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ASSESSING THE MIGRATION AND TRANSFORMATION OF PESTICIDES IN THE SUBSURFACE: THE ROLE OF EXPERT SYSTEMS

by

A.S. Crowe and J.P. Mutch

The Groundwater Contamination Project
National Water Research Institute
Canada Centre for Inland Waters
Burlington, Ontario, Canada
L7R 4A6

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ABSTRACT

The expert system described here is designed to aid regulatory personnel in their assessment of the potential for pesticides to contaminate the soil and groundwater environment. The expert system, known as EXPRES (EXpert system for Pesticide Regulatory Evaluation Simulations), consist 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 model. 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 les possibilités qu'ont les pesticides de contaminer le sol et l'eau souterraine. Le système expert, appelé EXPRES (EXpert system for Pesticide Regulatory Evaluation Simulations), est constitué des modèles numériques existants qui sont utilisés pour simuler le transport et la transformation des pesticides dans la zone insaturée; ces modèles sont couplés à un système basé sur la connaissance qui guide l'utilisateur dans le choix de toute l'information nécessaire pour établir les profils géologiques, physiques, climatiques, hydrogéologiques, pédologiques et agricoles de régions agricoles typiques du Canada, conformément aux exigences du modèle pour le pesticide. Le système expert est conçu comme un outil de gestion pour faciliter les décisions en matière de réglementation, et non comme un outil de recherche. Ainsi, son but n'est pas de fournir de l'information sur les processus qui règlent le devenir des pesticides dans les milieux poreux, mais de fournir une évaluation des dangers potentiels et d'indiquer si une étude plus poussée est justifiée.

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 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 develope 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 paper outlines the two year program currently being undertaken by the Groundwater Contamination Project to development the expert system, and also provides the reader with a brief overview of expert systems.

PERSPECTIVE-GESTION

La Division des pesticides de la Direction des produits chimiques commerciaux d'Environnement Canada doit évaluer les dangers pour l'environnement liés à un pesticide et à ses produits de transformation avant que l'utilisation de ce pesticide par le public soit approuvée. Une des préoccupations précises de la Division des pesticides est la possibilité qu'un pesticide contamine les ressources d'eau souterraine. Bien qu'il existe à l'heure actuelle un certain nombre de modèles qui peuvent prévoir le transport et la transformation des pesticides sous la surface du sol, le personnel chargé de la réglementation ne possède pas, de manière générale, l'expertise nécessaire pour utiliser judicieusement ces modèles. La Division des pesticides a fait appel au personnel du Projet de contamination des eaux souterraines, INRE, pour mettre au point un système expert qui peut être utilisé pour faciliter l'évaluation du potentiel de contamination des eaux souterraines par les pesticides. De plus, ce système expert peut être utilisé pour identifier le développement agricole qui peut être ou ne pas être durable. Le présent article décrit le programme de deux ans qui a été entrepris par le Projet sur la contamination des eaux souterraines pour mettre au point le système expert et donne également au lecteur un bref aperçu des systèmes experts.

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National Water Research Institute
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KEYWORDS

expert systems, knowledge-based systems, pesticides, pesticide registration, transport modelling

INTRODUCTION

Pesticides are, by design, poisons which are introduced into our environment in order to kill target species of plants or organisms. Although pesticides will enhance crop production and the quality of the crop through the control of pests, there are environmental risks associated with their use. For example, several recent studies focusing upon the transport and transformation of the pesticide aldicarb in the subsurface (Zaki et al., 1982; Jones, 1985; Harkin et al., 1986; Jones and Marquardt, 1987; Jones et al., 1987; Priddle et al., 1987; 1988) provide strong evidence that pesticides can cause the contamination of groundwater even if the recommended application procedures are followed. The possibility of groundwater contamination is of special concern in rural areas of Canada where 82% of the rural population rely on groundwater as a source of domestic water supply (Hess, 1986).

All pesticides used in Canada undergo extensive testing to ensure that they and their degradation products present minimal risks to the environment before being registered for public use (Agriculture Canada, 1987). However, regulatory personnel typically have little predictive capability in how a pesticide behaves in the subsurface. Numerous models currently exist for predicting the distribution and concentration of a pesticide in the subsurface. For example, several well known models are LEACHM (Wagenet and Hutson, 1986; 1987), PRZM (Carsel et al., 1984; 1985), GLEAMS (Leonard et al., 1987), MOUSE (Pacenka and Steenhuis, 1984; Steenhuis et al., 1987), CMIS/CMLS (Nofziger and Hornsby, 1986, 1987), VULPEST (Villeneuve et al.,

1987). The application of these models in a regulatory framework is limited because, first, specialized knowledge is required in order to assess the transport and transformation of pesticides in the unsaturated soil zone because they are governed by a complex set of chemical, biological and physical processes, second, the numerical framework upon which the models are based are generally complex and typically can only be operated by a trained modeller, and third, the models require a specialized set of physical and chemical data which are not generally obtained during typical field studies. Therefore, these models can not readily be used by regulatory personnel who are assigned the task of assessing the effects of a pesticide on the quality of the groundwater. Thus, there is a need to develop or adapt a model which is sufficiently sophisticated for simulating the major processes controlling the fate of pesticides, and yet can easily and accurately be used by the regulatory personnel.

A recent development that transfers the decision making requirements associated with computer modelling technology from a complex science to a practical tool for non-specialist is the expert system. Because expert systems are designed to assist the user in solving a complex problem that is beyond the user's present level of knowledge in either the field of interest or in computing ability, expert systems represent an attractive tool for providing regulatory personnel with the capability of assessing the impact of pesticides in the groundwater environment. Although expert systems technology has not been widely applied to the field of groundwater contamination, the systems that have been developed illustrate that expert systems can be a valuable tool for assisting a non-specialist with complex technical problems. For example, the EROKEY expert system (McClymont and Schwartz, 1987) was constructed to assist the user in preparing input data for a contaminant transport model and to help the user design a monitoring strategy. This expert system will supply input data if requested by the user, check the values of the input data for consistency, and provide concentration distributions for a contaminant plume at a specified time. The GEOTOX expert system (Wilson et al., 1986; Mikroudis and Fang, 1986) was designed to assess hazardous waste sites in order to prioritize remedial measures on a cost-effective basis.

