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

J.P. Mutch AND A.S. Crose

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PHASE TWO REPORT
DEVELOPMENT OF THE BASIC EXPERT SYSTEM

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

by

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June 1990
NWRI Contribution #90-82

ABSTRACT

The expert system described herein is designed to aid regulatory personnel in their assessment of the potential for pesticides to contaminate the soil and shallow groundwater environment. The expert system, known as EXPRES (EXpert system for Pesticide Regulatory Evaluation Simulations), consists of existing numerical models 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 choice of all the necessary information for characterizing the geological, physical, climatic, hydrogeological, pedological and agricultural settings of typical agricultural regions across Canada, as required by the pesticide models. The expert system 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, its purpose is not to provide insight into the processes that control the fate of pesticides in porous media, but to provide an assessment of the potential hazards and to identify if further study is warranted.

RÉSUMÉ

Le système expert décrit ici est conçu pour aider le personnel chargé de la réglementation à évaluer la capacité des pesticides de contaminer les sols et les eaux souterraines peu profondes. Le système expert EXPRES (EXpert system for Pesticide Regulatory Evaluation Simulations) se compose de modèles numériques existants qui sont utilisés pour simuler le transport et la transformation de pesticides dans la zone non saturée, lesquels modèles sont jumelés à un système à base de connaissances qui guide l'utilisateur pour choisir toute l'information nécessaire à la caractérisation des contextes géologiques, physiques, climatiques, hydrogologiques, pédologiques et agricoles des régions agricoles types du Canada, selon les besoins des modèles de pesticide. Le système expert est conçu pour être utilisé comme un outil de gestion permettant de prendre des décisions stratégiques, et non comme un outil de recherche. Il ne sert donc pas à mieux comprendre les processus qui régissent le devenir des pesticides dans les milieux poreux, mais à évaluer les dangers potentiels et à déterminer si l'étude mérite d'être approfondie.

MANAGEMENT PERSPECTIVE

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 on the Pesticide Division is the potential for a pesticide to contaminate groundwater resources. Although a number of 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. In addition, this expert system can be used for the identification of agricultural development which may or may not be sustainable. This report outlines the two year program currently being undertaken by the Groundwater Contamination Project to develop the expert system. This report deals specifically with Phase 2 of the project, describing the modifications made to the pesticide transport and transformation models, and the development of the user-system interface for the expert system.

PERSPECTIVE DE GESTION

La Division des pesticides de la Direction des produits chimiques commerciaux, Environnement Canada, est chargée d'évaluer les dangers environnementaux associés aux pesticides et à leurs produits de transformation avant que leur utilisation publique ne soit approuvée. Une préoccupation particulière de la Division est la possibilité qu'un pesticide contamine des ressources en eau souterraine. Même s'il existe actuellement certains modèles qui peuvent prévoir le transport et la transformation des pesticides dans le sol, le personnel chargé de la réglementation n'ont en général pas les compétences requises pour utiliser ces modèles avec précision. L'équipe du Projet de contamination des eaux souterraines, INRE, a été approchée par la Division des pesticides pour identifier les types de développement agricole susceptibles d'être viables. Ce rapport décrit le programme de deux ans qu'est à mettre sur pied l'équipe du Projet de contamination des eaux souterraines pour mettre au point le système expert. Il traite en particulier de la phase 2 du projet, décrivant les modifications apportées aux modèles de transport et de transformation des pesticides, ainsi que la mise au point de l'interface utilisateur-système destinée au système expert.

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1. INTRODUCTION

Pesticides have been used extensively to enhance both crop production and quality. However, the use of pesticides is not without environmental risk. In particular, the contamination of shallow groundwater resources has occurred all too frequently. For example, several recent studies examining the 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., 1988; 1989; 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, subject 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.

The EXPRES expert system is designed to aid regulatory personnel with their evaluation of the possible detrimental effects of pesticides on the quality of groundwater. EXPRES is actually a knowledge-based system coupled to 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 designed to replace the current procedures 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 associated with a new pesticide;
- (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 to be 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 respect to both 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.

The objectives of Phase Two of the project are to make the necessary modifications to the pesticide transport and transformation model, incorporating required processes such as surface runoff and erosion, and to develop the basic data entry system for the expert system. This report describes the development of the EXPRES expert system to date. The report presents a brief

review of expert systems, and the components of the EXPRES expert system. Modifications made to the two pesticide transport and transformation models are also discussed, and a description of the data entry system for EXPRES is given.

2. 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 manner that, through an interactive process between the expert system 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) and the project proposal (Crowe and Jackson, 1989). The reader requiring a more detailed description is referred to these two publications.

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 is composed of 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

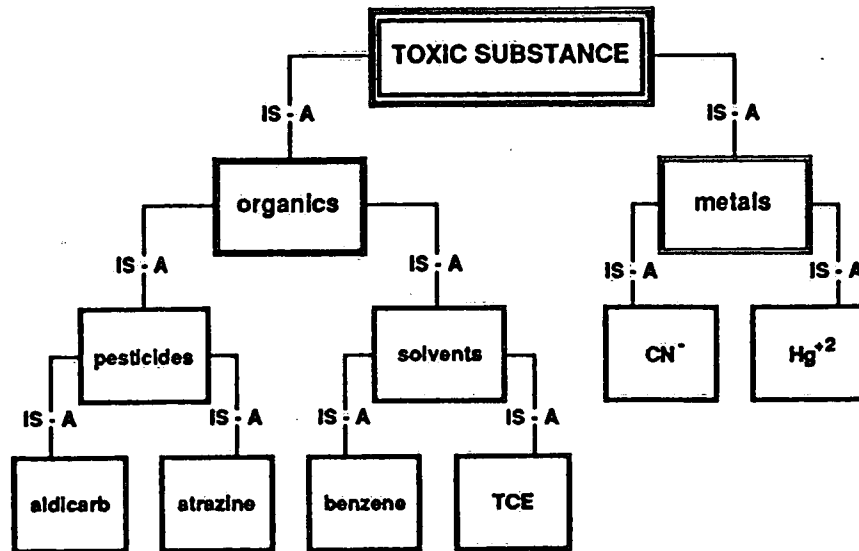
may be either high quality information, such as exact values, or it may be heuristically derived information based upon inferences and relations.

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 of any one of these structures, they are more commonly constructed using 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.

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. Representation of knowledge within an expert system: (a) production rules forming a reasoning strategy, (b) a schematic net, (c) a frame.

3. AN EXPERT SYSTEM FOR PESTICIDE REGULATORY DECISIONS

The EXPRES (EXpert system for Pesticide Regulatory Evaluation Simulations) expert system is designed as a management tool to be used as an aid in making policy decisions regarding the benefits and risks associated with the use of a proposed pesticide, and specifically, to ensure that the quality of groundwater in agricultural areas is maintained. Because EXPRES is not intended for use as a research tool, its primary objective is to provide a general assessment of the potential hazards to the shallow groundwater regime associated with the use of 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 EXPRES expert system, and the biological, chemical and physical processes that must be incorporated into the transport and transformation model are discussed in the following sections.

