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AN EXPERT SYSTEM FOR ASSESSING THE MIGRATION AND TRANSFORMATION OF PESTICIDES IN THE SUBSURFACE

by
A.S. Crowe, J.P. Mutch
and R.E. Jackson

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

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MANAGEMENT PERSPECTIVE

The Pesticide Division of the Commercial Chemicals Branch is required to assess the potential for a pesticide and its degradation products to adversely affect the soil and shallow groundwater environment before approval is given to allow public use of the pesticide. Because of the limited knowledge that the staff of the Pesticide Division have in the field of pesticide transport in the subsurface, they requested that the Groundwater Contamination Project, NWRI, develop an expert system that can be used to aid in the assessment of the potential for groundwater contamination by pesticides. This reports outlines the program to be taken by the Groundwater Contamination Project during the next two years to develop the expert system.

PERSPECTIVE-GESTION

Le Division des pesticides de la Direction des produits chimiques commerciaux doit d'abord évaluer dans quelle mesure un pesticide donné et ses produits de dégradation peuvent exercer un effet néfaste sur le sol et les environnements où les eaux souterraines sont peu profondes, avant d'approuver l'utilisation de ce pesticide par le grand public. Comme le personnel de la Division des pesticides possède des connaissances limitées dans le domaine du transport des pesticides dans le sous-sol, il a demandé aux personnes de l'INRE chargées du Projet d'étude de la contamination des eaux souterraines d'élaborer un système expert qui faciliterait l'évaluation des risques de contamination des eaux souterraines par les pesticides. Ce rapport décrit brièvement le programme qui, au cours des deux prochaines années, sera entrepris dans le cadre du Projet d'étude de la contamination des eaux souterraines dans le but d'élaborer un système expert.

RÉSUMÉ

Les eaux souterraines constituent une importante source d'eau domestique au Canada, plus particulièrement en milieu rural. Les études portant sur le devenir des pesticides dans le sous-sol ont fourni de solides données permettant d'établir que les pesticides risquent de contaminer sérieusement les aquifères peu profonds en milieu rural. Il faudra donc, avant d'approuver l'utilisation générale d'un pesticide, mettre au point des techniques qui permettront d'évaluer dans quelle mesure ce pesticide et ses produits de dégradation risquent de contaminer les eaux souterraines. Typiquement, les personnes chargées de l'application des règlements, qui évaluent les effets des pesticides sur la qualité des eaux souterraines, ne possèdent pas le niveau de connaissances nécessaire pour faire une modélisation numérique du transport et du devenir des pesticides dans le sous-sol. C'est pour cette raison que nous procédons actuellement à l'élaboration d'un système expert en vue d'aider ces personnes à évaluer les effets des pesticides sur le sol et sur les environnements où les eaux souterraines sont peu profondes. Le système expert comprendra un modèle numérique que l'on pourra utiliser pour simuler le transport et la transformation des pesticides dans la zone vadeuse, ainsi qu'un système basé sur des connaissances qui guidera l'utilisateur lors de la sélection de toutes les informations requises pour caractériser le contexte géologique, physique, climatique, hydrogéologique, pédologique et agricole des

zones d'agriculture situées un peu partout au Canada, qui seront nécessaires pour réaliser une simulation. Le système expert a été conçu en vue d'être utilisé comme outil de gestion qui facilitera le processus décisionnel en matière de politiques, et n'est pas destiné à servir d'outil de recherche. Le but du système expert n'est donc pas de donner un aperçu des processus régissant le transport et le devenir des pesticides dans des milieux poreux, mais plutôt de faire une évaluation rapide et générale des risques possibles et de déterminer s'il y a lieu d'effectuer d'autres études.

ABSTRACT

Groundwater is an important source of domestic water supply in Canada, and is especially so in rural areas. Studies focusing upon the fate of pesticides within the subsurface provide strong evidence that pesticides have the potential to cause serious contamination of shallow aquifers in rural areas. Thus, techniques are required that can assess the potential for a pesticide and its degradation products to contaminate groundwater before the pesticide is approved for general use. Typically, the regulatory staff who evaluate the effects of pesticide on groundwater quality do not have the level of knowledge required for numerical modelling of the transport and fate of pesticides in the subsurface. Therefore, an expert system is being constructed to aid regulatory personnel in their assessment of pesticides on the soil and shallow groundwater environment. The expert system will consist of an existing numerical model, which can be 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 all the necessary information for characterizing the geological, physical, climatic, hydrogeological, pedological and agricultural settings of typical agricultural zones across Canada required for a simulation. 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, the purpose of the expert system is not to provide insight into the processes that control the transport and fate of pesticides in porous media, but to provide a quick and general assessment of the potential hazards and to identify if further study is warranted.

INTRODUCTION

Groundwater is an important source of domestic water supply in Canada. Hess (1986) estimated that 26% of Canadians and 38% of the municipalities in Canada (up to 100% in P.E.I.) were dependent upon groundwater for their drinking water. The importance of groundwater increases dramatically in rural areas where 82% of the rural population rely on groundwater (Hess, 1986). Because groundwater is an important source of drinking water for farms and small towns, serious health problems could occur if the groundwater in rural areas becomes contaminated. A particular area of concern deals with the fate of pesticides following their application. Some pesticides may enter the groundwater even if the methods of application are acceptable. For example, several studies focusing upon the transport and fate 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 have the potential to cause serious contamination of groundwater and related health problems in rural areas. Therefore, it is imperative that techniques be developed to assess the effect of a pesticide and its degradation products before it is approved for public use.