This paper describes the framework of an expert system which is designed to provide regulatory personnel with a tool for evaluating the transport and transformation of pesticides in the subsurface environment in order to identify potential groundwater problems. The expert system is known as EXPRES; EXpert system for Pesticide Regulation Evaluation Simulations. The expert system is actually a knowledge-based system coupled to a pesticide transport and transformation code, and because it is an expert system, it is designed such that staff not trained in the use pesticide transport models can easily use, and obtain reliable information from, the models. EXPRES is designed as a management tool to be used as an aid in making policy decisions. 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 in order 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-monitoring registration is needed.

The specific tasks undertaken by the expert system include:

(1) providing regulatory personnel with a method of obtaining the geological, hydrogeological and computing 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.

This paper describes the feasibility and advantages of an expert system approach to assessing the potential for pesticides to contaminate groundwater, as well as an outline of how such an expert system could be constructed.

REGISTRATION OF PESTICIDES IN CANADA

Pesticides (herbicides, insecticides, fungicides) are used extensively in Canada to enhance the quantity and quality of agricultural crops. In order to minimize potential risks to the environment, all pesticides used in Canada are registered for a particular crop, a specific pest and a specific usage. Environment Canada, in conjunction with Agriculture Canada, Health and Welfare Canada, and the Department of Fisheries and Oceans, are responsible for establishing the pesticide regulations in Canada. Environment Canada's role is to estimate the environmental risks associated with pesticide usage. Specifically, Environment Canada's responsibility is to identify, and minimize or prevent deleterious impacts on non-target species, communities and ecosystems. Environment Canada is also responsible for assessing the potential for contamination of surface water and groundwater due to pesticide usage.

The registration requirements and procedures for demonstrating that a pesticide and its transformation products are environmentally safe are outlined by a set of guidelines prepared jointly by Agriculture Canada, Environment Canada and the Department of Fisheries and Oceans (Agriculture Canada, 1987). In general, registration requires that the manufacturer submit, first, a description of the components and environmental chemistry of the pesticide and its transformation products, including degradation pathways and rate constants, second, a discussion of the persistence and mobility of the pesticide and its transformation products in the environment according to the specific uses of the pesticide, and third an assessment of the toxicity of the pesticideto non-target species. Environment Canada evaluates the results of these studies (i.e. mobility, persistence) to assess the affect that the pesticide will have on the environment.

In order to protect the environment from the detrimental effects of pesticide usage, Environment Canada undertakes a three phase program consisting of (1) a pre-registration evaluation, which determines, and advises on, the environmental risks associated with new pesticides, (2) a regulatory re-evaluation, which assesses, and provides advice on, the environmental risks for existing pesticides, and (3) a post-registration monitoring and research, program which identifies pesticides which need to be assessed under actual field conditions.

The risks analysis for a pesticide is divided into four stages. The first stage focuses upon environmental exposure by examining the persistence, mobility, accumulation and transformation of the pesticide in air, water and soils and the effects of exposure of non-target organisms to the pesticide, within different geographical, climatic, hydrological and pedological settings. The fate of pesticides in the subsurface is governed by three factors that control its concentration, mobility, persistence and potential for accumulation. These factors are (1) the chemical properties of the pesticide, (2) the characteristics of the sites across Canada (physical, climatic, hydrogeological, pedological), and (3) method of pesticide application and quantities used in each region. In order to specifically assess the potential for a pesticide to contaminate groundwater, the following laboratory and field studies are required to be undertaken by the manufacturer:

(1) vapour pressure and volatilization;
(2) hydrolysis;
(3) phototransformation on soil and in water;
(4) solubility in water;
(5) octanol/water partitioning coefficient;
(6) adsorption/desorption from soil;
(7) leaching;
(8) biotransformation (aerobic and anaerobic) in soil and water;

(9) terrestrial field dissipation and accumulation (field studies).
Environment Canada reviews the data obtained from these studies to determine the risks associated with the pesticide when released into the environment. A detailed description of the data required, and the procedures for obtaining these data, are presented in Agriculture Canada (1987). The second stage involves administrating environmentally focused toxicological tests to determine the effects of the pesticide on selected organisms. The third stage of the risk analysis procedure is the integration and comparison of the exposure data and the toxicological hazard data to determine the effects of the pesticide on selected organisms under various environmental conditions. The final stage of the procedure involves the application of guidelines to assess the risk associated with a pesticide. Once Environment Canada has completed its environmental assessment of the pesticide, the risks and benefits of the usgage of the pesticide are evaluated by Agriculture Canada for the purpose of deciding whether or not the pesticide should be registered.

Because each registration is different in terms of (1) the chemistry of the pesticide, (2) the proposed application procedures and quantities, and (3) the climatic, agricultural, hydrogeological and geographical settings, the guidelines are designed to be flexible. Hence, the evaluation and acceptance or rejection of data is based upon scientific judgement designed to reflect these variations rather than enforcing a ridgid criteria. Also, 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. In order to reduce the amount of uncertainty that exists, the data supplied by the manufacturers are analyzed through a series of worst-case scenarios at the different sites and under various conditions. However, the total number of possible senarios is too numerous for all to be tested.

The expert system discussed in this paper is designed to aid regulatory personnel within Environment Canada in their assessment of the potential for a pesticide to contaminate groundwater. The application of the expert system is not intended to replace any part of the existing registration procedure, rather it will be used in conjunction with existing environmental risk analysis procedures.

AN OVERVIEW OF EXPERT SYSTEMS

Expert systems (also known as knowledge-based expert systems) are a class of computer programs which fall within the field of artificial intelligence. Generally, expert systems functions 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. The difference between an expert and a layman is that an expert has acquired a great deal of knowledge through a high level of study, training, insight and personal experience during their life, whereas a general practitioner does not have either the specific training or experience to confidently assess a problem. The human expertise which is encoded into an expert system includes knowledge, experience, judgement and problem-solving ability.

Currently, as illustrated by Figure 1, there are two conventional approaches to undertaking a complex problem that requires the application of a numerical model. If the person with the problem, known as the client, has access to the appropriate numerical codes, the client can prepare the required input data set, run the model and use the results of the simulations as a basis for conclusions. However, in most cases the client does not have the expertise to either (1) use the models, (2) adequately ensure that the input data are accurate and consistent and (3) check the results of the simulations for accuracy or provide a meaningful interpretation of the results. Thus, the client will usually approach an expert, such as a numerical modeller, with expertise in both the framework upon which the models are based and the application of these numerical models. The

client converses with the modeller to describe the objectives of the study and the available data (Figure 1). The modeller then chooses an appropriate code, synthesizes the data, runs the model and verifies and interprets the results of the simulations. The pertinent information is then passed to the client through a discussion of the modelling results. An expert system approach (Figure 1) basically undertakes the same series of steps, but without the necessity of actually approaching an expert. The expert system will in effect converse with the client, prompting the client and providing explanations and suggestions if necessary, in order to obtain the information required to undertake a simulation. The expert system will then decide upon the most appropriate method of solving the problem, and will check the input data received from the client and evaluate the results of the simulation. The results, including an interpretation and explanation, are conveyed to the client by the expert system. Although there will be some problems that can not be adequately handled by an expert system, in most cases a properly constructed expert system can duplicate the knowledge of human experts. Thus, the advantages of an expert system are (1) a considerable reduction in time between requesting a simulation and obtaining the results, (2) a dramatic reduction in costs by avoiding the expert's fees, and (3) the expert system can act as an education tool as it guides the user through the simulation.