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 that simulate the fate of a pesticide in the subsurface to accurately use these complex codes. Therefore, the following criteria are being 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 four parts; (1) the inference engine, (2) the user-system interface, (3) the pesticide transport and reaction model, and (4) the information and knowledge data bases.

3.1 THE INFERENCE ENGINE

The inference engine contains the programming statements that 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 will also evaluate the results produced by the simulation model. The reasoning strategy is based on the application of the appropriate production rules, frames and semantic 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 will perform internal checks to ensure accuracy and consistency among all values entered and will convert the results of a simulation into an easily interpretable form. The data update module will allow the existing data bases to be modified or expanded with the addition of new facts or knowledge.

3.2 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 will provide 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 transport and transformation models. The user-system interface prompts the user for simulation options required by the models

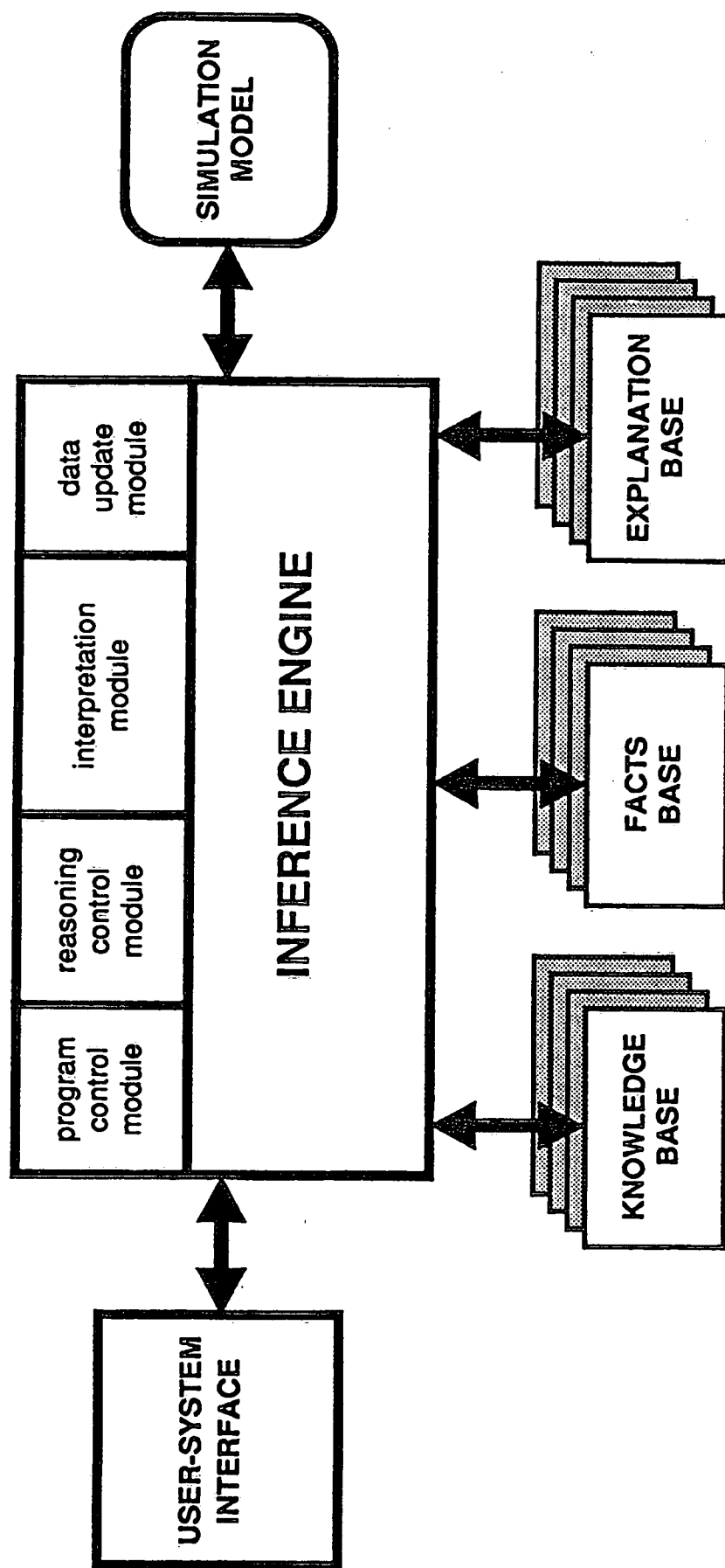


Fig.2. General architecture of an expert system.

and for data characterizing a pesticide and the site of application. If the user is uncertain as to the information being requested, definitions, explanations, and assistance from the explanation data base will be 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 may also be available to the user from the knowledge base to aid in the selection of an appropriate value for the requested information.

The user-system interface will automatically provide typical values for the physical, climatic, hydrological and pedological setting of agricultural areas from the information stored within the facts data base. The user then has the option of modifying any or all of 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. Screens also allow the user to enter information in any order and to quickly review previously entered data if desired.

A second important feature of the user-system interface module is that it will convey both quantitative and qualitative information to the user from the output of the simulation model. Output will take the form of both tables of numbers and graphical output to help visualize trends, anomalies and relationships among variables. To help novice users understand the critical output from the model, EXPRES will also contain various levels of decision-making support for aiding in the interpretation of the simulation results. In ascending order of support, these levels will be:

- (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).

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.3. A typical screen for data entry via the user-system interface.

A more detailed description of the actual functioning of the user-system interface is given in Sections 5.1 and 5.2.

3.3 THE SIMULATION MODEL

3.3.1 MODEL REQUIREMENTS AND SELECTION

A numerical model is used to simulate pesticide transport and transformation within the unsaturated zone. The accuracy of the predictions depends upon how realistically the numerical 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 and erosion. Chemical and biological processes that affect the chemical character of the pesticide include transformation/degradation (hydrolysis, oxidation, microbial transformation, phototransformation), adsorption, plant uptake and volatilization of the pesticide.

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.

Of the models reviewed in the Phase One Report (Mutch and Crowe, 1989), 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 model for a particular simulation must take into account the objectives of the simulation, the availability of data and the execution time required for the simulation. When field data are characterized in sufficient detail, LEACHM will provide a more detailed analysis of the fate of a pesticide and associated daughter products with respect to both time and depth. The use of PRZM is more appropriated when a more qualitative assessment of the potential for a pesticide to contaminate groundwater is required, or when the field data are not characterized in detail. Even though the more complex model (LEACHM) describes the processes affecting pesticide transport and transformation in more detail, 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.

3.3.2 PRZM - PESTICIDE ROOT ZONE MODEL

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 curve number approach developed by

the Soil Conservation Service, 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 80286-based personal computer with a math co-processor, is less than ten minutes.