The transport and fate of pesticides in both the unsaturated soil zone and the shallow groundwater regime is governed by a complex set of chemical, biological and physical processes. Predicting the distribution and concentration of a pesticide is a highly specialized task which generally requires applying computer models. While numerous models currently exist to handle this task, including LEACHM (Wagenet and Hutson, 1986; 1987), PRZM (Carsel et al., 1984; 1985), MOUSE (Pacenka and Steenhuis, 1984; Steenhuis et al., 1987), CMIS/CMLS (Nofziger and Hornsby, 1986, 1987) and VULPEST (Villeneuve et al., 1987), the general application of these models is limited because, first, the theoretical framework upon which the models are based are generally complex and typically they can only be operated by a trained modeller, and second, the models require a specialized set of physical and chemical field data which are not readily 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 the pesticide on the quality of the groundwater. Thus, there is a need to develop or adapt a model which is sufficiently sophisticated to simulate the major processes controlling the migration and 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-experts 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, they represent an attractive tool for providing the user with the capability of assessing basic problems. An expert system for the transport and fate of pesticides would be an important regulatory tool for assessing the impact of pesticides on the groundwater environment.

This paper describes an expert system under development by the Groundwater Contamination Project of the National Water Research Institute for the Pesticide Division, Commercial Chemicals Branch. The primary purpose of the expert system is to provide regulatory personnel with a tool for evaluating the fate of pesticides on the soil and shallow groundwater environment in order to identify potential groundwater problems. Specifically, it is designed to:

(1) provide regulatory personnel with a method of obtaining the geological, hydrogeological and computing modelling expertise required for their assessments;

(2) predict migration rates and concentrations of pesticides in the unsaturated zone with time and depth;

(3) determine the concentration of pesticide reaching the water table and the time required for the pesticide to reach the water table;

(4) be easy to use by staff not trained in the use pesticide transport models.

The expert system will be designed as a management tool to be used as an aid in making policy decisions and not for use as a research tool. Thus, the application of the expert system is not to provide insight into the processes that control the transport and fate of pesticides in porous media, but to provide a quick and general assessment of the potential hazards and to identify if further study (e.g. field testing) is warranted.

AN OVERVIEW OF EXPERT SYSTEMS

Expert systems (also known as *knowledge-based systems*) are a class of computer programs which fall within the field of artificial intelligence (Figure 1). Generally, expert systems function by encoding the decision-making abilities of a specialist, or "expert", in a particular field of endeavour into a computer program in such a way that the user can be confidently guided through the necessary steps required to solve a complex problem. This human expertise which is encoded into an expert system includes *knowledge*, *experience* and *problem-solving ability*. Although expert systems are computer programs, there are significant differences between the conventional computer programs and expert systems. For example, conventional computer programs that model pesticide transport will input quantitative data which are typically numbers, manipulate these data with FORTRAN statements and finally present the results. 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.

An important feature of expert systems is that they are based upon informational concepts rather than quantitative data. Information is divided into two groups; *information* and *knowledge*. Information includes all the quantitative data, facts and figures obtained from textbooks, manuals, laboratory and field experiments, etc. Knowledge is more qualitative in nature and it includes a collection of facts, insights, hunches and best procedures for solving a problem. An important type of information used in expert systems is the "rule-of-thumb" knowledge or *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 nets and frames reduce the number of rules required.

Expert systems which are based upon production rules (known as rule-based systems) consist of "IF-THEN" conditional statements that when data accumulated for a particular problem matches the data in the "IF" part of the rule, leads to the undertaking of the statements in the "THEN" part of the rule. An example of a production rule is:

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

The three types of production rules are based upon the action taken within the "THEN" part of the rule when the conditions stated in the "IF" part of the rule are true. These are:

(1) Inference Rules: When the data gathered for a problem matches the conditions stated within the "IF" part of the rule, the statements within the "THEN" portion of the rule 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 "IF" part of the rule, the statements within the "THEN" portion of the rule expresses an intermediate or final conclusion.
(eg. IF conc. of aldicarb >9 µg/L THEN the groundwater is hazardous)

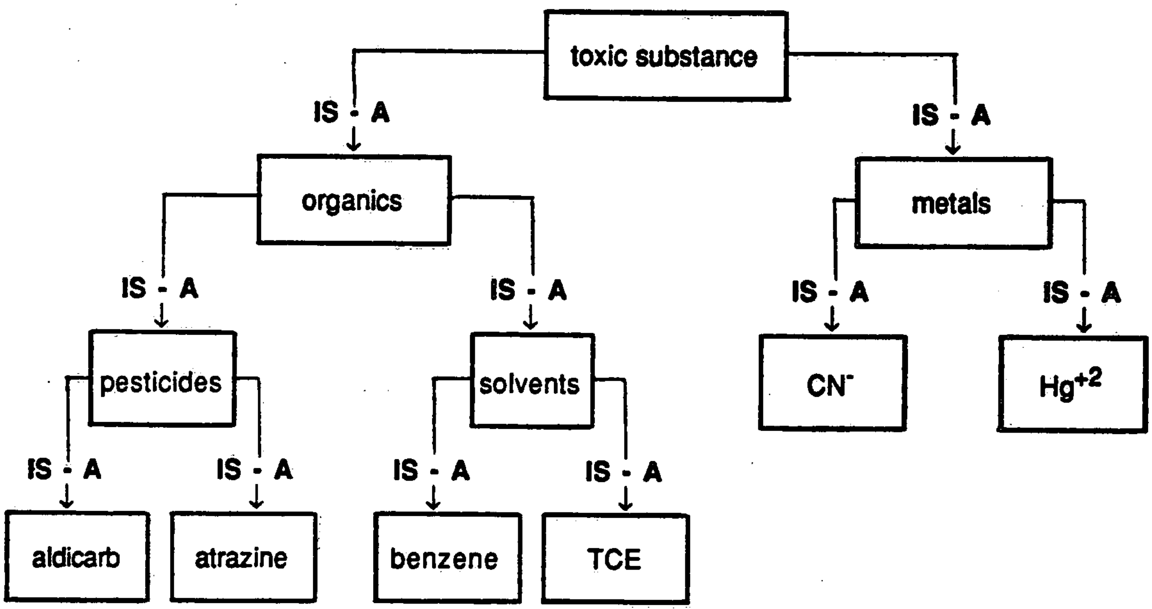
(2) Situation - Action Rules: When the data gathered for a problem matches the conditions stated within the "IF" part of the rule, the statements within the "THEN" portion of the rule take a particular action.
(eg. IF this groundwater is used for drinking THEN take remedial action)

The linking of production rules forms a reasoning strategy. This linking process is known as *chaining*, and rules can be linked by either forward chaining or backward chaining. An example of chaining is:

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

With forward chaining, the expert system uses a series of rules to arrive at a particular result according to information given as input. An example of forward chaining, using the above example, information on the presence of aldicarb and then its concentration is used to determine if the groundwater is contaminated.Backward chaining starts with a goal to be resolved by requesting the necessary information. For example, with backward chaining, to determine if the groundwater is contaminated, the expert system must first know if aldicarb has been detected and if so, at what concentration.

