and only if accurate input characterization data are available.

The use of complex pesticide models requires a specialized knowledge in both the processes that control pesticide transport and transformation, and in the use of numerical models. The application of more complex models by a broad range of those who can make use of these models, is therefore, difficult. A means of overcoming the difficulties involved in applying complex models has been proposed by Crowe and Mutch (1990), where an expert system is being developed to aid pesticide regulatory personnel in their evaluation of the possible detrimental affects of a pesticide on groundwater quality when applied to different agricultural settings across Canada. The expert system will guide regulatory personnel through the development of the input data set required by a pesticide transport and transformation model. The expert system will also perform the necessary tasks in running the model, and will provide regulatory personnel with an interpretation of the results of the simulation.

A management model (PRZM) and a research model (LEACHM) were chosen for inclusion in the expert system (Mutch and Crowe, 1989). PRZM allows for quick executions of the system when a number of "what if" scenarios are being investigated, and would also be used by the system when surface runoff or erosion are important, or when detailed characterization data are not available. The use of LEACHM permits a more detailed evaluation to be performed on the processes and environmental factors controlling the fate of the pesticide in the unsaturated zone. LEACHM would be employed after the worst case or typical case scenarios were identified with the PRZM model. LEACHM would also give the expert system the ability to simulate metabolites generated from the parent pesticide.

Based on the review of the existing pesticide models presented herein, and from the conclusions drawn by Mutch and Crowe (1989), it is evident that for a general range of applications, PRZM and LEACHM, are the most useful and flexible models in their respective classification categories. Although the two models represent the physical and chemical processes that control the fate of a pesticides in the subsurface, the mathematical framework upon which these models simulate the flow of water and transport of a pesticide is very different. For example, these differences include: (1) PRZM uses a lumped parameter representation; LEACHM employs a distributed parameter representation, (2) PRZM simulates the flow of water with a water balance approach; LEACHM solves for the distribution of hydraulic heads with Richards equation, and (3) PRZM uses numerical dispersion generated during the execution of the code to simulate hydrodynamic dispersion; LEACHM actually solves the hydrodynamic dispersion equation by using values of dispersivity and molecular diffusion, and corrects for numerical dispersion created. Because the approach taken by PRZM in representing water flow and pesticide transport is less detailed, it is instructive to know whether simulations undertaken with PRZM actually provide meaningful results. Simulations were conducted with the two models to give an indication of the typical predictive information provided by the two models.

Similar reference data sets were compiled for the two models. Two year simulations were preformed on a soil column with the water table set at a depth of 2.5 metres. Conceptually, the soil column was broken into two zones. Parameters assigned to the first 50 centimetres were representative of the root zone, while parameters assigned to the remaining two metres were representative of the below root zone layers. The soil column itself, was divided into 50, 5 cm compartments in the PRZM model, and 25, 10 cm compartments in the LEACHM data set.

The soil profile and parameters assigned to the hydrogeological, climatic, and agricultural setting are hypothetical to the extent that the specific values for these parameters are not derived from a particular field site. Rather, the values are typical of conditions which would exist at a variety of sites on Prince Edward Island (MacDougall et al., 1981). Crop management and chemical parameters for the simulations are representative of values that would be appropriate for an application of aldicarb to a potato crop on Prince Edward Island (Priddle et al. 1987;1988;1989, Mutch, 1989).

A single pesticide application (2 kg/ha) was applied to a pesticide free column on day 1, and incorporated to a depth of 10 centimetres. Precipitation in the amount of 3 millimetres per day was applied. The pesticide had a solubility of 6000 mg/L and an organic carbon partition coefficient of 5 L/kg. Degradation of the pesticide was not consider in the simulations presented.

The soil would be classified as a sandy-loam with a bulk density of 1.2 g/cm^3 in the root zone and 1.5 g/cm^3 in the below root zone layers. The saturated hydraulic conductivity was set at 700 mm/day and 100 mm/day for the root and below root zone layers, respectively, in LEACHM, while in the PRZM model the field capacity and wilting points were set to 0.30 and 0.10, respectively. Plants were present in the simulations, however, pesticide uptake by the plant roots was not considered. The layered soil representation described above was used as this representation approximates conditions found in the field.

It should be noted that in the simulations conducted, the models were not calibrated to produce similar results, beyond providing similar input data sets to the two models. The models have different water flow representations and describe various processes in differing amounts of detail. It would therefore, not be expected that the two models would produce the same results, without a calibration of the parameters (e.g. dispersion, field capacity, etc.) of one model against the results of the other. The results presented, simply provide an indication of the type of output that can be expected from the two models.