3.3.3 LEACHM - LEACHING ESTIMATION AND CHEMISTRY MODEL

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. LEACHM 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 rate constants may be varied as a function of depth.

The time step in LEACHM 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 LEACHM are, firstly, a lengthy execution time (eg. 5 hours for a one year simulation with 45 soil compartments, on a 80286-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 of the LEACHM model 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. These modifications are discussed in more detail in Section 4.

3.4 THE DATA BASES

The fourth 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 will also contain 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 that will be 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.

The information that will be 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 will be accessed to provide a typical range of values, and to allow the user to follow the expert system's reasoning strategy, check the entered values for consistency with previously entered information, and to aid the user in understanding the conclusions and recommendations. The type of information that will be contained within this data base includes:

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

The facts data base will be 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 will be 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 will, however, be 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 will be 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 will be comprised of the physical and chemical characteristics of existing pesticides. It will be 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.

To date, the production rules required to operate the PRZM model in a basic expert system have been encoded into the knowledge base of EXPRES. Typical model parameters for

an application of the pesticide, aldicarb, to potatoes on Prince Edward Island have been incorporated into the facts data base. This data base has been prepared for program testing and demonstration purposes only. Additional information for the PEI agricultural setting s well as the other agricultural zones will be developed during later phases of the development of the EXPRES expert system.

4. MODIFICATIONS TO THE PESTICIDE TRANSPORT AND TRANSFORMATION MODELS

Several modifications were made to the two pesticide transport and transformation models prior to their incorporation into EXPRES. The modifications made to PRZM include:

- (1) reading climatological data from a common meteorological file;
- (2) reading input parameters from an input file created by EXPRES.

The modifications made to LEACHM include:

- (1) reading climatological data from a common meteorological file;
- (2) reading input parameters from an input file created by EXPRES;
- (3) estimating potential evapotranspiration from mean daily temperatures when measured pan evaporation data is not available;
- (4) adding a snowmelt subroutine;
- (5) accounting for surface runoff and erosion losses of both water and pesticide.

Only a relatively minor modification was made to PRZM, allowing it to read climatological data from a meteorological data file that is common to both PRZM and LEACHM.

Because the LEACHM model will be selected for execution when a more detailed evaluation is desired, more extensive modifications were made to this model. These modifications allow LEACHM to meet more of the criteria established for the selection of the simulation model. Originally, LEACHM read climatological data only on days for which there was a precipitation or irrigation event. The climatological data was read from the input data file, necessitating the duplication of the some times lengthy climatological data in each input data set. LEACHM was modified to read climatological data on a daily basis from an external climatological data file, eliminating the need to duplicate the climatological data in each input data set. LEACHM now reads the mean daily temperature, total daily precipitation and total daily pan evaporation values (when available).

Daily temperature values are necessary to accommodate two additional modifications that were made to LEACHM. The first is the addition of an empirical method for estimating daily potential evapotranspiration values when measured pan evaporation data are unavailable. When daily pan evaporation values are not available, a default value of -99.0 is placed in the climatological file, signalling the model to use the empirical function to estimate daily potential

evapotranspiration from the mean daily temperature. When measured daily pan evaporation values are available, the model accepts these data from the climatological data file. The daily pan values are then reduced by a pan evaporation coefficient in a manner similar to that which is done when estimating daily lake evaporation (Linsley et al., 1982).

The second modification to LEACHM, which requires the use of the mean daily temperature is a snowmelt subroutine. The snowmelt subroutine is incorporated directly into the LEACHM model and acts to both accumulate any precipitation or melt any accumulated snow depending upon whether the mean daily temperature is less than or greater than 0°C. The precipitation that falls when the temperature is less than 0°C is accumulated as snowfall (snow pack storage) and remains unavailable for infiltration into the soil until the mean daily temperature rises above 0°C. When the temperature rises above 0°C, the model will estimate the amount of snowmelt that will occur on that day and will add this amount to any additional precipitation that may fall on that day. The estimation of the amount of snowmelt is based on a simple linear relationship relating the amount of snowmelt to the mean daily temperature (Linsley et al., 1982).

Modifications have also been made to the LEACHM model that allow the model to simulate surface runoff and erosional losses of both water and pesticide in a manner similar to that used in the PRZM model. Erosional losses are determined with a modified Universal Soil Loss Equation (MUSLE) approach (Williams and Brendt, 1977), and surface runoff is calculated with a curve number approach developed by the USDA Soil Conservation Service (Haith and Loehr, 1979). The curve number approach for estimating surface runoff partitions precipitation between surface runoff and water available for infiltration. Carsel et al. (1984) defend the use of this method in their model (PRZM), stating that the method relates the amount of runoff to the soil type, land use and management practices, and is a reliable procedure that has been developed by the USDA. Pesticide lost via erosion (adsorption of the pesticide to eroded soil particles) is related to the amount of surface runoff and a number of factors that consider the type of soil, the setting, the crop planted and the farm management practices. The equation is further refined with an empirical enrichment ratio that takes into account the amount of organic matter lost with the eroded soil since, in general, pesticides are most strongly sorbed to the organic matter in the soil.

5. THE EXPRES USER-SYSTEM INTERFACE

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 most 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.