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:



Thus, 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, or 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:

CLIMATE DATA

	rainfall:	evaporation:	humidity:	temperature:
Jan	______	______	______	______
Feb	______	______	______	______
Mar	______	______	______	______
Apr	______	______	______	______
May	______	______	______	______
etc.				

Here, any climatic data for a particular place can be readily retrieved or modified by entering the keyword "CLIMATE DATA".

The user - system interface conveys the encoded expertise to the user via a *dialogue format*, which is analogous to a conversation between an expert and a client. 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 as data bases. The user responds to these prompts by entering information as numbers, words, or a simple "YES - NO" or "TRUE - FALSE". 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 using frames via templates at the computer screen for input of common information.

An expert system also contains an explanation module which is designed to help the user understand the question or requested information by offering choices of values, explanations or definitions and it will check the entered values for consistency with previously entered information.

The major components comprising the architecture of an expert system is illustrated by Figure 2. The Program Control Unit contains statements which affect the general control of the expert system, the order in which they are linked, the reasoning strategy and evaluation of production rules, and the user - system interface. Access to the Knowledge Base and Information Base is controlled by the Program Control Unit. The Knowledge Base includes all the rules, nets and frames, plus the questions, explanations and definitions contained in the help module, as well as the conclusions and recommendations based upon an evaluation of the information supplied by the user. The Information Base is the data bases of facts, figures, etc supplied by the programmer. It also accumulates information entered by the user, generated by the Knowledge Base or calculated during the data manipulation stage. The Data Manipulation component of the expert system is a mathematical model, unique to each expert system, that does the actual simulations or calculations.

Expert systems are computer programs and thus are constructed with programming languages. The two groups of programming languages that comprise the present expert systems are knowledge engineering 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 expert systems without the domain-specific knowledge data base. Because expert system shells are existing expert systems, they lack the generality and the flexibility required to adapt it to another problem. 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 regular programming languages. These include symbolic manipulation languages or artificial intelligence languages, such as LISP or PROLOG and conventional programming languages, such as FORTRAN, C or PASCAL. Because they are programming languages they offer greater flexibility in the design and construction of expert systems and expert system shells.

AN EXPERT SYSTEM FOR PESTICIDES REGULATORY DECISIONS

The purpose of the expert system is to provide regulatory personnel within the Pesticide Division with a tool that will aid in their evaluation of the fate of pesticides in the subsurface in order to ensure that the quality of the groundwater is maintained. The expert system will be designed as a management tool to be used in making policy decisions regarding balancing the benefits and risks of a proposed pesticide, and not as a research tool. Thus, the objective of the expert system is not to provide insight into the processes that control the transport and fate of pesticides in porous media, but 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 will be towards examining "worst-case" and "typical-case" scenarios of pesticide application in agricultural regions across Canada.

The important criteria to be used to construct the expert system and the required biological, chemical and physical processes that the model should incorporate is discussed as follows. The expert system should be designed to be easy to use, even by those not familiar with using the numerical models which simulate pesticide transport in the subsurface. Therefore, several important criteria will be addressed during the design and construction of the expert system. These criteria include:

(1) the system must be usable by those with minimal computer skills and knowledge of pesticide transport in groundwater flow regimes;
(2) the user should be able to effectively use the expert system 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 general architecture for the expert system for assessing the effects of pesticides on the subsurface is illustrated by Figure 3. The expert system is actually composed of three parts; the Program Control Unit, the Pesticide Transport and Reaction Model, and the Information and Knowledge Bases. The purpose and design of the Program Control Unit, which includes the User Interface Module are essentially the same as that discussed in the previous section. The User Interface Module is an interactive program that will guide the user through the entry of data required by the transport model. For example, information concerning the chemical characteristics of a pesticide, the application procedure, the physical setting of the field site and the hydrological properties of the soil environment, is entered by having the user respond to a series of questions. Should the user be unfamiliar with any of the requested information, the expert system will provide either an explanation about the required data or recommend typical values which could be used.

The second part of the expert system consists of amass transport and reaction model for predicting pesticide migration and concentrations in the subsurface. In order to accurately predict the transport of pesticides in the subsurface, the mathematical framework of this expert system must be based on the accepted scientific principles that describe the important biological, chemical and physical processes that affect the transport and fate of the pesticides. The important processes that will be considered in the model include:

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

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

These physical and chemical processes controlling the transport and degradation of pesticides are affected by a number of environmental factors which must be considered by the model. These 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/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.

Currently, there are several pesticide transport and reaction models that simulate many of these processes. Rather than developing a new pesticide transport and reaction model, an existing model will be modified to suit our needs. This will not only reduce the time required to arrive at a final product, but by using an widely accepted model, the important processes will be included in the model and these will be verified through previous use. The criteria for choosing a pesticide model for the 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) predict the degradation products and their concentrations within the subsurface;

(4) transport and react pesticides in the flow regime based on generally accepted scientific principals;

(5) be currently a widely accepted and verified model;

(6) be programmed in such a way as to ensure 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.

