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PHASE ONE REPORT
A REVIEW AND ANALYSIS EXISTING PESTICIDE TRANSPORT AND TRANSFORMATION MODELS

by
J.P. Mutch
and
A.S. Crowe

Rivers Research Branch
National Water Research Institute
Canada Centre for Inland Waters
Burlington, Ontario, Canada
L7R 4A6

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ABSTRACT

The application of existing pesticide transport models within a regulatory framework has been limited because (1) the use of these models often requires specialized knowledge in the theory and modeling of pesticide transport in the unsaturated zone, and (2) the models require a specialized set of physical and chemical field data. Regulatory personnel who are assigned the task of assessing the environmental risks associated with a new pesticide generally do not have this specialized knowledge and information available to them.

An expert system is being developed which will be employed to bridge the gap between pesticide models and regulatory personnel, not versed in the use of these models. A major component of the expert system will be a numerical model that can simulate the fate of pesticides in the unsaturated zone. Rather than developing a new model, an existing code will be chosen and modified to suit the specific requirements of the expert system.

Fifteen existing models that have been documented were reviewed with regard to their possible incorporation into the expert system. The selection of a model is based upon both the physical, chemical and biological processes simulated by the model as well as its suitability to be effectively used from a regulatory perspective. Generally, the models can be classified into two groups. The first group of models, known as screening models are simple assessment model, providing only a relative index of the potential for the pesticide to leach to the water table. The models do not actually simulate the processes involved and do not quantify the amount or rate of pesticide leaching.

They are therefore, not suitable for incorporation into the expert system. The second group of models, the research-management models, are better suited for the expert system. Although certain simplifying assumptions are made, the models simulate the processes that control the fate of a pesticide in the subsurface and provide quantitative estimates of the amount and rate of pesticide leaching.

Two of the pesticide models, LEACHM and PRZM were chosen as the models that most closely meet the design criteria established for the expert system. Both models are one-dimensional, finite difference models that simulate advective and dispersive transport of the pesticide. Attenuation processes such as degradation, sorption, plant uptake are also simulated. LEACHM is the more detailed of the two, simulating water flow with a direct solution to Richards equation. However, execution times are lengthy in comparison to the PRZM model. PRZM uses a simplified water balance and also includes a simulation of surface runoff and erosion. By including the two models, the expert system can take advantage of the strengths of each model and provide regulatory personnel with a useful tool to aid in policy decisions regarding the registration of pesticides.

RÉSUMÉ

On n'a pu utiliser les modèles de dispersion des pesticides actuels, dans un cadre de réglementation, parce que (1) ces modèles nécessitent souvent une connaissance spécialisée de la théorie et de la modélisation de la dispersion des pesticides dans la zone d'aération, et (2) il faut avoir une série spécialisée de données physiques et chimiques pratiques.

Les employés chargés de la réglementation qui doivent évaluer les risques environnementaux associés à un nouveau pesticide n'ont pas, en général, cette connaissance et ces renseignements spécialisés. On met au point un système expert qui permettra de combler cette lacune et qui pourra être utilisé par des employés qui n'ont pas l'expérience de l'utilisation de ces modèles. Un modèle numérique qui peut simuler le devenir des pesticides dans la zone d'aération sera une composante importante du système expert. Plutôt que d'élaborer un nouveau modèle, on choisira un code actuel et on le modifiera pour répondre aux besoins particuliers du système expert.

On a étudié 15 modèles actuels, pourvus de toute la documentation voulue, dans le but de les incorporer éventuellement au système expert. Les processus physiques, chimiques et biologiques simulés par le modèle, ainsi que la facilité d'utilisation du modèle dans une perspective de réglementation constituaient les critères de sélection d'un modèle. En général, on peut classer les modèles en deux groupes. Le premier groupe de modèles, qu'on appelle modèles de sélection sont de simples modèles d'évaluation qui se contentent de donner un indice relatif du potentiel d'infiltration du pesticide dans

la nappe phréatique. Ces modèles ne simulent pas les processus en cause et ne quantifient ni l'infiltration du pesticide ni sa vitesse d'infiltration. Il n'est donc pas approprié de les incorporer au système expert. Le deuxième groupe de modèles, les modèles de recherche et de gestion, conviennent mieux au système expert. Même si certaines hypothèses de départ y sont simplifiées, ces modèles simulent les processus de devenir d'un pesticide dans le sous-sol et donnent des estimations quantitatives de l'infiltration et de la vitesse d'infiltration du pesticide.

Les deux modèles relatifs aux pesticides, LEACHM et PRZM que l'on a choisis sont ceux qui répondent le mieux aux critères établis pour le système expert. Ce sont des modèles à une dimension, aux différences finies, qui simulent l'advection et la dispersion du pesticide. On y simule aussi les modes atténuateurs, par exemple la transformation biochimique, la sorption, et l'absorption par les plantes. LEACHM, qui est le plus détaillé des deux modèles, simule le débit de l'eau en donnant une solution directe à l'équation de Richards. Cependant, les durées d'exécution sont plus longues que pour le modèle PRZM. Le PRZM utilise un bilan hydrique simplifié et comprend aussi une simulation de l'écoulement de surface et de l'érosion. Grâce à ces deux modèles, le système expert peut bénéficier des points forts de chacun d'eux et donner aux employés chargés de la réglementation un outil capable de les aider à prendre des décisions en matière de lignes directrices sur les permis à accorder aux pesticides.

MANAGEMENT PERSPECTIVE

The prevention of ground water contamination by agricultural pesticides requires a through assessment of the fate of the pesticides in the subsurface before they are registered for commercial use. With the complexity of the processes that control the fate of pesticides in the subsurface, it is necessary to use sophisticated computer models to simulate the transport and transformation of the pesticides in the subsurface. However, regulatory personnel within the Pesticide Division of the Commercial Chemicals Branch, who are assigned the task of performing this assessment, generally do not have experience in the use of these models and do not have access to the specialized data sets required by the models.

The Groundwater Contamination Project, RRB, NWRI, is developing an expert system on behalf of the Pesticide Division of Environment Canada which will be employed to bridge the gap between the pesticide models and regulatory personnel. The project will take two years to complete and is being funded by the Pesticide Division. This report presents the results of Phase I of the project.

Fifteen existing models were reviewed with regard to their possible incorporation into the expert system. The selection of a model was based upon both the physical, chemical and biological processes simulated by the model, as well as its suitability for effective used from a regulatory perspective. Two of the pesticide models, LEACHM and PRZM, were chosen as the models that most closely

meet the design criteria established for the expert system. By including the two models, the expert system can take advantage of the strengths of each model and provide regulatory personnel with a useful tool to aid in policy decisions regarding the registration of pesticides.

RÉSUMÉ ADMINISTRATIF

Pour empêcher les pesticides agricoles de contaminer les eaux souterraines, il faut bien évaluer le devenir des pesticides dans le sous-sol avant de leur accorder un permis à des fins commerciales. Comme il s'agit là d'un processus complexe, il faut utiliser des modèles informatiques élaborés pour simuler la dispersion et la transformation des pesticides dans le sous-sol. Cependant, les employés chargés de la réglementation, à la Division des pesticides de la Direction des produits chimiques commerciaux, qui doivent effectuer cette évaluation, n'ont pas en général l'expérience de l'utilisation de ces modèles et n'ont pas accès aux séries de données spécialisées qu'il faut avoir quand on utilise ces modèles.

Grâce au projet sur la contamination des eaux souterraines, de la Direction de la recherche sur les cours d'eau, INRE, on met au point un système expert pour la Division des pesticides d'Environnement Canada, système qui permettra de combler cette lacune. Le projet durera deux ans et son coût est assumé par la Division des pesticides. Le présent rapport donne les résultats de la phase I du projet.

On a examiné 15 modèles dans le but de les incorporer éventuellement au système expert. Les critères de sélection d'un modèle comprenaient les processus physiques, chimiques et biologiques que le modèle pouvait simuler, ainsi que sa facilité d'utilisation dans une perspective de réglementation. Les deux modèles relatifs aux pesticides, LEACHM et PRZM, que l'on a retenus sont ceux qui répondent le mieux aux critères établis pour le système expert. Grâce à ces

deux modèles, le système expert peut bénéficier des points forts de chaque modèle et donner aux employés chargés de la réglementation un outil capable de les aider à prendre des décisions en matière de lignes directrices sur les permis à accorder aux pesticides.

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1. INTRODUCTION

Ground water is a very important source of domestic water in Canada, particularly in rural areas. Hess (1986) estimates that 26 % of all Canadians and 38 % of the municipalities in Canada rely on ground water supplies for their domestic needs. In rural areas this number increases to 82 %, while on Prince Edward Island 100 % of the domestic water needs are satisfied by ground water. The widespread use of agricultural chemicals in rural areas and the detection of pesticides in some domestic and municipal water supplies have raised concerns about the possibility of ground water contamination by agricultural pesticides.

Contamination caused by agricultural pesticides raises additional concerns not generally associated with the more obvious sources of pollution, such as landfill leachate, chemical or petroleum spills, or industrial discharges (all quasi-point sources). The areal extent to which pesticides are applied makes containment of the source, and remedial action (e.g. pump and treat), in the event of contamination, impractical. The emphasis must therefore be placed on prevention of contamination rather than relying on remedial measures in the event that contamination does occur.

When chemical pesticides were first introduced, little concern was given to the potential for these pesticides to leach to the ground water table. However, with the increasing sensitivity of analytical testing equipment, and the realization that these chemical may leach to the water table, numerous cases of ground water contamination by pesticides have been discovered. An EPA report, discussed by Bouwer (1989), states that of approximately 45000 wells tested in problem areas, more than 5500 had concentrations of at least one pesticide in excess of the recommended drinking water limit, and an additional 5500 wells had traces of at least one pesticide from a group of 73 different pesticides. The EPA report also states that 46 different pesticides have been found in the ground water of 26 U.S. states where it has been shown that "normal" agricultural practices where followed in the use of the pesticide.

As an illustrative example, the contamination of ground water supplies by the pesticide aldicarb has been studied by many investigators (Jones, 1985; Harkin et al., 1986; Pacenka et al., 1987; Jones et al.,1987; Priddle et al., 1987;1988). Aldicarb was first detected in domestic wells on Long Island, New York in 1979, and in a survey of 8404 Long Island wells, aldicarb was found in excess of the New York state recommended drinking water limit of 7 ppb in 13.5 % (1135) of the wells tested (Moye and Miles, 1988). The maximum concentration in this survey was more than 70 times the recommended drinking water limit. Since 1979, aldicarb contamination has also been reported in a number of U.S. states and Canadian provinces.

With strong evidence that pesticides have the potential to cause serious contamination problems even when recommended application procedures are followed, it is imperative that techniques be developed to assess the migration and transformation of a pesticide, and its toxic degradation products, in the subsurface before these pesticides are registered and available for commercial use. All pesticides used in Canada undergo extensive testing to ensure that they and their degradation products present minimal risks to the environment before they are registered for public use. However, a thorough knowledge of the processes that determine the fate of the pesticide in the subsurface is required for this assessment. The physical, chemical and biological processes that control the transport and transformation of a pesticide in the subsurface are varied and complex, and as yet are not completely understood. However, with the aid of certain simplifying assumptions, computer models have been developed that provide reasonable approximations of the transport and transformation of a pesticide in the subsurface.

