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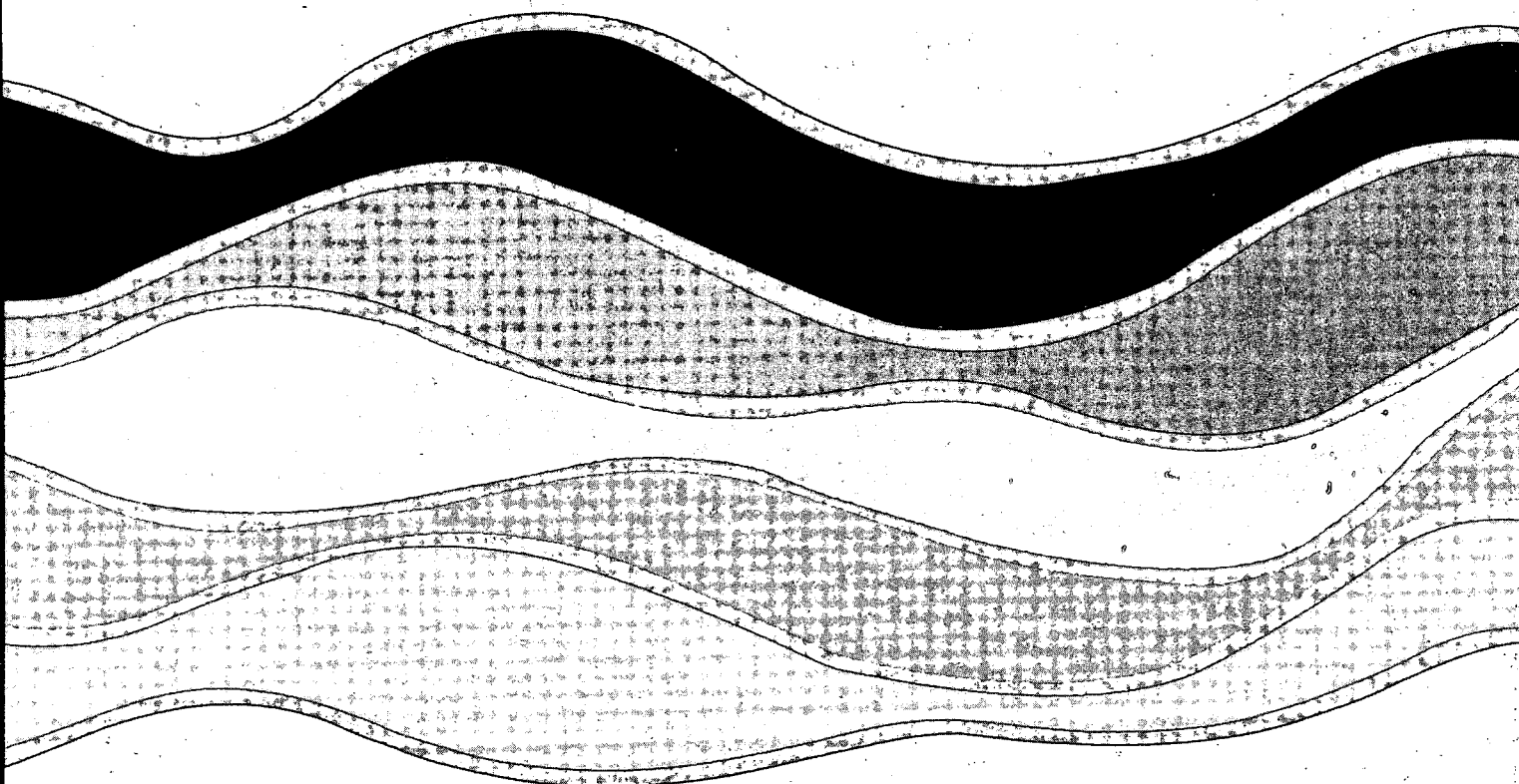
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**EXPRES: AN EXPERT SYSTEM FOR ASSESSING THE
FATE OF PESTICIDES IN THE SUBSURFACE**

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EXPRES: AN EXPERT SYSTEM FOR ASSESSING THE
FATE OF PESTICIDES IN THE SUBSURFACE

by

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MANAGEMENT PRESPECTIVE

The Pesticide Division of the Commercial Chemicals Branch, Environment Canada, is required to assess the environmental hazards associated with a pesticide and its transformation products before it is approved for public use. One specific concern of the Pesticide Division is the potential for a pesticide to contaminate groundwater resources. Although a number of computer models currently exist that can predict the transport and transformation of pesticides in the subsurface, generally, regulatory personnel do not have the expertise required to accurately utilize these models. The Groundwater Contamination Project, NWRI, was approached by the Pesticide Division to develop an expert system that can be used to aid in the assessment of the potential for groundwater contamination by pesticides. This expert system, known as EXPRES (EXpert system for Pesticide Regulatory Evaluation and Simulation) can be used for the identification of agricultural development which may or may not be sustainable. This paper outlines the design, development and operation of the expert system, and also provides the reader with a brief overview of EXPRES.

PERSPECTIVES GESTION

La Division des pesticides de la Direction des produits chimiques commerciaux d'Environnement Canada évalue les risques environnementaux associés à un pesticide et à ses produits de transformation avant d'approuver son utilisation par la population. Elle s'intéresse particulièrement aux risques de contamination des eaux souterraines par un pesticide. Bien qu'il existe plusieurs modèles informatisés pour prévoir le transport et la transformation des pesticides dans les eaux souterraines, le personnel chargé de l'application de la réglementation ne possède généralement pas le savoir-faire pour bien les utiliser. La Division des pesticides a demandé au personnel affecté au Projet de contamination des eaux souterraines de l'INRE de mettre au point un système expert pour évaluer le potentiel de contamination des eaux souterraines par les pesticides. Ce système expert, appelé EXPRES (système expert pour les simulations de l'évaluation réglementaire des pesticides), peut être utilisé pour identifier les activités de développement agricole durable. Le présent rapport décrit la conception, la mise au point et le fonctionnement du système expert et en donne un bref aperçu au lecteur.

ABSTRACT

This paper describes an expert system, known as EXPRES (EXpert system for Pesticide Regulatory Evaluation Simulations), which is designed to aid regulatory personnel in their assessment of the potential for pesticides to contaminate the soil and groundwater environment. EXPRES consists of two existing numerical models (PRZM and LEACHM) which are used to simulate the transport and transformation of pesticides in the unsaturated zone, coupled with a knowledge-based system that guides the user through the selection of all the necessary information to construct input data sets for these models. Specific tasks undertaken by EXPRES include: (1) supplying the geological, physical, climatic, hydrogeological, pedological and agricultural settings of typical agricultural regions across Canada as required by the pesticide models, (2) predicting migration rates and concentrations of pesticides in the unsaturated zone with time and depth, (3) determining the concentration of pesticide reaching the water table and the time required for the pesticide to reach the water table, and (4) aiding the user with an interpretation of the results of the simulations.

RÉSUMÉ

Ce rapport décrit le système expert EXPRES (système expert pour les simulations de l'évaluation réglementaire des pesticides), conçu pour aider le personnel chargé de l'application de la réglementation à évaluer le potentiel des pesticides à contaminer le sol et les eaux souterraines. EXPRES comprend deux modèles numériques existants (PRZM et LEACHM) utilisés pour simuler le transport et la transformation des pesticides dans la zone non saturée, et un système axé sur une banque de connaissances qui, par la sélection de toutes les données nécessaires, permet à l'utilisateur de créer des fichiers d'entrée pour ces modèles. Le système expert EXPRES a pour fonction de 1) fournir des données géologiques, physiques, climatiques, hydrogéologiques, pédologiques et agricoles des régions agricoles typiques du Canada requises pour construire les modèles des pesticides, 2) prévoir les vitesses de migration et les concentrations de pesticides dans la zone non saturée, en fonction du temps et de la profondeur, 3) déterminer la concentration de pesticides qui atteint la nappe phréatique et le temps requis à ces pesticides pour atteindre la nappe phréatique, et 4) aider l'utilisateur à interpréter les résultats des simulations.

Introduction

Pesticides have been used extensively to enhance both crop production and quality. However, the use of pesticides is not without environmental risks. In particular, the contamination of shallow groundwater resources has occurred all too frequently. For example, several recent studies examining only one pesticide, aldicarb, and its transformation products, have shown that this pesticide can lead to the contamination of groundwater even when recommended application procedures are followed (Zaki et al., 1982; Jones, 1985; Harkin et al., 1986; Jones and Marquardt, 1987; Jones et al., 1987; Priddle et al., 1987; 1988; Mutch et al., 1990).

Before a pesticide is registered for public use in Canada, the following federal government agencies; Agriculture Canada, Environment Canada, Health and Welfare Canada and the Department of Fisheries and Oceans, expose all new pesticides to extensive testing to ensure that the pesticides, and their degradation products, present minimal risks to the environment (Agriculture Canada, 1987; Crowe and Mutch, 1990). Of particular concern during the assessment of the environmental risks associated with a pesticide, is the persistence, mobility, accumulation and transformation/degradation of the pesticide in the subsurface. Several numerical models that are capable of predicting the distribution and concentration of a pesticide in the subsurface currently exist (see review by Mutch and Crowe, 1990). However, the application of these models in a regulatory framework is limited because, firstly, the transport and transformation of a pesticide is governed by a complex set of chemical, biological and physical processes, and a specialized knowledge of these processes is required in order to accurately assess the fate of pesticides in the unsaturated soil zone. Secondly, the numerical framework upon which the models are based is generally complex and typically can only be operated by a trained modeller. Thirdly, the models require a specialized set of physical and chemical data which is not generally obtained during typical field studies. Therefore, there is a need to develop or modify an existing numerical model so that it will have a sufficient level of realism in its simulation of the major processes controlling the fate of pesticides, enabling it to assess the effects of a pesticide on the quality of the groundwater, and yet be easily and accurately used within a regulatory environment.