Although expert systems are computer programs, there are significant differences between conventional computer programs and expert systems. Conventional computer programs that are focused towards modelling or automating particular processes or tasks, execute a set of procedures that have been prescribed by the programmer, and are well suited for routine and exacting tasks. For example, a pesticide transport model will input quantitative data which are typically numbers, manipulate these data according to a prescribed set of FORTRAN statements and finally present specific results for the given problem. Expert systems extend conventional programming techniques by including a decision-making ability into the code. Expert systems input information (rather than just data), evaluate, interpret and may suggest alternatives based upon the input information. The data are manipulated in the same manner as a conventional program, however the results are evaluated for accuracy and recommendations may be presented.

During the 1980's, there has been a dramatic increase in the applications of expert systems, especially in engineering and sciences, as evidenced by the variety of papers presented at conferences (eg. Sriram and Adey, 1986; 1987). Although computers and programming languages are well adapted to the precise methods of solving or calculating quantitative problems, they are not well adapted to programming on the basis of imprecision and interpretation. Much work has focused upon the reasoning processes used to construct expert systems, and the following is a brief review of these concepts. For detailed information the reader is referred to an introductory text (eg. Addis, 1985; Alty and Coombs, 1984; Davis and Lenat, 1982; Hoyes-Roth et al., 1983; Waterman, 1986; Weiss and Kulikowski, 1984; Winston, 1984).

Expert systems are characterized by their use of large data bases of both informational concepts and quantitative data. Information is divided into two groups; facts and knowledge. Facts includes the quantitative data obtained from textbooks, manuals, laboratory and field experiments, etc. Facts can be divided into either observed facts, which are given data, or derived facts, which are deduced through a direct mode of inference. Knowledge is more qualitative in nature and it includes a collection of facts, insights, hunches and best procedures or rules for solving a problem. An important type of knowledge used in expert systems is heuristic knowledge. This is 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.

Expert systems are classified according to the manner in which knowledge is represented. There are three structures that can be used to represent knowledge, these being (1) production rules, (2) semantic nets and (3) frames. Expert systems can be constructed entirely with one of these structures. However, more commonly they are composed of a combination of rules, nets and

frames because this combination of structures reduce the number of rules required to construct an expert system.

Expert systems which are based upon production rules (known as rule-based systems) consist of "IF-THEN" conditional statements. When data accumulated for a particular problem matches the conditions stated in the "IF" part of the rule (known as the condition or premise), the statements in the "THEN" part of the rule (known as the action or consequence) are executed. An example of a production rule is:

IF aldicarb is detected in groundwater **THEN** the water is contaminated

Production rules are classified on the basis of the probability of the consequence being true based on the uncertainty associated with interpreting the condition. Production rules are either:

(1) Categorical Rules:
The consequences are an exact result of the condition being true.
(eg. IF aldicarb is detected in groundwater THEN the groundwater is contaminated)

(2) Probabilistic Rules:
The consequences have uncertainty associated with the interpretation of the condition.
(eg. IF aldicarb is detected in groundwater THEN the groundwater may be toxic)

In the above examples, the first is a categorical production rule because the presence of aldicarb in groundwater automatically implies that the groundwater is contaminated. However, the second is probabilistic because toxicity is not due to simply the identification of aldicarb in the groundwater, but rather to its concentration in groundwater.

Also, production rules can be subdivided into three types based upon the action taken within the consequence portion of the rule when the conditions stated in the conditional portion of the rule are true. Both categorical and probabilistic rules are subdivided into the following three types of rules:

(1) Inference Rules:
When the data gathered for a problem matches the conditions stated within the premise, the consequence adds to or replaces data.
(eg. IF the soil is sand THEN its hydraulic conductivity is ~ 10^{-2} cm/s)

(2) Premise - Conclusion Rules:
When the data gathered for a problem matches the conditions stated within the premise, the consequence expresses an intermediate or final conclusion.
(eg. IF conc. of aldicarb >9 µg/L THEN the groundwater is hazardous)

(2) Situation - Action Rules:
When the data gathered for a problem matches the conditions stated within the premise, the consequence is a particular action.
(eg. IF this groundwater is used for drinking THEN take remedial action)

The linking or chaining of production rules forms the reasoning strategy. Rules can be linked by either forward chaining or backward chaining. In the application of the two types of chaining, forward chaining is generally used as a diagnostic tool where as backward chaining is used as an interpretive tool. With forward chaining, an expert system makes use of a series of rules to arrive at a particular consequence according to a series of conditions and information given as input. The following example of forward chaining uses the given information on the presence and

concentration of aldicarb in the groundwater, in order to diagnose wheter or not the groundwater is contaminated and must be decontaminated:

> **IF** aldicarb is detected in groundwater **THEN** test its concentration
> **IF** its concentration is > 9 µg/L **THEN** groundwater is contaminated
> **IF** the groundwater is contaminated **THEN** take remedial action

Backward chaining starts with one or more given consequences to be resolved and determines what conditions must be met and information provided in order to reach the consequences. An example of backward chaining is, given that the groundwater is contaminated with aldicarb (the consequence), determine the possible causes and processes (the conditions) that led to the contamination:

> **IF** groundwater contains aldicarb **THEN** was it transported by groundwater
> **IF** it migrated with groundwater **THEN** what is flow direction and velocity
> **IF** the flow characteristics are known **THEN** where is the aldicarb source
> **IF** the source is known **THEN** what caused its persistence

The second structure for representing knowledge is the semantic net. Semantic nets are used to represent non-rule-based knowledge according to an association among objects, events or concepts. The data are associated by "IS-A" links within hierarchial networks. An example of a hierarchial network of facts within a semantic net is illustrated by Figure 2. The information that can be implicitly inferred from this semantic net is that aldicarb, as well as all other pesticides, are hazardous in drinking water, and that toxic substances include aldicarb.