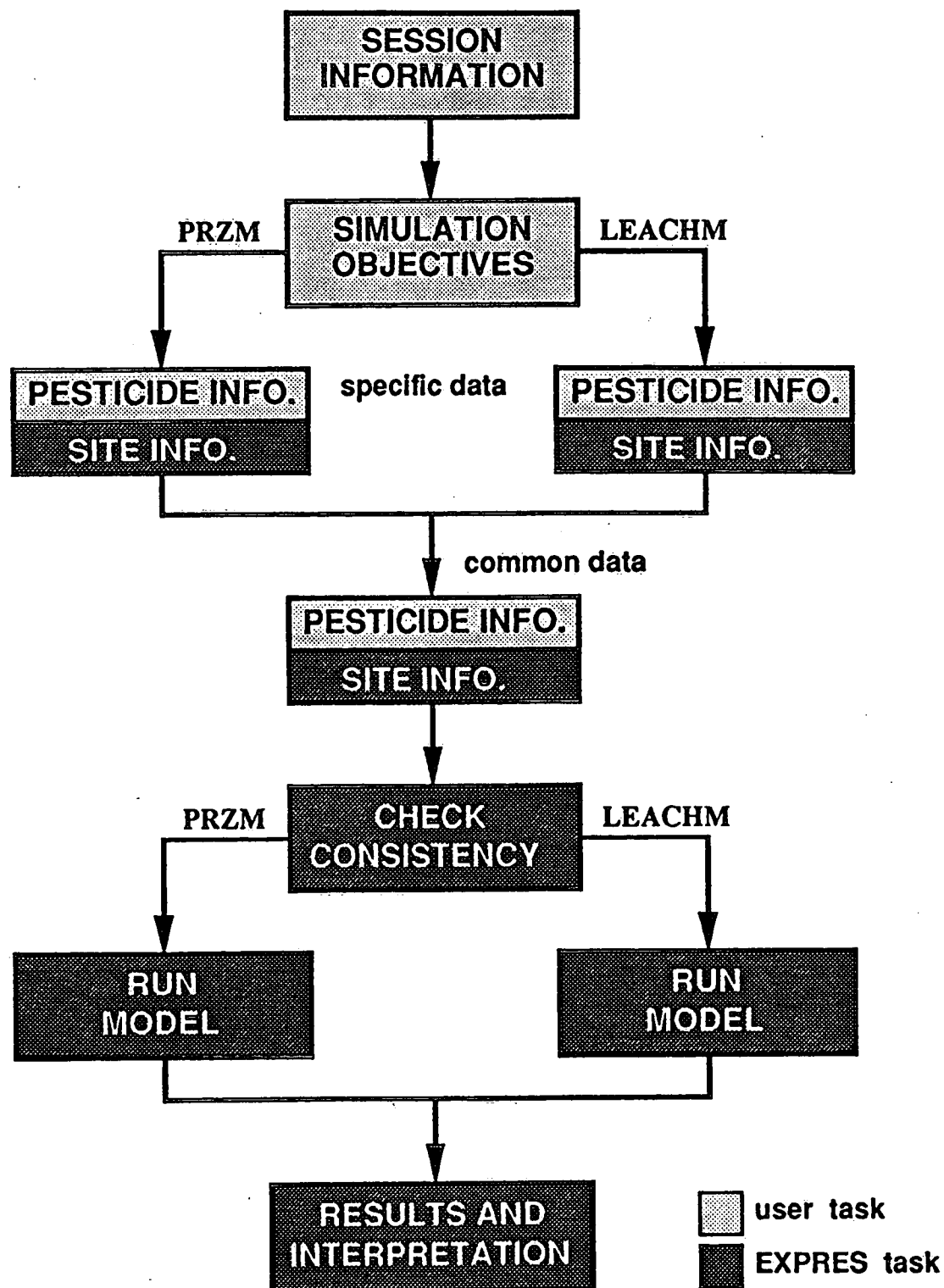


Fig.4. Basic operations undertaken within EXPRES.

5.1 DEVELOPMENT OF THE INPUT DATA SET

All user-system interactions, including the general operation of EXPRES, take place via screens. The screen shown previously (see 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

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<div style="border: 1px solid black; padding: 10px; margin-bottom: 10px;"> <h3 style="text-align: center; margin: 0;">SESSION INFORMATION</h3> </div> <div style="display: flex; justify-content: space-between;"> <div style="width: 45%;"> <div style="border: 1px solid black; padding: 5px; margin-bottom: 10px;"> <h4 style="margin: 0;">INTRODUCTION</h4> <ul style="list-style-type: none"> [] Discuss Instructions [] Overview of EXPRES [♦] Example Session </div> <div style="border: 1px solid black; padding: 5px;"> <h4 style="margin: 0;">FILES</h4> <ul style="list-style-type: none"> [] Modify an Existing File <div style="border: 1px solid black; height: 30px; width: 100%; margin-top: 5px;"></div> [] Create a New File <div style="border: 1px solid black; height: 30px; width: 100%; margin-top: 5px;"></div> [] Session Notes </div> </div> </div>			

Fig.5. Screen for entering session information.

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

EXPRES

SIMULATION OBJECTIONS

SPECIFIC OBJECTIONS

[] Run a scenario

[♦] Sensitivity analysis

DAUGHTER PRODUCTS

[♦] Simulated

[] Not simulated

NEED RESULTS

[♦] Quickly (i.e. < 1 hour)

[] No preference

COMPUTER

[♦] 80286

[] 80386

Approximate Simulation Length (days):

Fig.6. Screen for entering simulation objectives.

25

rules	
	set MODEL = PRZM
1 a	if (COMPUTER = 80286) then
	set CUTOFF_DAYS = 150
1 b	elseif (COMPUTER = 80386) then
	set CUTOFF_DAYS = 600
	endif
2 a	if (SIMULATION_LENGTH <= CUTOFF_DAYS) then
	set MODEL = LEACHM
2 b	elseif (SIMULATION_LENGTH > CUTOFF_DAYS) then
3 a	if (DAUGHTER_PRODUCTS = YES and
	QUICK_RESULTS = NO) then
	set MODEL = LEACHM
3 b	elseif (DAUGHTER_PRODUCTS = YES and
	QUICK_RESULTS = YES) then
	write "Simulation of daughter products takes > 1 hour.
	Do you require: (A) results quickly or
	(B) daughter products? "
4 a	if (ANSWER = A) then
	set MODEL = PRZM
4 b	elseif (ANSWER = B) then
	set MODEL = LEACHM
	endif
	endif
5 a	if (PERFORM_SENSITIVITY_ANALYSES = YES and
	QUICK_RESULTS = NO) then
	set MODEL = LEACHM
5 b	elseif (PERFORM_SENSITIVITY_ANALYSES = YES and
	QUICK_RESULTS = YES) then
	write "Sensitivity analyses should be done with detailed
	model to be informative, but this will take > 1 hour.
	Do you still require results quickly: YES or NO? "
6 a	if (ANSWER = YES) then
	set MODEL = PRZM
6 b	elseif (ANSWER = NO) then
	set MODEL = LEACHM
	endif
	endif
	endif

Fig.7. Reasoning strategy for model select within EXPRES.

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

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

Fig.8. Screen for entering general information for a simulation.

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				

Fig.9. Screen for entering user-supplied data (eg. pesticide parameters).

29

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.10. Screen for displaying EXPRES-supplied data (eg. cropping periods).

The figure shows three overlapping screenshots of the EXPRES software interface, illustrating the pull-down menus used for data entry assistance. Each screenshot has a menu bar with 'Next-Pg', 'Previous-Pg', 'Default-Values', 'Run', 'Exit-EXPRES', 'Help', and 'Instructions'.

Top Screenshot (a) Parameter Definition: The 'EXPRES' menu is open, showing 'DEFINITION', 'EXPLANATION', and 'ASSISTANCE'. The 'DEFINITION' option is selected. A text box defines K_{oc} as the organic carbon partition coefficient, a proportionality constant describing partitioning of pesticide between the amount dissolved and the amount sorbed to organic matter in the soil. Below this is a table with columns 'Chemical Number' and 'Chemical Name'.

Chemical Number	Chemical Name
1	
2	
3	
4	

Middle Screenshot (b) Parameter Explanation: The 'EXPRES' menu is open, showing 'DEFINITION', 'EXPLANATION', and 'ASSISTANCE'. The 'EXPLANATION' option is selected. A text box explains the generally used distribution coefficient K_d with the equation $C_s = K_d \cdot C_w$. It also states that K_d is dependent on clay fraction and organic content, with the equation $K = K_{oc} \cdot f_{oc}$. Therefore, $C_s = K_{oc} \cdot f_{oc} \cdot C_w$. Below this is a table with columns 'Chemical Number' and 'Chemical Name'.