Expert systems represent an attractive tool for overcoming the difficulties involved with the application of these complex pesticide models by regulatory personnel who are assigned the task of assessing the fate of pesticides in the subsurface. Generally, expert systems are designed to assist non-specialists in solving complex problems that are beyond their present level of knowledge in either the field of interest or in computing ability.

This paper describes an expert system which is designed to aid regulatory personnel with their evaluation of the possible detrimental effects of pesticides on the quality of groundwater. The expert system, known as EXPRES; EXpert system for Pesticide Regulatory Evaluation Simulations, is actually a knowledge-based system combined with a pesticide transport and

transformation code. It is designed to guide a user through the development of the input data set required by a pesticide transport and transformation model, execute the model and provide an interpretation of the potential for groundwater contamination. EXPRES is designed as a management tool to be used as an aid in making policy decisions. Thus, the use of the expert system is not intended to replace the current procedure for pesticide evaluation and registration. Rather, it is intended that the expert system will be used in conjunction with current procedures. The goals of EXPRES are to:

- (1) provide a quick and general assessment of potential environmental hazards;
- (2) identify if further field or laboratory study is warranted;
- (3) define specific regions or sites where field testing is required;
- (4) identify locations where post-registration monitoring is needed.

In order to meet these goals, the specific tasks undertaken by the expert system include:

- (1) providing regulatory personnel with a method of obtaining the geological, hydrogeological and computer modelling expertise required for their assessments;
- (2) predicting migration rates and concentrations of pesticides in the unsaturated zone with time and depth;
- (3) determining the concentration of pesticide reaching the water table and the time required for the pesticide to reach the water table;
- (4) aiding the user with an interpretation of the results of the simulations.

An overview of expert systems

Generally, expert systems (also known as knowledge-based expert systems) function by encoding the decision-making abilities of a specialist, or "expert", in a particular field of endeavour into a computer program in such a way that, through an interactive process between the program and the user, a general practitioner or layman can be confidently guided through the necessary steps required to solve a complex problem. Human expertise which is encoded into an expert system includes knowledge, experience, judgement and problem-solving abilities that has been acquired through years of training and personal experience. This section presents a brief overview of the general concepts of an expert system used in the construction of EXPRES and is summarized from Crowe and Mutch (1990). The reader requiring a more detailed description is referred to Crowe and Mutch (1990).

There are significant differences between conventional computer programs and expert systems. Conventional computer programs execute a prescribed set of procedures as defined by the programmer and thus, are well suited for routine (i.e. repetitive) and exacting (i.e. mathematical calculation) tasks. For example, a typical numerical model will input quantitative data (typically numbers), manipulate these data according to a prescribed set of programming statements, and

present the results in a specific format. Expert systems extend conventional programming techniques by including decision-making and interpretive abilities into the code. Expert systems input information (rather than just data) and have the ability to evaluate, interpret, and to suggest alternatives, based upon the input goals of the study. Recommendations and interpretations, in addition to quantitative information, are presented at the end of a simulation.

The two main features characterizing an expert system are, firstly, their use of large informational data bases, and secondly, their representation of knowledge. Information can be divided into facts and knowledge. Facts include the quantitative data obtained from textbooks, manuals, laboratory and field experiments, etc. Facts can be further subdivided into observed facts (given data) or derived facts (deduced through a direct mode of inference). Knowledge is more qualitative in nature and it includes a collection of facts, insights, hunches and problem solving rules or procedures, including heuristic knowledge, which is derived from experience gained through solving problems in the past. The information contained within an expert system may be either high quality information, such as exact values, or it may be heuristically derived based upon the inferences and relations.

Three structures are typically used to represent knowledge: (1) production rules, (2) semantic nets and (3) frames (Figure 1). Although expert systems may be constructed entirely with any one of these structures, they are more commonly composed of a combination of rules, nets and frames. Production rules consist of "IF-THEN" conditional statements, such that when information for a particular problem matches the conditions stated in the "IF" portion of the rule (known as the condition or premise), the statements in the "THEN" portion of the rule (known as the action or consequence) are executed. The linking of rules forms a reasoning strategy that can be used as either a diagnostic tool or an interpretive tool. Semantic nets are used to represent non-rule-based knowledge according to an association among objects, events or concepts where the data are associated by "IS-A" links within a hierarchical network. Frames are used to group or categorize non-rule based knowledge that is characterized by a number of attributes or related parameters and typically take the form of mini-data bases where these data are entered or retrieved via a keyword.

An expert system for pesticide regulatory decisions

The EXPRES expert system (EXpert system for Pesticide Regulatory Evaluation Simulations) is designed as a management tool to be used as an aid in making policy decisions regarding the benefits and risks of a proposed pesticide, and specifically, to ensure that the quality of the groundwater in agricultural areas is maintained. Because EXPRES is not intended for use as a research tool, its primary objective is to provide an assessment of the potential hazards to the shallow groundwater regime associated with a particular pesticide, and to identify if further study (e.g. field testing) is warranted. It is not intended to provide insight into the processes that control

the transport and transformation of pesticides in porous media. The important criteria for constructing the expert system and the biological, chemical and physical processes incorporated into the transport and transformation model are discussed in this section.

The objective of using an expert system framework for the evaluation of the fate of pesticides in the subsurface is to allow those not proficient in the use of numerical models which simulate pesticide transport in the subsurface to accurately use these complex codes. Therefore, the following criteria are addressed in the design and construction of the EXPRES expert system:

- (1) the system must be easily used by those with minimal computer skills and knowledge of pesticide transport in the subsurface;
- (2) upon introduction to the expert system, the user should be able to effectively use the system within a relatively short time;
- (3) it should run quickly and efficiently on a personal computer;
- (4) parameters required by the pesticide model should be readily available from data bases or easily entered into the system via a dialogue format;
- (5) corrections and changes during data entry should be easy to fix;
- (6) it must check the accuracy and consistency of user-supplied data, with identification and/or suggestions for missing values;
- (7) the user should be provided with an evaluation and interpretation of critical output from the simulation model, in an informative, useful and easily understood form;
- (8) the data bases should be complete;
- (9) the data bases should be constructed so that they can be easily modified and updated.

The general architecture of the EXPRES expert system is illustrated by Figure 2. EXPRES is composed of three parts; (1) the inference engine, (2) the user - system interface, and (4) the information and knowledge data bases. An important component of the knowledge base is the pesticide transport and reaction models which will be discussed in a separate section.

The Inference Engine

The inference engine contains the programming statements which affect the general control of EXPRES. The inference engine is divided into several modules, each controlling specific operations. The program control module regulates the basic computer operations of EXPRES, and determines how, and in what order, the procedures are undertaken, such as linking the pesticide transport model, printing or plotting the results of the simulations, and searching the data bases. The reasoning control module manages the reasoning strategy required to compose a data set characterizing the physical setting, climatic conditions and agricultural practices of a particular site. It also evaluates the results produced by the simulation model. The reasoning strategy is based on the application of the appropriate production rules, frames and sematic nets. The interpretation module translates the user's entries into a form that can be used by the expert system to select rules

to control the operation of EXPRES, prompts the user for further information and composes an input data set for the simulation model. In addition, this module performs internal checks to ensure accuracy and consistency among all the entered values and converts the results of a simulation to an easily interpretable form. The data update module allows the existing data bases to be modified or expanded with the addition of new facts or knowledge.

The User - System Interface

The second component of EXPRES is the user - system interface. It is an interactive program that guides the user through the entry of data required by the pesticide transport models within EXPRES and provides assistance on interpreting the results obtained from the model. By entering data interactively, the user is not required to have knowledge or experience in programming, or in the use of the operating system or pesticide models. The user - system interface prompts the user for simulation options required by the models and for data characterizing a pesticide. If the user is uncertain as to the information being requested, then definitions, explanations, and assistance from the explanation data base are provided to the user. If the requested information is unavailable, the user - system interface will assist the user in obtaining the required information by displaying typical values or options stored in the facts data base. Heuristic or empirically derived estimation techniques are also available to the user from the knowledge base to aid in the selection of an appropriate value for requested information.

The user - system interface automatically provides typical values for the physical, climatic, hydrological and pedological setting of agricultural areas from the information stored within the facts data base. The user has the option to modify these default values. Generally, the user enters or modifies the data and information presented by EXPRES in frames. A frame, or a collection of frames and prompts, presented by EXPRES on a computer monitor is known as a screen, such as the one illustrated by Figure 3. Screens allow considerable information to be entered quickly and efficiently when compared to the time and effort required to enter the same data via a series of prompts from a user - system interface. Also, screens allow the user to enter information in any order and to review previously entered data quickly.

A second important feature of the user - system interface module is that it conveys both quantitative and qualitative output from the simulation model to the user. Output takes the form of tables of numbers and/or graphics to help visualize trends, anomalies and relationships among variables. Also, to help novice users understand the critical output from the model, EXPRES contains various levels of decision-making support for aiding in the interpretation of the simulation results. In ascending order of support, these levels are:

- (1) simple presentation of results in tabular form;
- (2) graphical presentation of results (eg. concentration with depth at a specific time);

- (3) explanations of what is represented by the graphs (eg. pesticide will reach the water table before it completely degrades);
- (4) recommendations regarding further simulations (eg. change the value of hydraulic conductivity by an order of magnitude to see if pesticide will still not contaminate groundwater).