The third structure for representing knowledge is a frame. Frames are used to group or categorize non-rule based knowledge that is characterized by a number of attributes or related parameters. Data are grouped into mini-data bases in a fill-in-the-blanks type of statements and these data are entered or retrieved via a keyword. Frames makes the association of information more explicit than rule-based systems. An example of a frame is shown by Figure 3. Here, any climatic data for a particular place can be readily retrieved or modified by entering the keyword "CLIMATE DATA".

The major components comprising the architecture of an expert system are illustrated in Figure 4. The main component of an expert system is the inference engine. The inference engine basically controls the execution of the expert system, links all of its operations and searches the data bases through a number of modules in response to input provided by a user. The program control module links the various modules and components of the expert system and determines how, and in what order, the procedures are undertaken. The reasoning control module accesses the rules in the knowledge base and controls the reasoning strategy. The interpretation module transforms the user's entries, according to input data, explanations and program options, into a form where rules can be selected, as well as preparing the data for, and interpreting the results of, the numerical simulation unit, and it also checks and verifies the user's entries and results of the simulations for accuracy and consistency. The data update module allows for the modification of existing data or the addition new data to the knowledge, facts and explanations bases.

The user - system interface conveys the encoded expertise to the user via an interactive terminal session or a dialogue format, which is analogous to a conversation between an expert and

a client. By entering data this way, the user is not required to have knowledge of programming, the operating system or modelling. This dialogue format takes the form of either prompts or questions to the user for required data and choice of simulation options, or as menus or tables from which values are chosen via the retrieval of information which is stored in the data bases. The user responds to these prompts by entering information as numbers, words, or as simple "YES - NO" responses. There are problems associated with an expert system which is based entirely on rules. If considerable information is required and entered via responses to prompts, then considerable time will be spent answering the questions. In addition, the user can not volunteer information at any time, cannot return to a previous question and typically a question must be answered before the expert system will allow the user to continue. These problems can be over come by the use of frames for entering common information.

Generally, data within an expert system can be grouped into three data base known as, the knowledge base, facts base and explanation base. The knowledge base includes all the rules, nets and frames that are used to relate the facts and concepts describing a domain or a reasoning methodology. The facts data base contains all the quantitative information for a given domain. An expert system also contains an explanation data base comprised of explanations and definitions which are used by the inference engine to (1) help the user understand the question or requested information during input by offering choices of values, explanations or definitions, (2) allow the user to follow the expert system's reasoning strategy, (3) check the entered values for consistency with previously entered information, and (4) aid the user's understanding of the conclusions and recommendations based upon an evaluation of the information supplied by the user. Interpretation of data or reasoning is not undertaken within the data bases; these functions occur only within the inference engine.

The simulation unit of the expert system is a mathematical model, unique to each expert system, that does the actual simulations or predictions according to the purpose of the expert system. For example, if the expert system is designed to aid in the assessment of pesticide transport through the subsurface, the model will be a pesticide transport and transformation code. The inference engine will construct an input data set for the simulation model from the user's input and from information contained within the data bases.

Expert systems are computer programs and thus are constructed with programming languages. The three groups of programming languages commonly used in the construction of expert systems are knowledge engineering languages, symbolic manipulation languages and regular programming languages. Knowledge engineering languages, also known as expert system shells, are computer programs that are designed specifically to construct expert systems. Typically, they are existing knowledge-based expert systems without a domain-specific knowledge data base. Because shells are existing expert systems, they lack the generality and the flexibility required for adaption to another problem. A specific problem arises when trying to design an expert system that incorporates an existing simulation model within the framework of an existing expert system shell because an expert system shell currently does not exist that can drive a simulation model. Hence, expert system shells are generally good only for a simple or restricted class of applications. A second group of programming languages that comprise expert systems, are the symbolic manipulation languages or artificial intelligence languages, such as LISP or PROLOG. The symbolic manipulation languages are most applicable to expert systems that include negligible calculations, and hence they are difficult to apply to engineering or scientific problems. A similar problem exists with these languages because most existing simulation models are programmed in conventional computer languages. The third group of computing languages are the conventional programming languages, such as FORTRAN, C or PASCAL. Conventional programming languages offer greater flexibility in the design and construction of expert systems and expert system shells, especially when existing simulation models are to be incorporated into an expert system.

AN EXPERT SYSTEM FOR PESTICIDES REGULATORY DECISIONS

The purpose of the EXPRES expert system (EXpert system for Pesticide Regulation Evaluation Simulations) is to provide regulatory personnel with a tool that will aid in their evaluation of the fate of pesticides in the subsurface, and specifically, to ensure that the quality of the groundwater in agricultural areas is maintained. EXPRES 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 is not intended for use as a research tool. Thus, the objective of the expert system is not to provide insight into the processes that control the transport and transformation of pesticides in porous media, but rather, its purpose is to provide a quick and general 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. Because the model will be used as an aid in making policy decisions regarding balancing the risks and benefits of the pesticide, the orientation of the model is towards examining "worst-case" and "typical-case" scenarios of pesticide application in agricultural regions across Canada. The important criteria for constructing the expert system and the required biological, chemical and physical processes that the model should incorporate are discussed in this section.

The most important characteristic of EXPRES is that it should be designed to be easy to use by those not experienced in the use of numerical models which simulate pesticide transport in the subsurface. Therefore, there are several important criteria that must be addressed during the design and construction of the expert system. These criteria include:

(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 program should be readily available from data bases or easily entered into the system via a dialogue format;
(5) the data bases should be complete;
(6) corrections and changes during data entry should be easy to fix;
(7) output should be informative, useful and easily understood;
(8) the program should be written in a manner that will allow for easy modification;
(9) data base should be constructed so that they can easily be modified and updated.

The use of an expert system approach by regulatory personnel for evaluating the potential for pesticides to contaminate groundwater offers several advantages over the approach of contacting an outside expert to perform this work or undertaking the task in-house by someone who does not have the expertise to ensure the accuracy of the results. Advantages of EXPRES include:

(1) complex modelling codes can be used by those not familiar with this technology;
(2) reduced costs and time associated with not having to contact an outside consultant;
(3) a test of the accuracy and consistency of user-supplied data, with identification and/or suggestions for missing values;
(4) an evaluation and interpretation of critical output from the simulation model;
(5) a systematic evaluation of the potential for a pesticide to contaminant groundwater through a sensitivity analysis of parameters affecting the fate of pesticides in the unsaturated zone;
(6) data bases containing information characterizing field sites and pesticides can be stored for future reference;
(7) it can be used as an educational tool for teaching basic concepts about pesticide transport and transformation.