Typical pesticide transport models that fall into this group include LEACHM (Wagenet and Hutson, 1986; 1987), PRZM (Carsel et al., 1984; 1985), MOUSE (Pacenka and Steenhuis, 1984; Steenhuis et al., 1987) and CMIS/CMLS (Nofziger and Hornsby, 1986, 1987). Pesticide transport models simulate pesticide transport only through the unsaturated zone. However, two models (PRZM and GLEAMS) will account for lateral loss (runoff) of water and solute at the ground surface. 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 are lumped parameter models, in which the subsurface is represented as a series of compartmentalized storage elements that simulate water and solute flux through the unsaturated zone with a simplified water balance. However, LEACHM represents the subsurface as a distributed parameter model to solve the solute transport equation. Most models account for the major physical, chemical and biological processes affecting the transport and degradation of pesticides in the unsaturated zone. The models require input data from four general area; climatic conditions, soil parameters, chemical characteristics of the pesticide and farm management practices. The models range in complexity from basic education models (eg. MOUSE) to sophisticated research models (eg. LEACHM), with a corresponding increase in the accuracy in the prediction of pesticide transport. Advantages offered by the more complex models are often offset by an increase in run-times and difficulty in formulating the input data sets. The models are deterministic, however, stochastic techniques have been employed in VULPEST (Villeneuve et al., 1987).

It should be noted that while the current pesticide transport and transformation models can be applied to an actual field site, they generally do not accurately reproduce the measured field distribution of pesticides with depth (Hornsby et al., 1988). There is typically too much spatial heterogeneity in the soil profile to be accurately reproduced by the model, and thus the model will not give a good match to pesticide concentrations with depth at any specific time. However, fluxes to the water table over time are reasonably reproduced by the models.

The current models that simulate the transport and transformation of pesticides (with the exception of PRZM) 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 the expert system 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 transport by surface runoff.

Other important components of the expert system are the Knowledge Base and the Information Base, which form the "expert's" contribution to the system. For clarification, these two bases are illustrated as three module, Production Rules, Data Bases and Explanation Module, on Figure 3 and each is discussed below.

The information contained within the Data Bases Module comprise detailed information regarding, first, the physical, climatic, hydrogeological and agricultural setting of typical agricultural zones across Canada, and second, the chemical characteristic of pesticides.

The first data base will comprise all data describing a series of typical agricultural zones across Canada. These data are required for the pesticide transport and transformation model. For example, typical agricultural zones could 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 data will characterize the physical, climatic, hydrogeological and agricultural setting of agricultural zones. 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 be guided, however, by experience from a variety of field studies undertaken within a particular zone. The expert system will have a data base containing the hydrological, physical, climatic and agricultural data describing these agricultural zones which can be recalled by the user to test the environmental effects of applying the pesticide in these agricultural zones. 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, the expert system will be designed such that the parameters comprising a typical agricultural zone can easily be modified by the user for a particular simulation.

The second data base, containing the chemical characteristics of pesticides, will be accessed by the user when information for a new pesticide is required by the model but does not exist. By looking at similar pesticides in this data base, the user will be able to approximate the required data for the new pesticide. An important feature in the design of this data base is that it must allow values contained in the data base to be easily be modified, new data to be included as it becomes available and new pesticides to be added to the data base.

The Production Rules Module basically consists of encoded expertise or knowledge that will guide a user in the choice of parameters for a simulation and is based upon the concepts presented in the previous section. It provides the link between the user and the expert's information and knowledge for guiding the user through their choice of parameters and options for undertaking a pesticide transport and degradation simulation.

The Explanation Module is similar to a data base in that it consists of encoded information provided by an expert that will help a user in the choice of parameters for a simulation when the information requested by the production rules is not understood by 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) evaluation of plausible values and relationships among the chosen parameters;
(5) time-dependant simulation parameters.

DEVELOPMENT OF THE EXPERT SYSTEM FOR PESTICIDES

The development of the expert system for assessing the impact of pesticides on groundwater quality will occur over two years and will progress through seven phases, as summarized by Figure 4. Throughout its the development, the expert system will undergo an intensive verification to ensure that the arithmetic calculations are correct, the transport and reaction processes are handled correctly, the information in the data bases is correct, and the input and output are meaningful and clear. The following is a brief description of the objectives and tasks for each phase of the project.

Phase 1: Preliminary Studies

The objectives of Phase 1 are to:

(1) formulate the design criteria for the expert system;
(2) undertake a review of existing pesticide transport models;
(3) choose a pesticide transport model which can be easily modified to fulfil the objects of this study;
(4) review available data and sources of data that are required by the model.

All of the activities undertaken in Phase 1 will provide the background information necessary to design the expert system. Once the basic design requirements have been determined, existing pesticide transport models will be evaluated in order to determine which model best fits the needs of our expert system.

Phase 2: Initial Development of the Expert System

The objectives of Phase 2, the initial development of the expert system, are to:

(1) incorporate the required processes into the model;
(2) develop the software to make it into an expert system;
(3) modify the system to allow it to execute on a personal computer.

The actual development of the expert system will occur in two stages. The first stage will focus on the development of the pesticide transport and reaction model that was chosen during Phase 1 of the project. It is expected that the model will require some modifications in order to include additional processes, to allow it to run on a personal computer, and to adapt it to the expert system. The expert system will require code to be written that will account for total pesticide available to move across or transform on the ground surface due to application procedures, phototransformation etc. While the transport model will be essentially complete, the dialogue format for data entry and help options to assist the user will be very basic. The primary goal to be attained by the end of stage 1 (Phases 1 - 3) is to produce a model which can be used to determine what modifications or further work should be done. The second stage (Phases 4 - 7) involves incorporating the recommended changes into the model and preparation of the user's manual. It is anticipated that most of the actual programming will be done in FORTRAN. However, MICROSOFT C or Windows will be required to produce the dialogue format at the screen to interface between the user and the transport code.

Phase 3: Initial Development of the Data Base

The objectives for this phase of the project are to:

(1) construct data bases containing the physical, chemical and biological parameters which characterize the soil, groundwater, crops and climate in a typical agricultural zone;

(2) construct a data base of the chemical properties of a pesticide;

(3) construct the data bases in a manner which will easily allow expansion to include other agricultural zones and updated as new data become available.