The Data Bases

The third component of EXPRES is the three information data bases; the knowledge, explanation and the facts data bases (see Figure 2). The knowledge base contains the production rules which are used to relate the facts and concepts describing a domain or a reasoning methodology. The knowledge base contains the encoded expertise. This information is accessed via the reasoning control module of the inference engine to provide assistance to the user in the choice of parameters and options required for a pesticide transport and transformation simulation. The knowledge base also contains the production rules used for performing internal checks and for an interpretation of the results of a simulation via the interpretation module. Specifically, the type of information stored within the knowledge base includes:

- (1) all production rules for constructing the input data set for the simulation model;
- (2) rules for checking the plausibility of the values of the selected parameters;
- (3) production rules for interpreting the results of a simulation;
- (4) the models for simulating pesticide transport and transformation.

Because of the importance of the simulation of the transport and transformation of pesticides in the subsurface, the following section will discuss the simulation models in detail.

Information stored within the explanation base consists of encoded definitions and explanations, as well as elaborations designed to help the user understand the question or information being requested. In addition, this data base is accessed to provide a typical range of values, allows the user to follow the expert system's reasoning strategy, checks the entered values for consistency with previously entered information, and aids the user in understanding the conclusions and recommendations. The type of information within this data base includes:

- (1) definitions, explanations and tutorial information for the requested input parameters;
- (2) examples of similar data or situations;
- (3) recommended values;
- (4) time-dependent simulation parameters.

The facts data base is comprised of detailed information required by the simulation model to describe the physical, climatic, hydrogeological and agricultural setting of eleven typical agricultural zones across Canada (eg. an orchard in central British Columbia, a wheat field in Saskatchewan, a corn field in Ontario, a potato field in P.E.I., etc.). The characterization of these typical agricultural zones is hypothetical to the extent that the basic model parameters are not

derived from a particular field or orchard. The choice of parameters used to define the typical agricultural zones is, however, guided by experience from a variety of field studies undertaken within a particular zone. Because there is considerable variation in the physical, hydrogeological, climatic and agricultural settings on a local scale, the parameters assigned to a typical agricultural zone may not adequately represent all potential sites within the zone. Therefore, EXPRES is designed such that the parameters comprising a typical agricultural zone can be easily modified by the user for a particular simulation.

A second set of data in the facts data base is comprised of the chemical characteristics of existing pesticides. It is accessed by the user when information for a new pesticide is required by the model but is not available to the user. By examining a family of similar pesticides in this data base, the user will be able to approximate the required data for the new pesticide.

The Simulation Models

The simulation of the transport and transformation of pesticides within the unsaturated zone is undertaken with a numerical model. The accuracy of the predictions depend upon how realistically the model is able to reproduce the physical, chemical and biological processes that control the transport and transformation of the pesticides in the field. Thus, the mathematical framework of this model must be based upon accepted scientific principles that describe these processes. Physical processes controlling the transport of the pesticide include pesticide flux through the soil surface, advective and dispersive transport of dissolved pesticide, and pesticide loss due to surface runoff. Chemical and biological processes which affect the chemical character of the pesticide include chemical speciation (dissociation/association), adsorption, plant uptake, transformation/degradation (microbial transformation, phototransformation, hydrolysis, oxidation), and volatilization.

Several pesticide transport and transformation models that could meet the needs of EXPRES currently exist, and these models were evaluated for their potential incorporation into the expert system. The criteria defined for selecting a model for EXPRES are that the model must:

- (1) predict migration rates and concentrations of pesticides in the unsaturated zone with time and depth;
- (2) determine the concentration at, and time required for a pesticide to reach, the water table;
- (3) simulate the transport, and predict concentrations, of the transformation products;
- (4) be based on generally accepted scientific principles that govern the transport and transformation of pesticides;
- (5) be a widely accepted and verified computer code;
- (6) be programmed in such a way as to ensure that modifications can be made easily;
- (7) be compatible with the U.S. EPA models in terms of processes considered and with the assumptions, logistics and limitations inherent in the framework of their models.

Most existing models account for the major chemical, biological and physical processes that control pesticide transport and transformation in the unsaturated zone. Examples of these models include PESTAN (Enfield et al., 1982), SESOIL (Bonazountas and Wager, 1984), PRZM (Carsel et al., 1984; 1985), MOUSE (Pacinka and Steenhuis, 1984; Steenhuis et al., 1987), LEACHM (Wagenet and Hutson, 1986; 1987), CMIS/CMLS (Nofziger and Hornsby, 1986, 1987), GLEAMS (Leonard et al., 1987) and VULPEST (Villeneuve et al., 1987). The extent to which the models describe the basic processes influencing the migration and transformation of pesticides varies considerably among the models. Although there is a corresponding increase in the accuracy of the prediction of the fate of a pesticide with each increase in the level of complexity, often the advantages offered by the more complex models are offset by an increase in execution time and difficulty in formulating the input data sets.

Of the models reviewed (Mutch and Crowe, 1989, 1990), the model best suited for use in an expert system designed to assist in regulatory decisions on pesticide registration is the management model PRZM. A research model, LEACHM, was also selected because it provides a detailed description of the processes involved in the transport and transformation of pesticides in the unsaturated zone, thus it is preferable to a management model when a detailed evaluation of the transport or transformation processes is desired.

The choice between the use of the PRZM or LEACHM models for a simulation must take into account the objectives of a simulation, the availability of data and the execution time for a simulation. When field data are characterized in sufficient detail, LEACHM will allow for a detailed analysis of the fate of a pesticide and associated daughter products with respect to both time and depth. PRZM is more valuable when a more qualitative assessment of the potential for a pesticide to contaminate groundwater is required, and when the field data are not characterized in detail. Even though a more complex model (LEACHM) describes the processes affecting pesticide transport and transformation in more detail than PRZM, LEACHM will not provide more accurate results or additional insight if the input data necessary to accurately characterize a process at a particular site are not available.

The PRZM model, Pesticide Root Zone Model, (Carsel et al., 1984, 1985) simulates one-dimensional, pesticide transport under transient conditions. Although the model is based on an advective-dispersion equation, it employs a lumped parameter approach in which the unsaturated zone is divided into a series of compartments or storage elements. At each time step, the flux of water and solutes is cycled through the series of elements by maintaining a simplified representation of the water balance within each compartment (eg. flux is simulated with a "tipping bucket" concept). Infiltration and percolation of water is dependent upon two soil parameters, field capacity and wilting point. Compartments below the root zone quickly reach, and are maintained at

field capacity, simply flushing existing water in the compartment to the next lower compartment and eventually to the water table.

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 curve number approach and a modified Universal Soil Loss Equation, 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 from either pan evaporation data or is empirically estimated from daily temperature data. Plant uptake of pesticide is related to the transpiration rate in the model. Numerical dispersion created during the computation procedure is used to represent actual hydrodynamic dispersion. Equilibrium adsorption (linear and reversible) and first-order degradation are included but are restricted to a single pesticide species.

The size of the time step in PRZM is constant and is set at one day. Output from the model may include total and dissolved pesticide concentrations in each compartment, soil moisture contents and various pesticide and water flux parameters. Execution time for a one year simulation, on a 286-based personal computer with a math co-processor, is less than ten minutes.

LEACHM, Leaching Estimation And CHemistry Model, (Wagenet and Hutson, 1986, 1987) actually refers to a group of three solute transport models: LEACHMN (nitrogen), LEACHMS (inorganic salts) and LEACHMP (pesticides). Only the code that focuses upon pesticides, LEACHMP, is included in EXPRES. LEACHMP can be used to simulate the one-dimensional transport of a parent pesticide and up to three daughter products in the unsaturated zone under transient conditions, with multiple pesticide applications and user selected boundary conditions. The unsaturated zone is represented by as many as 45 soil compartments, with the ability to vary the values of physical, biological and chemical parameters assigned to each compartment, thus allowing simulations of the fate of pesticides in multi-layered soils. The flow of water within the model is based on a direct solution to the Richards equation, (Darcy's law and the continuity equation for the unsaturated zone), and is undertaken by a finite difference technique. Flow of water is controlled by characteristic curves defined for the soil which relate the retentivity and conductivity of the soil to the existing matric potential. Attenuation of the pesticide and daughter products are represented by equations describing equilibrium sorption and volatilization (both linear and reversible), and chemical and/or biological degradation (first-order), with individual adsorption, volatilization and degradation parameters assigned to each. The degradation rates parameters may be varied as a function of depth.

The time step in LEACHMP is variable, ranging from a minimum value of 1.0×10^{-7} to 5.0×10^{-2} of a day and is calculated at the beginning of each time step to meet certain criteria defined in the model (i.e. a specified maximum water flux). Output from the model includes current and cumulative concentrations for each of the pesticide species in each soil compartment, both water

and pesticide flux below prescribed depths, and cumulative mass balance checks to ensure that the simulations are accurate.

The primary disadvantages of LEACHMP are, firstly, a lengthy execution time (eg. 5 hours for a one year simulation with 45 soil compartments, on a 286-based personal computer with a math co-processor), and secondly, a large input data set required to characterize the existing conditions and objectives of the simulation. Other limitations with LEACHMP were removed as part of this study by modifying the original code (Wagenet and Hutson, 1987) to account for snowmelt, pesticide loss by surface runoff and the erosion, and estimation of pan evaporation (if unavailable) based on temperature data.

Operation of EXPRES

EXPRES is designed to operate on a 80286-based personal computer. Minimum hardware requirements include a 80286 math co-processor, a 20MB hard disk, a monochrome monitor, 640KB of memory and a CGA graphics card. Software for EXPRES is implemented within a DOS environment. Rather than using an expert system development shell, such as NEXPERT or KEE, or a symbolic manipulation language, such as LISP or PROLOG, development software for EXPRES consists of Microsoft® C for the user - system interface and inference engine, and Microsoft® FORTRAN for the simulation models (PRZM and LEACHM). A conventional programming language was used in the development of EXPRES because existing expert system shells typically lack the generality and flexibility required for adaption to specific problems other than those for which the shells were originally designed. In addition, it is difficult to couple expert system shells to existing simulation models programmed in FORTRAN, and EXPRES does not require the complex reasoning strategy of existing shells. Advantages offered by "C" in the construction of the expert system are that it can:

- (1) provide input data screens that allows data to be entered easily and efficiently;
- (2) produce screens which are visually pleasing and non-intimidating to a novice user;
- (3) provide a link among data bases, spread sheets, graphics and FORTRAN programs;
- (4) allow the construction of pull-down menus and screen overlays;
- (5) it is a common and widely used programming language.