Several computer models currently exist for predicting the distribution and concentration of a pesticide in the subsurface. However, the application of these models in a regulatory framework is limited because (1) the use of these models often requires specialized knowledge in the theory and modeling of pesticide transport in the unsaturated zone, and (2) the models require a specialized set of physical and chemical field data. Regulatory personnel who are assigned the task of assessing the environmental risks

associated with a new pesticide generally do not have this specialized knowledge and information available to them. It is therefore necessary to adapt these models in such a manner that they remain sufficiently sophisticated to simulate the major processes controlling the migration and transformation of pesticides, and yet, are easily and accurately used by regulatory personnel.

It is proposed that an expert system be employed to bridge the gap between pesticide models and regulatory personnel not versed in the use of these models. Generally, expert systems function by encoding the expertise of a specialist 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. The encoded expertise takes the form of prompts to the user for required data and choice of simulation options. The expert system responds to requests for assistance from the user to explain the information requested by the system and will retrieve information that it has stored in its data bases to assist the user in parameter selection for the model. The expert system thereby assists the user in solving complex problems that are beyond the user's present level of knowledge in either the field of interest or in computing ability.

For this study, the expert system will be designed as a management tool and will be structured to provide a general assessment of the potential hazards of an application of a pesticide, to identify if further research (e.g. field testing) is required in the pesticide registration process. Specifically, the expert system for pesticide regulatory decisions will provide predictions on the rate of pesticide migration as well as the concentration of the pesticide in the unsaturated soil profile. Estimates will also be provided for the amount and time required for a pesticide to reach the water table.

The entire project will take two years and the work is divided into a number of phases (see Appendix A). A more detailed description of the work to be completed in each phase is given in Crowe et al. (1989). This report describes the results of the work conducted for Phase 1. The specific objects for Phase 1 (Review of Existing Pesticide Models) 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 easily be modified to meet the criteria set for the expert system.

2. AN EXPERT SYSTEM FOR PESTICIDE REGULATORY PERSONNEL

2.1 A GENERAL OVERVIEW OF EXPERT SYSTEMS

An expert system (also known as a knowledge-based system) can be defined as a computer program that mimics the knowledge, reasoning, and possibly the linguistic skills of an human expert, in a particular field of endeavour (Miller, 1989; Schildt, 1987).

Expert systems differ from conventional computer programs in a number of respects. Conventional programs generally take a set of numeric or alpha-numeric input data, manipulate the data in a predetermined pattern, and present the results with no interpretation or evaluation. The expert system also manipulates numeric data in the conventional format. However, they differ from conventional computer programs in that they have the ability to evaluate and interpret input and output data, suggesting alternatives where appropriate, and making recommendations based on the model results.

Expert systems operate by having the knowledge, experience and problem solving abilities of an "expert" encoded into the computer software. Expert systems apply the knowledge, rules and judgement, garnered from human experts, to solve problems using logical rules of inference, in addition to the conventional algorithmic calculations. Expert systems can guide those with only a modest level of knowledge and experience in a particular field through a lengthy and complex problem by providing the user with access to a body of problem-specific knowledge.

An important feature of expert systems is that they are based on informational concepts rather than just quantitative data. The data encoded in the expert system may take the form of either facts or knowledge. Facts include all the quantitative data obtained from public sources such as textbooks, manuals, laboratory and field experiments, etc. Knowledge is more qualitative in nature and is comprised of a collection of facts, insights, hunches and problem solving techniques and methodologies. An important component of the knowledge base is the "rule of thumb" knowledge or heuristic knowledge. Heuristic knowledge is a set of rules or information that are not formulated as a result of ordinary, accepted knowledge, but is information held by an expert and derived from experience gained through years of problem solving.

2.2 DESIGN OF AN EXPERT SYSTEM FOR PESTICIDE REGULATORY PERSONNEL

The objective in the design of the expert system for the Pesticide Division of Environment Canada is to provide regulatory personnel with a tool that will aid in their evaluation of the fate of pesticides in the subsurface, to ensure that ground water quality in agricultural areas is maintained. The expert system will therefore, be designed as a management tool to aid in making policy decisions during the registration process and is not intended for use as a research tool. Thus, the function of the expert system is not to provide insight into the processes that control the fate of a pesticide in a porous media, but is to provide a quick and general assessment of the potential hazards to the shallow ground water regime associated with the application of a 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.

2.2.1 GENERAL DESIGN CRITERIA

The expert system is designed for use by Pesticide Division regulatory personnel who may not have experience in the use of numerical models that simulate the transport and transformation of pesticides in the subsurface. As a result there are several important design criteria that the expert system must meet:

(1) the system must be easily used by those with minimal computer skills and knowledge of pesticide transport in the subsurface;
(2) on introduction to the system, personnel should be able to effectively use the system in a relatively short time;
(3) it should run quickly and efficiently on a personal computer;
(4) parameters required by the model should be readily available from data bases or easily entered into the system via a dialogue format;
(5) the data bases should be as complete as possible;
(6) corrections and changes during data entry should be easily accommodated;
(7) output from the expert system should be informative and easily understood;
(8) the program should be written in a manner that will allow for easy modification;
(9) data bases should be constructed so that they can be easily updated and modified.

2.2.2 STRUCTURE AND DESIGN CRITERIA OF THE EXPERT SYSTEM FOR PESTICIDE REGULATORY PERSONNEL

The specific architecture for the expert system being designed to assess the effects of pesticides on the subsurface is illustrated in Figure 1. The expert system is composed of four parts; the Inference Engine (IE), the User-System Interface (USI), the Pesticide Transport and Transformation Model, and the Knowledge, Facts and Explanation Bases.

2.2.2.1 THE INFERENCE ENGINE

The Inference Engine contains statements which affect the general control of the expert system. The Inference Engine consists of four modules. The first, a program control module, controls the basic computer operations as they are needed by the expert system. These operations include the linking of the various components of the expert system, reading of the data bases, printing or displaying output, etc. The second module, the reasoning control module, regulates the reasoning strategy and evaluation of the results from the transport model through the application of appropriate production rules. The interpretation module translates the user's responses into a format that can be understood by the expert system. For example, input data are translated to form an input data set for the transport module, explanations or requests for data access the appropriate data base, input data are checked for consistency among previously entered values and results from the transport model are converted to easily interpreted output. The final module, the data update module, is used to modify existing data or to add new values to the Knowledge, Facts, or Explanation data bases.

2.2.2.2 THE USER-SYSTEM INTERFACE

The User-System Interface will be an interactive program designed to guide the user through the entry of data required by the pesticide transport model. The module will prompt the user for information pertaining to the physical setting of the site, the chemical properties of the pesticide, and the hydrological properties of the soil at the site. Should the user be unfamiliar with any of the requested information, the expert system, through

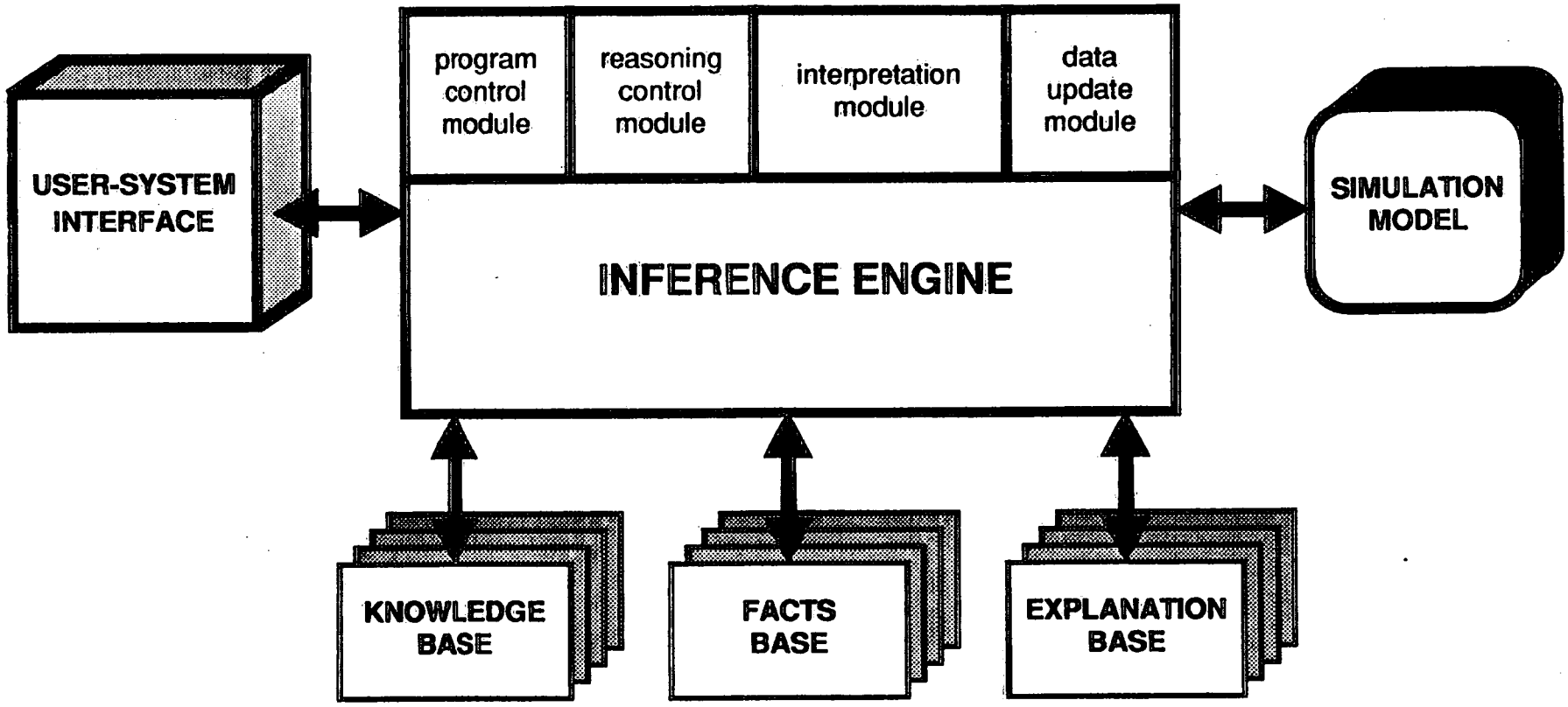

Figure 1. Architecture of the expert system.

the User-System Interface, will provide an explanation of the information required and possibly recommend typical values that may be used. When appropriate, the expert system will automatically supply required data from its information data bases according to the information already entered by the user. The user will then have the option to modify the data, if desired. The expert system will also perform internal checks to ensure the consistency of data entered.

