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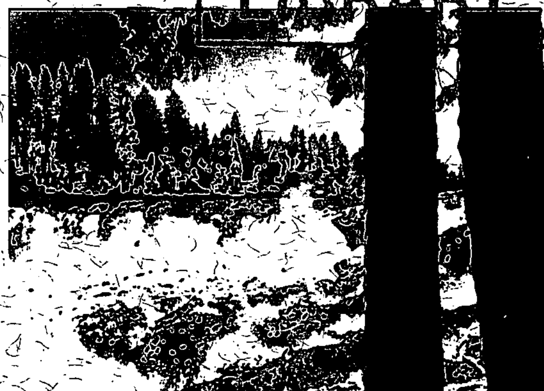
# EXPRES: An Expert System for Assessing the Fate of Pesticides in the Subsurface

## Users' Manual

J.P. Mutch, A.S. Crowe and O. Resler





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NATIONAL WATER RESEARCH INSTITUTE
CANADA CENTRE FOR INLAND WATERS
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# Abstract

The EXPRES expert system is designed to aid regulatory personnel in their assessment of the potential for pesticides to contaminate the soil and shallow groundwater environment. EXPRES (EXpert system for Pesticide Regulatory Evaluations and Simulations) consists of one screening assessment and two mathematical simulation models. The screening assessment model (LP/LI) allows users to perform a quick and general assessment of the relative potential for a particular pesticide to contaminate shallow groundwater. The two mathematical models (PRZM and LEACHM) simulate the transport and transformation of pesticides in the unsaturated zone. EXPRES couples these pesticide models to a knowledge-based system that guides users through the choice of all the information required to execute the models and assists them in the interpretation of the predicted results. The information required by the models consists of data that characterize the physical, hydrogeological, pedological, and meteorological characteristics of the agricultural regions being simulated. EXPRES includes a data base that contains the data required by the models to characterize 22 typical agricultural regions across Canada. This report discusses the EXPRES expert system and will serve as a users' manual for the expert system.

# Résumé

Le système expert EXPRES devrait aider le personnel chargé de la réglementation à évaluer, pour les pesticides, le potentiel de contamination des sols et de la nappe phréatique peu profonde. EXPRES (EXpert system for Pesticide Regulatory Evaluations and Simulations) comprend un modèle d'examen préalable et deux modèles de simulation mathématique. Le modèle d'examen préalable (LP/LI) permet à l'usager d'effectuer, pour un pesticide donné, une évaluation rapide et générale du potentiel relatif de contamination de la nappe phréatique peu profonde. Les deux modèles mathématiques (PRZM et LEACHM) simulent le transport et la transformation des pesticides dans la zone non saturée. Ces modèles sont associés à une base de connaissances qui guide l'utilisateur dans le choix des données nécessaires à l'exécution des modèles et l'aide à interpréter les résultats prévus par le système. L'information requise pour les modèles comprend des données caractérisant les conditions géologiques, physiques, climatiques, hydrogéologiques, pédologiques et agricoles du site faisant l'objet d'une simulation. Le système EXPRES comporte une base de données contenant l'information nécessaire aux modèles pour caractériser 22 régions agricoles types au Canada. Le présent document traite du système EXPRES et servira ainsi de guide de l'utilisateur.

# Introduction

Pesticides are, by design, poisons that are deliberately introduced into the environment to kill target plants or organisms. The use of pesticides will enhance both crop quality and production through the control of harmful pests. However, there are environmental risks associated with the use of pesticides. Several studies focusing on the transport and transformation of the pesticide aldicarb in the subsurface (Zaki et al. 1982, Jones 1985, Harkin et al. 1986, Jones and Marquardt 1987, Jones et al. 1987, Priddle et al. 1987 and 1988) provide strong evidence that pesticides can cause groundwater contamination, even when the recommended application procedures are followed. The implications of this finding are of particular concern in rural areas, where 82% of rural Canadians rely on groundwater as a source for their domestic water supply (Hess 1986). It is in these rural areas that the potential for groundwater contamination by pesticides is greatest, because of the widespread use of pesticides in these areas.

Currently, all pesticides used in Canada undergo extensive testing before their registration to ensure that they, and their degradation products, present minimal risks to the environment (Crowe and Mutch 1990). However, a greater emphasis must be placed on the prevention of the contamination of groundwater by pesticides because of (1) the potential health risks associated with the ingestion of pesticide-contaminated groundwater, (2) the potential extent of the problem, and (3) the impracticality of remediating a contaminated groundwater resource. Therefore, regulatory personnel must be given the means of more accurately assessing the fate of a pesticide in the subsurface during the registration process, before the release of the pesticide for public use.

Pesticide assessment models capable of simulating the fate of pesticides in the subsurface are currently available, and would aid regulatory personnel in their assessment of the potential impact of a pesticide on the subsurface environment. However, the application of many of these pesticide models within a regulatory framework has been limited because (1) the assessment models generally require the user to have a specialized knowledge of the physical, chemical, and biological processes controlling the transport and transformation of a pesticide in the unsaturated zone, (2) the numerical framework upon which the models are based is often complex and typically can be operated only by a trained modeller, (3) the models require a specialized set of physical and chemical data that are not generally obtained during typical field or laboratory studies, and (4) there is currently no means of ensuring that the input data supplied to the pesticide models, and the results calculated by these models, are accurate and meaningful. Thus, there is a need to find a solution that will allow regulatory personnel to use these pesticide models accurately and efficiently in the assessment of the impact of a pesticide on groundwater quality. The development of an expert system approach to assessing the potential for groundwater contamination with these models provides a method for overcoming many of these problems.