An expert system relies on the data bases for the parameters required for the simulations. Because the model predictions will be only as good as the quality of the data bases, the development and verification of the data bases is critical for the success of the expert system. Therefore, it is anticipated that the design and construction of the data bases will take as long as programming the expert system. The development of the data bases will be undertaken in two stages. The first stage will focus on the design and the construction of very simplified data bases for the purpose of testing and validating the pesticide transport model. At this time, only the data bases containing information describing the chemical characteristic of the pesticides and the typical agricultural zones will be constructed. Because these data bases are used for validating and testing the model, they will contain the information for only one pesticide and one agricultural zone. However, the information required to define a pesticide and an agricultural zone will be complete. Finalization of the data bases, which will essentially add more pesticides and agricultural zones to the existing data bases, will be complete during stage 2 in the development of the data bases for the expert system.

Phase 4: Verification of the Expert System

The objectives of Phase 4, the verification of the expert system, are to:

(1) undertake an internal verification of the model;

(2) submit the expert system to regulatory staff and to provide instruction on how to use the expert system so that they may identify problems, limitations, confusion, etc. with the code.

Verification is an important step in the development of a model because it will ensure that the numbers calculated by the model are both meaningful and accurate. This testing procedure will ensure that (1) the arithmetic calculations are correct, (2) the physical and chemical processes are simulated correctly, (3) the simulation options and dialogue format work correctly, (4) information required by the expert system will be in the data bases, and (5) the output is meaningful and clear. At this time, verification will focus on the transport and transformation model and on the shell of the expert system, but not the data bases. The model will be verified by comparing simulation results to those observed in the field. Because the data bases will not be complete at this time, this initial verification will focus on reproducing the fate of at least one pesticide in one agricultural zone. This verification step will ensure that the expert system will undertake the required calculations and that the regulatory personnel who will use the model are comfortable with the way in which the expert system functions.

Phase 5: Finalization of the Data Bases

The objectives of this phase, the finalization of the data bases, are to:

(1) finalize the data bases containing parameters which characterize the soil, groundwater, crops and climate in typical agricultural zones across Canada;

(2) finalize the data bases of the chemical properties of pesticides;

(3) construct a hydrological data base for use by the modeller if help is required;

(4) design the data base in a manner which will allow it to be easily modified.

The three data bases that are required by the expert system were designed during stage 1 of the data base development. The second stage in the development of the data bases focus upon two data bases: (1) the physical, climatic, hydrogeological and agricultural setting of typical agricultural zones across Canada, and (2) the chemical characteristic of pesticides. The data bases used to verify the model (Phase 4) which contain the physical, chemical and biological parameters characterizing one typical agricultural zone and one pesticide will be expanded to include several sites and pesticides.

Phase 6: Finalization of the Expert System

The objectives of Phase 6 are to:

(1) incorporate changes noted by the Pesticide Division into the expert system and its data bases;

(2) upgrade the dialogue procedure for entering data with enhanced screens, questions and help functions;

(3) enhance the output of the final results calculated by the expert system.

This stage in the development of the expert system is designed to, first, correct any problems identified during the verification process, and secondly, to ensure that the dialogue format for input is complete. Most of the time allocated to this phase will focus upon improving the visual input at the terminal and ensuring that any questions that the user may have can be addressed by the expert system.

Phase 7: Project Finalization

The objectives for the final phase of the project are to:

(1) incorporate any final changes, as recommended by the Pesticide Division, into the model;

(2) prepare a user's manual for the expert system.

This phase of the project is designed to, first, ensure that any final modifications are included in the expert system, and secondly, prepare a user's manual describing the operation of the expert system. The user's manual will provide a thorough description of the theoretical framework of the transport and reaction processes, information contained within the data bases, and a description of the input data required by the model. The manual will also provide detailed information on the coding of the expert system and the data bases to allow changes to be undertaken. In addition, example data sets, terminal sessions, a full description of the input parameters and a discussion of the output will be included. Limitations and restrictions on the application of the expert system will be included.

CONCLUSIONS

Because of the potential for contamination of groundwater by pesticides, regulatory personnel must have the means of assessing the potential for a pesticide to contaminate groundwater 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 they require considerable physical and chemical input data to undertake a simulation. An expert system is being developed which will aid the regulatory personnel in their assessment on the potential detrimental affects of pesticides on the soil and shallow groundwater environment. The expert system will providing the user encode expertise in the areas of geology, hydrogeology and numerical modelling that is required to undertake their simulations with a current pesticide transport code. 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, the purpose of the expert system is to provide only a quick and general assessment of the potential hazards and to identify if further study is warranted.