Breakthrough curves for the pesticide at the water table are presented in Figure 5, while concentration profiles for the two models at different times throughout the simulations are displayed in Figures 6 and 7. Although the magnitude of the concentrations of the breakthrough curves differ for the two models, the shape of the two sets of breakthrough curves, the travel time and the relative reduction in concentration of each set are not significantly different. The degree to which PRZM is compartmentalized (50 compartments), allows the model to produce results that are in close agreement with those provided by LEACHM (see Figures 5 through 7). The simplified water balance in the PRZM model, although estimating water flow in the unsaturated zone based on a simplified black box type of approximation, provides results that are in good agreement with those predicted by the more complex model (LEACHM) for simulations in sandy soils, where percolation through the soil

profile is relatively quick. However, in tighter soils, where water movement is more restricted, and where the upward movement of water can occur in response to evaporational losses, the ability of LEACHM to simulate the upward movement of water in the soil profile will result in a more accurate simulation of the transport and transformation of the pesticide in the subsurface (Jones, 1989).

Thus, a model which simulates the complex physical system in some detail may not necessarily produce significantly better results than a less complex model, such as PRZM. In some circumstances the advantages offered by using a model such as LEACHM may be limitted to sensitivity analyses studies that focus upon the importance of the controlling physical and chemical processes that affect the fate of pesticides in the subsurface.

CONCLUSIONS

Existing pesticide transport and transformation models offer a wide range of applications, from general mapping of area that may be susceptible to groundwater contamination, to detailed site assessments. In choosing the most appropriate model for a particular application the following points should be considered; (1) the specific objectives of the study, (2) the knowledge and experience of the user in modelling pesticides in the unsaturated zone, (3) the assumptions inherent in, and the limitations imposed by, the number and descriptive detail of processes included in the model, (4) both the ease of use, and the ease of interpretation of model results, and (5) the availability of accurate input characterization data. If conflicts arise in any of the considerations outlined above, a reevaluation of the study objectives may be required. Although there are a wide variety of models available that are applicable to many different situations, one model may not satisfy all the selection criteria. In some situations, it may be appropriate to select more than one model with which to perform the simulations, as is the case in Crowe and Mutch (1990).

Pesticide models are divided into two groups based upon the approach that the models take. The first, screening models, compare physical and chemical characteristics of the site and pesticide to the properties of other pesticides and sites where groundwater contamination is known to have occurred. The assessment of the potential for a pesticide to contaminate groundwater is given on a relative basis with respect to other pesticides that are known to have contaminated groundwater supplies. The models do not attempt to simulate the processes involved and do not quantify either the amount, or rate, of pesticide leaching to the water table. The second group, mathematical models, attempt to describe the major processes affecting the fate of pesticides in the subsurface with mathematical representations. These models generally provide estimates on both the amount and rate of pesticide leaching to the water table. Mathematical models are further subdivided into either educational, management, or research models. The number of processes included in the models, the level to which these processes are described, the amount of input data required, and the difficulty in using the models, all increase from educational models, through management models, to research models. The range of applications for the mathematical models is varied. These models may provide information ranging from instructional guidance (educational models) to a detailed site assessments (research models).

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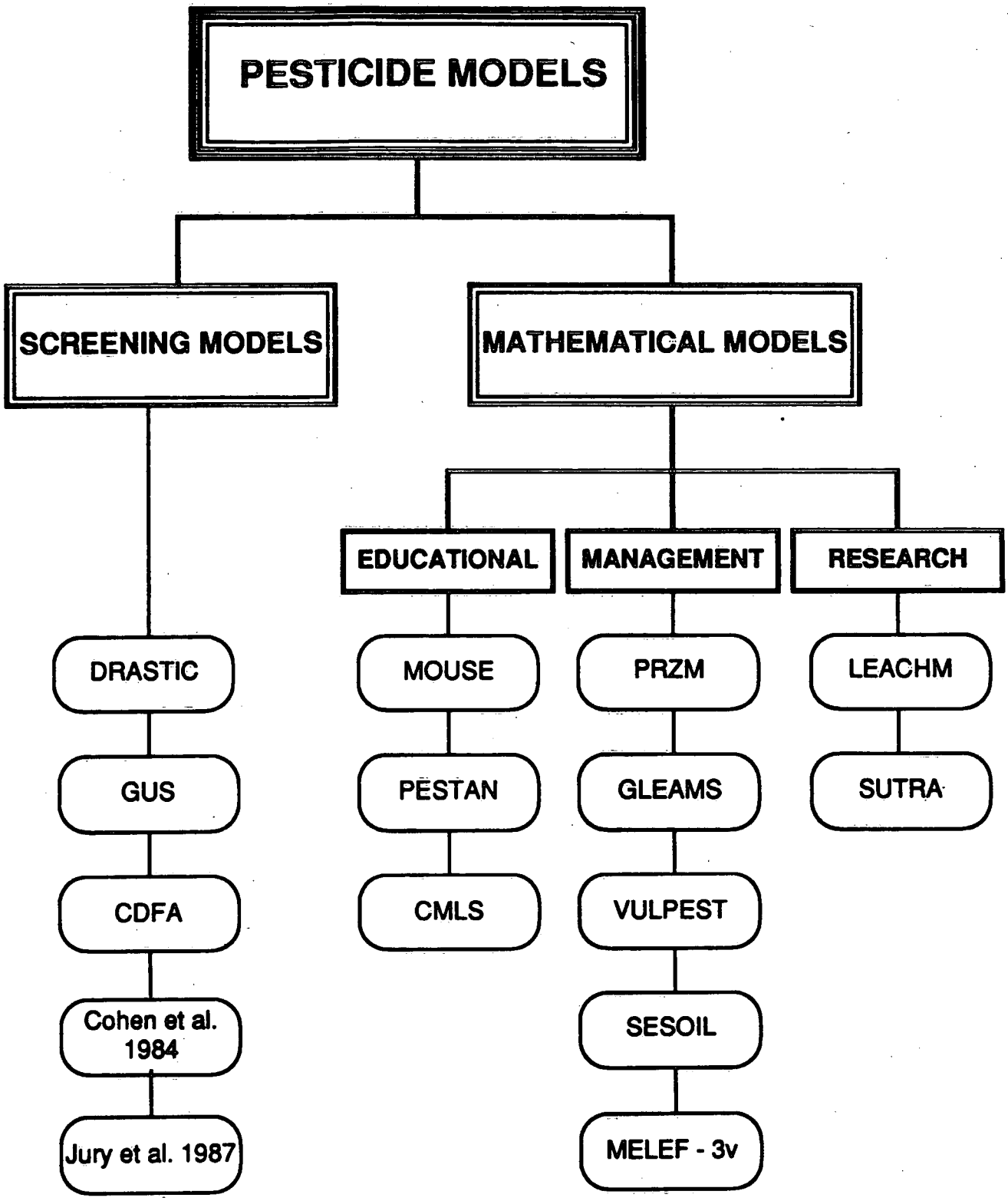
LIST OF FIGURES