Chemical Number	Chemical Name
1	
2	
3	
4	

Bottom Screenshot (c) Parameters Assistance: The 'EXPRES' menu is open, showing 'DEFINITION', 'EXPLANATION', and 'ASSISTANCE'. The 'ASSISTANCE' option is selected. A text box provides four methods to estimate K_{oc} :

- (1) $\log K_{oc} = 3.01 - 0.356 \cdot \log WS$
- (2) $\log K_{oc} = 0.402 \cdot \log K_{ow} + 1.071$
- (3) $\log K_{oc} = 2.352 \cdot \log R_1 + 0.705$
- (4) $\log K_{oc} = 0.0085 \cdot \text{mol.wt.} + 0.132$

Below this is a table with columns 'Chemical Number' and 'Chemical Name'.

Chemical Number	Chemical Name
1	
2	
3	
4	

Fig.11. Screen illustrating the pull-down menus used to aid the user with data entry: (a) parameter definition, (b) parameter explanation, (c) parameters assistance.

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. After all the consistency checks have been performed, EXPRES runs either the PRZM or LEACHM model. Table A.1 in Appendix A list the parameters required by the two pesticide transport and transformation model.

5.2 EVALUATION AND INTERPRETATION OF OUTPUT

Following the execution of either PRZM or LEACHM, control is returned to EXPRES and the expert system will modify the output produced by the models to present the results of a simulation in a manner in which the user can clearly understand and interpret the results. The two types of output available with EXPRES are, concentration profiles (pesticide concentrations throughout the soil profile at different times), and time series representations of the pesticide concentration at the water table or other specified depths. A more detailed list of the variables that may be specified for inclusion in the output data files is given in Table B.1 of Appendix B.

Typical examples of each type of output from EXPRES are illustrated with an application of the models evaluating the potential for the pesticide, aldicarb, to contaminate groundwater beneath potato fields on Prince Edward Island, Canada. This problem has been well documented (Priddle et al., 1988, 1989; Mutch et al., 1990). The simulations were performed using a simplified data set for demonstration purposes as the detailed data base characterizing a potato field on Prince Edward Island will be developed during the next phase of the project.

Profiles of the total aldicarb concentration with depth in the soil column are shown by Figure 12 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

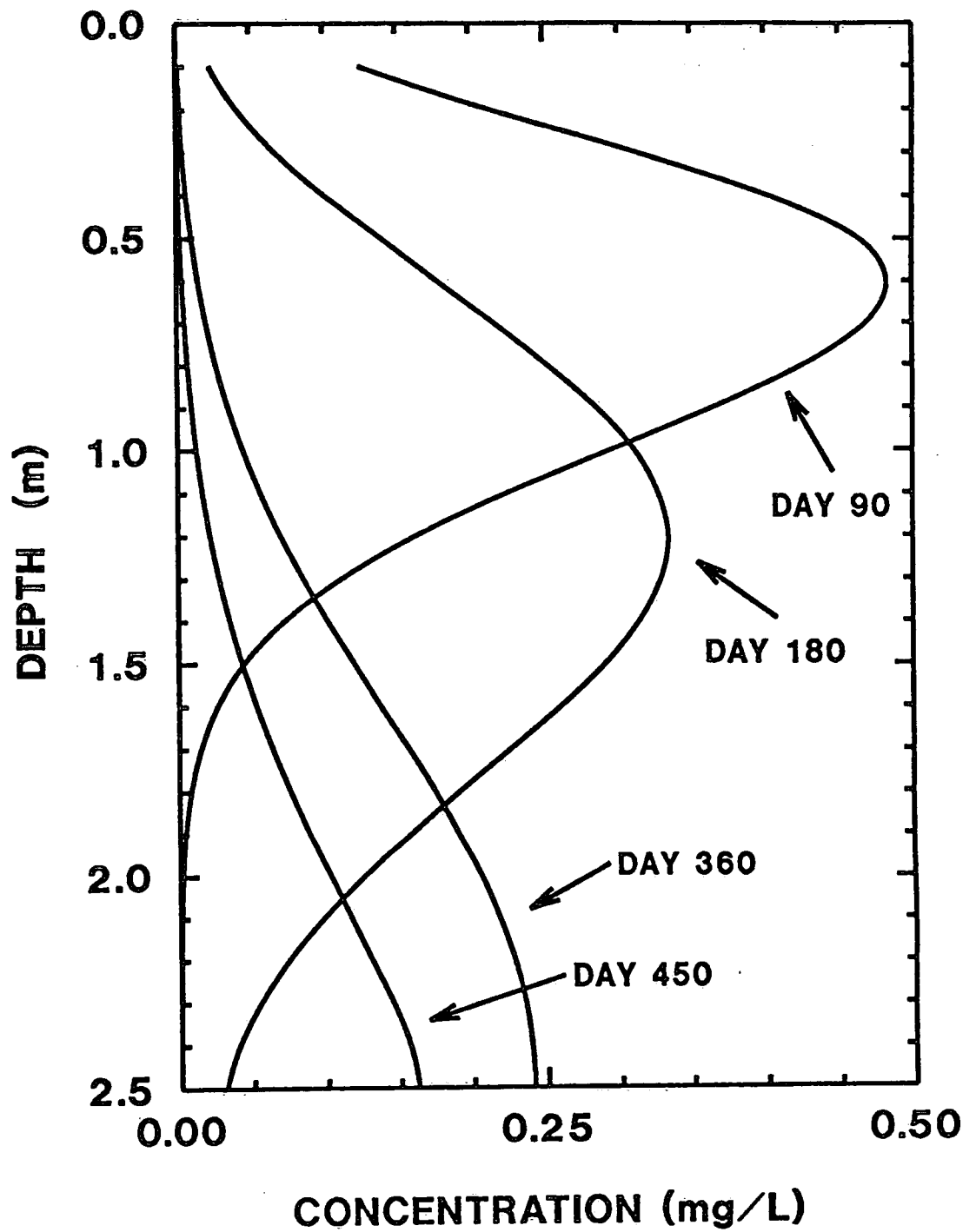


Fig.12. Typical graphical output from EXPRES: Concentration profile showing concentration vs. depth at selected days.

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 the 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 13 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 time required 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 the 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 ("typical case" to "worst case") for a sensitivity analysis but 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 analysis will not be undertaken by EXPRES. Rather, the user will be required to note the appropriate range of values for the particular parameter, and then at times 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, who can then re-execute the model. Thus, a series of individual graphs, such as Figure 12 or 13, can be superimposed upon one another to depict the relative influence of the variation in values of the chosen parameter.