The general architecture of the EXPRES expert system illustrated by Figure 4. EXPRES is composed of four parts; (1) the inference engine, (2) the pesticide transport and reaction model, (3) the information and knowledge bases, and (4) the user - system interface.

The inference engine contains the programming statements which affect the general control of the expert system. The program control module controls the basic computer operations such as linking the pesticide transport model, printing or plotting the results of the simulations, etc. The reasoning control module basically controls the reasoning strategy required to compose a data set characterizing the physical setting, climatic conditions and agricultural practices of a particular site, and controls the evaluation of 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 responses to the expert system's questions into a form that can be used by the expert system to either prompt the user for further information or compose an input data set for the simulation model. In addition, the module performs internal checks to ensure consistency among all the entered values and converts the results of a simulation to an easily interpretable form. The data update module is used to modify or update the information in the existing EXPRES data bases. Additional information that characterize the field sites or the environmental chemistryof the pesticides may be added to the facts or knowledge data bases, and new explanations or examples may be added to the explanation data base.

The user - system interface module is an interactive program that guides the user through the entry of data required by the pesticide transport model within EXPRES and provides assistance on interpreting the results obtained from the model. The module prompts the user for information pertaining to the chemical characteristics of a pesticide, the procedures followed to apply the pesticide, the physical and climatic setting of the field site and the hydrological properties of the soil environment. Should the user be unfamiliar with any of the requested information, EXPRES will provide either an explanation about the required data and/or recommend typical values which may be used. The user will then have the option to modify these data. A second important feature of the user - system interface module is that it provides both quantitative and qualitative output from the simulation model. Output is conveyed to the user in the standard form of tables of numbers. Also, to help less experienced persons understand the critical output form the model, EXPRES provides interpretations, evaluations and predictions based on these results. An important feature of the user - system interface is that it is coupled to graphics to help visualize trends, anomalies and relationships among variables.

The third part of EXPRES consists of a model that can be used to predict the transport and transformation of pesticides in the unsaturated zone. In order to accurately predict the transport of pesticides in the subsurface, the mathematical framework of this model must be based on the accepted scientific principles that describe the important biological, chemical and physical processes that control the transport and fate of the pesticides. These important processes include:

(1) transport of dissolved pesticide:
- advective transport of dissolved mass;
- dispersion of the mass;
- percent mass loss due to surface runoff and pesticide flux through the surface;

(2) changes to chemical character of the pesticide:
- chemical speciation (dissociation/association);
- adsorption (linear, reversible, instantaneous equilibrium);
- first-order degradation (hydrolysis, microbial transformation, phototransformation);
- volatilization.

The physical, chemical and biological processes controlling the transport and degradation of pesticides in the subsurface are in turn affected by a number of environmental factors which must be considered by the model. These factors include the:

(1) moisture profile through the unsaturated zone;

(2) depth to the water table;
(3) hydraulic properties of the soil and aquifer;
(4) recharge rates at the ground surface;
(5) temperature of air and water;
(6) thickness of soil zone;
(7) plant uptake;
(8) water fluxes at surface and depth;
(9) pH of the soil-water environment;
(10) pesticide fluxes at the ground surface.

Rather than developing a new pesticide transport and reaction model, existing models have been chosen and modified to fulfil the needs of the expert system. This not only reduces the time required to arrive at a final product, but by using a widely accepted model, this ensures that the important processes are included in the model and that the model will have been verified through previous use. Currently, there are several pesticide transport and reaction models that simulate many of these processes. Because of the importance of this component of EXPRES, the choice of the pesticide transport model is discussed in detail in the next section. However, the criteria used to choose a model for the EXPRES expert system 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 pesticide to reach, the water table;
(3) simulate the transport, and predict concentrations, of the degradation products;
(4) be based on generally accepted scientific principals that govern the transport and transformation of pesticides;
(5) be currently 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.

The fourth component of EXPRES is the information data bases, which essentially form the "expert's" contribution to the system. The expert system requires three data bases, a Knowledge Bases, a Facts Base and an Explanation Base (Figure 4).

The Knowledge Base contains the production rules, which basically consists of encoded expertise or knowledge that guides a user through a simulation. This base provides two functions. First, it is accessed through the reasoning control module of the inference engine (user - system interface) to provide the link between the user and the expert's information and knowledge to assist the user in their choice of parameters and options for undertaking a pesticide transport and degradation simulation. Second, production rules are used for internal checks and for output interpretation through 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) checks for plausible values and relationships among chosen parameters;
(3) production rules for interpreting the results of a simulation.

Information stored in the Explanation Base consists of encoded explanations and elaborations provided by an expert that can aid a user in the choice of parameters for a simulation when the information requested by the production rules is not understood by the user or is not available to the user. The type of information within this data base includes:

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

The Facts Data Base is comprised of detailed information that describes, first, the physical, climatic, hydrogeological and agricultural setting of typical agricultural zones across Canada, and second, the chemical characteristic of pesticides. An important feature in the design of these data bases is that it must allow values contained in the data bases to be easily modified, new data to be included as they becomes available and new pesticides to be added to the data bases, through the data update module contained in the inference engine. These data are required by the pesticide transport and transformation model.

The first set of data in the Facts Data Base contains information to characterize typical agricultural zones. These agricultural zones include:

(1) an orchard in central British Columbia;
(2) a berry field in the Fraser River Delta, B.C.;
(3) a grain field in the Peace River District of Alberta;
(4) a sugar beet field in southern Alberta;
(5) a wheat field in Saskatchewan;
(6) a grape vineyard in the Niagara region of Ontario;
(7) a corn field in Ontario;
(8) a potato field in Quebec;
(9) a potato field in P.E.I.;
(10) a forest zone in New Brunswick;
(11) an orchard in central Nova Scotia.

The characterization of these typical agricultural zones are 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 guided, however, 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 easily be modified by the user for a particular simulation.

The second set of data in the Facts Data Base, containing the chemical characteristics of pesticides, is accessed by the user when information for a new pesticide is required by the model but does not exist. By looking at a family of similar pesticides in this data base, the user will be able to approximate the required data for the new pesticide.