PESTICIDE MODELS
SCREENING MODELS
MATHEMATICAL MODELS
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RESEARCH
DRASTIC
GUS
CDFA
Cohen et al. 1984
Jury et al. 1987
MOUSE
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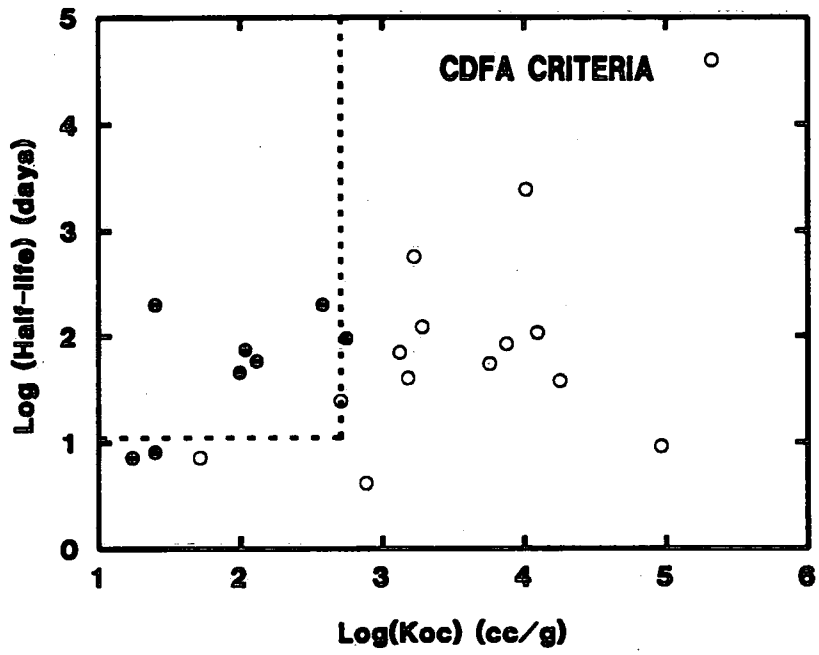