The basic operations undertaken within EXPRES, their order of implementation, and whether the operations require prompts from the user or are handled internally by EXPRES, are illustrated by Figure 4. This figure illustrates how EXPRES branches to, firstly, obtain model specific data for either PRZM or LEACHM, and secondly, to run a specific model, depending upon the simulation objectives. Because much of the input data are common to the two models, branching is not undertaken by EXPRES for all the required data. One group of input data (pesticide characteristics) are entered through prompts to the user, and another group of data (site

characteristics) are retrieved as default values via EXPRES. Finally, EXPRES will display output and evaluate the results from the models depending upon the goal of the pesticide evaluation simulation. These operations are described in more detail below.

All user - system interactions, including the general operation of EXPRES, take place via screens. The screen shown previously (Figure 3) and those that follow are representative of the screens used by EXPRES. A series of commands and pull-down menus that are accessed through the command line located at the top of the screen provides the user with control of EXPRES. Movement among the screens is handled with the commands *Next-Pg* and *Previous-Pg*, while movement among variables within a screen is controlled by the arrow keys. Default values for the hydrological, meteorological and soil parameters, which are stored in the facts data base, are accessed via the *Default-Values* command. Upon completion of the input data set, execution of a simulation model is undertaken with the *Run* command. The user may exit EXPRES at any time through the *Exit-EXPRES* command, saving the data set in either a complete or incomplete state. The *Help* command provides additional information for parameters presented on the EXPRES screens. The *Instructions* command provides a pull-down menu describing the basic operation of EXPRES.

As an input data set for the simulation models is created by EXPRES, all user supplied or default values are saved as an ASCII file. Because all information is saved upon exiting from EXPRES, the user may leave EXPRES at any time, with or without the completion of a data set. Upon re-entering EXPRES, the user may recall the existing data, by specifying the name of the ASCII file, and may then either run the existing scenario (if complete), modify the scenario, or complete the data set. One of the first screens displayed by EXPRES is a request for session information (Figure 5). EXPRES requests that the user enter the name of a current file if an existing data set is being recalled, or enter a new file name if a new pesticide is being investigated. Also, three types of introductory information may be obtained which would enable a novice user to become familiar with EXPRES. Firstly, information is available that discusses the instructions on the operation of EXPRES, including moving through the screens, entering data, running a simulation and interpreting the results. Secondly, an overview of EXPRES, consisting of the purpose, applications, limitations of EXPRES and the simulation models PRZM and LEACHM, may be recalled. Thirdly, the user may be lead through an example session in which all the user requested information, in addition to the default values, is supplied.

The selection and application of a pesticide model by EXPRES is primarily based upon the objectives of a simulation. Although not a primary factor in influencing the accuracy of a simulation, the required execution time must be considered when deciding which model should be run. The execution of LEACHM on a 80286-based PC is typically of sufficient length that simulations can only be run during an "over-night" situation. However, the processes are

sufficiently simplified within PRZM so that this model typically performs a simulation in less than an hour. As a result, selection of the PRZM model is most applicable when a number of "what if" scenarios are to be investigated (i.e. what if the hydraulic conductivity was an order of magnitude greater at a specific site than reported for the agricultural zone), or for determining what combination of parameters produce a worst-case scenario. Simulations performed with the LEACHM model are more applicable when assessing the relative influence of each parameter on the transport and transformation of a pesticide through a sensitivity analysis, or in undertaking a detailed investigation of the worst-case scenario determined with the PRZM model.

The simulation objectives are defined by the user (Figure 6) and based on these choices, EXPRES will choose the most appropriate model (PRZM or LEACHM) to use in the evaluation. The user has the option of performing either a single simulation (*Run a scenario*) or a series of simulations where the value of an individual parameter is varied systematically over a plausible range of values to determine the response of the system to a small error in the value of one of the parameters (*Sensitivity analysis*). The user also specifies whether the results are desired within an hour (*Quickly*) or can be produced over several hours (*No preference*). The user also specifies whether or not daughter products are to be simulated. EXPRES then considers information on the approximate length of the simulation and the computational power of the PC's processor (80286 or 80386) when making the selection of the appropriate model.

The reasoning strategy for the selection of either the PRZM or LEACHM model is illustrated by Figure 7. This reasoning strategy is typical of that used within EXPRES. Based on the choices illustrated by Figure 6, EXPRES would indicate that LEACHM is the most appropriate model for undertaking a sensitivity analysis which considers daughter products. However, with a 80286-base PC, the user would be informed that the results cannot be produced with LEACHM in less than an hour. Therefore, the user is requested to re-examine his objectives by either indicating that the simulations may take more than one hour, or that if the results must be made available within an hour, then a sensitivity analysis considering the fate of daughter products can not be performed.

There are two general groups of data required by EXPRES; data which must be supplied by the user and default values supplied by EXPRES (Figure 8). The first group consists of user supplied data that describes the user's choice of an agricultural zone of interest, the chemical characteristics of the pesticide, and the form of output from the simulation models. Because EXPRES is designed to be used when evaluating a new pesticide, the pesticide data would not be in the existing data base, and hence, the user must enter the required information into empty frames within a screen (Figure 9). Based upon the user's choice of an agricultural zone (eg. a potato field in PEI), EXPRES supplies a second group of data, which are default parameters describing the soil, crop and meteorological conditions for the chosen agricultural zone. An example of a screen

in which default values have been placed into the appropriate frames is illustrated by Figure 10. Although most of the data entered by the user or retrieved from the facts data base are common to both PRZM and LEACHM, some values are model specific. However, the process of determining which data are required for which model is handled internally within EXPRES, and hence, is transparent to the user.

The registration of each new pesticide is different in terms of (1) the chemistry of the pesticide, (2) the proposed application procedures and quantities, and (3) the meteorological, agricultural, hydrological, and geographical conditions of the site of intended use. Because the variability inherent in these factors, both from region to region and within a specific site, leads to considerable uncertainty as to what will happen when a pesticide is used at an actual field site, the creation of data sets for the simulation models is designed to be flexible. In order to reduce the amount of uncertainty that exists, the data supplied by the manufacturers can be analyzed through a series of worst-case scenarios at the different sites and under various conditions. The user may change any of the default values characterizing an agricultural zone, and undertake the simulations as a sensitivity analysis.

An important feature of EXPRES is that it is designed with an on-line help facility to aid the user in the selection and entry of data. EXPRES incorporates pull-down menus, accessed through the *Help* command located on the command line at the top of each screen, to provide the user with information on parameters in the form of a *Definition*, *Explanation* and *Assistance* (Figure 11). The *Definition* facility will give a brief definition of a parameter, while additional information about a parameter is provided through the *Explanation* facility, which discusses where or how a value may be used or obtained. *Assistance* provides examples of recommended values or empirical equations which may be used to estimate the value of a parameter.

After the user has entered all the data required to undertake a pesticide transport and transformation simulation, EXPRES uses a series of rules to check the consistency and validity of the data selected or modified by the user. For example, values of parameters must be within realistic bounds (eg. the user can not change precipitation by a factor of 10), indicate that the hydraulic conductivity of a sandy soil is 10^{-9} cm/s, or have a planting date later than the harvesting date. Consistency checks are initiated when the user changes a default value.

Following the consistency check, EXPRES runs either PRZM or LEACHM and modifies the output produced by these models to present the results of a simulation in a manner in which the user can clearly understand and interpret the results. EXPRES will display model-specific screens that allow the user to choose the type of output desired. The two types of output are, firstly, concentration profiles, which show pesticide concentrations through the soil profile at different times, and secondly, summary files, which depict time series representations of pesticide concentrations at the water table.

These two types of output from EXPRES are illustrated through its application to an evaluation of the potential for the pesticide aldicarb to contaminate groundwater beneath potato fields on Prince Edward Island, Canada. This problem has been well documented through previous studies (Priddle et al., 1988, 1989; Mutch et al., 1990). The soil profile and parameters assigned to the hydrogeological, climatic and agricultural setting do not represent a specific site on Prince Edward Island (PEI), rather the values represent an agricultural zone, whose parameters are typical of the conditions which may exist at a variety of potato growing areas on PEI. A single pesticide application (2 kg/ha) was applied to a sandy-loam soil and incorporated to a depth of 10 cm. The pesticide has a solubility of 6000 mg/L, an organic carbon partition coefficient of 5 L/kg and there is assumed no degradation or pesticide uptake by the roots of the plants. The soil column is comprised of a 50 cm root zone and a 200 cm vadose zone extending below the root zone, with soil bulk densities of 1.2 gm/cm³ and 1.5 gm/cm³, respectively. The water table is at a depth of 2.5 m. Because PRZM and LEACHM use different numerical representations to transport water through a soil column, there are soil parameters specific to each model. A saturated hydraulic conductivity of 70.0 cm/d for the root zone, and 10.0 cm/d for below root zone is used by LEACHM, while field capacity and wilting point values of 0.30 and 0.10, respectively, are required by PRZM. A uniform rainfall of 3 mm per day was applied in the simulations. The soil column is divided into 25-10 cm compartments for LEACHM and 50-5 cm compartments for PRZM.