PESTICIDE TRANSPORT/TRANSFORMATION MODELS

Most existing models account for the major chemical, biological and physical processes that simulate pesticide transport and transformation in the unsaturated zone. Examples of these models include LEACHM (Wagenet and Hutson, 1986; 1987), PRZM (Carsel et al., 1984; 1985), MOUSE (Pacenka and Steenhuis, 1984; Steenhuis et al., 1987), GLEAMS (Leonard et al., 1987), SESOIL (Bonazountas and Wager, 1984) and CMIS/CMLS (Nofziger and Hornsby, 1986, 1987). A general discussion of pesticide transport and transformation models is presented in this section. Particular emphasis is placed on the models that are most applicable to the EXPRES expert system.

Pesticide transport models simulate the migration of pesticide through the unsaturated zone only. Pesticide transport is based on a solution to the one-dimension form of the advective-dispersive solute transport equation under transient conditions. In general, these models represent the unsaturated zone as a series of compartmentalized storage elements. With the exception of LEACHM, the models are lumped parameter models, in which water and solute flux through the unsaturated zone is simulated by a simplified water balance among the storage elements. Layered soils are represented by assigning different physical, chemical and biological parameters to the storage elements. Although LEACHM represents the subsurface as a series of compartments,

water and solute transport is simulated as a distributed parameter model by the solution of the solute transport equation. All models with the exception of VULPEST (Villeneuve et al., 1987), are deterministic; VULPEST employs stochastic techniques in its simulation. Most models account for the major physical, chemical and biological processes affecting the transport and degradation of pesticides in the unsaturated zone, such as advection, dispersion, chemical speciation, first-order degradation, adsorption (linear, reversible and instantaneous local equilibrium) and plant uptake (as a function of the rate of transpiration). These processes and an overview of pesticide transport and transformation models are presented by Mutch and Crowe (1989, 1990). Only three models (PRZM, MOUSE and GLEAMS) will account for lateral loss (runoff) of water and solute at the ground surface. All models are designed primarily for relatively non-volatile compounds. With the exception of LEACHM, none of the models account for volatilization losses and transport in the soil profile. The models require input data from four general areas; climatic conditions, soil parameters, chemical characteristics of the pesticide and farm management practices.

While the models attempt to describe the major processes influencing the migration and transformation of pesticides, the extent to which they describe these processes varies considerably. The models range in complexity from basic education models (eg. CMLS), through an intermediate management-level model (eg. PRZM), to sophisticated research models (eg. LEACHM). With each increase in the level of complexity, there is a corresponding increase in the accuracy of the prediction of pesticide transport. Advantages offered by the more complex models are often offset by an increase in execution time and difficulty in formulating the input data sets.

Of all the models reviewed (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 (eg. LEACHM) should also be considered for inclusion because the simulation of the processes involved in the transport and transformation of pesticides in the unsaturated zone would make this more preferable to a management model when a detailed evaluation of transport or transformation processes is desired. To highlight the differences between the models, a brief description of these two pesticide transport models (PRZM and LEACHM), which are incorporated into EXPRES is presented as follows. The reader is referred to the user's manual prepared by the authors of the codes or to Mutch and Crowe (1989, 1990) for a detailed description of the two pesticide models.

PRZM - Pesticide Root Zone Model

The PRZM model (Carsel et al., 1984) was developed by the U.S. EPA, and is classified as a management model. It simulates one-dimensional, solute transport under transient conditions. Although the model is based on an advective-dispersion equation, it employees 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. The flow of water is simulated under the following simple rules:

(1) any water which infiltrates into a soil compartment in excess of the field capacity will be drained to the compartment below within one day;
(2) moisture between the wilting point and field capacity in the root zone compartments is available for evapotranspiration;
(3) the moisture content of a soil compartment cannot fall below the 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 the universal soil loss equation (Modified USLE), 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. 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. The solution to the set of equations representing the balances for each compartment is undertaken by the finite difference technique. Numerical dispersion created during the numerical solution of the equations is used to represent actual hydrodynamic dispersion. Execution times, on a 286-based personal computer, for a one year simulation are less than ten minutes.

Output from the model may include total and dissolved pesticide concentrations in each compartment, soil moisture content and various pesticide and water flux parameters.

LEACHM - Leaching Estimation and Chemistry Model

The LEACHM code (Wagenet and Hutson, 1987) actually encompasses three solute transport models: LEACHMN (nitrogen), LEACHMS (inorganic salts) and LEACHMP (pesticides). The following discussion will be limited to the LEACHMP model.

LEACHMP is classified as a research/management solute transport model. The objective when formulating LEACHMP was to develop a model that would simulate natural processes in sufficient detail to provide useful and accurate results while restricting the amount and complexity of input data. It was also intended that the output be organized to allow for quick and simple interpretation, and hence provide managers with a tool that is easily used and understood.

LEACHMP can be used to simulate one-dimensional, pesticide transport in the unsaturated zone under transient of climate conditions, with multiple pesticide applications and user selected boundary conditions. The unsaturated zone is represented by as many as 45 soil nodes, each with different values of physical, biological and chemical parameters assigned, thus giving the model the ability to simulate 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 the finite difference technique. Flow is controlled by characteristic curves defined for the soil which relate the retentivity and conductivity of the soil to the existing matric potential. Pesticide attenuation is represented by equations describing equilibrium sorption (linear and reversible), volatilization, and chemical and/or biological degradation (first order).

Processes simulated and information provided by LEACHMP includes:

(1) the migration of two daughter products as they are formed due to the transformation of a parent pesticide, with individual adsorption and degradation parameters assigned to each;
(2) the characteristic curves for a particular soil;
(3) plant growth;
(4) evaporation and transpiration;
(5) plant uptake of water and pesticide;
(6) water flux, flux density, water contents and matric potentials for each soil compartment according to the surface and bottom boundary conditions specified by the user;
(7) chemical and/or biological degradation (first order) and volatilization;
(8) the solute flux and concentrations;
(9) flow of heat in the soil profile and temperature distribution in the soil profile;
(10) the degradation rate constants as a function of the temperature profile.

The time step in LEACHMP is variable, ranging from a minimum value of 1.0×10^{-7} of a day 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 totals for each of the pesticide species in each soil compartment, both water and pesticide flux below a prescribed depth, and mass balance checks for the totals to ensure that the simulations are accurate.

Disadvantages of LEACHMP are the lengthy execution times (eg. 5 hours for a one year simulation with 45 soil compartments, on a 286-based personal computer), lengthy input data to characterize the objectives of the simulation and the site, the lack of surface runoff, and the use of field-average values for model parameters which represent the spatial and temporal variability of a natural system.