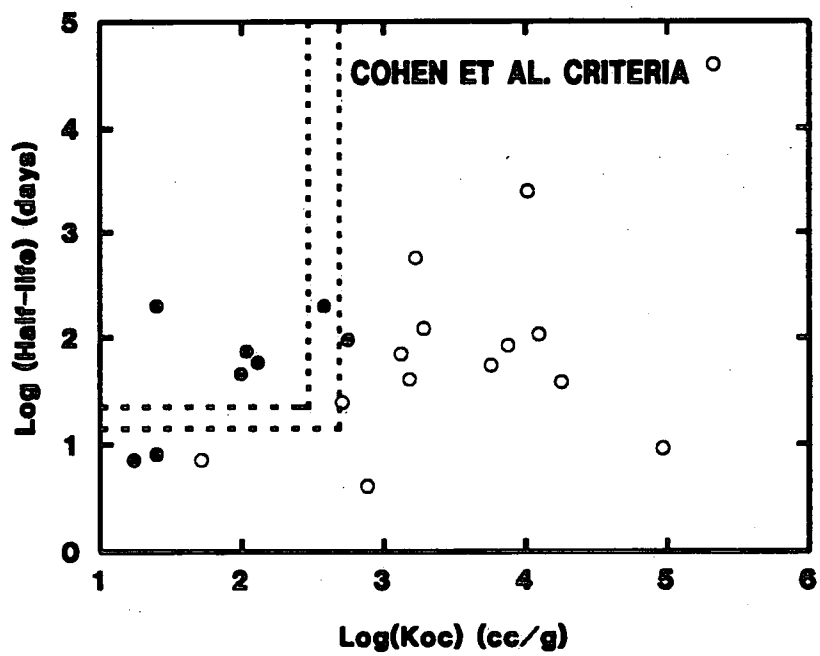
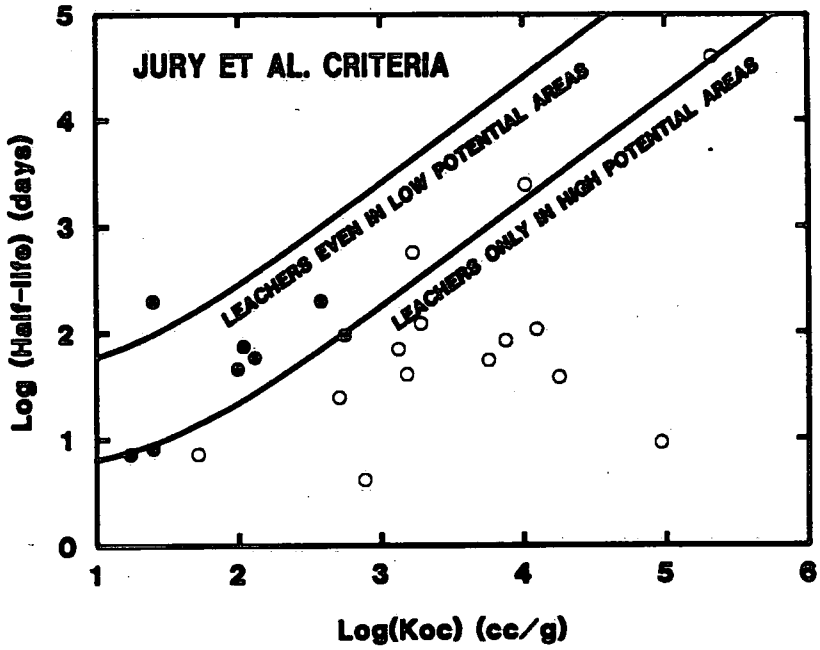
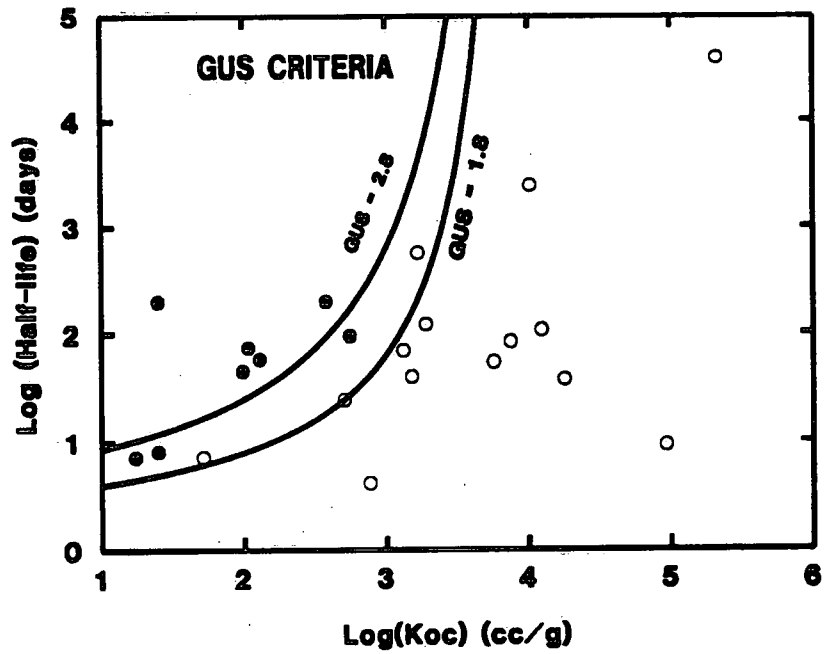
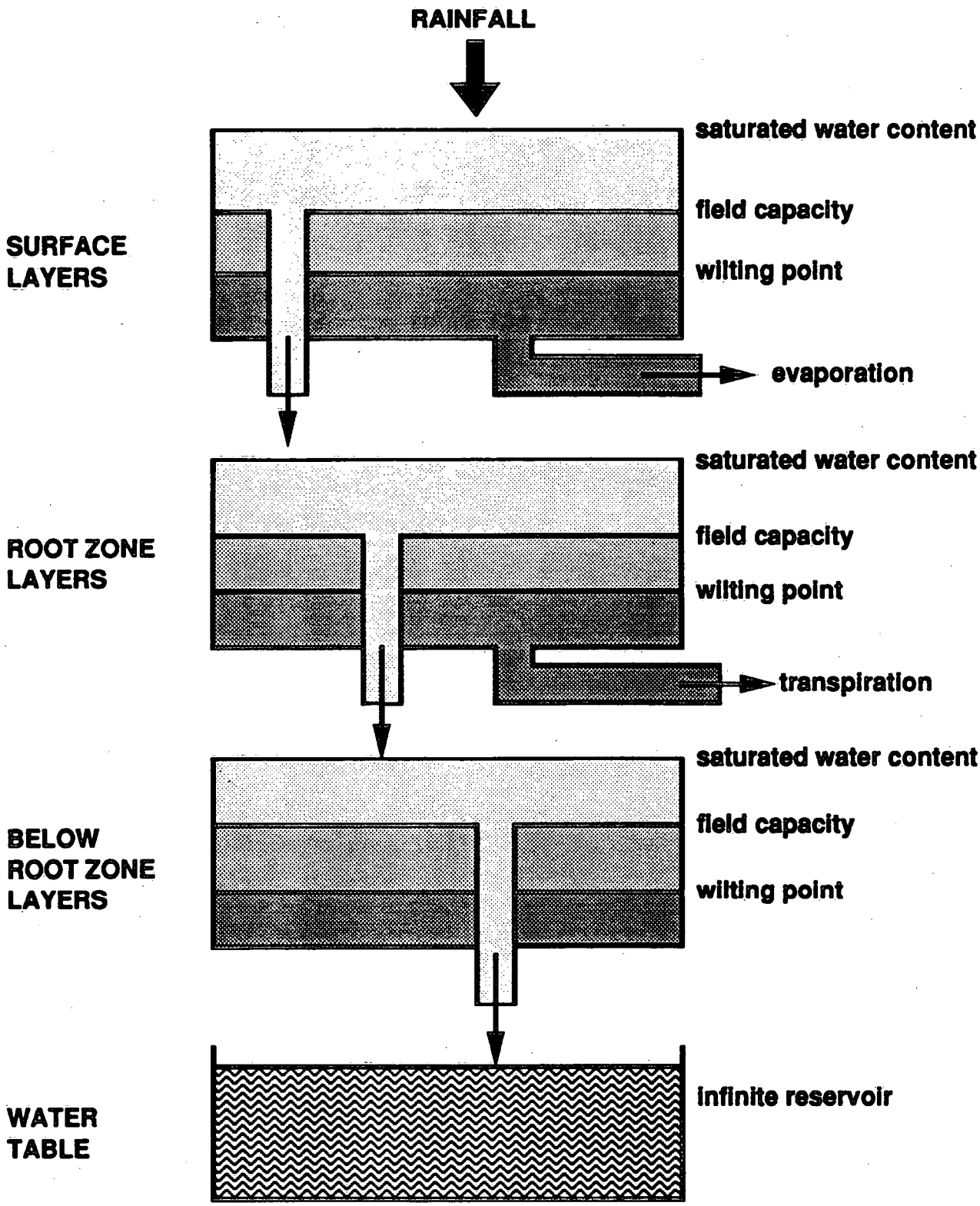
CMLS
PRZM
GLEAMS
VULPEST
SESOIL
MELEF - 3v
LEACHM
SUTRA