This report describes an expert system that was developed by the Groundwater Contamination Project of the National Water Research Institute for the Pesticides Division of the Commercial Chemicals Branch of Environment Canada. The expert system has been named EXPRES (EXpert system for Pesticide Regulatory Evaluations and Simulations). EXPRES allows regulatory personnel to use existing pesticide models to help them assess the potential environmental risks associated with new pesticides seeking registration. The description of the structure and operation of the expert system that is provided in this manual is specific to EXPRES Version 2.1 (February 1993).

To assess and/or simulate the fate of pesticides in the subsurface, one must first become familiar with the various physical, chemical, and biological processes that influence the mobility, persistence, and retention of a pesticide in the unsaturated zone. Chapter 2 presents a brief overview of these principles. Chapter 3 provides an overview of pesticide models that are capable of assessing the potential impact of a pesticide on the subsurface environment. The selection criteria used in choosing the pesticide models incorporated into the EXPRES expert system are also discussed, and an overview of the three pesticide assessment models included in EXPRES is presented. Chapter 4 is a summary of the conceptual framework of expert systems, including the methods used in encoding domain-specific knowledge. The structure and operation of EXPRES are discussed in Chapters 5 and 6, respectively. Chapter 7 discusses simulations undertaken with EXPRES showing different applications for the expert system. The conclusions and recommendations drawn from the project are presented in Chapter 8. The contents of this report will provide the reader with information on the operation of EXPRES, and on the types of analyses that are possible with the expert system.

# Theory of Pesticide Transport and Transformation in the Unsaturated Zone

Simulating the transport and transformation of a pesticide in the unsaturated zone is a difficult task because many physical, chemical, and biological factors control the fate of pesticides there. These factors can generally be categorized as either transport processes (processes and mechanisms that transport the pesticide and its degradation products through the unsaturated porous medium) or attenuation processes (processes that act to attenuate or retard the movement of the pesticide). A review of these processes is provided in this chapter.

## TRANSPORT OF PESTICIDES IN A POROUS MEDIUM

The three primary mechanisms involved in the transport of pesticides are advection (mass flow), solute diffusion/dispersion, and 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 water table. The second mechanism, solute diffusion/dispersion, accounts for chemical and mechanical mixing of the pesticide in solution as it moves through the porous media in the subsurface. Diffusion/dispersion has the net effect of spreading the pesticide over a larger area, thus decreasing concentrations at the centre of mass of the pesticide. However, this tends to increase concentrations at the outer edge of the contaminate plume. The third mechanism, vapour diffusion, acts in a manner similar to that of solute diffusion, and is an important process for highly volatile pesticides in contact with air.

Secondary processes such as surface runoff and erosion 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 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 primary mechanisms is expressed in the solute transport equation

$$\frac{\partial(c \cdot \theta)}{\partial t} = -\frac{\partial(q \cdot c)}{\partial z} + \frac{\partial}{\partial z}[D_d(\theta,v) \cdot \frac{\partial c}{\partial z}] \pm \eta(z,t) \qquad (1)$$

where c is the dissolved solute concentration, $\theta$ is the water content of the soil, q is the water flux across a unit area per unit time, $D_d(\theta,v)$ is the diffusion/dispersion coefficient, v is the average linear groundwater velocity, z is the depth, t is the time, and $\eta(z,t)$ is a source/sink term that accounts for the processes that act to attenuate the migration of the pesticide. A derivation of this equation can be found in Hillel (1980b).

The bulk flow of water is the primary factor in determining the velocity with which a pesticide is transported in the unsaturated zone. The flow of water in the unsaturated zone, as 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 (subatmospheric) pressure potentials arising from the affinity of water for the surfaces of the soil particles. The negative suction potentials ($\phi$) that arise are generally reported as equivalent positive values and are referred to as matric suction ($\psi$), signifying that a positive matric suction value actually represents a negative matric potential ($-\phi = \psi$). With this convention in mind, the flow of water in the unsaturated zone occurs from areas of low matric suction to areas of high matric suction. In the unsaturated zone, water is transmitted both in the pores that are saturated at a 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. At the transition point between saturated and unsaturated conditions, capillary forces holding the water in the pores of the soil are exceeded as suction forces develop. Water in the largest, most conductive pores is the first to drain. As suction forces continue to develop, the capillary forces in successively smaller pores are exceeded, and they in turn drain, further reducing the size of the conductive pathways for the flow of water. This has the effect of reducing the hydraulic conductivity of the soil ($K(\theta)$). To complicate matters further, the conductivity relationship (relating $K(\theta)$ to $\psi$) is hysteretic, with different curves for wetting and drying fronts. The same phenomenon is observed in the retentivity curve that relates the matric suction of a soil to its volumetric soil-water content.

The conductivity and retentivity curves, discussed above, are complex for a given soil. However, simplified empirical relationships have been developed for the conductivity and retentivity curves by measuring the relationship between $K(\theta)$ and $\psi$, and between $\theta$ and $\psi$ in the laboratory and under field conditions (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 advective transport of a pesticide is controlled by the distribution of the hydraulic head (h) within the subsurface. The equation that describes the distribution of the hydraulic head and water content in the unsaturated zone is known as Richards equation. Richards equation couples the continuity equation (conservation of mass) with Darcy's Law, and is given by

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K(\theta) \cdot \frac{\partial h}{\partial z}\right) \pm \eta(z,t) \tag{2}$$

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

## ATTENUATION OF PESTICIDES

The source/sink term, $\eta(z,t)$, in Equation 1 represents several processes that act to attenuate the transport of pesticides in the subsurface. Attenuation of a pesticide can occur as the result of the following three groups of processes: (1) partitioning of the pesticide, (2) transformation or degradation of the pesticide, and (3) plant processes. A general description of these processes follows.