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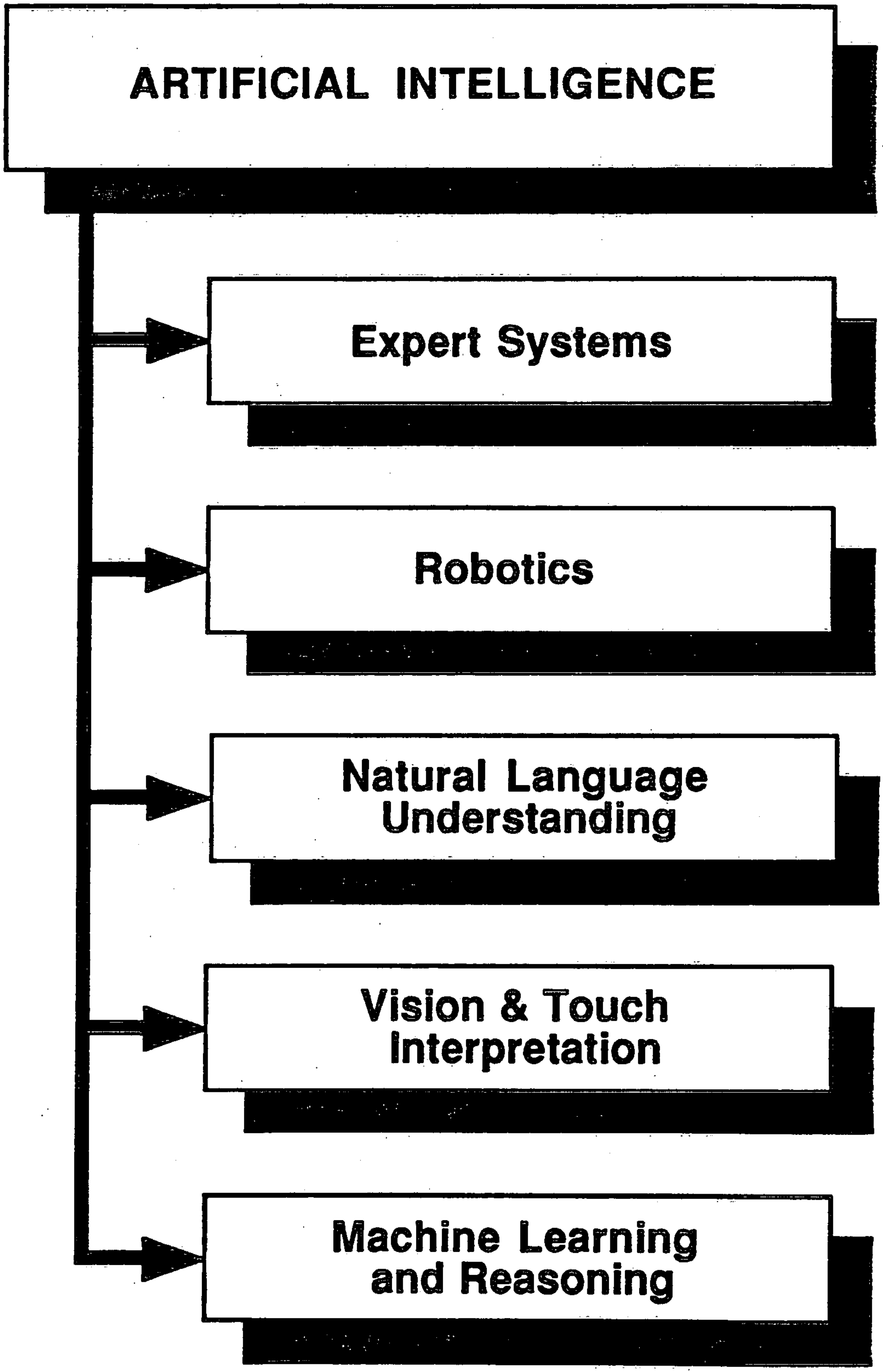

Figure 1. Subdisciplines of artificial intelligence.

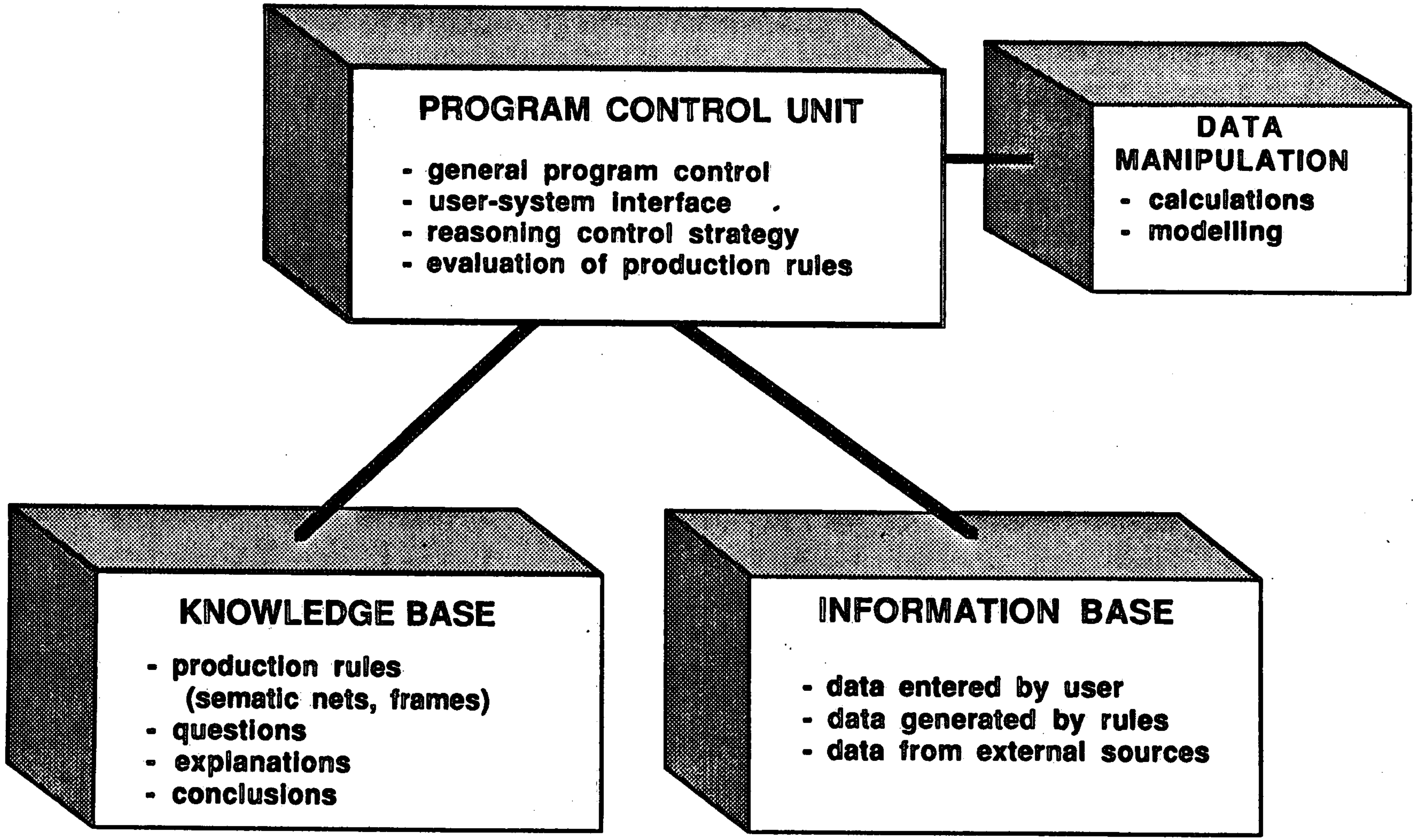

Figure 2. General architecture of an expert system.