Both of the models have been tested against both field and laboratory data, and the accuracy of the model predictions has been verified. It should be noted that while current pesticide transport and transformation models can be applied to an actual field site, they generally do not accurately reproduce a measured pesticide concentration profile obtained from the field (Hornsby et al., 1988). There is typically too much spatial heterogeneity in the soil profile for the model to accurately reproduce the observed pesticide concentrations with depth at a specific time. However, fluxes to the water table over time are reasonably reproduced (Hornsby et al., 1988).

The current models that simulate the transport and transformation of pesticides (with the exception of PRZM, MOUSE and GLEAMS) are only focused towards the subsurface environment. The amount of pesticide that is available at the soil surface to move downward towards the water table is dependent upon the pesticide application procedure and processes affecting this amount of pesticide. Therefore, as part of the expert system, a module will be incorporated into the program which will enquire of the user information regarding how the pesticide is applied and processes affecting the amount of pesticide. Once these parameters are chosen, the model will then compute the flux through the soil surface. The pesticide transport and transformation portion of EXPRES will then calculate the distribution of pesticide within the soil profile. This module will consider:

(1) methods of application (areal spraying, direct incorporation into soil, etc.);
(2) rates of application;
(3) type of applications (single, multiple, long, short);
(4) pesticide loses due to surface runoff.

CONCLUSIONS

Because of the potential for contamination of groundwater by pesticides, regulatory personnel must have the means of assessing the migration of a pesticide 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. The expert system will provide the user with encoded expertise in the areas of geology, hydrogeology and numerical modelling that is required to undertake a simulation with the chosen pesticide transport code. 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 an assessment of the potential hazards and to identify if further study is warranted.

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FIGURES

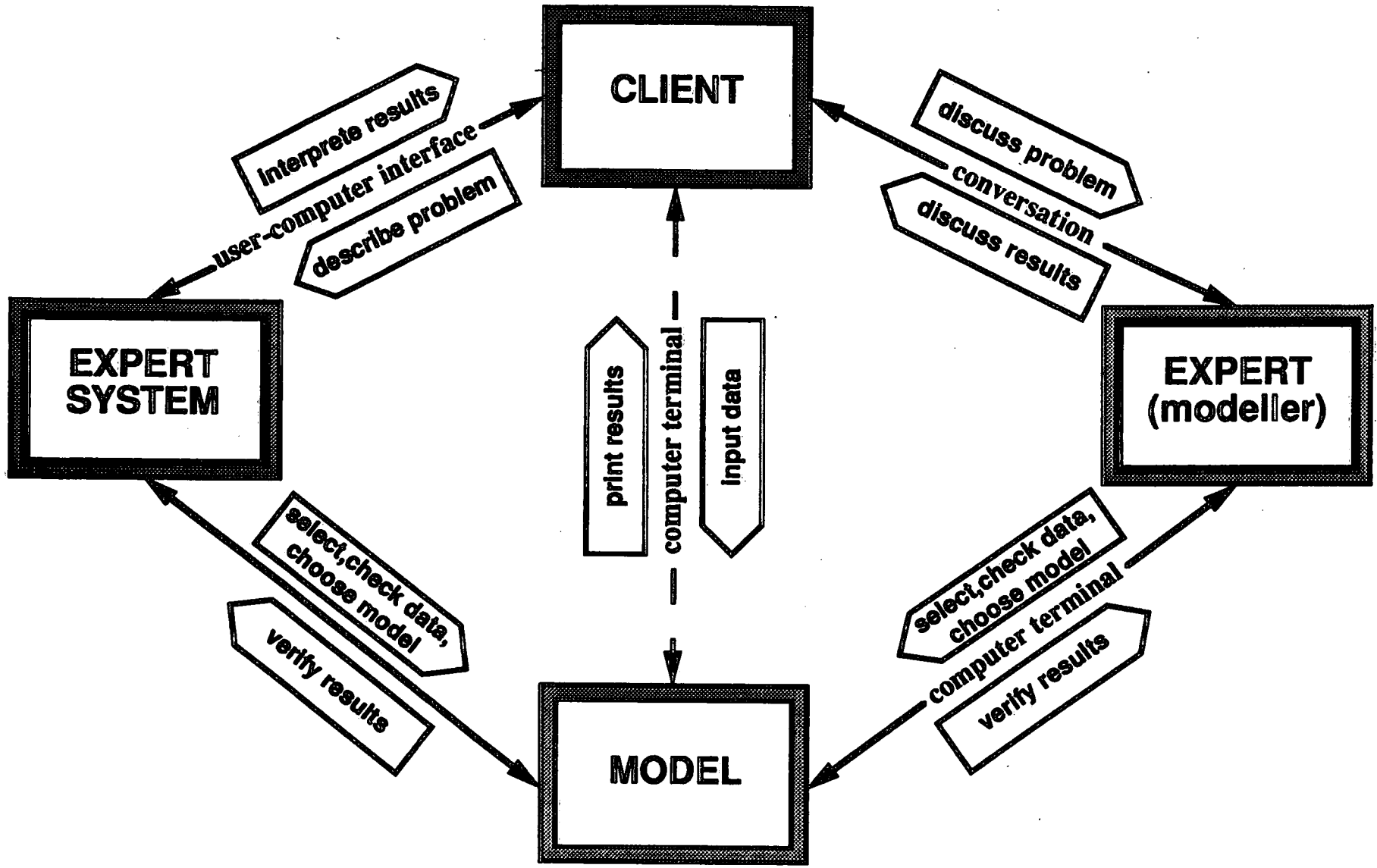
CLIENT
EXPERT SYSTEM
EXPERT (modeller)
MODEL
interprete results
user-computer interface
describe problem
discuss problem
conversation
discuss results
print results
computer terminal
input data
select,check data, choose model
verify results
select,check data, choose model
computer terminal
verify results

Fig 1.