An illustrative example, a sensitivity analysis on the reaction rate constants

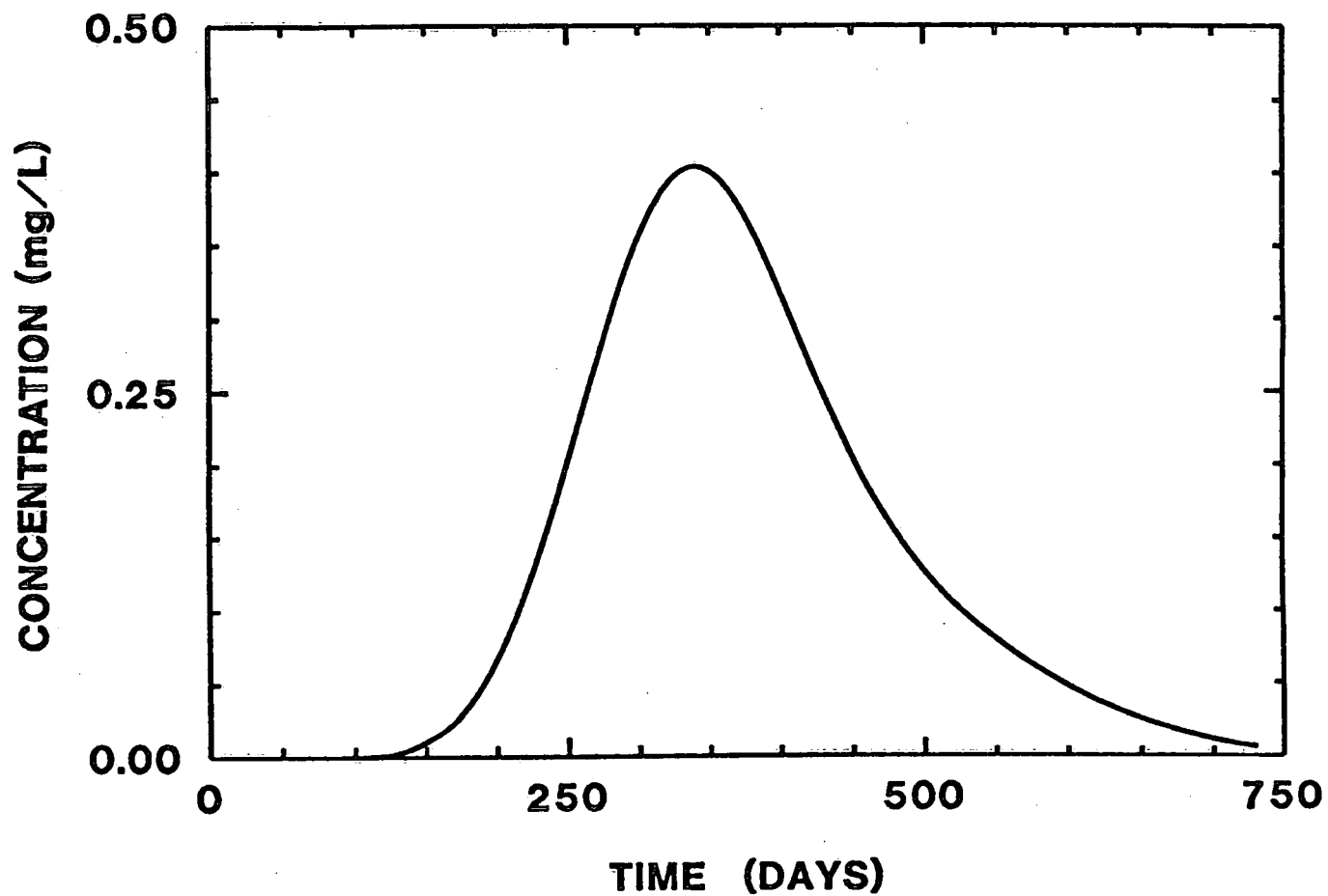
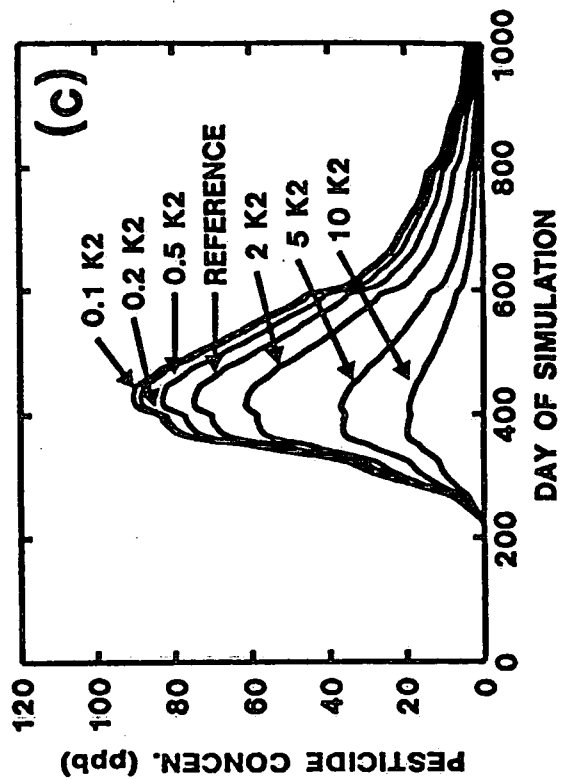
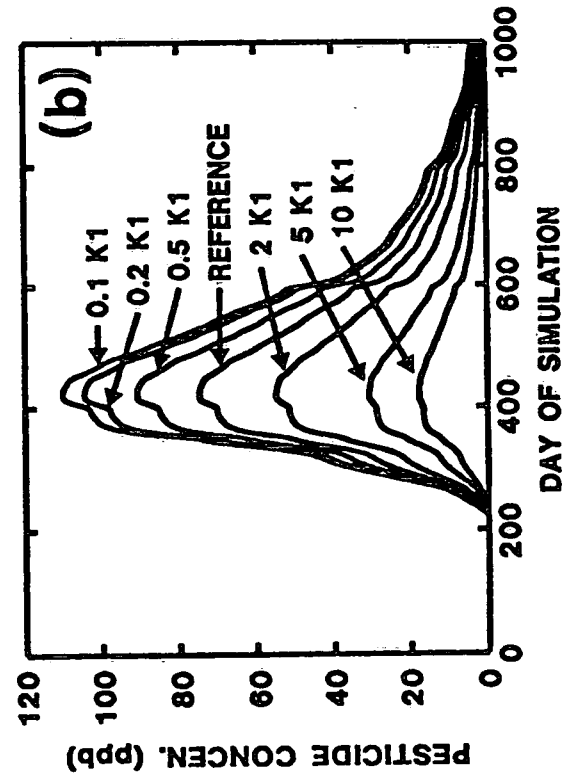
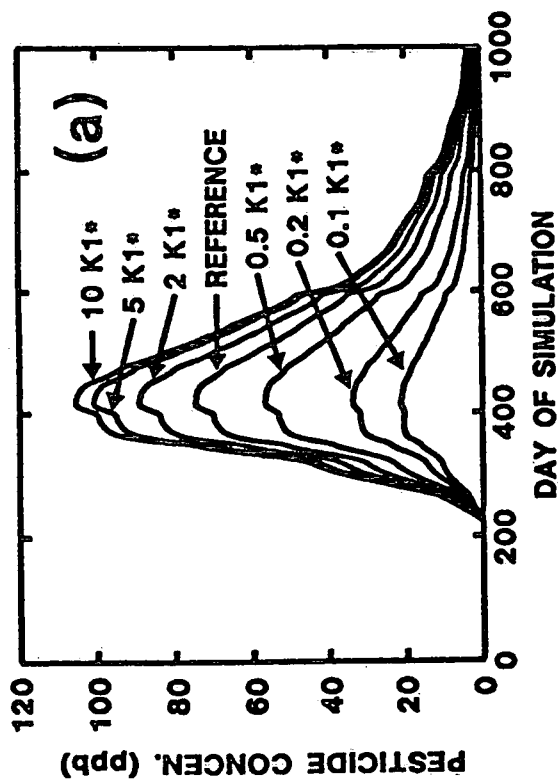