### Partitioning of the Pesticide

Partitioning of a pesticide between its dissolved and solid phase occurs by the adsorption of the dissolved pesticide onto the surface of soil minerals and/or organic matter present in the soil matrix. The processes involved in the adsorption of organic chemicals (in this case, 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).

For pesticides, it is often assumed 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 pesticide concentration, c, by a distribution (or partition) coefficient, $K_D$.

$$c_s = K_D \cdot c \tag{3}$$

The amount, composition, and cation exchange capacity of the clay fraction strongly affect the adsorption of pesticides with permanent positive charges (such as paraquat and diquat). However, no correlation has been observed between the percent clay and the amount of nonpolar organic adsorption (Jury 1986). A positive linear relationship does, however, exist between the organic carbon content of a soil and the adsorption of organics (i.e., pesticides) to that soil (Jury 1986). The distribution coefficient, $K_D$, is related to the amount of organic carbon present in a soil (Karickhoff et al. 1979). The relationship is represented by

$$K_D = K_{oc} \cdot f_{oc} \tag{4}$$

where $K_{oc}$ is the 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 $f_{oc}$ is the fractional organic carbon content in the soil.

Jury (1986) reviews the practical limitations of using these adsorption representations. 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 .5 ppb 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 compounds studied (aromatic and chlorinated hydrocarbons) at 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 remaining sorbed to the soil particles (and out of the aqueous phase) tends to be higher than that predicted by these adsorption models.

Another 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 dissolved and gaseous phases. Dissolved-vapour phase partitioning is similar to the dissolved-solid partitioning of the pesticide. The concentration of the pesticide in the gaseous phase, $c_g$ (also known as vapour density), is linearly related to the pesticide concentration in the dissolved phase, c, by Henry's Law:

$$c_g = H \cdot c \tag{5}$$

where H is a dimensionless partition coefficient known as Henry's Law constant.

**Transformation Processes**

The processes controlling the transformation of pesticides in the unsaturated zone are of importance in determining persistence and hence the contamination potential of the pesticide. Even if the physical processes are in place to transport a pesticide to the water table, the pesticide will not be considered as a 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 nonpersistent 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 chemical must be given sufficient mobility during its effective lifetime in the subsurface environment to move it through the soil profile to the water table. As the persistence of a pesticide increases, the timing of rainfall and/or irrigation events becomes less critical in determining the contamination potential of the pesticide.

Transformation processes encompass both chemical and biological processes that control the fate of a pesticide. These processes may be either biologically or nonbiologically mediated. Biologically mediated processes are catalyzed by enzymes and include processes such as biologically mediated hydrolysis and oxidation-reduction (redox) reactions. The chemical reactions tend to occur at faster rates in the surface and root zone layers, where microbial populations are higher, than they do at greater depths, where the microbial population tends to decline significantly (Jury and Valentine 1986). Significant factors influencing biologically mediated processes are those that act to control both the availability of the substrate and the size and activity of the microbial population. Nonbiologically mediated processes include strictly chemical and photochemical reactions. Chemical hydrolysis and redox reactions may also occur without the aid of biological catalysts, while photochemical reactions require the adsorption of light (photons) to catalyze the reactions. Photochemical reactions are therefore only potentially important at and/or near the soil surface. Thus, pesticides incorporated in the soil are not significantly affected by these reactions (Valentine 1986).

Difficulties arise when trying to determine the degradation and/or transformation rates 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 a pesticide in the soil. It is possible that the disappearance of a portion of the pesticide may be misinterpreted as a transformation loss when the disappearance may be due to other processes (e.g., bound chemical residues). In such a case, the rate constants will be overestimated.

Most mathematical representations of degradation and transformation are greatly simplified. The processes discussed above are lumped together and represented as either first-order or second-order rate reactions that account for the overall effective disappearance of a pesticide. First-order equations are 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 over time. Measurements of the active microbial biomass are often required in the determination of the second-order rate constants for biotic processes, and are more difficult to obtain.

The limitations imposed by these rate constants must be recognized. The assumptions and simplifications inherent in the determination of these rate constants prevent their use from providing anything more than an empirical approximation. First-order equations, considering only the chemical concentration of the pesticide, 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) provides a more accurate and less site-specific result. The determination of rate constants is often performed in the laboratory, where conditions are controlled. However, these conditions may vary greatly from those found in the field. Closer approximations will result if the rate constants are determined under conditions that closely resemble those found in the field.

**Plant Processes Influencing Pesticide Transport**

The processes affecting the fate of a pesticide in the soil (i.e., transport, sorption, and transformation of solutes) also occur within the plant (Donigian and Rao 1986). 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, that are dissolved in the soil water are taken up with the soil moisture by either passive or selective processes. 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 of pesticide withdrawn to the transpiration rate may not be appropriate in some instances. Although the understanding of these processes is incomplete, it is well known that the extraction of water and the uptake of 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 cause the flux of water and pesticide to reverse in the root zone, drawing the pesticide back towards the surface.

# Pesticide Assessment Models

Pesticide assessment models have developed along two paths, and as a result can be classified into two broad categories, as either screening or mathematical models. The two categories vary widely according to (1) the approach taken for an assessment, (2) the level of detail incorporated into the descriptions of the processes controlling the fate of pesticide in the subsurface, and (3) the intended use of the models. Screening models provide a relative assessment of the leaching potential of a pesticide or site (i.e., relative to other pesticides or sites). Mathematical models simulate the processes controlling the migration and transformation of pesticides in the subsurface. The general characteristics of models included in the two categories are discussed in this chapter.