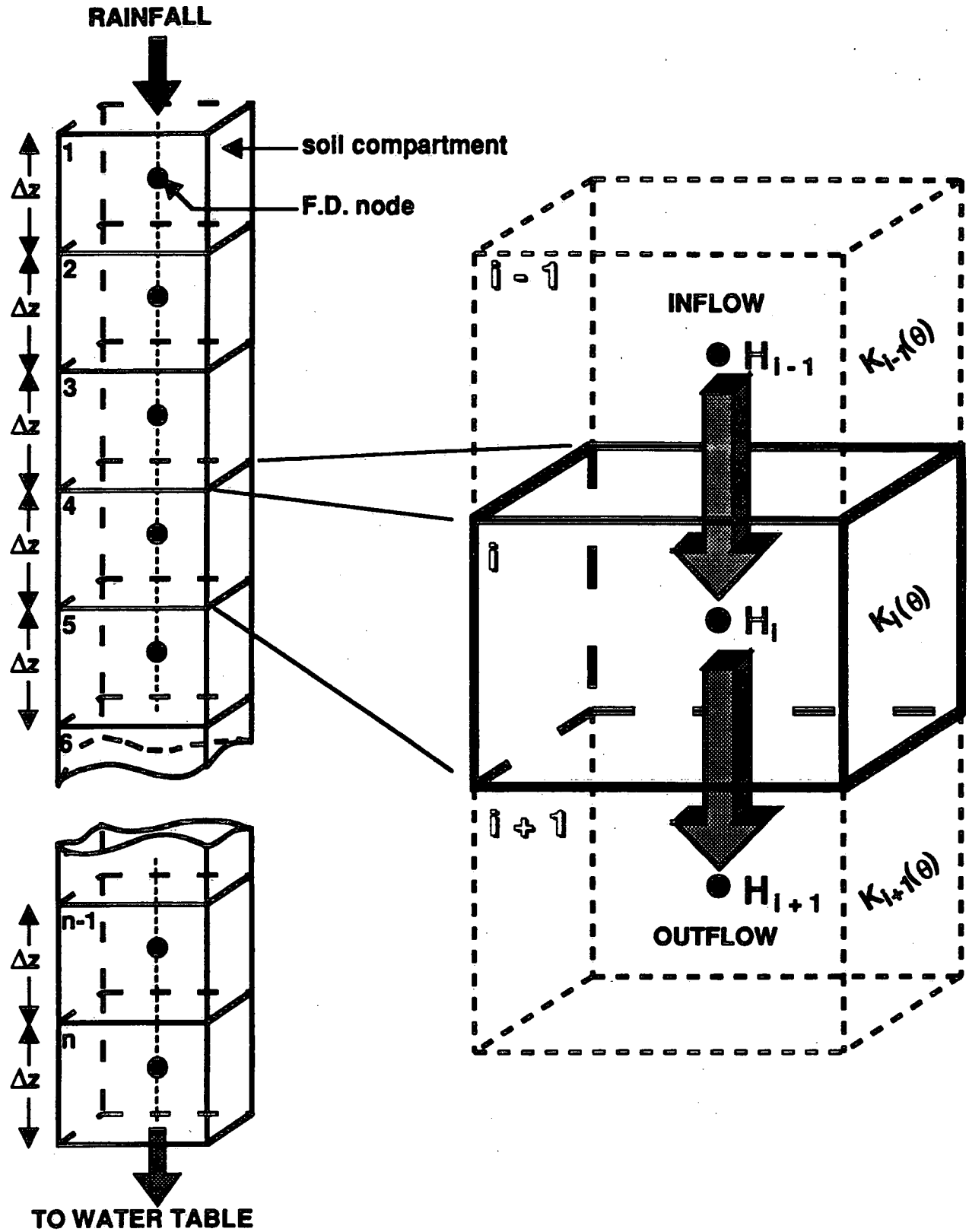

CDFA CRITERIA
Log (Half-life) (days)
Log(Koc) (cc/g)
0
1
2
3
4
5
6

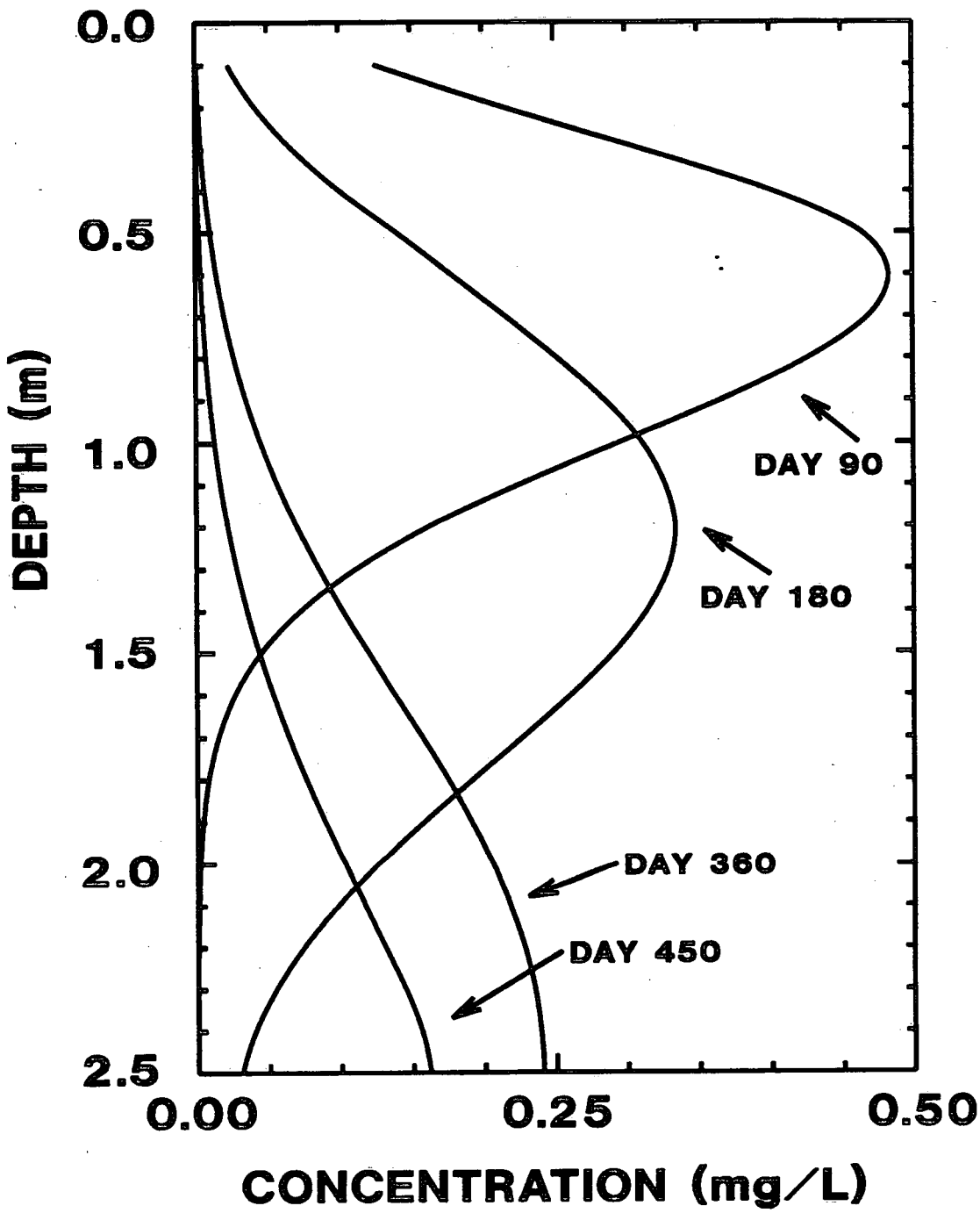