2.2.2.3 SOLUTE TRANSPORT AND TRANSFORMATION MODEL

The third part of the expert system consists of a Pesticide Transport and Transformation Model that predicts the fate of a pesticide in the unsaturated zone. Rather than developing a new model, an existing model will be chosen and modified to meet the needs of the expert system. This will not only reduce the time required to arrive at a final product, but by using a widely accepted model, it will ensure that the important processes are included in the model and they will have been verified through previous use. The criteria for choosing the model for the expert system are as follows:

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

In order to accurately predict the transport of pesticides in the subsurface, the mathematical framework for the transport and reaction model must be based on the accepted scientific principles that describe the processes that control the transport and transformation of the pesticides in the unsaturated zone. These important process include:

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

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

The physical, chemical and biological processes controlling the fate of pesticides in the subsurface are in turn affected by a number of environmental factors that must be considered by the pesticide model. These environmental 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 at depth;
(9) pH of the soil and water environments;
(10) pesticide fluxes at the ground surface.

2.2.2.4 FACTS, KNOWLEDGE AND EXPLANATION DATA BASES

The forth component of the expert system consists of the three information data bases, which form the "expert's" contribution to the system. The data contained in the Facts Base is comprised of detailed information regarding, first, the physical, climatic, hydrogeological and agricultural setting of typical agricultural zones across Canada, and second, the chemical characteristics of pesticides.

All data necessary to describe a series of typical agricultural zones across Canada will be included in the Facts Base. 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 Nova Scotia.

The characterization of these typical agricultural zones will be hypothetical to the extent that the basic model parameters are not derived from a particular field or orchard. The choice of parameters used to define the typical agricultural zones will, however, be guided by experience from a variety of field studies undertaken within a particular zone. Because there is considerable variation in the physical, hydrological, 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. The expert system will therefore be designed such that the existing parameters describing a typical agricultural zone can be easily modified by the user for a particular simulation.

The Facts Base will also contain data describing the chemical characteristics of a group of pesticides. It will be accessed by the user when information for a new pesticide is required by the model that does not already exist. By looking at a family of similar pesticides in the data base, the user will be able to approximate the required data for the new pesticide. The expert system must also allow pesticide parameter values contained in the data base to be easily modified, and allow new data to be included in the data base as it becomes available. It should also allow for the addition of new pesticides to the data base.

The production rules will be stored in the Knowledge Base, to be accessed by the reasoning control module of the Inference Engine when necessary. This information is the encoded expertise or knowledge that will guide the user through the choice of parameters and options for a particular pesticide transport and transformation simulation. The type of information within the Knowledge Base includes:

(1) all production rules;
(2) evaluations of plausible values and relationships among the chosen parameters.

Information contained within the Explanation Base is used to assist the user in the choice of model parameters when the information requested by the User-System Interface module is not understood, or is not available to the user. Information contained within the Explanation Base includes:

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

3. THEORY OF PESTICIDE TRANSPORT IN THE UNSATURATED ZONE

The transport and transformation of a pesticide in the unsaturated one is complicated because they are controlled by many physical, chemical and biological factors. However, these factors can be categorized into two groups; transport processes and attenuation processes. The first group is comprised of the processes and mechanisms that transport the pesticide and its degradation products through the unsaturated porous medium. The second roup includes those processes that act to attenuate or retard the movement of the chemicals. These processes must be understood before any attempt can be made to accurately simulate the fate of pesticides in the subsurface. The two groups of processes are discussed in this chapter.

3.1 TRANSPORT OF PESTICIDES IN A POROUS MEDIUM

The three mechanisms involved in the transport of pesticides are:

(1) advection (mass flow);
(2) liquid diffusion/dispersion;
(3) vapour diffusion.

The first, advective (mass) flow, considers the passive transport of dissolved solutes with the bulk flow of water. In the unsaturated zone, emphasis is placed on the vertical movement (leaching) of the pesticides towards the ground water table. The second mechanism, liquid diffusion/dispersion, accounts for chemical and mechanical mixing of the pesticide in the subsurface. These processes have the net effect of spreading the pesticide over an increasingly larger area, thus, decreasing concentrations at the centre of mass of the pesticide but increasing it beyond the centre of mass. Vapour diffusion, the third mechanism, acts in a similar manner to the liquid diffusion for the portion of the pesticide in the vapour phase. This mechanism becomes more important with pesticides that are highly volatile.

Secondary processes, such as surface runoff, erosion, and volatilization, may become significant in the transport of some pesticides under certain conditions. However, Donigian and Rao (1986) quote several references in concluding that runoff and erosional losses of pesticides in agricultural applications usually account for only a small percentage of the total pesticide application. This finding is supported by Carsel et al. (1988) and Jones et al. (1986).

Mathematically, the relationship among these three mechanisms is expressed as the solute transport equation:

$$\frac{\partial(c^*\Theta)}{\partial t} = -\frac{\partial(q^*c)}{\partial z} + \frac{\partial}{\partial z}(D_d(\Theta,v)^*\frac{\partial c}{\partial z}) + S \qquad (3.1)$$

where:

c = the dissolved solute concentration,
q = the flux across a unit area per unit time,
$D_d(\Theta,v)$ = the diffusion/dispersion coefficient, and
S = a source/sink term.

Generally, this equation indicates that the change in the concentration of the pesticide in the soil water with time is determined by assuming that the solute advective flux is proportional to, first, the bulk movement of the water and secondly, the concentration gradient of the pesticide in the bulk soil solution. The final term in the solute transport equation is a source/sink term that accounts for the processes that act to attenuate the migration of the pesticide. A more detailed derivation of this

equation can be found in Hillel (1980b).

Because the bulk movement of water is a major factor determining the direction of pesticide transport and the speed at which pesticide migration occurs, it is important to understand how water travels through an unsaturated porous medium. Water flow in the unsaturated zone, as is the case with saturated flow, occurs due to the presence of a potential energy gradient. Flow occurs in the direction of the decreasing energy potential, and the rate of flow (flux) is proportional to the potential gradient.

However, in the unsaturated zone soil-water is also subjected to negative (sub-atmospheric) pressure potentials arising from the affinity of water for the surfaces of the soil particles. The negative suction potentials (ϕ) that arise are generally reported as an equivalent positive value, and are referred to as matric suction (ψ), signifying that a positive matric suction value actually represent a negative matric potential ($-\phi = \Psi$). With this convention in mind, water flow in the unsaturated zone occurs from areas of low matric suction to areas of high matric suction. Water flow in the unsaturated zone occurs in both the pore space of those pores that are saturated at the given matric suction, and along the hydration film covering the solid particles in those pores that are not completely saturated (Hillel, 1980b).

The most significant difference between saturated and unsaturated flow is the dependence of the unsaturated hydraulic conductivity on the matric potential of the soil. As conditions change from saturated to unsaturated, capillary forces holding the water in the larger pores are exceeded as suction forces develop, and water in the largest, most conductive, pores is the first to drain. As suction continues to develop, the capillary forces in successively smaller pores are exceeded, and they in turn drain, further reducing the size of the water conducting pathways and the hydraulic conductivity of the soil.

To complicate matters further, the conductivity relationship (relating the hydraulic conductivity (K) of a soil to its matric suction (ψ)) is hysteretic, with different curves for wetting and drying fronts. The same phenomenon is observed in the retentivity curve which relates the matric suction (ψ) of a soil to its volumetric soil-water content (Θ).

The conductivity and retentivity curves, discussed above, are complex for a given soil. However, simplified empirical relationships have been developed by measuring these soil parameters in the laboratory, or under field conditions (see Hillel (1980b)). Empirical regression equations have also been proposed to facilitate the development of the conductivity and retentivity relationships based on a few pertinent soil parameters (Hutson and Cass, 1987; Wagenet and Hutson, 1987).

The Richards equation requires that the velocity of the ground water be known before the pesticide concentration can be calculated. In order to calculate the ground water velocity or the flux across a unit area per unit time, the distribution of hydraulic head within the subsurface must be known. The equation that describes the distribution of hydraulic head and water content in the unsaturated zone, known as Richards equation, couples the continuity equation (conservation of mass) with Darcy's Law. This equation is:

$$\frac{\partial \Theta}{\partial t} = \frac{\partial}{\partial z}\left(K(\Theta)^*\frac{\partial H}{\partial z}\right)+S(z,t) \qquad (3.2)$$

where:

Θ = the soil water content,
$K(\Theta)$ = the hydraulic conductivity,
H = the hydraulic head,
z = the depth,
t = time, and
S(z,t) = represents possible sources and sinks for water gain and/or loss.

The reader is referred to Hillel (1980b) and Wagenet and Hutson (1987) for a detailed discussion of the development of Richards equation.

3.2 ATTENUATION OF PESTICIDES IN AN UNSATURATED POROUS MEDIUM

Additional terms must be added to Equation 3.2 to account for the processes that attenuate the transport of pesticides in the subsurface. Attenuation of pesticides can occur as the result of the following three groups of processes,

(1) partitioning of the pesticide;
(2) transformation or degradation of the pesticide;
(3) plant processes.

3.2.1 PARTITIONING OF THE PESTICIDE

The presence of a chemical in a three phase system, such as in an unsaturated soil, will result in the partitioning of that chemical between its liquid, solid, and gaseous phases.

Partitioning of a pesticide between its dissolved and solid phase occurs by the adsorption of the pesticide on the surface of soil minerals, and/or organic matter present in the soil matrix. The processes involved in the adsorption of organic (i.e. pesticides) are varied and complex, and prevent the development of a detailed mathematical description of adsorption. However, a number of simplified adsorption isotherms (including Langmuir, Freundlich, and BET) have been developed to relate the sorbed chemical concentration to the dissolved concentration in the liquid phase (Bohn et al., 1979).

It is often assumed, for pesticides, that the adsorption relationship is linear, instantaneous, and reversible at low concentrations (Carsel et al., 1984: Jury, 1986; Wagenet and Hutson, 1987). The concentration of the sorbed phase, c_s, is related to the dissolved concentration, c, by a distribution (or partition) coefficient, K_D.

$$c_s = K_D * c \qquad (3.3)$$

The amount, composition, and cation exchange capacity of the clay fraction strongly affects the adsorption of pesticides with permanent positive charges (such as paraquat and diquat), but no correlation has been observed between the percent clay and the amount of non-polar organic adsorption (Jury, 1986).

A positive linear relationship does however, exist between the organic matter content of a soil and the adsorption of organics (i.e. pesticides) to that soil (Jury, 1986). The distribution coefficient, K_D, defining the partitioning of the sorbed and dissolved states of the pesticide, is related to the amount of organic matter present in a soil (Karickhoff et al., 1979), and is given by:

$$K_D = K_{OC} * f_{oc} \qquad (3.4)$$

where:

K_{OC} = organic carbon partition coefficient, defined as the amount of pesticide sorbed per gram of organic carbon, divided by the amount of pesticide per gram of solution, and

f_{OC} = fraction organic carbon content.

Jury (1986) reviews the practical limitations of using these adsorption representations. The adsorption models are assumed to be linear. However, no single K_D value describes the partitioning between the sorbed and dissolved states over the

entire range of possible concentrations. The results of experiments conducted by Karickhoff et al. (1979), on the sorption of hydrophobic compounds (water solubilities between 500 ppt and 1800 ppm) on pond and river sediments do, however, indicate that the linear adsorption isotherm is a good approximation for the observed sorption of the compounds studied (aromatic and chlorinated hydrocarbons) for trace concentrations.