## SCREENING MODELS

Screening models are elementary models that make use of a few of the physical characteristics of a site and/or chemical properties of a pesticide to provide a quick and general assessment of the potential for groundwater contamination by a pesticide. The assessment is made on a relative basis. Most screening models operate by comparing two or more chemical characteristics of a pesticide with the properties of other pesticides that are known to have caused groundwater contamination. Screening models may also compare the hydrogeologic properties of a site to other sites where the contamination of the groundwater is known to have occurred. Screening models do not use complex mathematical representations for the processes that are occurring in the subsurface, and therefore they do not simulate the transport and transformation of a pesticide. As a result, screening models are unable to quantify the amount of pesticide that leaches or the rate at which it leaches to the water table. Screening models can be subdivided into three groups based on the information that is required for an assessment (Fig. 1). A description of each follows.

### Group 1: Site Assessment Models

Group 1 screening models assess the vulnerability of a site to groundwater contamination by pesticides, based solely upon the physical characteristics of the site. The models provide only a relative indication of whether an area is more susceptible to groundwater contamination than another area. Group 1 screening models consider only one aspect of the potential for contamination (i.e., the hydrogeological characteristics of the site). Because they do not consider any of the properties of the pesticide, they cannot

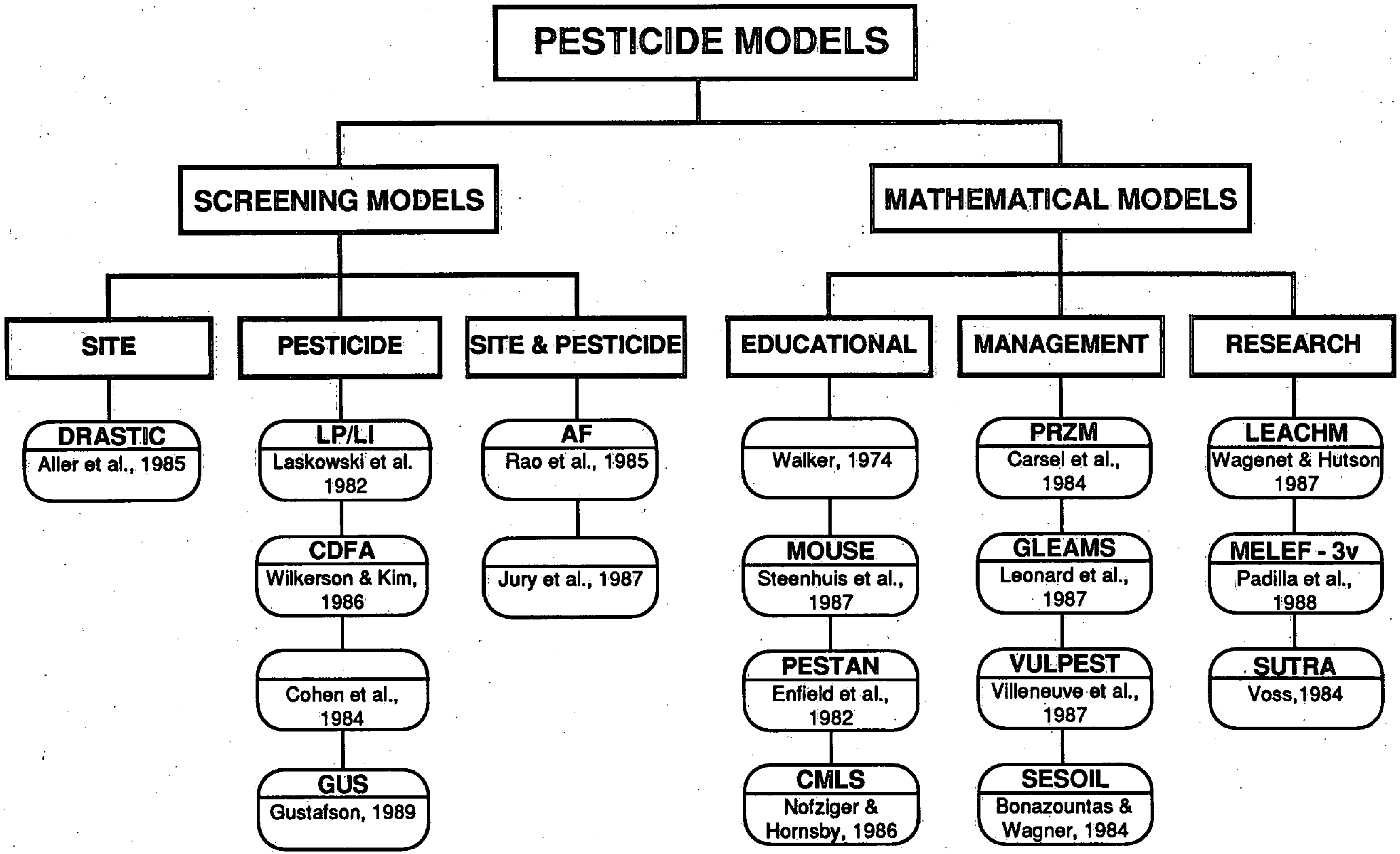



Figure 1. Classification of pesticide assessment models.

specifically indicate whether the application of a given pesticide has the potential to result in groundwater contamination or not. Because the models do not consider the specific properties of the pesticide, the vulnerability assessment is performed, in effect, assuming the pesticide is a highly soluble, nondegrading, nonadsorbing chemical (a "worst-case" scenario). In reality, however, the adsorption and degradation of a pesticide generally have a significant effect on the amount of pesticide that leaches and the rate at which it leaches to the water table. For example, even if the physical conditions exist to transport a pesticide to the water table, the pesticide will not contaminate the groundwater if it degrades or volatilizes to a sufficient extent before reaching the water table. In essence, these models only assess the presence, or lack thereof, of the physical characteristics that would make a site susceptible to groundwater contamination. Group 1 screening models are most applicable for use in preliminary groundwater contamination susceptibility mapping, where no specific pesticide has yet been identified for investigation.