Profiles of total aldicarb concentrations with depth in the soil column are shown by Figure 12a at 90, 180, 360 and 450 days since the application of the pesticide. Although the values used to construct these plots were obtained by the LEACHM model, similar profiles would be obtained if EXPRES had chosen the PRZM code. This type of a graph highlights two important features of pesticide transport and transformation within the unsaturated zone. Firstly, as time following pesticide application increases, the centre of mass of the pesticide moves downward through the soil column due to physical transport. Secondly, as the pesticide migrates downward, the maximum concentration decreases due to dispersion (peaks broaden as mass is spread over a larger area) and the transformation (chemical or biological reactions, i.e. oxidation, hydrolysis, etc.) of the pesticide. Thus, from a concentration profile, in addition to observing the time required for the pesticide to reach the water table and its concentration once it reaches the water table, concentrations at various times and depths within a soil column also can be obtained.

Figure 12b illustrates a plot of a temporal record of the total pesticide concentrations at the water table. In this example, the graph was plotted using the summary file output obtained with the PRZM model. A similar graph could be produced with a simulation using LEACHM. Although this graph is basically a summary of the total aldicarb concentration at the water table during a 750 day period of time, it provides two useful pieces of information. Firstly, it illustrates the times for

the pesticide to first reach the water table (95 days), the time for the peak concentration to reach the water table (340 days), and time for the pesticide to completely move through the soil column (approximately 800 days). Secondly, it provides information on the concentrations of total aldicarb at the water table at any time since the pesticide was applied.

The user can also choose to have EXPRES undertake a sensitivity analysis on most of the site characterizing and pesticide parameters. Once a parameter is chosen by the user, EXPRES will indicate a range of plausible values (values appropriate for a "typical case" scenario to values appropriate for a "worst case" scenario) for a sensitivity analysis. Because sensitivity analyses are most appropriately undertaken with the LEACHM model, and because this model typically requires several hours of execution time, the actual sensitivity analyses are not undertaken by EXPRES. Rather, at time convenient to the user, the existing input data set may be recalled and the appropriate parameters may be modified (as recommended by EXPRES) by the user and EXPRES rerun. Thus, a series of individual graphs, such as Figure 12a or 12b, can be superimposed upon one another to depict the relative influence of the variation in values of the chosen parameter.

An example of a sensitivity analysis of the reaction rate constants (transformation and degradation) of aldicarb and its daughter products is shown by Figure 13. Transformation is defined as the change of a parent chemical that is of environmental concern to a daughter product which is also of environmental concern. Degradation is defined as the change of a parent chemical to a degradation product which is no longer of environmental concern. Because sensitivity analyses were run and the simulation included the formation and reaction of daughter products, EXPRES chose the LEACHM model to perform these calculations. The reactions simulated are the transformation (by oxidation) of the parent pesticide, aldicarb, to its toxic daughter product, aldicarb sulfoxide (Figure 13a), and the degradation (by hydrolysis) of aldicarb and aldicarb sulfoxide to their respective non-toxic daughter products, aldicarb oxime (Figure 13b), and aldicarb sulfoxide oxime (Figure 13c). These graphs show the effect of the change in the total concentration of the pesticide due to changes in the individual rate constants from a best case to a worst case (an order of magnitude higher or lower than the reference value). It can be seen that an increase in the oxidation reaction rate constant (K_1^*) will increase the total pesticide concentration at the water table but that an increase in the hydrolysis reaction rate constants (K_1 and K_2) will decrease the total pesticide concentration at the water table. Also, it can be noted that the change in the total pesticide concentration, due to an increase in the oxidation rate constant, K_1^* , is proportionally less than the corresponding decrease in the rate constant (Figure 13a). The reverse situation is true for the hydrolysis reaction rate constants, K_1 and K_2 , (Figures 13b and 13c, respectively). For conditions that exist on PEI, it can be seen that the total pesticide concentration is most sensitive (i.e. a relative small change in the reaction rate constant produces a relatively large change in the total pesticide concentration) to increasing values of the rate constants describing the

hydrolysis of aldicarb (K_1) and aldicarb sulfoxide (K_2), and to decreasing values of the oxidation rate constants aldicarb (K_1^*). In addition, the total pesticide concentration is least sensitive to the an increasing value of the oxidation rate constant for aldicarb (K_1^*) and decreasing values of the two rate constants describing the hydrolysis of aldicarb to aldicarb sulfoxide (K_1) and aldicarb sulfoxide to aldicarb sulfoxide oxime (K_2). Thus, in order to assess the environmental risks associated with uncertainty in the values of the transformation and degradation rate constants of aldicarb, the transformation rate constant for aldicarb should be over-estimated and the two degradation rate constants should be under-estimated.

Conclusions

Because of the potential for contamination of groundwater by pesticides, regulatory personnel must have the means of assessing the fate of a pesticide as it moves through the unsaturated zone to the water table before the pesticide is approved for general use. Although several models currently exist which can simulate the transport and transformation of pesticides in the subsurface, these models are typically quite complex and require considerable physical and chemical input data to undertake a simulation. An expert system, known as EXPRES, is designed to aid regulatory personnel in their assessment of the potential detrimental affects of pesticides on the soil and shallow groundwater environment. EXPRES is basically a knowledge-based system that is built around two existing pesticide models, PRZM and LEACHM. The expert system will provide the user with encoded expertise in the areas of geology, hydrogeology and numerical modelling that is required in undertaking a simulation with a pesticide transport model. EXPRES is designed to be used as a management tool to aid in policy decisions and is not intended for use as a research tool. Thus, the purpose of EXPRES is to provide only a general assessment of the potential hazards posed by a new pesticide and to identify if further study is warranted.

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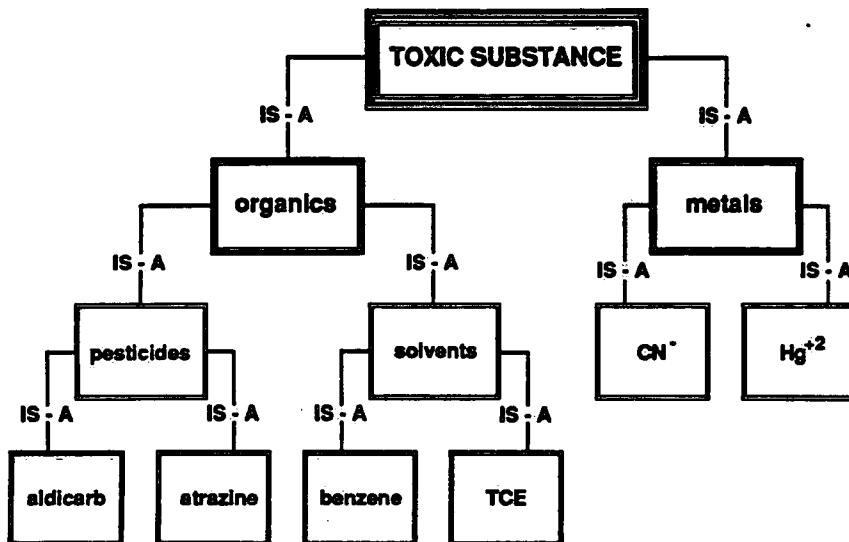
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a

IF aldicarb is detected in groundwater THEN tests its concentration
 IF its concentration is $>9 \mu\text{g/L}$ THEN the groundwater is contaminated
 IF groundwater is contaminated THEN undertake remedial measures

b



c

CLIMATIC DATA		Agricultural Zone 7-b		
	rainfall	temperature	evaporation	humidity
January	20.6	-14.8		
February	16.0	-12.1		
March	11.7	-4.3		
April	21.6	4.6		
May	31.4	11.0		
June	30.5	14.1		
July	42.7	16.7		
etc.				