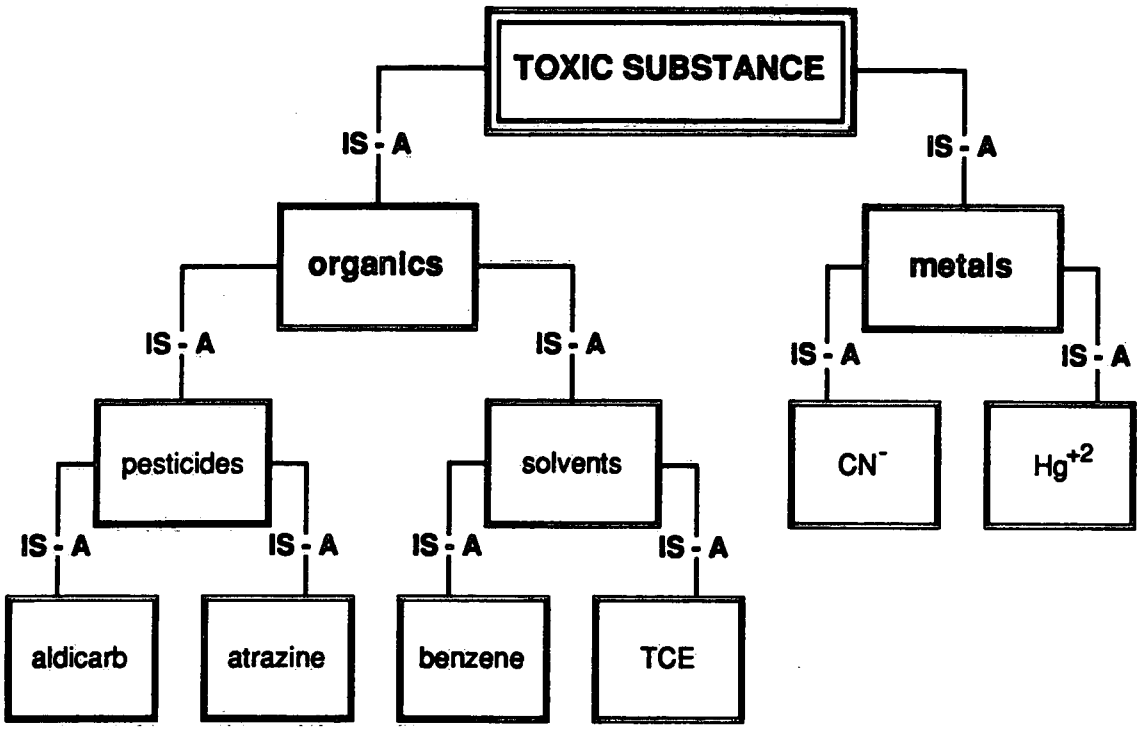
TOXIC SUBSTANCE
IS - A
IS - A
organics
metals
IS - A
IS - A
IS - A
IS - A
pesticides
solvents
CN⁻
Hg+2
IS - A
IS - A
IS - A
IS - A
aldicarb
atrazine
benzene
TCE

Fig 2.

CLIMATIC DATA

Agricultural Zone 7-b

	rainfall	humidity	evaporation	temperature
January				
February				
March				
April				
May				
etc.				

Fig. 3

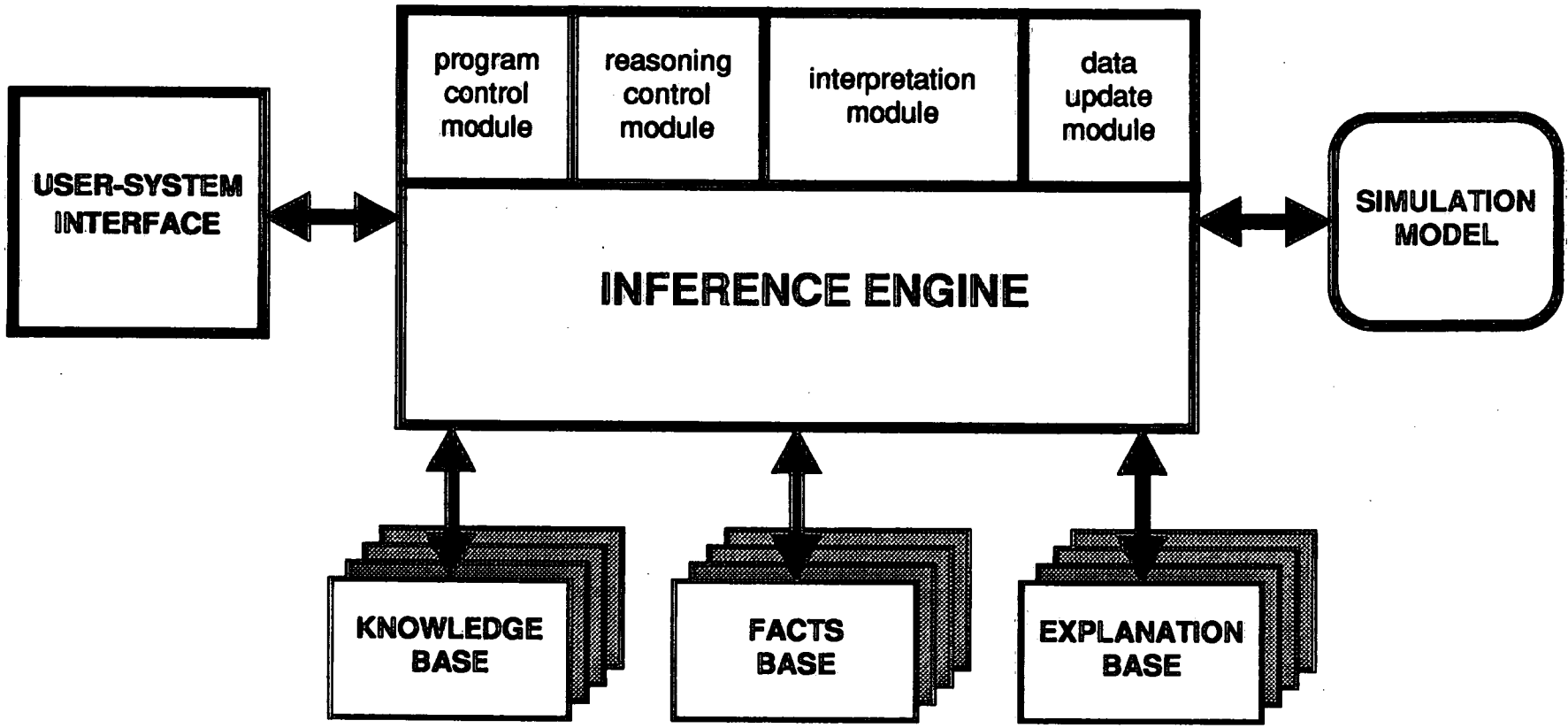
program control module
reasoning control module
interpretation module
data update module
USER-SYSTEM INTERFACE
INFERENCE ENGINE
SIMULATION MODEL
KNOWLEDGE BASE
FACTS BASE
EXPLANATION BASE

Fig 4.