### Group 2: Pesticide Assessment Models

Evaluations undertaken with Group 2 screening models are based solely upon the chemical properties of the pesticide, and generally indicate if a pesticide is likely to be a "leacher" or "non-leacher." Group 2 screening models provide only a relative assessment (with respect to other pesticides) of the potential for a given pesticide to leach to the water table. In effect, assessments with the Group 2 models assume that the site is homogeneous, permeable, with a significant amount of infiltration, and a fairly shallow water table (most favourable case for the leaching of a pesticide). Without considering any characteristics of the site where the pesticide may be applied (e.g., clayey soil vs. sandy soil; high recharge vs. low recharge), Group 2 models cannot indicate which sites may be susceptible to groundwater contamination. However, a relative ranking of pesticides provides valuable information. If a pesticide has a greater tendency to cause groundwater contamination at one site than other pesticides, it will generally also have a greater tendency to leach to the water table at other sites with different environmental conditions. Group 2 screening models are most applicable when a general assessment of the relative leaching potential of a particular pesticide is desired with respect to a large number of existing pesticides.

### Group 3: Site and Pesticide Assessment Models

The fate of pesticides in the subsurface, and therefore the potential for groundwater contamination at a specific site, is a function of both the physical characteristics of the site and the chemical properties of the pesticide. The third group of screening models considers both in assessing the potential for a pesticide to cause groundwater contamination problems at a particular site. Group 3 models could be used to (1) rank several pesticides at a given site, (2) rank several sites with respect to one particular pesticide, or (3) rank both a pesticide and site with respect to other pesticides used at other sites. This group of screening models provides a more accurate screening assessment of the potential of a given pesticide to contaminate the groundwater in a particular area. However, these models require considerably more data (both for the pesticide and the site) than do the models in the previous two groups. Due to the limiting assumptions upon which these screening models are based, they can provide only a relative ranking of the potential for groundwater contamination and cannot predict the severity or timing of the contamination.

## SELECTION OF A SCREENING MODEL

Screening models, by the nature of their design, contain limitations that restrict the type of assessment that can be undertaken. Specifically, these models

- do not simulate the processes involved in the transport and transformation of a pesticide in the unsaturated zone
- cannot predict pesticide concentrations at, or leaching rates to, the water table
- do not provide concentration profiles with time and/or depth
- assess pesticides only as a relative ranking and hence, will not indicate whether contamination is likely to occur at a specific site
- do not consider all environmental factors affecting the fate of pesticides (e.g., dispersion, soil pH, temperature)

However, screening model assessments offer several advantages that are not typically associated with models that simulate the processes controlling the fate of pesticides in the unsaturated zone. Specifically, these models

- can be used with ease and speed to assess the potential for groundwater contamination
- require few data, ones that are generally available from existing databases
- can be used by people without hydrogeological or contaminant expertise

These advantages make screening models attractive in certain situations. They may also be used to narrow the scope of a large investigation by identifying, and directing attention to, areas or pesticides that warrant additional study with more sophisticated models and/or field studies. These models may also be useful in prioritizing a proposed groundwater quality sampling program, or when insufficient data are available to justify the use of more complex models. In addition, a screening model assessment may be preferable to the assessment provided by a more complex mathematical model if only a general assessment of the potential for a pesticide to leach to the water table is required, or a determination of the susceptibility of a site to groundwater contamination. Their use is also preferable if the assessment of numerous sites and/or pesticides must be completed very quickly. A decision was made to incorporate a simple screening assessment model into EXPRES to make use of the advantages inherent in these models. This allows the user of EXPRES to overcome the limitations imposed by the more complex mathematically based models in certain circumstances. The screening model can be used within EXPRES as a preliminary evaluation step to determine whether a detailed investigation with the more mathematically complex model is warranted.

Seven pesticide screening models (Fig. 1) were identified and reviewed in Mutch and Crowe (1989) and Crowe and Mutch (1991a) for their possible inclusion in the EXPRES expert system.

Regulatory personnel using EXPRES will be responsible for assessing the potential detrimental effects associated with a pesticide on the groundwater environment in a number of locations across Canada. The intent is not to assess the potential vulnerability of a particular site, since there are potentially thousands of sites across the country where the pesticide will be used, but to assess the relative potential of a pesticide to leach to the water table. Thus, the ranking provided by the Group 2 screening models (based solely on the properties of the pesticide) is applicable to all sites on an equal basis. This provides a more useful assessment for regulatory personnel than would either a Group 1 or Group 3 screening model assessment, which would be focused on the environmental conditions found at a particular site. Therefore, a Group 2 screening model was incorporated into EXPRES.

In evaluating the Group 2 models, it was determined that the CDFA-based models (CDFA, GUS, and Cohen et al. 1984) were of limited value for fulfilling the objectives of EXPRES. First, they simply rank the pesticides either as "leachers," "potential leachers," or "non-leachers," and second, they do not consider all the important fundamental chemical properties of the pesticide (e.g., vapour pressure or aqueous solubility) that affect the amount of pesticide that can leach to the water table. The LP/LI screening model (Laskowski et al. 1982) was considered to be the most appropriate model for inclusion in EXPRES. A short description of the model follows.