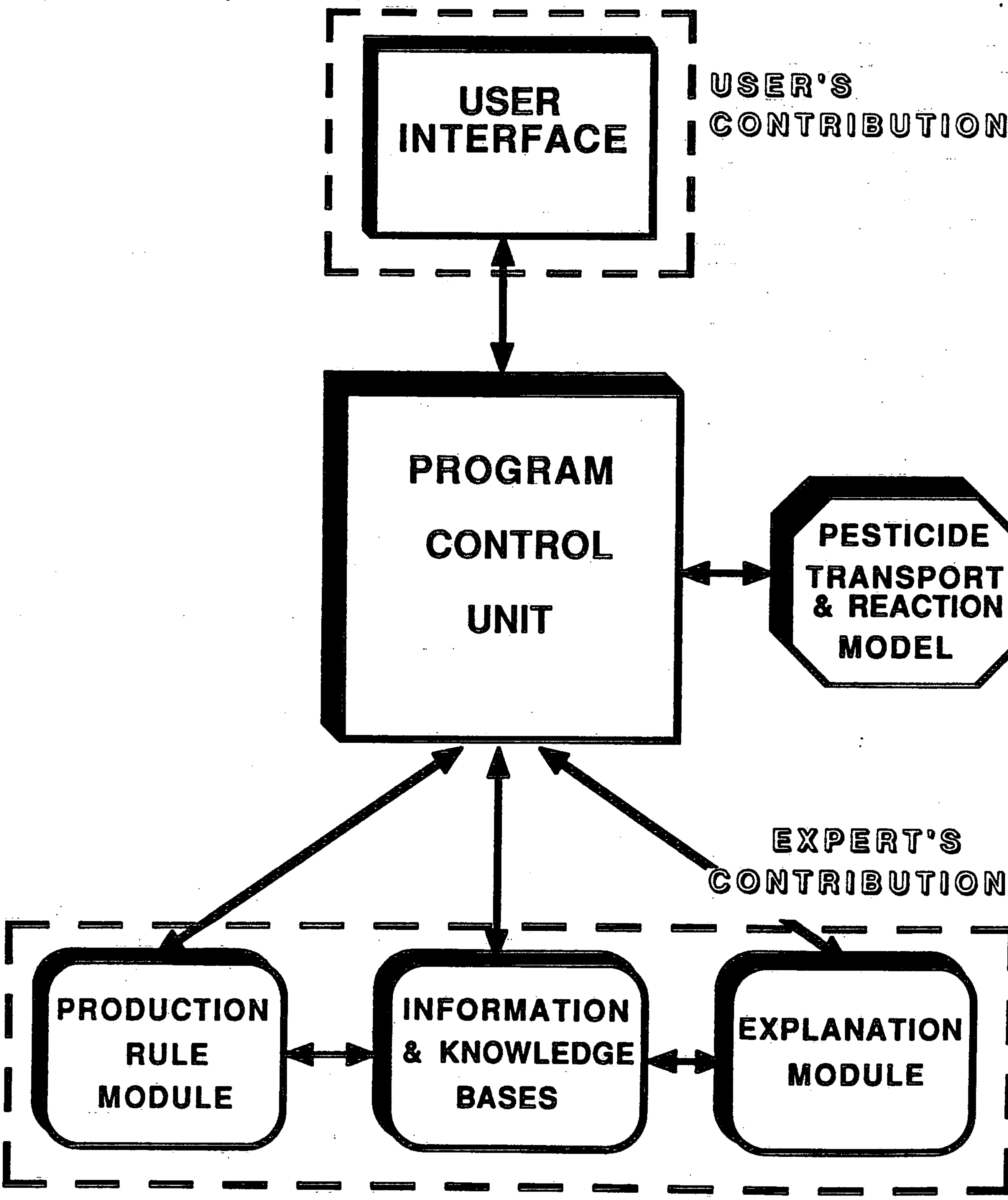

Figure 3. Schematic illustration of the components of the expert system for assessing the transport and transformation of pesticides in the subsurface.