COHEN ET AL. CRITERIA
Log (Half-life) (days)
Log(Koc) (cc/g)
0
1
2
3
4
5
6

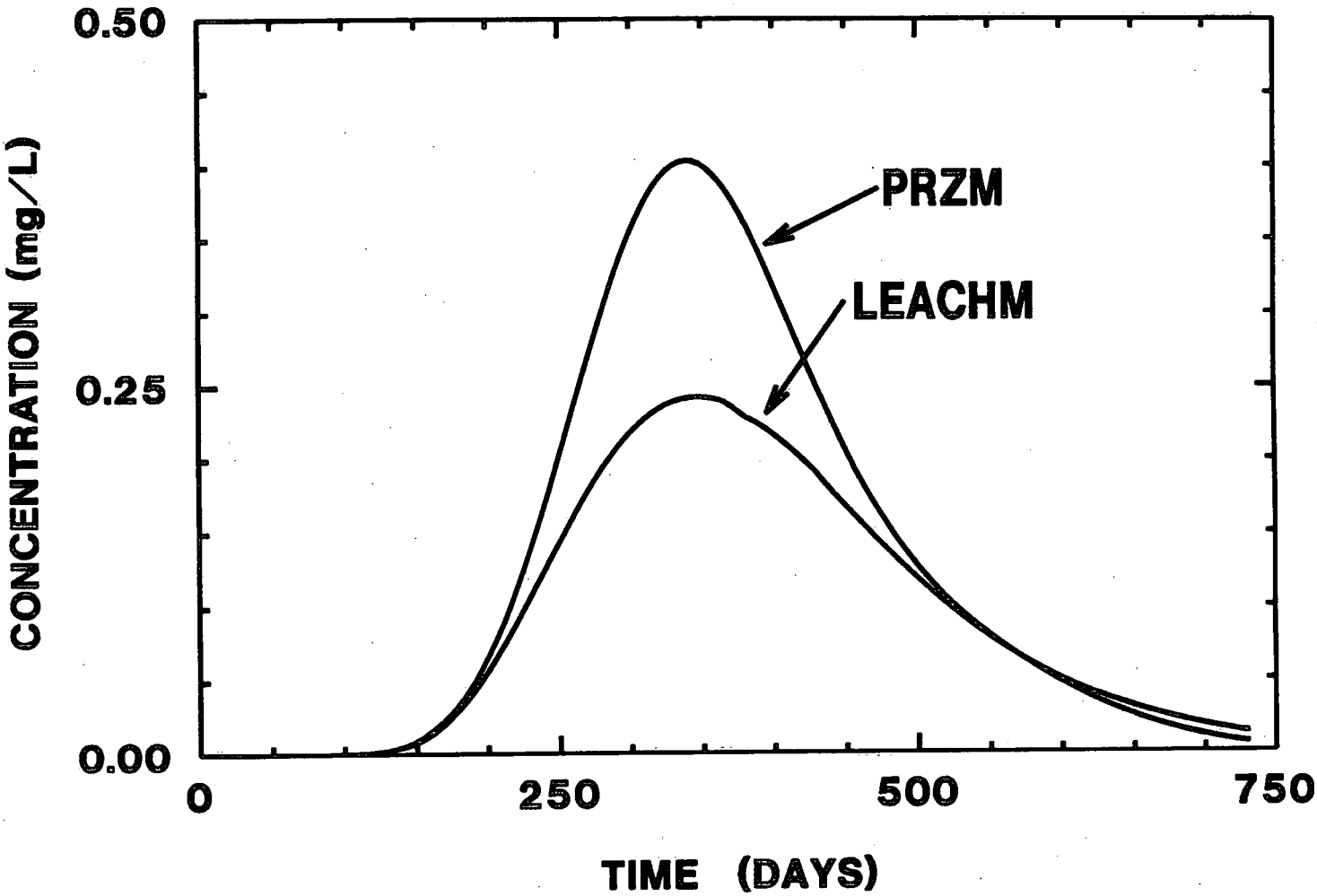

JURY ET AL. CRITERIA
LEACHERS EVEN IN LOW POTENTIAL AREAS
LEACHERS ONLY IN HIGH POTENTIAL AREAS
Log (Half-life) (days)
Log(Koc) (cc/g)
0
1
2
3
4
5
6