Fig.13. Typical graphical output from EXPRES: Summary file showing a time series of concentrations at the water table vs. days since pesticide was applied.

(transformation and degradation) of aldicarb and its daughter products is shown by Figure 14. 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 14a), and the degradation (by hydrolysis) of aldicarb and aldicarb sulfoxide to their respective non-toxic daughter products, aldicarb oxime (Figure 14b), and aldicarb sulfoxide oxime (Figure 14c). 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 rate reaction constants (K_1 and K_2) will result in a decrease in 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 14a). The reverse situation is true for the hydrolysis reaction rate constants, K_1 and K_2 , (Figures 14b and 14c, 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.



REFERENCE VALUES FOR RATE CONSTANTS		
	(0-0.4m)	(0.4-4.3m)
K1*	0.09082	0.01819
K1	0.04812	0.00962
K2	0.00374	0.00075

Fig.14. A sensitivity analysis of the influence of individual reaction rate constants on the total pesticide concentration at the water table: (a) transformation of aldicarb to aldicarb sulfoxide, (b) degradation aldicarb, (c) degradation of aldicarb sulfoxide.

6. 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.

Phase 3 of the development of the EXPRES expert system will concentrate on the development of the data bases required by the expert system. The first step in the development of the data bases (Phase 3) will place its emphasis on the development of a complete chemical data base for one pesticide and a complete data base describing the physical, hydrogeological and climatological setting for one particular agricultural zone. The intent is to develop a data base that may be used for testing and validating the expert system. Further development of these two data bases, as well as the explanation data base will occur in later phases of the project.

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APPENDIX A
INPUT PARAMETERS REQUIRED BY EXPRES

INPUT PARAMETERS REQUIRED BY EXPRES		
	PRZM	LEACHM
PROGRAM CONTROL		
EXISTING FILE NAME	X	X
SPECIFIC OBJECTIVE	X	X
RESULTS	X	X
DAUGHTER PRODUCTS SIMULATED	X	X
COMPUTER CHIP	X	X
APPROXIMATE SIMULATION LENGTH	X	X
UNITS	X	X
SIMULATION DATES	X	X
AGRICULTURAL ZONE	X	X
SUMMARY FILES GENERATED	X	X
OUTPUT PRINT FREQUENCY	X	X
COMPARTMENT REPORTING FREQUENCY	X	X
OUTPUT VARIABLES OF INTEREST	X	X
REPORTING DEPTHS		X
TABLES PRINTED		X
EROSIONAL LOSSES FLAG	X	X
PESTICIDE RESIDUE FLAG	X	X
PLANT ROOT GROWTH FLAG	X	X
PESTICIDE PARAMETERS		
PESTICIDE NAME	X	X
SOLUBILITY	X	X
ORGANIC CARBON PARTITION COEFFICIENT	X	X
PARENT/DAUGHTER		X
NUMBER OF PESTICIDE SPECIES	X	X
NUMBER OF PESTICIDE APPLICATIONS	X	X
APPLICATION DATE	X	X
APPLICATION RATE	X	X
DEPTH OF INCORPORATION	X	X
PESTICIDE APPLICATION METHOD	X	
PESTICIDE DECAY RATE ON FOLIGAGE	X	
FOLIAR EXTRACTION COEFFICIENT	X	
FOLIAR FILTRATION PARAMETER	X	
PESTICIDE DEGRADATION RATE IN SOIL	X	X
PESTICIDE TRANSFORMATION RATE IN SOIL		X
MOLECULAR DIFFUSION COEFFICIENT		X
MOLECULAR DIFFUSION CONSTANTS		X
DISPERSIVITY		X
DIFFUSION COEFFICIENT IN AIR		X
INITIAL PESTICIDE CONCENTRATIONS	X	X

INPUT PARAMETERS REQUIRED BY EXPRES cont.		
	PRZM	LEACHM
SOIL PARAMETERS		
NUMBER OF SOIL HORIONS	X	X
DEPTH TO WATER TABLE	X	X
TOTAL PROFILE DEPTH		X
BOTTOM BOUNDARY CONDITION		X
HORIZON THICKNESS	X	X
SURFACE/ROOT/BELOW ROOT ZONE	X	X
BULK DENSITY	X	X
ORGANIC CARBON CONTENT	X	X
FIELD CAPACITY	X	X
WILTING POINT	X	X
PERCENT SILT AND CLAY	X	X
STARTING THETA	X	X
AIR ENTRY VALUE		X
CAMPBELLS CONSTANT		X
SATURATED HYDRAULIC CONDUCTIVITY		X
ROOT FRACTION IN SOIL HORIZON		X
SOIL TEMPERATURE		X
MUSLE PARAMETERS (K,P,LS,C)	X	X
PARTICAL BULK DENSITIES	X	X
SOIL DRAINAGE PARAMETERS	X	
AREA OF FIELD	X	X
FARM MANAGEMENT AND CROP PARAMETERS		
NUMBER OF DIFFERENT CROPS	X	X
CROP NAMES	X	X
MAXIMUM INTERCEPTION STORAGE	X	
MAXIMUM ROOT DEPTH	X	
CROP COVER FRACTION	X	X
PESTICIDE UPTAKE EFFICIENCY FACTOR	X	X
PLANT DENSITY		X
MAXIMUM DRY FOLIAGE WEIGHT		X
CROP CONDITION AFTER HARVEST	X	X
CURVE NUMBER	X	X
NUMBER OF CROPPING PERIODS	X	X
PLANTING AND EMERGENCE DATES	X	
MATURITY AND HARVEST DATES	X	X
ROOT LENGTH		
MINIMUM ROOT WATER POTENTIAL		X
MAXIMUM ROOT WATER POTENTIAL		X
ROOT FLOW RESISTENCE TERM		X
MAXIMUM ACTUAL TRANSPIRATION		X