Fig 1

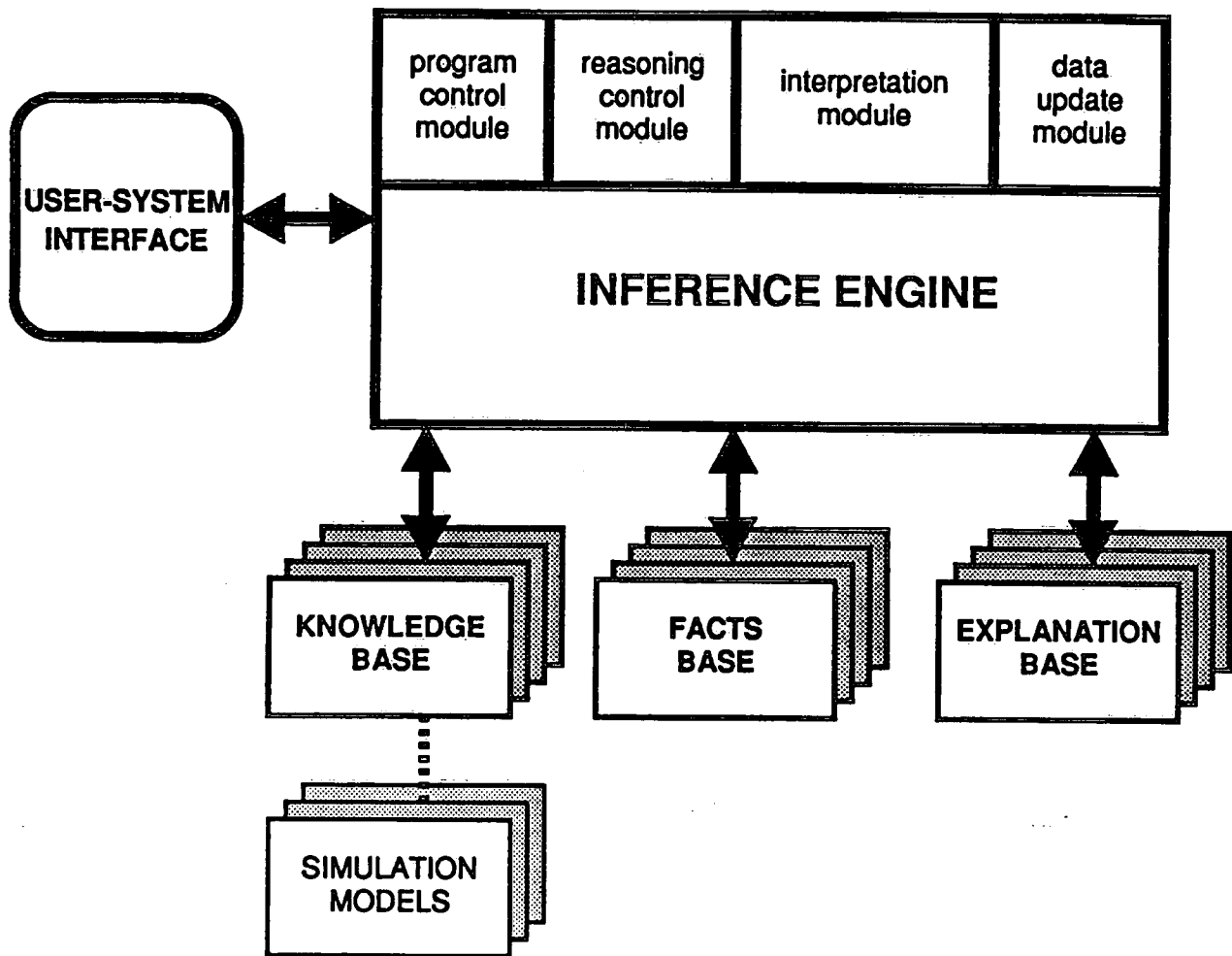


Fig 2

EXPRES

SOIL PARAMETERS

Number of Soil Parameters:

Depth to Water Table (m):

Horizon Number	Horizon Thickness (cm)	Surface (S) or Root (R) or Below Root (B)	Bulk Density (gm/cm ³)	Organic Carbon (%)
1	10.0	S	1.32	0.70
2	20.0	R	1.23	4.40
3	40.0	R	1.62	0.50
4	60.0	B	1.67	0.10
5	120.0	B	1.86	0.01

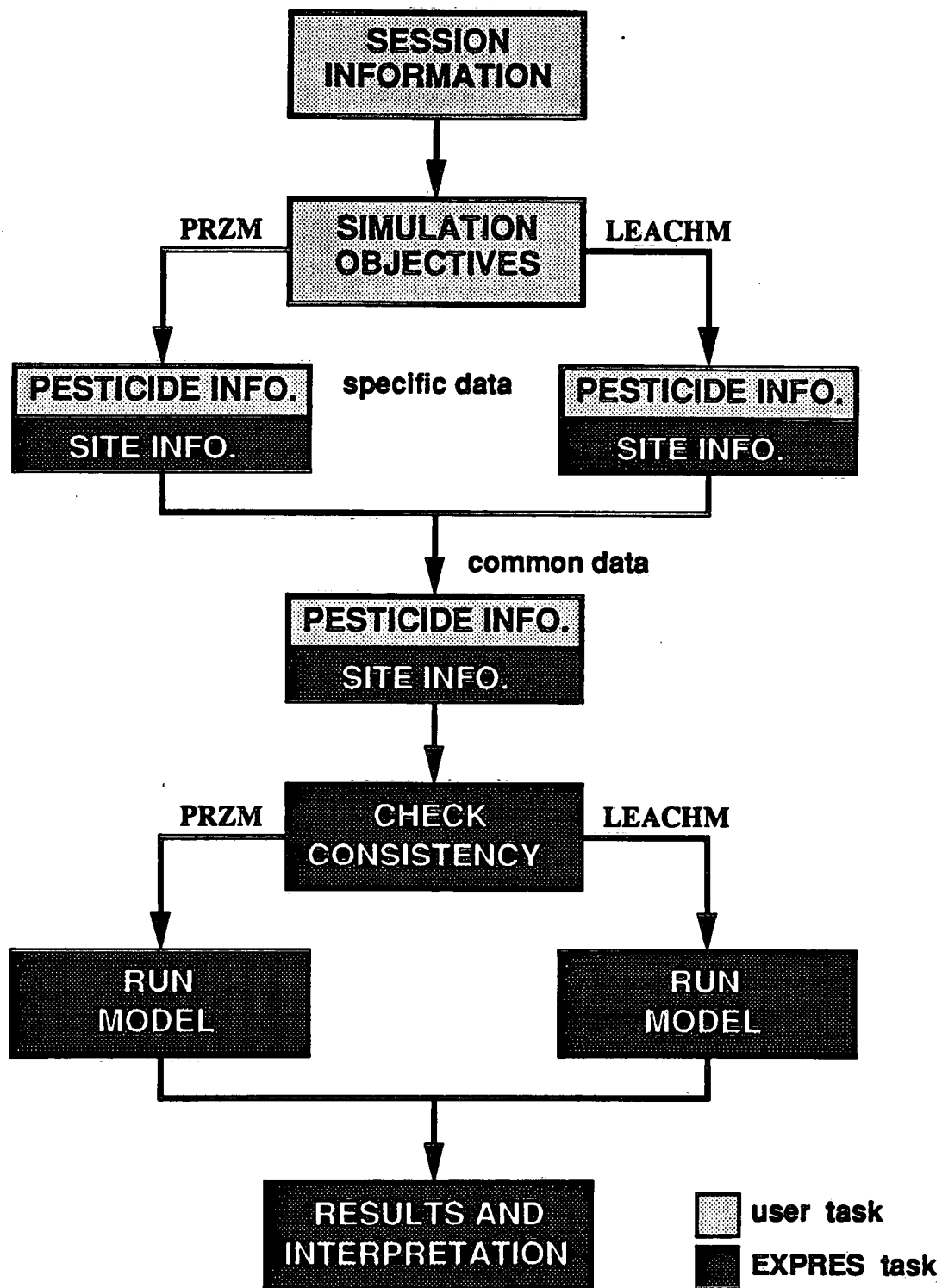


Fig 4

EXPRES

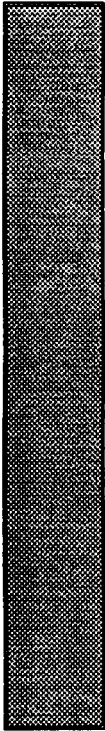
SESSION INFORMATION

INTRODUCTION

- [] Discuss Instructions
- [] Overview of EXPRES
- [♦] Example Session

FILES

- [] Modify an Existing File
- [] Create a New File
- [] Session Notes



EXPRES



SIMULATION OBJECTIONS

SPECIFIC OBJECTIVES

- ☐] Run a scenario
- ☐] Sensitivity analysis

NEED RESULTS

- ☐] Quickly (i.e. < 1 hour)
- ☐] No preference

DAUGHTER PRODUCTS

- ☐] Simulated
- ☐] Not simulated

COMPUTER

- ☐] 80286
- ☐] 80386

Approximate Simulation Length (days):


```

set MODEL = PRZM

If (COMPUTER = 80286) then
    set CUTOFF_DAYS = 150
else
    set CUTOFF_DAYS = 600
endif

If (APPROX_SIMULATION_LENGTH <= CUTOFF_DAYS) then
    set MODEL = LEACHM
else
    If (SIMULATE_DAUGHTER_PRODUCTS = YES .and.
        RESULTS_NEEDED_QUICKLY = YES ) then
        write "Daughter products must be simulated with
            the more detailed of the two models and
            the results cannot be produced < 1 hour.
            Do you still require results quickly: YES/NO?"
        If (ANSWER = NO) then
            set MODEL = LEACHM
        endif
    endif
endif

If (PERFORM_SENSITIVITY_ANALYSES = YES .and.
    RESULTS_NEEDED_QUICKLY = YES) then
    write "Sensitivity analyses should be performed with
        the more detailed model to be informative, but
        this will take more than 1 hour.
        Do you still require results quickly: YES/NO?"

    If (ANSWER = NO) then
        set MODEL = LEACHM
    endif
endif

If (RESULTS_NEEDED_QUICKLY = NO .and.
    (SIMULATE_DAUGHTER_PRODUCTS = YES .or.
    PERFORM_SENSITIVITY_ANALYSES = YES)) then
    set MODEL = LEACHM
endif
endif

```

Fig 7

EXPRES

GENERAL INFORMATION

UNITS

- ☐ Metric
☐ Imperial / US

SIMULATION DATES

Starting

Ending

SIMULATION PARAMETERS

User Supplied Parameters (Required)

- ☐ Agricultural Zone
☐ Pesticide Parameters
☒ Output Parameters

Default Parameters (Optional)

- ☐ Soil Parameters
☐ Crop Parameters
☐ Meteorological Parameters

EXPRES

EXPRES

PESTICIDE PARAMETERS

CHEMICAL SPECIES
 Number of Pesticides and
 Transformation Products to
 Simulate (maximum of 4):

Pesticide Number	Pesticide Name	Solubility (mg/L)	Koc (L/kg)	Parent (P) or Daughter (D)
1				
2				
3				
4				

EXPRES

CROPPING PERIODS

Number of Cropping Periods:

5

Crop Period	Crop Number	Planting Date (d · m · y)	Emergence Date (d · m · y)	Maturity Date (d · m · y)	Root Plant	Harvest Date (d · m · y)
1	1	010583	100683	010983	250983	101083
2	2	200584	150684	150884	100984	300984
3	3	100585	300585	200985	300985	071085
4	1	010586	100686	010986	250986	101086
5	2	200587	300587	150887	100987	300987