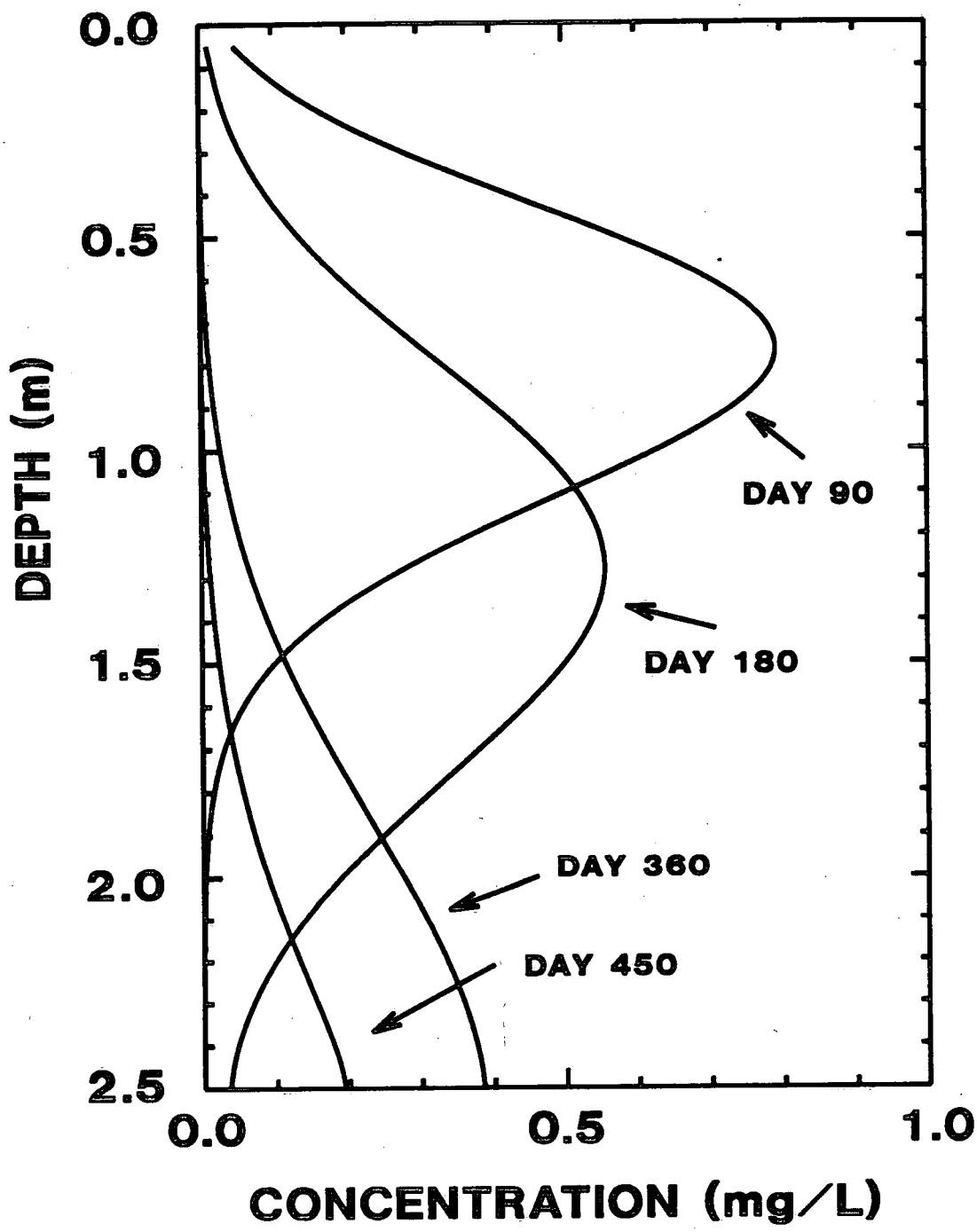

GUS CRITERIA
GUS = 2.8
GUS = 1.8
Log (Half-life) (days)
Log(Koc) (cc/g)
0
1
2
3
4
5
6


RAINFALL
saturated water content
field capacity
wilting point
SURFACE LAYERS
evaporation
saturated water content
field capacity
wilting point
ROOT ZONE LAYERS
transpiration
saturated water content
field capacity
wilting point
BELOW ROOT ZONE LAYERS
infinite reservoir
WATER TABLE


RAINFALL
soil compartment
F.D. node
Δz
1
2
3
4
5
6
n-1
n
TO WATER TABLE
i - 1
INFLOW
H_{i-1}
$K_{i-1}(\theta)$
i
H_i
$K_i(\theta)$
i + 1
H_{i+1}
$K_{i+1}(\theta)$
OUTFLOW


0.0
0.5
1.0
1.5
2.0
2.5
DEPTH (m)
DAY 90
DAY 180
DAY 360
DAY 450
0.00
0.25
0.50
CONCENTRATION (mg/L)


0.50
0.25
0.00
CONCENTRATION (mg/L)
PRZM
LEACHM
0
250
500
750
TIME (DAYS)


0.0
0.5
1.0
1.5
2.0
2.5
DEPTH (m)
DAY 90
DAY 180
DAY 360
DAY 450
0.0
0.5
1.0
CONCENTRATION (mg/L)