## The LP/LI Model

The LP/LI model (Laskowski et al. 1982) is a simple two-part screening model. It provides the user with a quick, and general, assessment of the potential for a pesticide to contaminate groundwater on a relative basis (with respect to other pesticides). The LP/LI model was chosen for incorporation into EXPRES for two reasons. First, it assesses the leaching potential of the pesticide solely on the basis of four chemical properties of the pesticide that influence its migration and transformation within the subsurface environment (i.e., organic carbon partition coefficient, pesticide half-life in soil, vapour pressure, aqueous solubility). Second, the model calculates a "ranking score" for the pesticide based on the values supplied for the four chemical properties of the pesticide. A relative assessment of the potential for the pesticide to leach to the water table is provided by comparing the ranking score of the test pesticide to those of other pesticides whose leaching histories are known.

The LP/LI model performs two assessments of the pesticide. The first, a leaching potential (LP) assessment, is a relative measure of the potential for the pesticide to leach to the water table. The second, a leaching index (LI) assessment, is a relative measure of the potential migration distance of the pesticide prior to its degradation in the subsurface. The equations used to calculate the ranking scores are

$$LP = S / (V_P \cdot K_{oc}) \tag{6}$$

$$LI = (S \cdot t_{1/2}) / (V_P \cdot K_{oc}) \tag{7}$$

where S is the aqueous solubility of the pesticide, $V_P$ is the vapour pressure of the pesticide, $t_{1/2}$ is the half-life of the pesticide in soil, and $K_{oc}$ is the organic carbon partition coefficient. As the ranking score of a pesticide increases, the potential for the pesticide to contaminate groundwater also increases.

The LP/LI model does not consider any of the characteristics of the site (e.g., clayey soil vs. sandy soil, high recharge vs. low recharge). Therefore, it cannot indicate whether the use of a given pesticide will actually have the potential to cause groundwater contamination at a particular site. In addition, it does not attempt to simulate the processes involved in controlling the fate of a pesticide in the subsurface and is therefore unable to quantify either the amount of pesticide that leaches or the rate at which it leaches towards the water table. However, the advantages of the LP/LI model outweigh the disadvantages in certain circumstances. Its use is appropriate when there are insufficient data to perform a more detailed assessment with the more complex simulation models. It can also be used to narrow the scope of a large investigation by identifying those pesticides that warrant additional study with a more sophisticated pesticide assessment model and/or field studies.

## MATHEMATICAL MODELS

In assessing the potential for groundwater contamination by pesticides, mathematical models attempt to simulate the major physical, chemical, and biological processes that are involved in the transport, attenuation, and transformation of the pesticides in the unsaturated zone. Therefore, in terms of pesticide assessment models, mathematical models are defined as models that quantify both the amount of pesticide that leaches and the rate at which it leaches through the soil profile to the water table, on a site-specific scale.

Mathematical models vary considerably in terms of the extent to which they describe the basic processes involved, the sensitivity and accuracy of the simulations, and the amount of input characterization data required. On the basis of these criteria, Wagenet (1986) has subdivided mathematical models into three groups: educational, management, and research (see Fig. 1).

### Group 1: Educational Models

Educational models are the simplest of the mathematical models and are applicable to only a limited number of situations. Generally, the governing processes are simplified to near ideal conditions. Typically, most of these models represent the subsurface as a uniform and homogeneous soil profile with a steady flow regime, and consider only the basic chemical and biological processes that influence the fate of pesticides (e.g., degradation, adsorption). The flow of water within the unsaturated zone is generally represented by a simplified water balance or lumped parameter approach, which does not simulate the upward migration of water due to evaporation. Therefore, these models are best suited for well-drained (e.g., coarse-grained) soils that allow for a quick downward migration of water. The amount of input characterization data required is restricted to a few parameters, which means that educational models generally consider little (if any) spatial variability in the hydrogeological and pedological character of the soil profile. Results from the models provide only qualitative information and may include the position of the solute front, the percentage of initial mass of pesticide remaining in the soil profile, etc. However, these models do not generally provide pesticide concentrations within the soil profile.

**Group 2: Management Models**

Management models allow for a greater variability in the physical character of the soil profile that is being simulated (i.e., allowing for a layered soil profile simulation under transient conditions), and consider more physical and chemical processes than do educational models. However, the application of these models is also limited because they either neglect certain processes (e.g., volatilization, transformation products), or represent these processes with simplified approximations (i.e., using a lumped parameter approach for the flow of water). As a result, these models cannot be used to provide detailed analyses or insights into the hydrological processes controlling the fate of a pesticide in the subsurface. However, they can provide semiquantitative assessments on the amount of pesticide that leaches and the rate at which it leaches to the water table. Management models require larger (but not restrictive) amounts of input characterization data. Because these models are intended to provide managerial guidance, they present their results in a manner that allows for a quick interpretation.

**Group 3: Research Models**

Research models attempt to describe the processes involved in as much detail as possible. As an example, research models may describe the flow of water in the unsaturated zone using a direct solution to Richards equation, while management and educational models may employ a simplified water balance. Research models often include processes not accounted for in management or educational models (e.g., volatilization, hydrodynamic dispersion, production and migration of transformation products). Because of the more detailed description included, they may be employed for detailed examinations into the influence that various factors have on the results predicted by the models. For example, they might be used to perform uncertainty analyses to determine which model parameters or processes are most influential in the fate of pesticides in the subsurface. However, the more detailed description often requires larger 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 when data are available to characterize the conditions being simulated with sufficient accuracy. However, their use is often more cumbersome (i.e., input data sets are more difficult to formulate, and they require considerably longer execution times). Typically, these models can provide the user with various pesticide storage and leaching rate values, as well as water contents and water flux values at different depths within the soil profile.