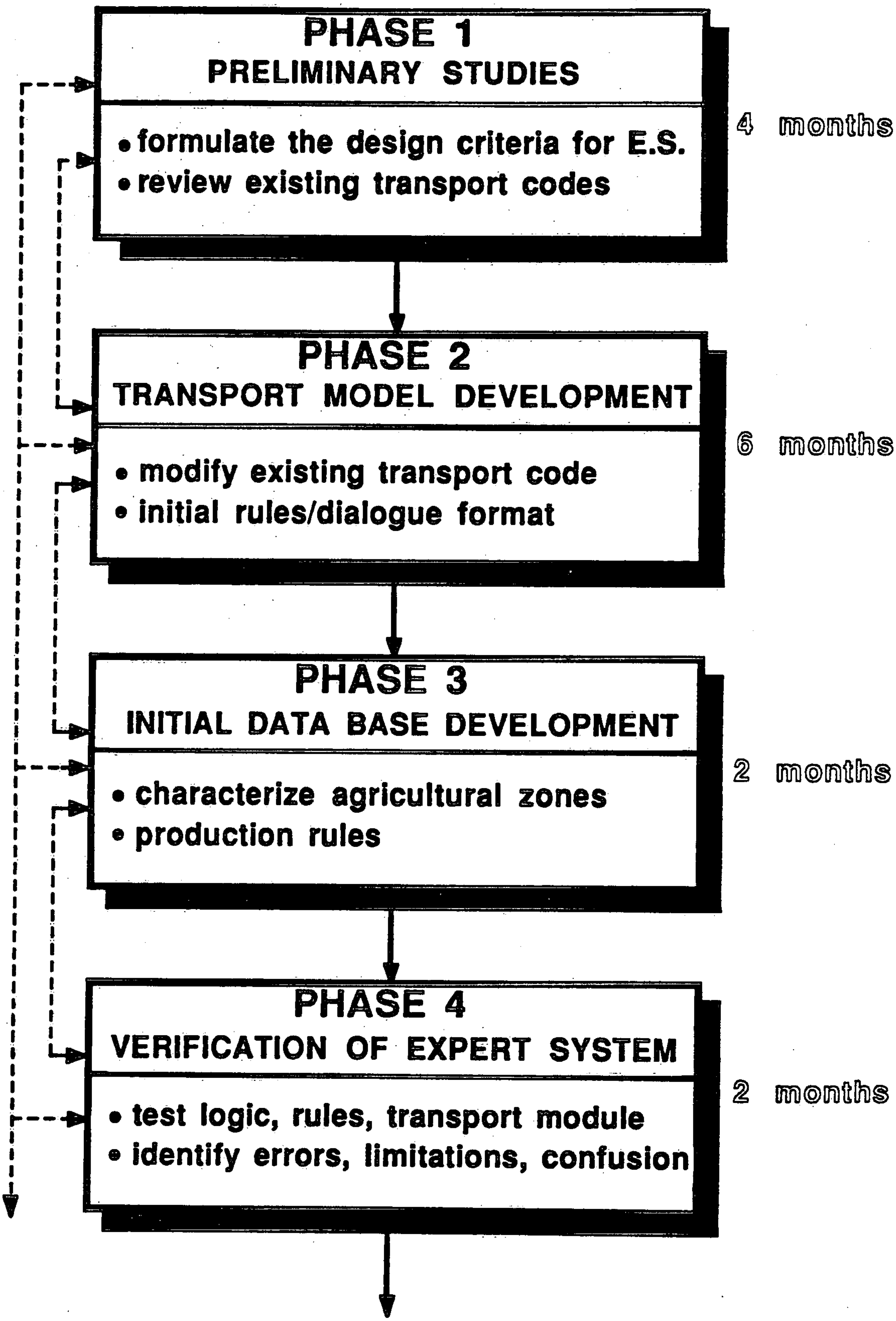

Figure 4. Project summary.

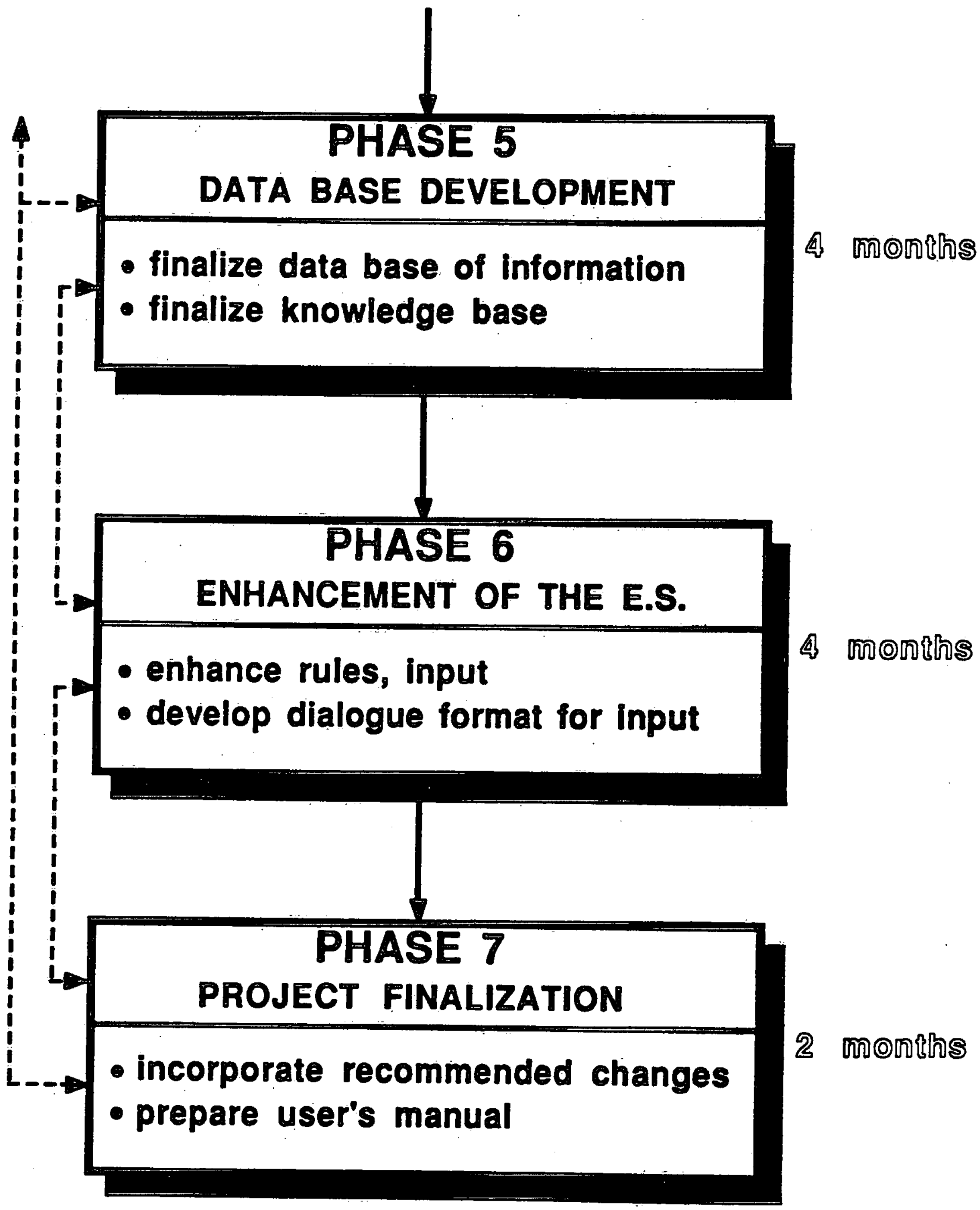

Figure 4. continued.