The adsorption isotherms are assumed to be reversible, however most pesticides exhibit a hysteretic adsorption- desorption isotherm. They provide a greater resistance to desorption than to adsorption, and are therefore, at least partially irreversible (Jury, 1986). Reversible models overestimate the amount of desorption as the pesticide is leached through the system. The amount of pesticide actually remaining sorbed to the soil particles (and out of the aqueous phase) tends to be higher than that predicted by these adsorption models.

The third assumption is that the adsorption processes are instantaneously at equilibrium. The validity of this assumption is dependent on the kinetics of the adsorption process and on the residence time of the adsorbing solute. In some instances, the time may be too short to establish equilibrium, and the actual adsorption would be lower than that predicted by the models.

The pesticide is also partitioned between its liquid and gaseous phases. Liquid-vapour partitioning is similar to the liquid-solid partitioning, as the concentration of the pesticide in the gaseous phase, c_g, is linearly related to the pesticide concentration in the liquid phase, c, by Henry's law,

$$c_g = K_H * c \qquad (3.5)$$

where : K_H = a dimensionless partition coefficient known as Henry's constant.

Solid-liquid partitioning, however, is a more important process in the transport of most pesticides than is the liquid-vapour partitioning of the chemical.

3.2.2 TRANSFORMATION PROCESSES

The processes controlling the transformation of pesticides are of prime importance in determining the contamination potential of the pesticide, as these processes determine the persistence of the chemical in the soil environment. Even if the physical processes are in place to transport a pesticide to the water table, the pesticide will not be considered as a potential contamination risk if it does not persist long enough to reach the water table.

Transformation processes are superimposed on the transport processes. The contamination potential of a non-persistent pesticide is, therefore, highly dependent on the timing of the rainfall and/or irrigation events in relation to the application date. If contamination is to occur, the pesticides must move quickly through the soil profile. Sufficient mobility must be given to the chemical during its effective life time in the environment to move it through the soil profile. As the persistence of a pesticide is increased, the timing of rainfall or irrigation events becomes less critical in determining the contamination potential of the chemical.

Transformation processes encompass both the chemical and biological processes that control the fate of a pesticide and may be either biologically or non-biologically mediated. For biologically mediated processes, the chemical reactions are catalyzed by enzymes and may include biologically mediated hydrolysis and oxidation-reduction (redox) reactions. Both reactions occur at faster rates in the surface and root zone layers where microbial populations are the highest (Jury and Valentine, 1986). The most significant factors influencing biologically mediated processes are those controlling the availability of the substrate, and the size, and activity of the microbial population.

Non-biologically mediated processes include strictly chemical and photochemical reactions. Chemical hydrolysis and redox reactions may occur without the aid of biological catalysts while photochemical reactions require the adsorption of light (photons) to catalyze the reactions. Photochemical reactions are therefore potentially important only at and near the soil surface. Pesticides incorporated in the soil are thus not significantly affected by these reactions (Valentine, 1986).

Difficulties arise when trying to determine the degradation rate of a pesticide. It is often difficult to distinguish between biotic and abiotic processes without extensive laboratory studies. There are many possible pathways and fates available to pesticides in the soil, and it is possible that the disappearance of a portion of the chemical may be misinterpreted as a transformation loss when in fact the disappearance may be due to other processes (i.e. bound chemical residues). In such cases, the rate constants will be overestimated.

Transformation rate constants are difficult to determine, and as a result, most mathematical representations are greatly simplified, lumping the processes together, and representing them as either first-order or second-order rate reactions to account for the effective disappearance of the pesticide.

First-order reaction equations are the most commonly used. Even when experimental data indicate that a more complex relationship is possible, first order reaction rates are often used because the determination of the first-order rate constant is relatively simple (Valentine and Schnoor, 1986). It requires only the measurement of the chemical concentration. Measurements of the active microbial biomass are often required in the determination of the second-order rate constant for biotic processes and are much more difficult to obtain.

The limitations imposed by these rate constants must be recognized. The assumptions and simplifications inherent in these constants prevent their use from providing anything more than empirical, engineering, approximations. First-order equations, considering only the chemical concentrations, are more site specific than higher order equations, where consideration is given to other factors in addition to the chemical concentration when determining the rate constant.

If the transformation pathway includes more than one transformation step, consideration of the individual rate constants for each step (rather than a single, lumped transformation step) provides more applicable, and less site specific results.

Determination of the rate constants is often performed in the laboratory, where conditions are controlled but may vary greatly from those found in the field. Closer approximations result if the rate constants are determined for field conditions.

3.2.3 PLANT PROCESSES INFLUENCING PESTICIDE TRANSPORT AND REMOVAL FROM THE UNSATURATED ZONE

The processes that occur in the soil (i.e. transport, sorption, and transformation of solutes) also occur within the plant (Donigian and Rao, 1986). Transport mechanisms within the plant result from the same pressure gradients as those in the soil and plants passively extract water from the soil while actively controlling the transpiration loss forced by atmospheric and soil-water potential differences. Nutrients and other chemicals, such as pesticides, dissolved in the soil-water are taken up at the same time by specific and non-specific selection processes. The extraction of water and the uptake of pesticides by the plant influence both the transport and transformation of pesticides in the soil. The withdrawal of water and pesticides by the plant reduces both the soil-water and pesticide content available for transport in the subsurface. The extraction of water by the plant may actually cause the flux of water and pesticide to reverse, drawing the pesticide back towards the surface. Hillel (1980a), however, states that the processes of water, nutrient and pesticide uptake by plants are largely independent and accounting for pesticide loss by relating the amount withdrawn to the transpiration rate may not be appropriate in some instances.

4. PESTICIDE TRANSPORT MODELS

This section contains a review of existing pesticide transport models. Fifteen models were identified and evaluated based on the criteria presented previously, and from this evaluation two models were chosen as being suitable for incorporation into the expert system.

In general, there are two groups of models available to assess the potential for ground water contamination by pesticides. The two groups are screening models and mathematical models.

4.1 SCREENING MODELS

Five of the 15 models identified are classified as screening models and are listed below.

(1) DRASTIC (Aller et al., 1985);
(2) GUS - Groundwater Ubiquity Score (Gustafson, 1989);
(3) CDFA screening model (Wilkerson and Kim, 1986);
(4) Cohen et al., 1984 screening model;
(5) Jury et al., 1987 screening model.

Screening models simply assess the potential for ground water contamination from a pesticide on a relative basis. Specifically, two or more chemical characteristics of the pesticide and/or hydrogeological properties of the application site are compared with similar pesticides and situations where contamination of the ground water was known to have occurred. The models do not actually simulate the physical, chemical, and biological processes involved in the transport of pesticides in the unsaturated zone and do not attempt to quantify the amount or rate of pesticide leaching to the ground water table. The models simply give a relative index of the potential for leaching of a pesticide with respect to other pesticides that have been known to contaminate ground water supplies. For example, based on previous experience it has been determined that pesticides with an organic carbon partition coefficient (K_{oc}) less than 512 cc/g, and a soil half-life greater than 11 days (CDFA criteria) have a high potential to leach to the water table. A pesticide with properties meeting these two criteria would be classified as a "leacher", with a high potential for ground water contamination. The chemical may then be restricted from use in certain areas.

After an initial review, all of the screening models were eliminated from further consideration, as they do not simulate the processes involved in the transport and transformation of a pesticide in the unsaturated zone. The screening models cannot predict pesticide concentrations or leaching rates at the ground water table, and therefore, these models do not meet the selection criteria set out for the expert system in Section 2.2.2.3.

4.2 MATHEMATICAL MODELS

The second group of pesticide transport models is the mathematical model. Ten of the 15 models identified are classified as mathematical models and are listed below.

(1) LEACHM - Leaching Estimation And Chemistry Model (Wagenet and Hutson, 1987);
(2) PRZM - Pesticide Root Zone Model (Carsel et al., 1984);
(3) MOUSE - Method Of Underground Solute Evaluation (Steenhuis et al., 1987);
(4) CMLS - Chemical Movement in Layered Soils (Nofziger and Hornsby, 1986);

(5) GLEAMS - Groundwater Loading Effects of Agricultural Management Systems (Leonard et al., 1987);
(6) SESOIL - SEasonal SOIL model (Bonazountas and Wagner, 1984);
(7) VULPEST - VULnerability to PESTicides (Villeneuve et al., 1987);
(8) PESTAN - PESTicide ANalytical model (Enfield et al., 1982);
(9) MELEF-3v (Padilla et al., 1988);
(10) SUTRA - Saturated - Unsaturated TRAnsport model (Voss, 1984).

In assessing the potential for ground water contamination by pesticides, mathematical models attempt to simulate the processes that are involved in the transport and transformation of the pesticides in the unsaturated zone of a soil. The models describe these processes with mathematical approximations that quantify both the amount and rate of pesticide leaching through the soil profile to the ground water table.

The existing mathematical models account for the major physical, chemical and biological processes affecting the transport and transformation of pesticides in the unsaturated zone. The models are all one-dimensional and generally simulate pesticide transport in the unsaturated zone based on an advective-dispersive equation for transient conditions.

The majority of the models use a simplified water flow representation for the unsaturated zone and are, to varying degrees, compartmentalized. This allows the models to simulate pesticide transport in layered soils by assigning different physical, chemical, and biological parameters to the different soil layers or horizons. A well mixed model representation is used to simulate solute transport.

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

The models are designed primarily for relatively nonvolatile compounds and generally do not account for volatilization losses and volatile transport in the soil profile. A few of the models account for the loss of pesticide due to surface runoff and erosion.

4.2.1 CLASSIFICATION OF MATHEMATICAL MODELS

Mathematical solute transport models are subdivided into one of three categories: educational, management, or research models. The categories are distinguished from each other based upon;

(1) the extent to which they describe the basic processes involved;
(2) the sensitivity and accuracy of the simulations;
(3) the amount of input characterization data required (Wagenet, 1986).

Figure 2 illustrates the classification categories for the 15 models identified.