## SELECTION OF A MATHEMATICAL MODEL

To predict the fate of pesticides in the subsurface accurately, the mathematical framework of a simulation model incorporated into EXPRES must be based on accepted scientific principles that describe the important physical, chemical, and biological processes that control the transport and transformation of a pesticide in the subsurface. The criteria used in the selection of an existing simulation model for inclusion in EXPRES are that it must

- be able to predict the migration rates and concentrations of the pesticide in the unsaturated zone with respect to both time and depth
- be able to determine the concentration at, and time required for a pesticide to reach, the water table
- be able to simulate the transport of daughter products and predict their concentrations
- be based on the accepted scientific principles that govern the transport and transformation of pesticides
- be currently a widely accepted and verified computer code

Eleven mathematical pesticide assessment models were identified and reviewed (Mutch and Crowe 1989, Crowe and Mutch 1991a) for possible inclusion in the EXPRES expert system (see Fig. 1).

After performing an evaluation of the mathematical models (Mutch and Crowe 1989), the PRZM (Carsel et al. 1984, 1985) and LEACHM (Wagenet and Hutson 1987) models were selected as best suited for inclusion in the expert system. LEACHM was selected because it was the most comprehensive model, describing the processes involved in greater detail than in any of the other models. Therefore, it should provide a more accurate simulation when sufficient data are available to characterize a site. However, execution times are lengthy with the LEACHM model (several hours are required for a one-year simulation on an 80286-based PC). Practical considerations may require a more expedient execution time for the assessment model when a number of "what if" scenarios are to be investigated. There may also be situations where a highly detailed simulation is not required, or where the use of a complex model is not warranted because of a lack of data. These practical considerations led to the inclusion of the PRZM model in the EXPRES expert system. PRZM is the best of the simplified water balance models. Its major advantages are that it can handle layered soils effectively, and it simulates transport below the root zone. In addition, PRZM includes a concise description of surface runoff and erosion processes. The choice between the use of the PRZM and LEACHM models for an assessment is based upon the objectives of the assessment (specified by the user), the availability of data, and on the time available to produce the results. Both simulation models require input data from four general areas: climatic conditions, soil parameters, chemical characteristics of the pesticide, and farm management practices.

An educational model was not included in EXPRES because PRZM uses essentially the same data and provides more useful results. The features included in the expert system, and its ease of use, will allow EXPRES to be used in an educational setting if desired.

## The PRZM Model

The PRZM (**P**esticide **R**oot **Z**one **M**odel) model (Carsel et al. 1984) simulates many of the physical, chemical, and biological processes controlling the fate of a pesticide in the unsaturated zone. PRZM is a management model, and as such, simulates a number of the processes included in the model with simplified representations. The unsaturated zone is divided into three layers. Runoff, erosion, precipitation, and snowmelt all interact with the surface layer. Evapotranspiration affects the water balance in the root zone layer, while there are no source or sink terms for water in the layer below the root zone, with the exception of the bottom of the soil profile. Each of the three layers is composed of a number of individual cells or compartments (an overall maximum of 50), and it is possible to assign different physical and chemical characteristics to each of these compartments. PRZM simulates the one-dimensional flow of water and solutes through the unsaturated zone under transient conditions. Although the model is based on an advective-dispersive equation, it employs a lumped parameter (tipping-bucket) approach in its representation of the flow of water through the soil compartments. The infiltration and percolation of water within the soil profile depend on two soil parameters: the field capacity and the wilting point of the soil. The flow of water is simulated according to the following simple drainage rules:

- Any water that infiltrates into a soil compartment in excess of the field capacity will be drained to the compartment below within one day.
- Moisture between the field capacity and the wilting point in the root zone compartments is available for evapotranspiration.
- The moisture content of a compartment cannot fall below its wilting point.

The transport of pesticides in the subsurface is calculated with a finite difference approximation to the solute transport equation (1). The water content (θ) and soil water velocity (v) terms are based on the lumped parameter description of the water balance given above, and are calculated according to the following:

$$\theta = SW_i/\Delta z \quad (8)$$

$$v = I_l \cdot \Delta z/\Delta t \quad (9)$$

where $SW_i$ is the soil-water content of compartment i, $\Delta z$ is the soil compartment depth, $I_i$ is the amount of percolation out of soil compartment i, and $\Delta t$ is the time step.

PRZM accounts for many of the processes affecting solute transport in the unsaturated zone. Surface runoff and soil erosion are simulated with a modified Soil Conservation Service curve number approach (Haith and Loehr 1979) and the Universal Soil Loss Equation (Williams and Berndt 1977), 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 either calculated from daily pan evaporation data or empirically estimated from daily temperature values. Plant uptake of the pesticide is related to the transpiration rate calculated by the model. Equilibrium adsorption (linear and reversible) and first-order degradation are included but are restricted to a single pesticide species. Only minor modifications were made to the PRZM model before its incorporation into the EXPRES expert system. The modifications enabled PRZM to read meteorological data from a common external file and to read the input characterization data from a file created by EXPRES.

The size of the time step in PRZM is constant and is set to one day. The solution to the set of water balance and solute transport equations for each soil compartment is undertaken by a finite difference technique. The numerical dispersion created during the solution is used to represent hydrodynamic dispersion that would occur in the field. Execution times for a one-year simulation require only a few minutes. Output from the model may include total, dissolved, and adsorbed pesticide concentration profiles with respect to both time and depth. A number of time series plots that depict the variations in the values of various water and pesticide parameters over time are also available.

The use of PRZM is most appropriate when a more general, quantitative assessment of the potential for a pesticide to contaminate groundwater is required, or when there are insufficient field data (e.g., typical soil profile data from a soil survey report) to warrant the use of the LEACHM model. The main disadvantages of the PRZM model are the simplified approach taken in describing the flow of water within the unsaturated zone, and the limitation of simulating the fate of only one pesticide species at a time (it does not simulate the fate of daughter products that may be generated during the breakdown of the parent pesticide). In addition, the model does not account for surface volatilization losses, and hydrodynamic dispersion is simulated with the numerical dispersion created during the solution of the approximated differential equations.