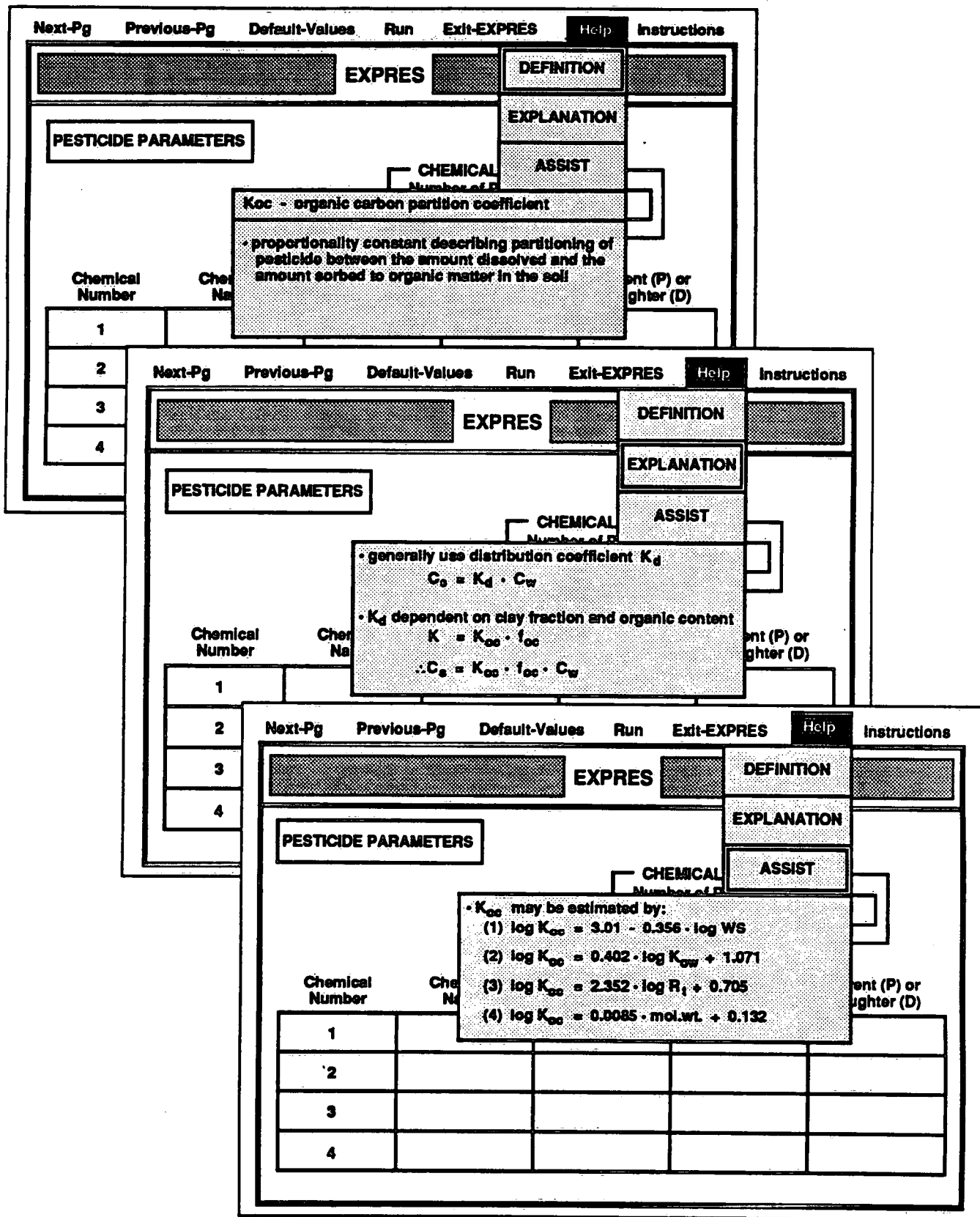


Fig 11

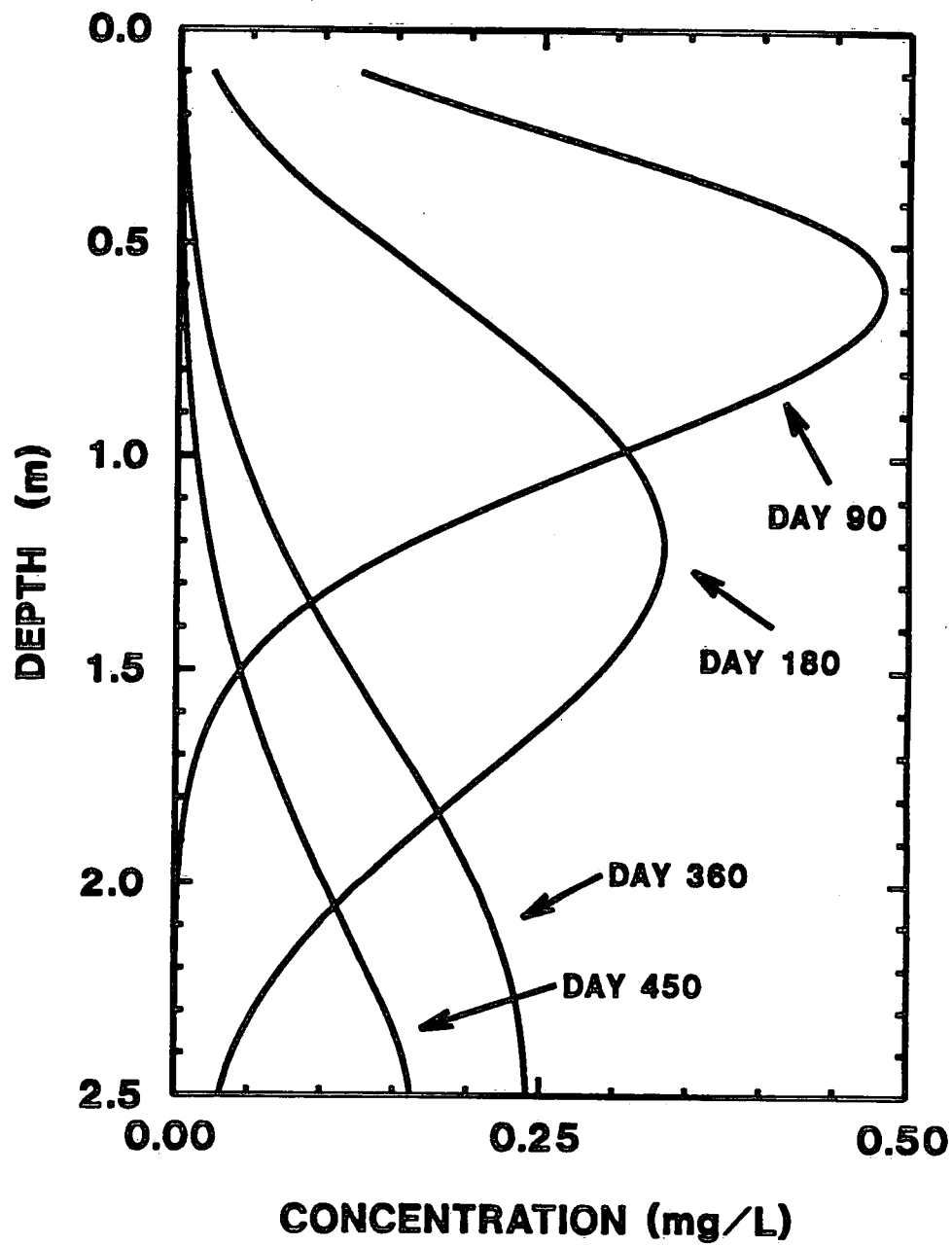


Fig 12a

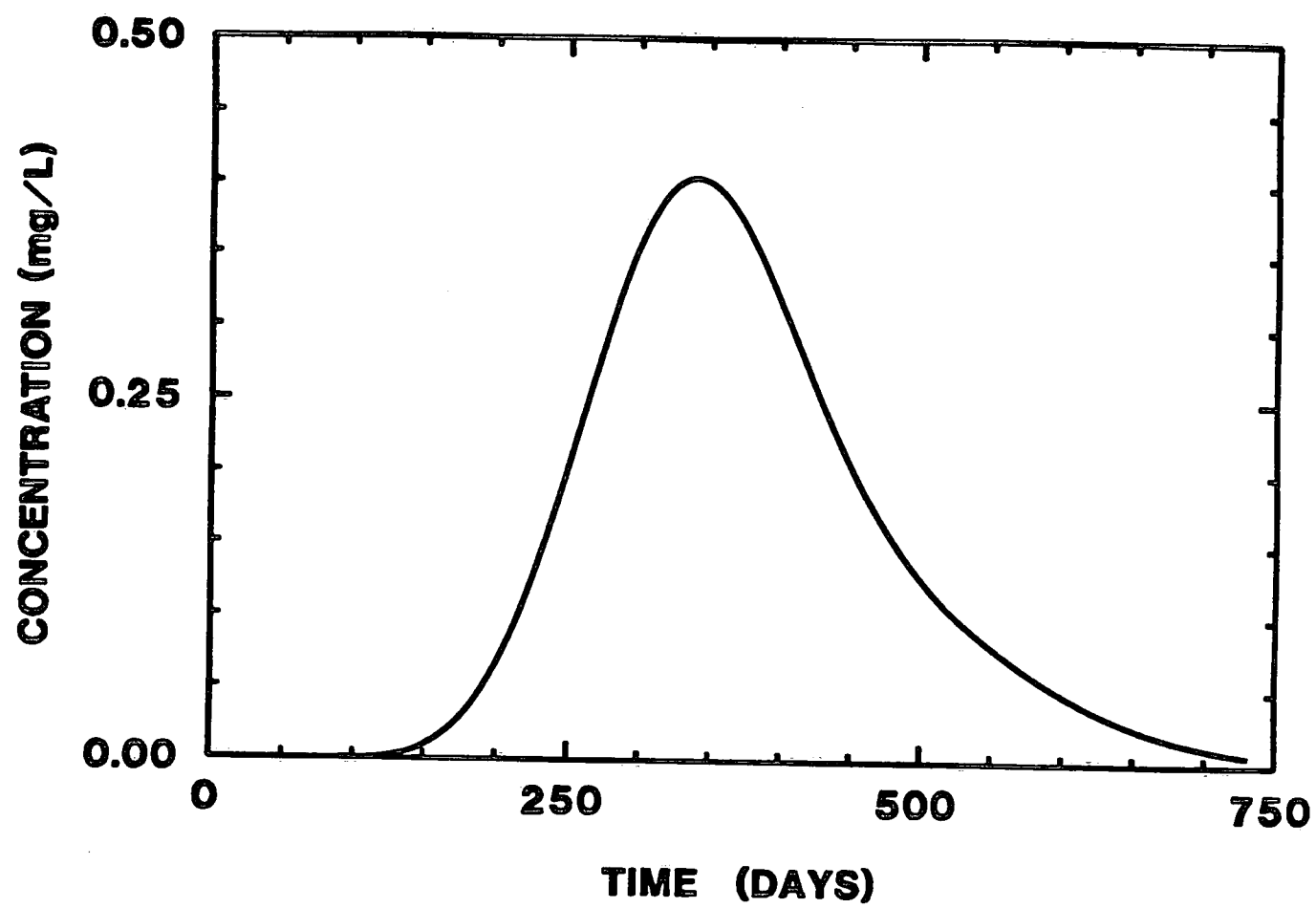
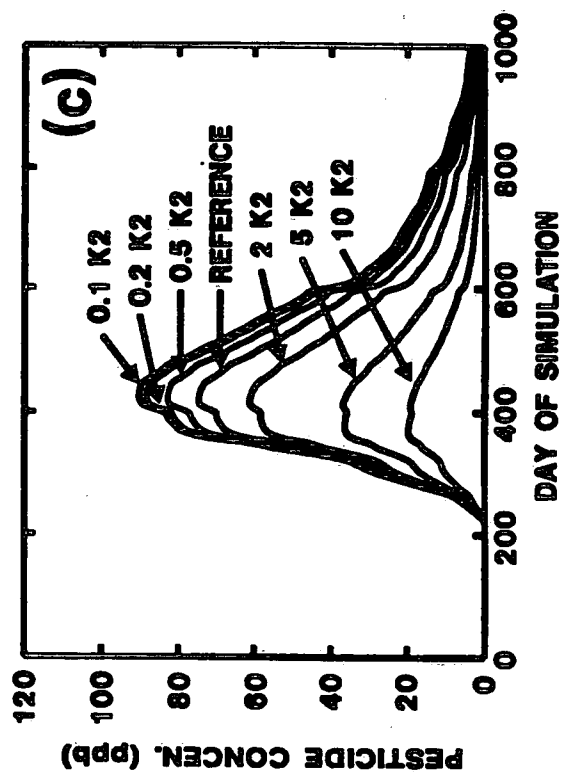
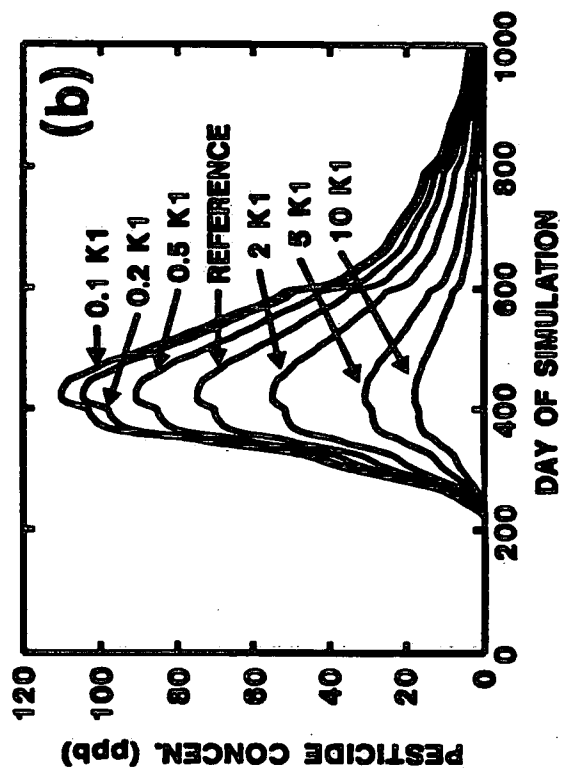
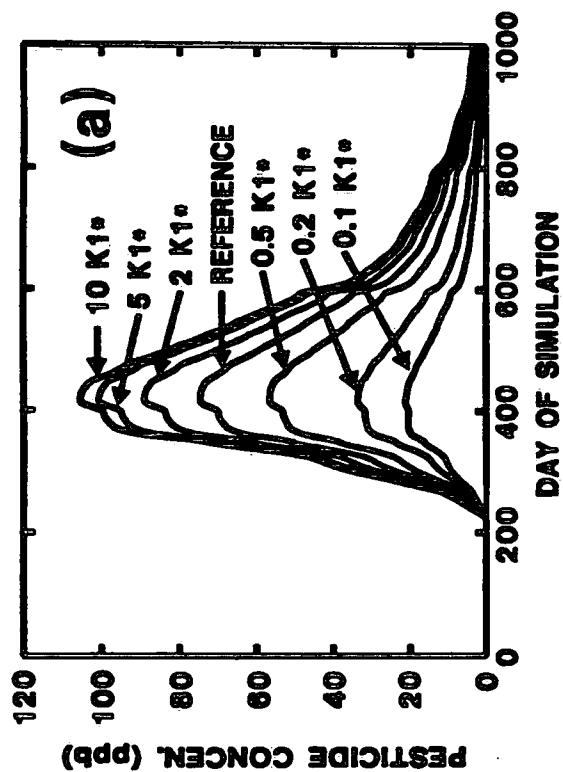


Fig 12 b