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

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

The third category is the research model. Research models attempt to describe the

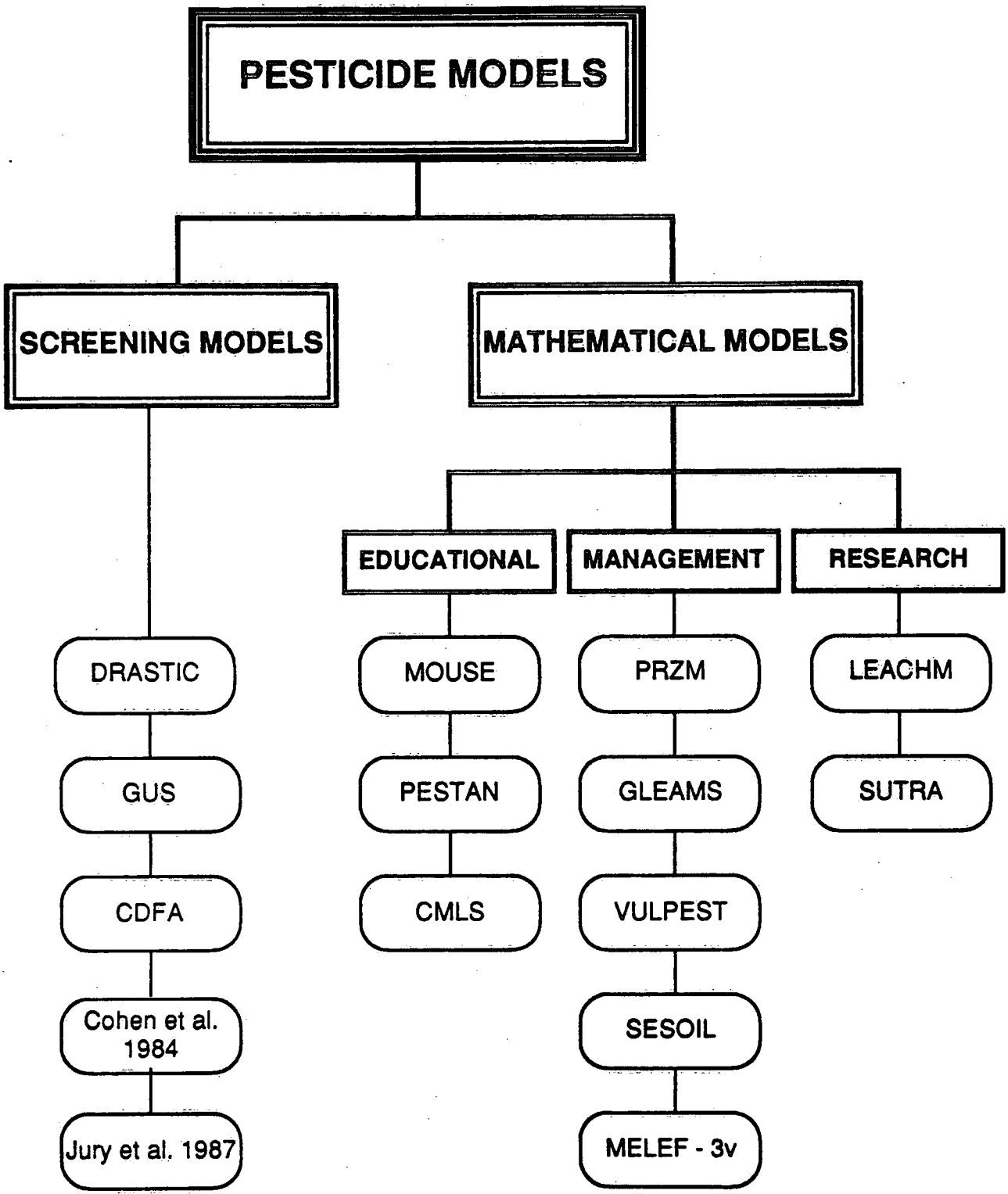

Figure 2. Classification of pesticide transport models.

processes in as much detail as possible. As an example, research models may describe water flow in the unsaturated zone using a direct solution to Richards equation, while management and educational models may employ a simplified water balance. As a result of the more detailed description, research models often require large amounts of input characterization data, some of which may not be readily available. Research models provide results that are more quantitatively accurate than the results from management models. However, their use is often more cumbersome (i.e. input data sets are more difficult to formulate, and they require considerably longer execution times).

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

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

4.2.2 AN INITIAL REVIEW OF THE MATHEMATICAL MODELS

Several of the mathematical models were also eliminated from further consideration during an initial review of the mathematical models. The reasons for eliminating each of the models are summarized below.

PESTAN (Enfield et al., 1982) - is a one-dimensional, solute transport model based on an analytical solution. The model assumes steady state, one-dimensional flow within a homogeneous soil profile. The model cannot accurately simulate situations were there are large variations in the seasonal rainfall or where the solute transport is occurring through a layered soil. The model is also restricted in its applicability by the use of an analytical solution.

MOUSE (Steenhuis et al., 1987) - is a one-dimensional model based upon a simplified water flow representation. MOUSE tracks the position of the solute peak according to the water flux moving past the solute peak and dispersion around the peak is calculated according to an error function representation. The model assumes only four layers and its ability to vary soil, biological and hydraulic parameters with depth is limited.

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

CMLS (Nofziger and Hornsby, 1986) - calculates the movement and position of a solute front only. The water flow and solute equations describe piston flow with no dispersion of the solute. In addition, CMLS does not calculate the chemical concentration profile, or leaching rate, of the pesticide, and therefore, fails to meet the design criteria set out for the expert system in Section 2.2.2.2.

SESOIL (Bonazountas and Wagner, 1984) - The solute transport subroutine in the SESOIL model can accommodate only four soil layers and this does not provide for

enough descretization for simulations in layered soils. In addition, the hydrological subroutine assumes a homogeneous soil profile and uses probability density functions for climatic variables, soil properties, and ground water elevations to determine long-term, "seasonal", averages for the components of the water balance. The use of a seasonally averaged components in the water flux may act to mask peak concentrations being leached to the water table that should be of concern. These conditions adversely affect the model's ability to simulate solute transport in layered soils, and therefore, the model is not recommended for inclusion in the expert system.

MELEF-3v is a one-dimensional, finite element, solute transport model. In addition to simulating mass transport in the unsaturated and saturated zones of a soil for unsteady conditions, the model also simulates heat flow. The time step in the model is variable depending on the conditions simulated and execution time may be long under certain conditions. The model, however, was eliminated from the selection process because it could not be shown from the literature search that this was a widely used and verified model based on an internationally accepted code and principles.

SUTRA (Voss, 1984) - is a two-dimensional, solute and thermal energy transport model for both the saturated and unsaturated zones. The model combines finite element and finite difference techniques and is very computationally intensive. Use of the model requires a mainframe computer and SUTRA has therefore been eliminated from further consideration for the expert system.

VULPEST (Villeneuve et al., 1987) - is a stochastic pesticide transport simulation model. The model actually uses a deterministic model within a stochastic (Monte Carlo) approach. VULPEST employs an analytical solution to a one-dimensional advective equation, and although the soil column can be separated into distinct layers, all model parameters remain constant in space and time for a given simulation. The spatial and temporal variation is accounted for by performing a number of simulations choosing model parameters for each simulation from a statistical distribution of the possible parameter values. A sufficient number of simulations are performed (1000-2000 simulations) and predicted results are assigned a statistical probability of occurrence. The model output provides stochastic breakthrough curves, maximum concentrations and the time of arrival, average annual concentration, and the accumulated mass for each Monte Carlo simulation. The results are presented in both data files and as graphical representations.

VULPEST was eliminated for several reasons. It uses an analytical solution that may restrict its applicability and it does not simulate the movement of any metabolites generated from the transformation of the parent pesticide. The model does not simulate dispersion and VULPEST uses monthly rainfall, evapotranspiration data to produce a simplified water balance. Average infiltration values and pore water velocities are generated, from which the solute transport can be calculated. The averaged values for the water balance may act to mask peak flux of pesticides to the ground water table. The stochastic approach requires an accurate distribution of field parameters that may require extensive field measurements.

GLEAMS (Leonard et al., 1987) is a modified version of CREAMS (Knisel, 1980), a surface runoff and erosion model. GLEAMS was created by expanding CREAMS to consider the vertical flux of pesticides and to determine the ground water loadings from pesticide applications.

GLEAMS is based on a transient, advective-dispersive equation and uses a simplified water balance. The model allows for up to seven soil layers or horizons, with the surface layer being set to a depth of 1 cm. All surface effects are limited to this surface layer. The surface runoff component in the model is based on a Soil Conservation Service curve number approach and evapotranspiration and plant uptake are considered. The upward movement of pesticide to the surface layer is simulated, however, volatilization from the surface layer is not simulated by GLEAMS. The model

simulates the movement of metabolites generated from the parent pesticide and different rate constants may be specified for pesticide located on the plant foliage, the soil surface and within the root zone.

There are several weaknesses in the GLEAMS model. It is applicable only to simulations within the root zone and is limited to the use of only seven soil compartments. This may create problems when simulating pesticide transport in layered soils. Surface volatilization is not simulated and GLEAMS, being derived from a surface runoff and erosion model, has a very lengthy and detailed description of these two processes and this requires a large amount of input characterization data.

4.3 PESTICIDE MODELS CONSIDERED FOR THE EXPERT SYSTEM

Four models were initially considered for the use in the expert system designed to assist in regulatory decisions for pesticide registration. These models were GLEAMS, VULPEST, LEACHM (Wagenet and Hutson, 1987) and PRZM (Carsel et al., 1984). GLEAMS and VULPEST were candidates for the expert system because GLEAMS had the most detailed description of surface runoff and erosion of all the models reviewed, while VULPEST can undertake simulations within a stochastic framework, providing information on the uncertainties of the predications. However, it is evident from Table 1, that the advantages offer by GLEAMS and VULPEST do not overcome their disadvantages. Both models were found to be lacking in some of the major processes that describe the fate of a pesticide in the subsurface. It was concluded that the two codes, LEACHM and PRZM, will more closely produce the desired level of accuracy required for the expert system. A more detailed description of these two models is given in the following sections.

4.3.1 LEACHM - LEACHING ESTIMATION AND CHEMISTRY MODEL (Wagenet and Hutson, 1987)

The LEACHM (Leaching Estimation And CHemistry Model) model was developed at Cornell University and is actually composed of three solute transport models: LEACHMN (nitrogen), LEACHMS (inorganic salts) and LEACHMP (pesticides). The object of this study is to simulate the transport of pesticides in the subsurface and as a result only the LEACHMP code will be considered in the following discussion. LEACHMP will henceforth be referred to as LEACHM.

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

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

$$\frac{\partial \Theta_i}{\partial t} = \frac{\partial}{\partial z}\left(K_i(\Theta)\frac{\partial H_i}{\partial z}\right) + U_i(\Theta) \qquad (4.1)$$

where:

Θ = the soil water content,
$K(\Theta)$ = the hydraulic conductivity,

Table 1. Charateristic of the pesticide transport models LEACHM, PRZM, GLEAMS and VULPEST.