INPUT PARAMETERS REQUIRED BY EXPRES cont.		
	PRZM	LEACHM
METEOROLOGICAL PARAMETERS		
NAME OF METEROLOGICAL STATION	X	X
MINIMUM DEPTH OF EVAPORATION	X	X
PAN EVAPORATION COEFFICIENT	X	X
SNOW MELT COEFFICIENT	X	X
AVERAGE DAYLIGHT HOURS	X	X
EROSIVE STORM DURATION	X	X
BAROMETRIC ENHANCEMENT FACTOR		X

APPENDIX B
AVAILABLE OUTPUT FROM EXPRES

OUTPUT PARAMETERS AVAILABLE FROM EXPRES SUMMARY FILES		
	PRZM	LEACHM
CONCENTRATION PROFILES		
TOTAL PESTICIDE CONCENTRATION	X	X
DISSOLVED PESTICIDE CONCENTRATION	X	X
ADSORBED PESTICIDE CONCENTRATION	X	X
GENERAL INFORMATION		
ECHO INPUT DATA	X	
CURRENT CONDITIONS	X	
RETENTIVITY AND CONDUCTIVITY DATA		X
MASS BALANCE	X	X
WATER FLUX AND STORAGE		
PLANT CANOPY	X	
SNOW PACK	X	
SURFACE LAYER	X	X
PLANT ROOTS		X
PROFILE	X	X
PROFILE SUMMARIES	X	X
PESTICIDE FLUX AND STORAGE		
PLANT CANOPY	X	
SNOW PACK	X	
SURFACE LAYER	X	X
PLANT ROOTS		X
PROFILE	X	X
PROFILE SUMMARIES	X	X

OUTPUT PARAMETERS AVAILABLE WITH EXPRES TIME SERIES FILES

WATER STORAGE AND FLUX

CROP INTERCEPTION	X	
SOIL WATER CONTENT	X	X
SNOWPACK STORAGE	X	
PRECIPITATION	X	X
SNOWFALL	X	X
CANOPY THROUGH FALL	X	X
PERCOLATION	X	X
EVAPOTRANSPIRATION	X	X

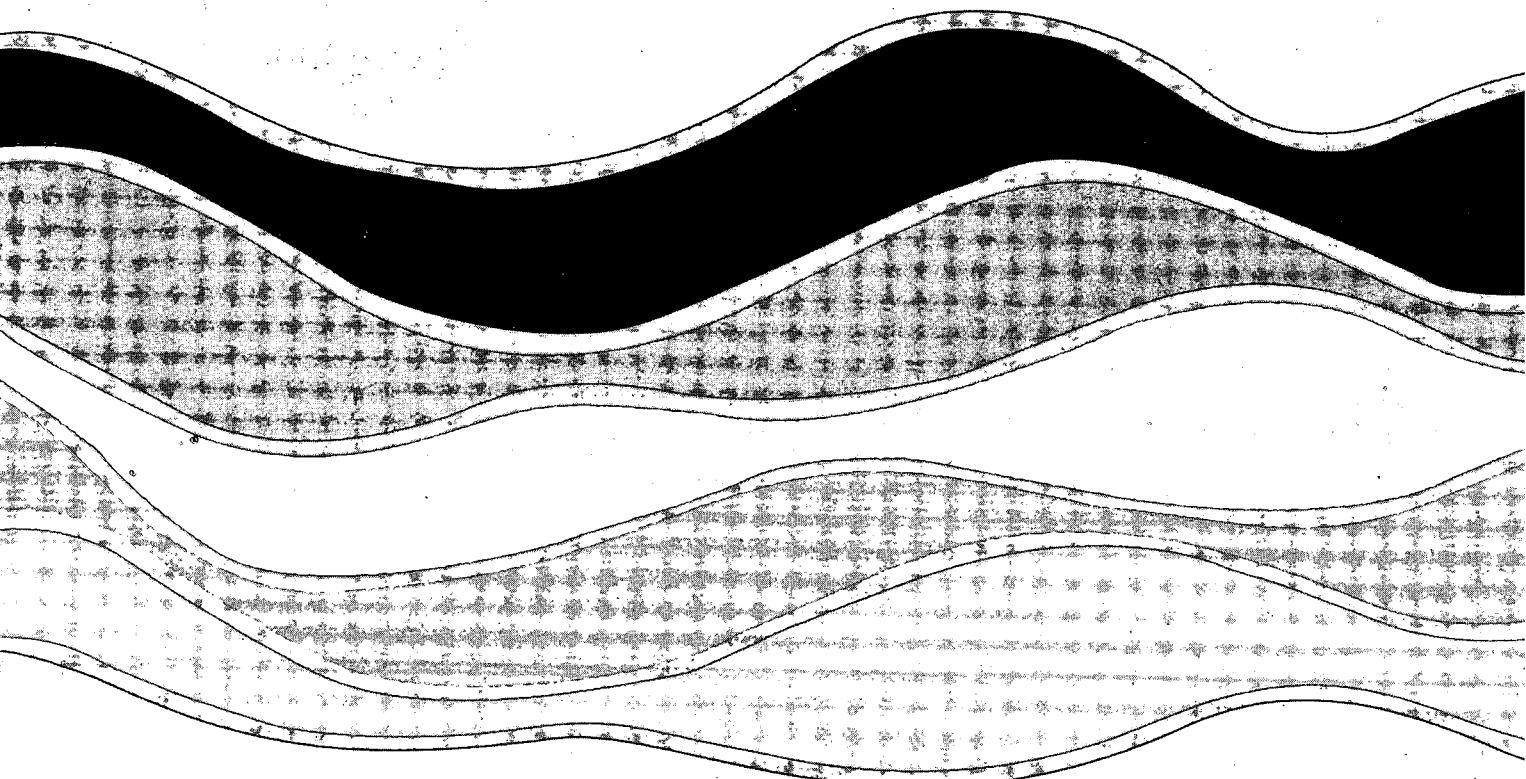
PESTICIDE STORAGE AND FLUX

FOLIAR PESTICIDE STORAGE	X	
TOTAL PESTICIDE IN SOIL COMPARTMENT	X	X
DISSOLVED PESTICIDE IN SOIL	X	X
TOTAL PESTICIDE APPLICATION	X	X
FOLIAR PESTICIDE DECAY LOSS	X	
NET PESTICIDE DIFFUSIVE FLUX	X	
PESTICIDE ADVECTIVE FLUX	X	X
PESTICIDE DECAY RATE	X	
PESTICIDE UPAKE	X	X
PESTICIDE RUNOFF LOSSES	X	X
PESTICIDE EROSION LOSSES	X	X
TOTAL PESTICIDE UPTAKE	X	X
TOTAL PESTICIDE DECAY RATE FOR ENTIRE PROFILE	X	X

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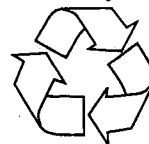
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