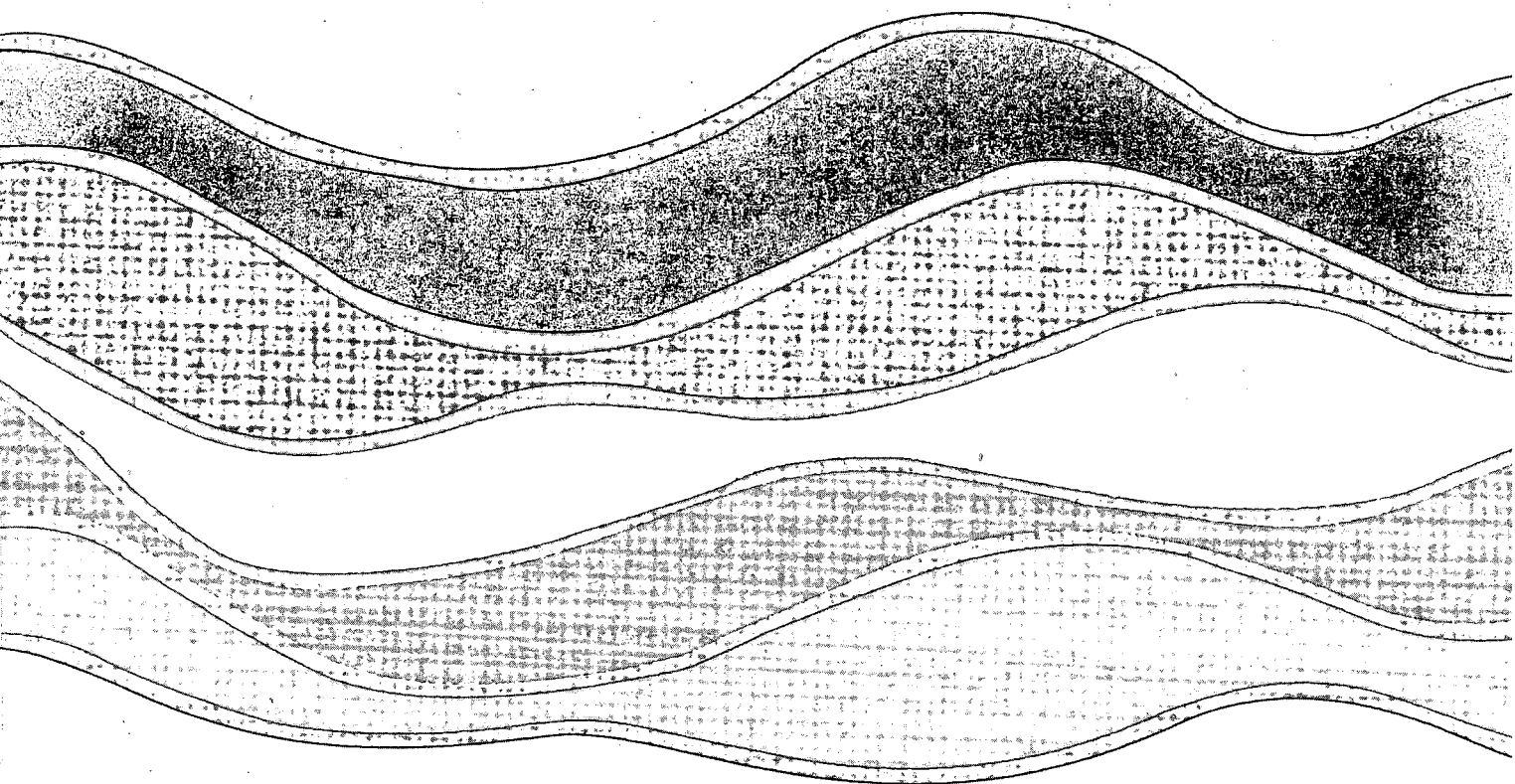


REFERENCE VALUES FOR RATE CONSTANTS			
	(0-0.4m)	(0.4-4.3m)	
K1*	0.09082	0.01819	
K1	0.04812	0.00982	
K2	0.00374	0.00075	

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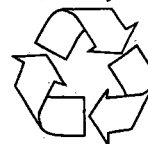
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