PROCESSES	LEACHM	PRZM	GLEAMS	VULPEST
ADVECTION	YES	YES	YES	YES
DISPERSION	YES	YES	YES	NO
MODEL CLASSIFICATION	RESEARCH	MANAGEMENT	MANAGEMENT	MANAGEMENT
TYPE OF MODEL	DETERMINISTIC	DETERMINISTIC and LUMPED PARAMETER	DETERMINISTIC	PROBABILISTIC (STOCHASTIC)
TYPE OF SOLUTION	FINITE DIFFERENCE	FINITE DIFFERENCE & LUMPED PARAMETER	FINITE DIFFERENCE	ANALYTICAL
SIMULATING CONDITIONS	TRANSIENT	TRANSIENT	TRANSIENT	STEADY STATE
WATER BALANCE	RICHARDS EQUATION	SIMPLIFIED	SIMPLIFIED	SIMPLIFIED
CHEMICAL SPECIATION	YES	NO	YES	NO
LAYERED SOILS	YES	YES	DIFFICULT	YES
RUNOFF/EROSION	NO	YES	YES	NO
SORPTION	LINEAR REV. EQUI.	LINEAR REV. EQUI.	LINEAR REV. EQUI.	LINEAR REV. EQUI.
EVAPOTRANSPIRATION	YES	YES	YES	YES
VOLATILIZATION	YES	NO	NO	NO
DEGRADATION	1st-ORDER	1st-ORDER	1st-ORDER	1st-ORDER
PLANT GROWTH	YES	YES	YES	NO
PLANT UPTAKE	YES	YES	YES	NO
SNOWMELT	YES	YES	YES	NO
SIZE OF THE TIME STEP	VARIABLE (SECONDS TO HOURS)	CONSTANT (1 DAY)	CONSTANT (1 DAY)	CONSTANT (1 DAY)
CLIMATIC DATA	DAILY/WEEKLY	DAILY	DAILY	MONTHLY
EXECUTION TIME	LENGHTY	MODERATE	MODERATE	MODERATE

H = the hydraulic head,
z = the depth of the soil compartment,
t = time, and
U(Θ) = represents possible sources and sinks for water gain and/or loss.

LEACHM employs a block-centered, finite difference approach to solving this equation. Basically, the unsaturated zone is divided into a series of nodes in the vertical direction, with the area surrounding each node representing a block or soil compartment (Figure 3). Within LEACHM, the node spacing (Δz) or size of each compartment is assumed constant. In finite difference notation for inflow and outflow from a soil compartment is described by Darcy's Law (Figure 3).

$$\text{inflow} = \left(\frac{K_{i-1}(\Theta) + K_i(\Theta)}{2}\right)\left(\frac{H_{i-1} - H_i}{\Delta z}\right) \qquad (4.2)$$

$$\text{outflow} = \left(\frac{K_i(\Theta) + K_{i+1}(\Theta)}{2}\right)\left(\frac{H_i - H_{i+1}}{\Delta z}\right) \qquad (4.3)$$

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

$$\left(\frac{K_{i-1}(\Theta) + K_i(\Theta)}{2} * \frac{H_{i-1} - H_i}{\Delta z}\right) - \left(\frac{K_i(\Theta) + K_{i+1}(\Theta)}{2} * \frac{H_i - H_{i+1}}{\Delta z}\right) \qquad (4.4)$$

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

$$\frac{\Theta_{i,t} - \Theta_{i,t-1}}{\Delta t} = \left(\frac{K_{i-1}(\Theta) + K_i(\Theta)}{2} * \frac{H_{i-1} - H_i}{\Delta z}\right) - \left(\frac{K_i(\Theta) + K_{i+1}(\Theta)}{2} * \frac{H_i - H_{i+1}}{\Delta z}\right) + U_i(t) \qquad (4.5)$$

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

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

$$q_{i,t} = K_{i,t} - K_i * \left(\frac{H_{i-1} - H_i}{2 * \Delta z}\right) \qquad (4.6)$$

Once the water flux density is known, the model calculates the change in the pesticide concentration with time within each soil compartment.

$$\frac{\partial c}{\partial t}(\rho K_D + \Theta + \varepsilon K_H) = \frac{\partial}{\partial z}\left([\Theta D(\Theta,q) + \varepsilon K_H D_{OG}]\frac{\partial c}{\partial z} - qc\right) + S \qquad (4.7)$$

where:

c = the dissolved solute concentration,
K_D = partition distribution coefficient,
ε = gas filled soil porosity,
K_H = Henry's Law constant,
q = the flux across a unit area per unit time,
$D(\Theta,q)$ = the liquid diffusion/dispersion coefficient,
D_{OG} = the vapour diffusion/dispersion coefficient,
S = a pesticide source/sink term.

The finite solute transport equation (4.7) is solved by the finite difference method within LEACHM. The finite difference approximation to equation (4.7) is developed in the same manner as the Richards equation. A detailed description of the theory and finite difference approximations used in the LEACHM model are presented in Wagenet and Hutson (1987).

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

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

Additional processes simulated by LEACHM include:

(1) the transport and transformation 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 that define water movement in a particular soil;
(3) plant growth;
(4) daily evaporation and transpiration;
(5) water and pesticide uptake;
(6) the water flux, flux density, water contents and matric potentials for each soil compartment at each time step according to the surface and bottom boundary conditions specified by the modeler;
(7) the amount of chemical and/or biological degradation;
(8) the solute flux and concentration profile;
(9) the 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 the LEACHM model is variable, ranging from $1x10^{-7}$ of a day to $1x10^{1.3}$ of a day. The value for the time step is calculated at the beginning of each time step to meet certain criteria set up within the model (i.e. a specified maximum water flux).

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

The LEACHM model has a few weaknesses in relation to its incorporation into the expert system. The main disadvantage is the lengthy execution times (eg. 5 hours for a one year simulation with 45 soil compartments, on a COMPAQ 286 - DESKPRO with a math co-processor). Other problems include the lack of a surface runoff and erosion simulator, and input data requirements, necessary to characterize the objectives of the simulation and the site are more extensive than for other models.

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

The PRZM model (Carsel et al., 1984) was developed by the U.S. EPA, and is classified as a management model. It also simulates one-dimensional water flow and solute transport under transient conditions and divides the unsaturated zone into a series of soil compartments. Although PRZM simulates are based on the advective-dispersive equation (equation(3.2)), water flow is represented as a lumped parameter model (rather than a distributed parameter model, as is the case with LEACHM). At each time step the flux of water and solutes is calculated and cycled through the soil compartments with a simplified lumped parameter representation for the water balance (eg. flux is simulated with a "tipping bucket" concept) (Figure 4). For example, the water storage in the PRZM model can be expressed for the three soil regions as:

SURFACE ZONE COMPARTMENTS:

$$SW_1 = SW_{1,t-1} + P + SM - I_1 - Q - E_1 \qquad (4.8)$$

ROOT ZONE COMPARTMENTS:

$$SW_i = SW_{i,t-1} + I_{i-1} - U_i - I_i \qquad (4.9)$$

BELOW ROOT ZONE COMPARTMENTS:

$$SW_i = SW_{i,t-1} + I_{i-1} - I_i \qquad (4.10)$$

where:

SW_i = soil water in layer i for the previous time step (cm),
P = precipitation minus crop interception (cm/day),
SM = snow melt (cm/day),
Q = runoff loss (cm/day),
E_i = evaporational losses (cm/day),
U_i = transpirational losses (cm/day), and
I_i = percolation out of soil compartment i.

Each of the three layers shown in Figure 4 may actually consist of several individual cells, each described by different physical and chemical parameters.

The percolation of water is dependent on two soil parameters, field capacity and wilting point. The flow of water is simulated according to the following simple drainage rules:

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

If $SW_i > FC_i$ then $I_i = SW_i - FC_i * \Delta z$, else $I_i = 0$

where:

FC_i = the water content of soil compartment i at field capacity, and
Δz = the thickness of the soil layer.

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

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

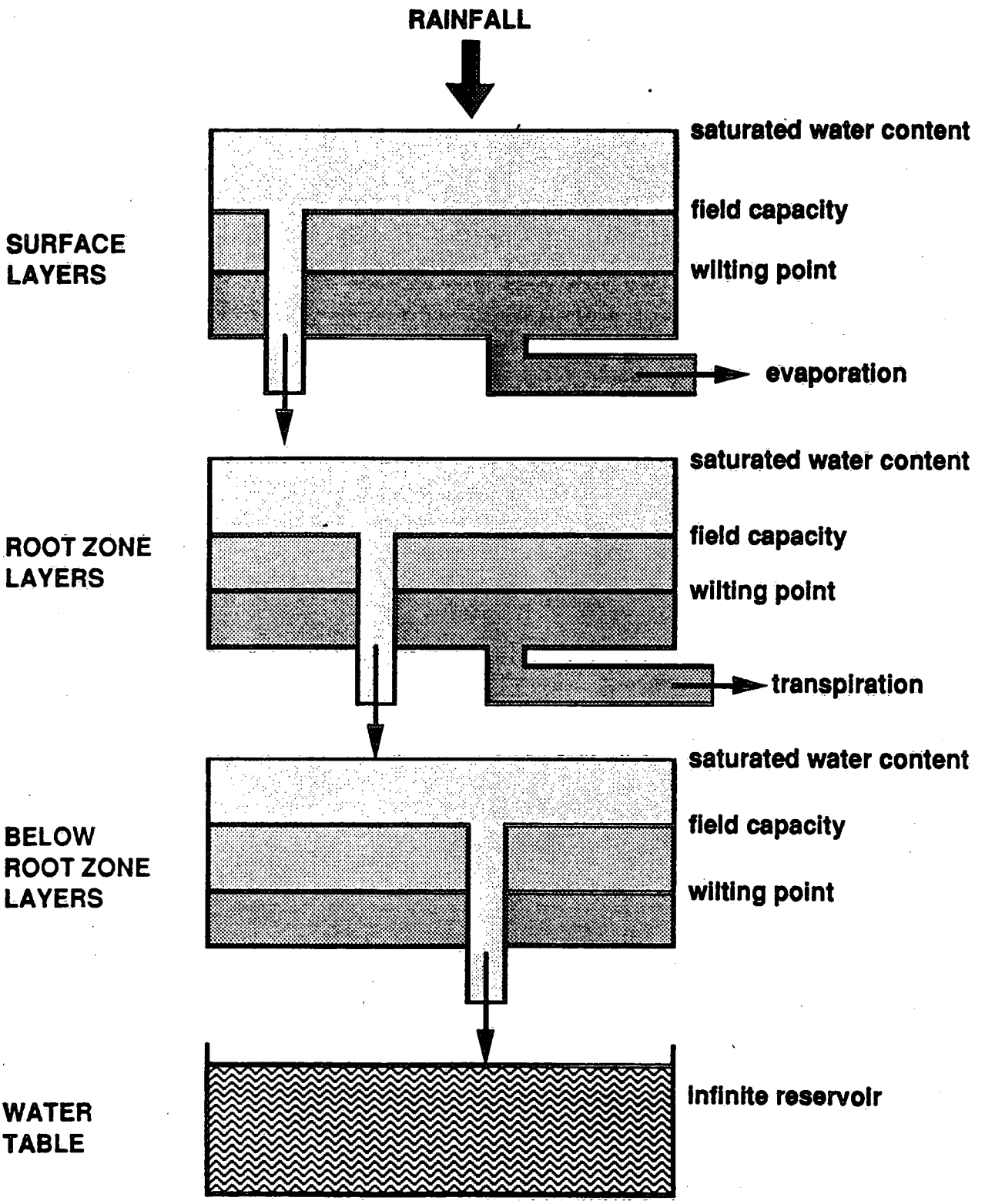

Figure 4. Representation of the flow of water within the PRZM model.

where:

$AWET_i$ = available water for evapotranspiration in soil compartment i,
WP_i = the water content of soil compartment i its wilting point.

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

SW_i is always $\geq WP_i$

Compartments below the root zone quickly reach, and are maintained at field capacity, simply flushing excess water in the compartment and eventually to the water table.

The transport of pesticides in the subsurface is calculated with a finite difference approximation to the solute transport equation (4.11). The soil water velocity term (v) and the water content term (Θ) are based on the lumped parameter description of the water balance given above.

$$\frac{\partial c\Theta}{\partial t} = \left(\frac{\partial D}{\partial z} \cdot \frac{\partial c\Theta}{\partial z}\right) - \frac{\partial (vc\Theta)}{\partial z} + S \qquad (4.11)$$

where:

c = the dissolved solute concentration,
Θ = the soil water content, ($\Theta = SW/\Delta z$)
D = the liquid diffusion/dispersion coefficient,
v = the soil water velocity, ($v = I * \Delta z/\Delta t$),
S = pesticide source/sink terms,
t = time, and
z = depth.

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, 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 daily pan evaporation data or is empirically estimated from the daily temperature. Plant uptake of pesticide is related to the transpiration rate in the model. 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 to 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 numerical solution of the equations is used to represent actual hydrodynamic dispersion. Execution times (on a COMPAQ 286-DESKPRO, with a math co-processor) for a one year simulation is less than ten minutes.

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

The main disadvantage of the PRZM model is the simplified approach to the transport of water and solute through the unsaturated zone. The processes are not described in as much detail as in the LEACHM model, however, execution times are considerably shorter and the amount of input data required by the model is not excessive and is generally available from existing data bases. Two disadvantages associated with PRZM are that the model does not account for surface volatilization losses of the pesticide and is restricted to the simulation of the parent pesticide only.

5. SELECTION OF A PESTICIDE TRANSPORT MODEL FOR THE PESTICIDE REGULATORY EXPERT SYSTEM

It is clear from a review of the available models that none of the models identified fully satisfies all the design criteria for the expert system. LEACHM is the most detailed of the models identified. Its description of the water balance is much closer to reality than is the simplified water balance descriptions in the other models and should therefore provide more accurate simulations. However, execution times with the LEACHM model are lengthy and runoff and erosion are not currently considered in the model.

PRZM is the best of the simplified water balance models. Its major advantages over the other simplified water balance models are that PRZM can handle layered soils effectively and also simulates transport below the root zone. In addition, it includes a description of surface runoff and erosion with very short and concise data requirements. The execution time of the PRZM model is much shorter than of the LEACHM model.

5.1 ADDITIONAL CRITERIA FOR MODEL SELECTION

The depth to which the models describe the processes involved the transport and transformation of pesticides in the unsaturated zone should be the primary concern. Because LEACHM is the most detailed of the models identified, it should be selected for the expert system. However, practical considerations may require a more expedient execution of the model and if the model is to be run a number of times to investigate possible "What If" scenarios, it may not be possible to use the LEACHM model. It was therefore decided that a second model should also be included in the expert system. PRZM, being the best of the simplified models, was chosen as the second model for the expert system.

It is intended that, based on general information supplied by the user, the expert system will make the decision of which model to run for a given simulation based on the objective of the simulation and the availability of data. If simulations are to be conducted to investigate several possible scenarios, the expert system will run the PRZM model to take advantage of the quick execution times. When a final set of conditions for the worst, or typical, case is determined the LEACHM model could then be run, and the results compared to those of earlier runs with the PRZM model.

Comparisons between LEACHM and PRZM results will be possible for sandy soils where the rate of water movement through the soil profile is fast. Jones (1989) quotes Hornsby as a reference in stating that the differences between the LEACHM and PRZM models will not be significant in sandy soils.

Larger differences between predicted results for the two models will however, occur in heavier soils where the infiltration process is much slower. The expert system will suggest that results from the LEACHM model should be used when soil properties suggest a heavy soil with slow infiltration.

The inclusion of the PRZM model is also important in that it is a U.S. EPA code. Decisions made by Canadian regulatory personnel will have to be supported and defended by comparing to results to those from the U.S. EPA regulatory process. Using PRZM in the expert system will provide for these comparisons without the need for running a U.S. EPA code outside the expert system for comparison purposes.

5.2 MODIFICATIONS TO THE EXISTING MODELS

The possibility of making modifications to the two models will be investigated. A concern of pesticide regulatory personnel is that as the models now stand, all use first-order kinetics to describe the degradation of pesticides in the soil. In reality, the raw data supplied to the Pesticide Division by the pesticide manufacturers, indicates that the degradation process does not generally conform to this first-order assumption. Two possible modifications will be investigated to deal with this concern. First, an additional subroutine

may be added to the expert system that will accept the raw data supplied to the Pesticide Division and the subroutine will then generate a degradation equation based on this data. The second alternative would be to allow the model to run initially for a short period of time (one or two days) with a first order reaction constant representing an initial fast degradation and then switch the rate constant to a slower degradation rate for the remainder of the simulation period.

A number of modifications may be made to the models individually. A runoff and erosion subroutine may be added to the LEACHM model while surface volatilization and mass balancing for degradation products may be added to the PRZM model.

6. CONCLUSION

The prevention of ground water contamination by agricultural pesticides requires a through assessment of the fate of the pesticides in the subsurface before they are registered for commercial use. With the complexity of the processes that control the fate of pesticides in the subsurface, it is necessary to use sophisticated computer models to simulate the transport and transformation of the pesticides in the subsurface. However, regulatory personnel assigned the task of preforming this assessment generally do not have experience in the use of these models and do not have access to the specialized data sets required by the models.

The construction of an expert system to bridge the gap between regulatory personnel and the pesticide transport models has been proposed. Fifteen pesticide transport models available for inclusion in the expert system were reviewed and analyzed for their applicability to the expert system. Of the 15 pesticide models identified two models, LEACHM and PRZM, were chosen for the incorporation in the expert system. Both models are one-dimensional, finite difference representations and simulate advective and dispersive transport, adsorption, degradation, plant growth and uptake and evaporation.

LEACHM was the most advanced model identified, describing the processes involved in greater detail than in the other models. For example, LEACHM uses a direct solution to Richards equation for water flow and is capable of following the fate of two daughter products in addition to the parent pesticide. However, execution times with LEACHM were much longer (>30 times) than simulations with the other models and LEACHM does not include surface runoff or erosional losses.

PRZM offers advantages that are lacking in the LEACHM model. The model includes a concise description of surface runoff and erosion and execution times with the model are much faster. PRZM is a U.S. EPA code and will therefore provide results that are comparable with regulatory studies performed in the U.S. This comparison will be required to support and defend any decisions made by Canadian regulatory personnel.

With the inclusion of the two models in the expert system, it is intended that based on introductory information provided, the expert system will decide which model will be run for the desired simulation.

The selection of the two models for the expert system brings to an end the work conducted for Phase 1 of the project. Work will now commence on Phase 2 of the project, which will see the construction of the basic framework for the expert system.

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RRB-89-88

PHASE ONE REPORT
A REVIEW AND ANALYSIS EXISTING PESTICIDE TRANSPORT AND TRANSFORMATION MODELS

by
J.P. Mutch
and
A.S. Crowe

Rivers Research Branch
National Water Research Institute
Canada Centre for Inland Waters
Burlington, Ontario, Canada
L7R 4A6

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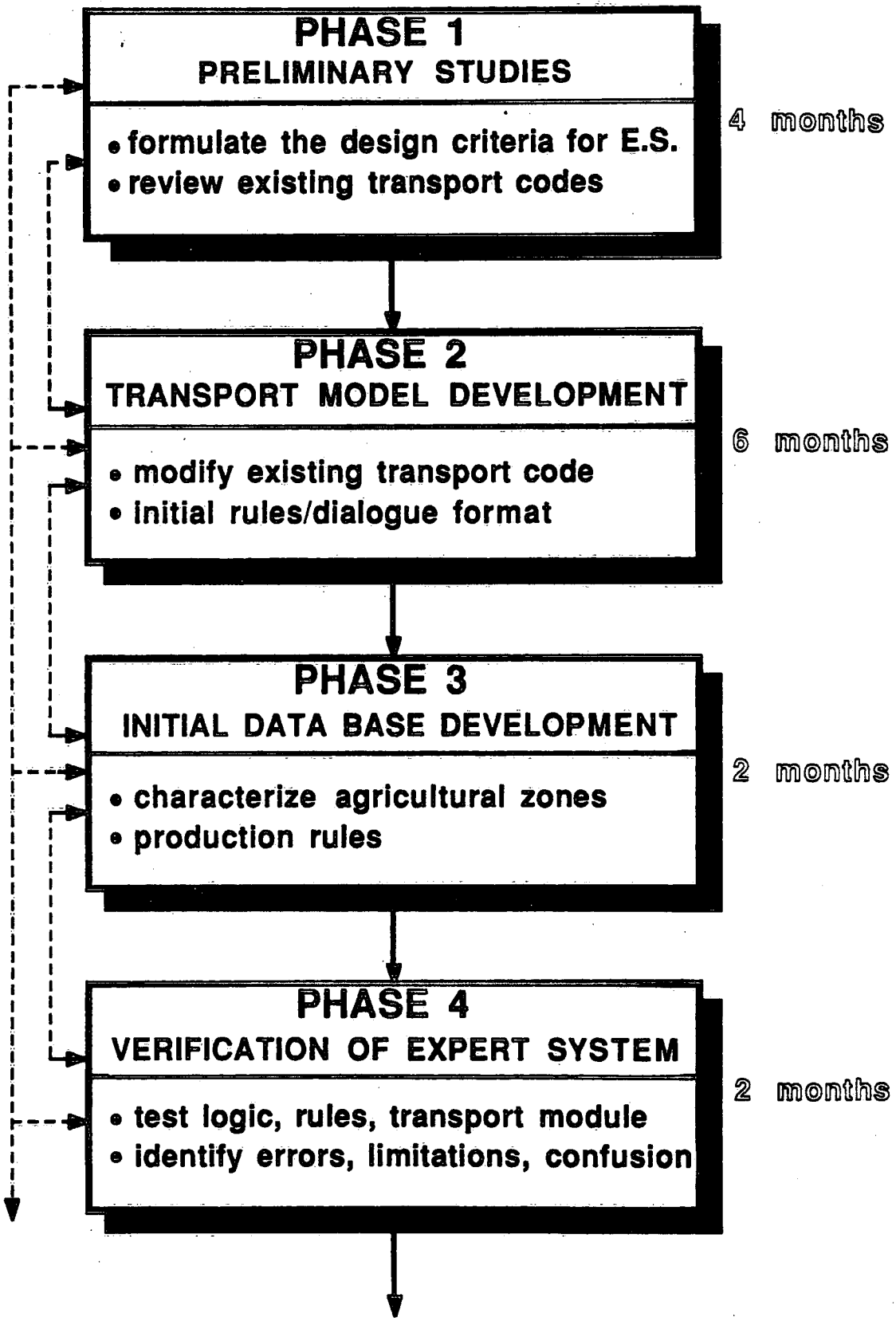
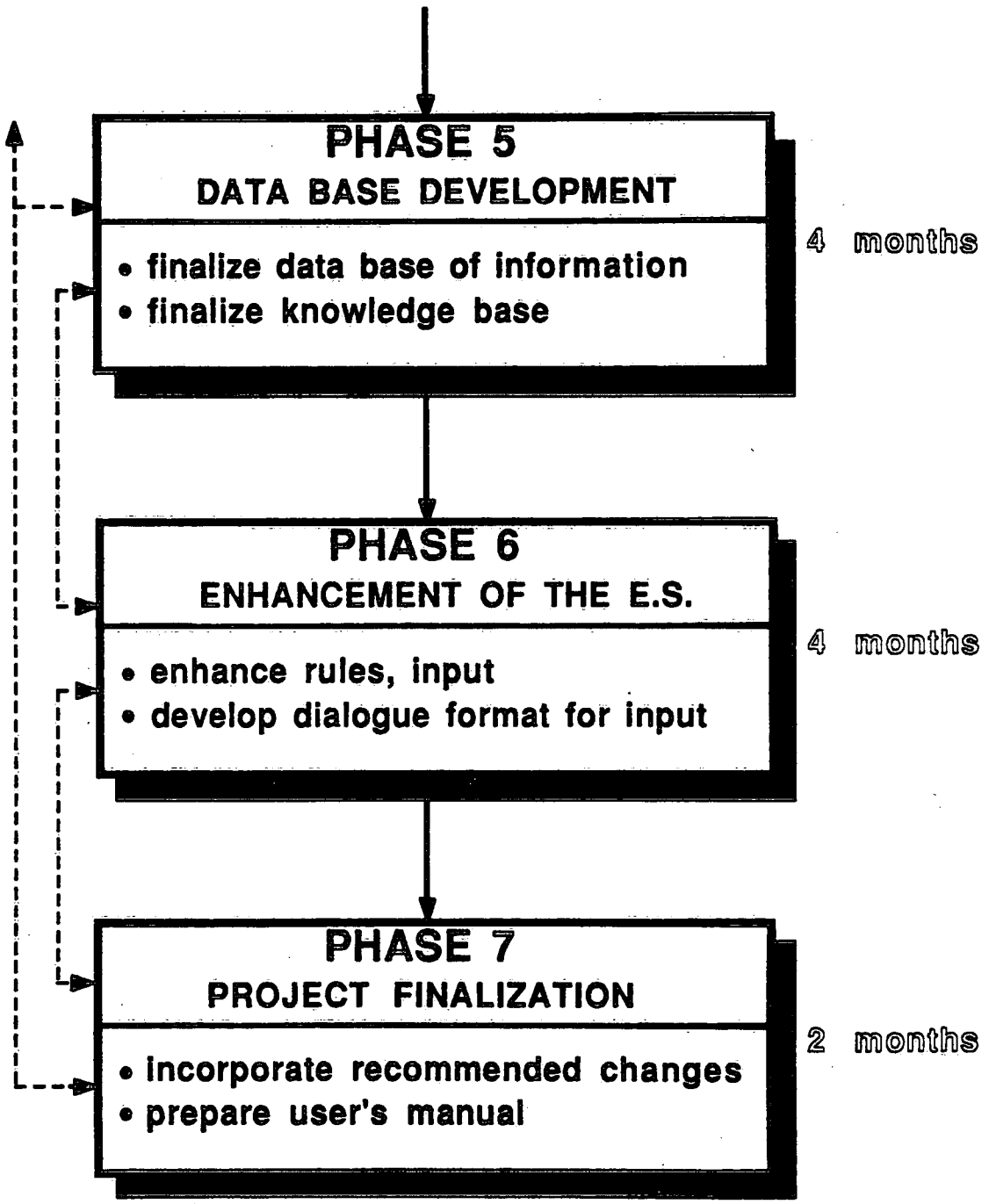
NWRI Contribution #89-172

APPENDIX A

PROJECT SUMMARY



Project summary: for the developement of the expert system. .



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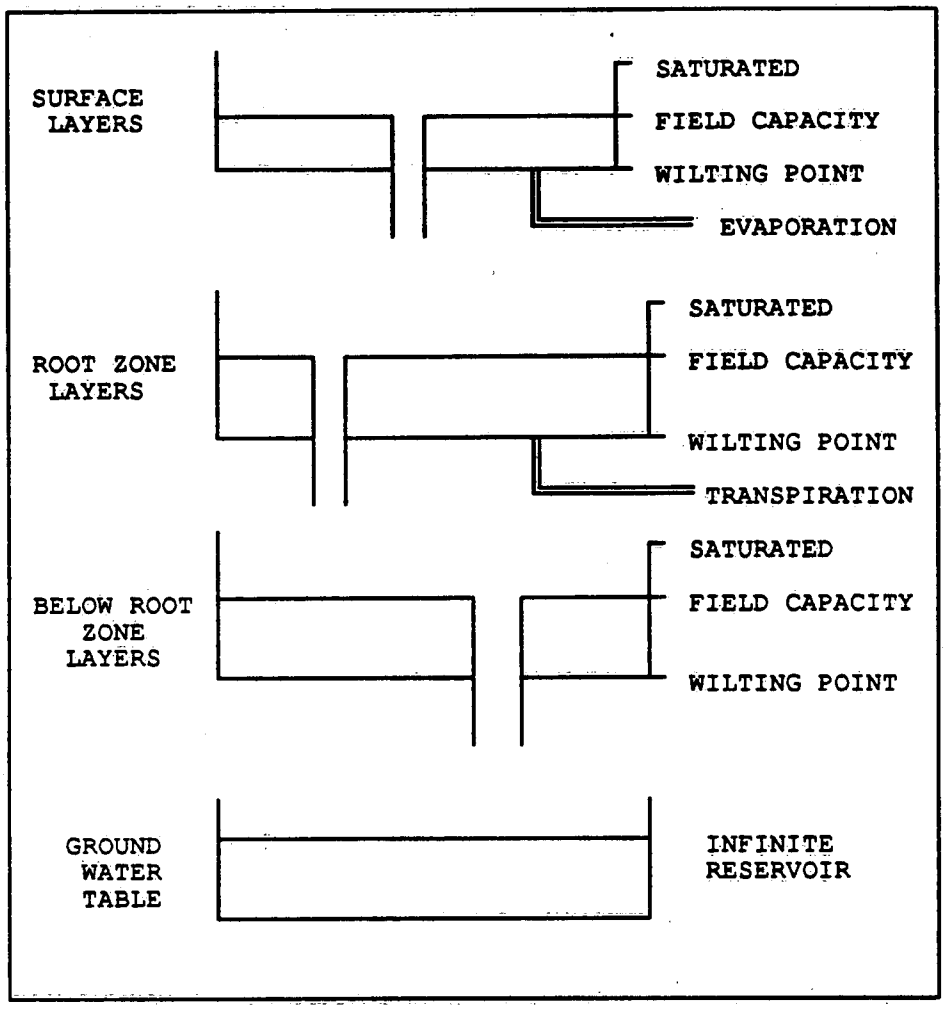

Figure 4. Representation of the flow of water within the PRZM model.

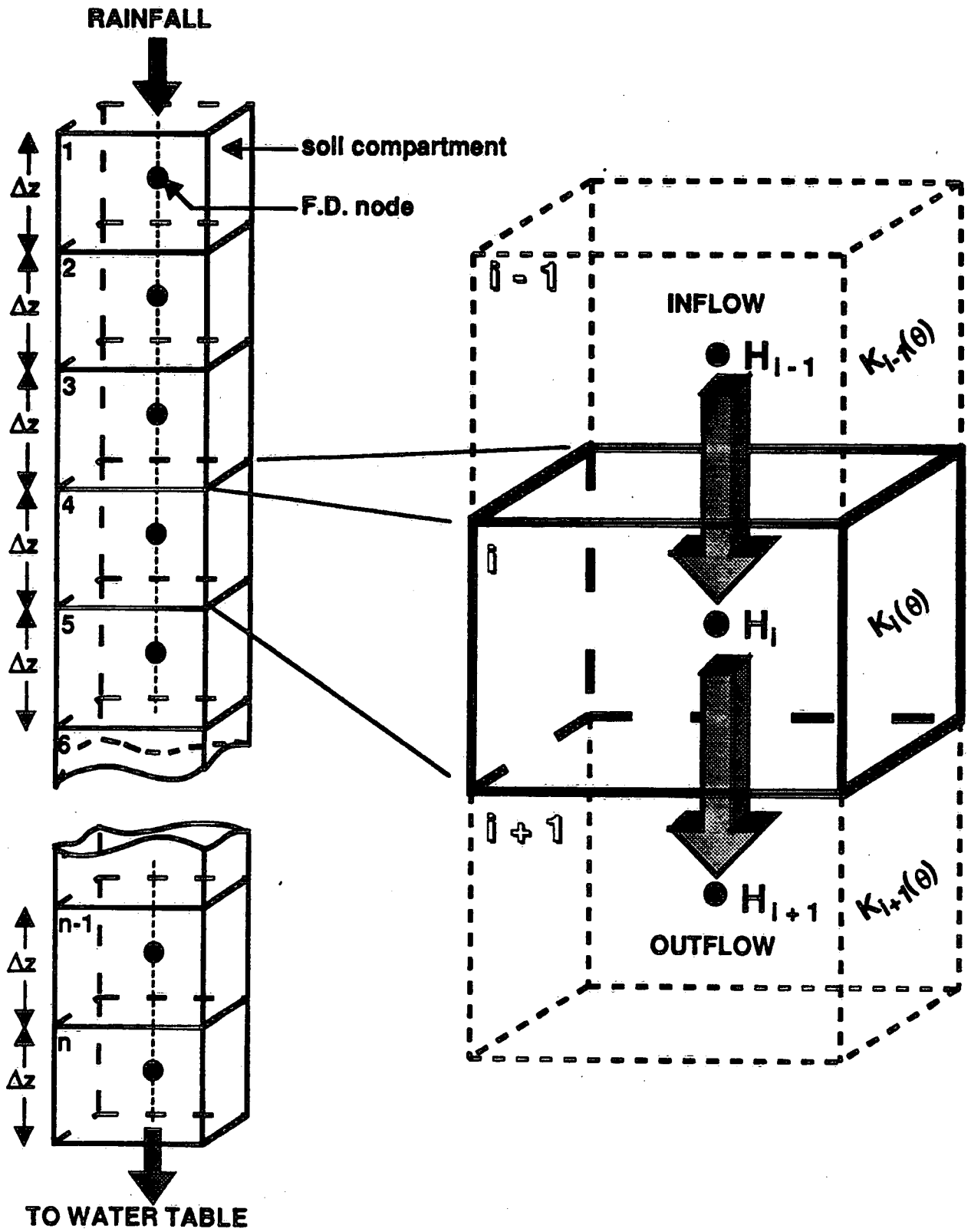

Figure 3. Representation of the flow of water within the LEACHM model.