**The LEACHM Model**

The LEACHM (Leaching Estimation And CHemistry Model) model (Wagenet and Hutson 1987) simulates the major processes involved in controlling the fate of pesticides in the unsaturated zone in as much detail as possible. The LEACHM model is composed of three solute transport models: LEACHMS (inorganic salts), LEACHMN (nitrogen), and LEACHMP (pesticides). Because the focus of this project is to simulate the fate of pesticides in the subsurface, the following description will deal solely with the LEACHMP code. LEACHMP will hereafter be referred to simply as LEACHM.

LEACHM can be used to simulate pesticide transport in the unsaturated zone under transient meteorological conditions, with multiple pesticide applications. The simulation of the flow of water within the model is based on a direct solution to a one-dimensional form of Richards equation, which more closely approximates the processes controlling the flow of water in an unsaturated soil (Equation 2). LEACHM divides the soil profile into a series of equally spaced compartments in the vertical direction. The flow of water is controlled by the characteristic curves defined for the soil, which relate the retentivity and conductivity of the soil to the existing matric potential in the soil profile. After solving Richards equation, LEACHM determines the water flux across each soil compartment boundary to calculate the advective transport of the pesticide. Once the water flux density is known, the model calculates the change in the pesticide concentration (c) with time (t) within each soil compartment, using a finite difference solution to the following solute transport equation:

$$\frac{\partial c}{\partial t}(\rho K_D + \theta + \epsilon H) = \frac{\partial}{\partial z}(\theta D_d(\theta,q) + \epsilon H D_{OG})\frac{\partial c}{\partial z} - qc \pm \eta(z,t) \qquad (10)$$

where $\epsilon$ is the gas-filled soil porosity, q is the water flux across a compartmental boundary, $\rho$ is the soil bulk density, H is the dimensionless Henry's Law constant, and $D_{OG}$ is the vapour diffusion/dispersion coefficient. LEACHM simulates hydrodynamic dispersion by allowing the user to specify diffusion and dispersion coefficients for the dissolved and vapour phase of the pesticide.

LEACHM can simulate as many as 50 soil compartments, and can assign different physical, biological, and chemical parameters to each, thus giving the model the ability to simulate water and solute transport in multilayered soils. The spatial and temporal variabilities that may occur at a field site are approximated by field-averaged values.

Pesticide attenuation is represented by equations describing equilibrium sorption (linear, reversible), and chemical and/or biological degradation (first-order). LEACHM includes a description of pesticide volatilization and is able to simulate the fate of up to four pesticide species (e.g., a parent pesticide and three daughter products, or other combinations). Additional processes simulated by LEACHM include (1) plant growth, (2) daily evaporation and transpiration, (3) water and pesticide uptake by the plant, (4) several surface and bottom boundary conditions, and (5) the flow of heat and distribution of temperature in the soil profile.

Several modifications were made to the LEACHM model before its incorporation into EXPRES. These changes include being made able to read the input characterization data from a file created by the expert system and the meteorological data (mean daily temperature, total daily precipitation, and total daily pan evaporation - when available) from a common external file. The daily temperature values are necessary to accommodate two additional modifications that were made to LEACHM. The first is the addition of an empirical method for estimating daily potential evapotranspiration values when measured pan evaporation data are unavailable. The second is the addition of a simplified snowmelt routine based on the mean daily temperature (degree-day approach).

The snowmelt and pan evaporation estimation techniques incorporated into LEACHM are identical to routines found in the PRZM model. LEACHM was also modified to allow the model to simulate surface runoff and erosional losses of both water and pesticide in a manner similar to that used in the PRZM model. Erosional losses are determined with a modified Universal Soil Loss Equation (MUSLE) (Williams and Berndt 1977), while surface runoff is calculated with a curve number approach developed by the USDA Soil Conservation Service (Haith and Loehr 1979). The output from the model includes current and cumulative totals for various pesticide and water parameter values in each soil compartment, and also at specified depths. Mass balance checks are also performed to ensure that the simulations are accurate. The reader will find more detail on the modifications made to the LEACHM model in Mutch and Crowe (1990a,b).

The greater level of detail included in the descriptions contained in the LEACHM model gives it the ability to provide a detailed assessment of the fate of a pesticide and its associated daughter products in the unsaturated zone, with respect to both time and depth. LEACHM can also be used to investigate the relative influence that the physical, chemical, and biological processes have on the fate of a pesticide in the subsurface (i.e., uncertainty analyses). However, LEACHM will not provide more accurate results, or additional insights, if the input data necessary to characterize accurately the environmental conditions at a particular site are not available.

The disadvantages of the LEACHM model are that it requires more input characterization data and much longer execution times than the PRZM model. Execution times can be lengthy because the time step is variable, and can range from $1 \times 10^{-7}$ of a day to $1 \times 10^{-1.3}$ of a day. It is calculated at the beginning of each time step to meet certain criteria set up within the model (e.g., a specified maximum water flux).

# An Overview of Expert Systems

Expert systems (also known as knowledge-based systems) are a class of computer programs that fall within the field of artificial intelligence. Generally, expert systems function by encoding the decision-making and interpretive abilities of a specialist, or "expert," in a particular subject into a computer program. The program is structured in such a way that through an interactive process, a general practitioner, or layperson, can be guided through the steps required to solve a complex problem. An expert system operates in much the same way as a conversation between an expert and a layperson in that the system prompts the user for information and objectives of the study. Should the user be unfamiliar with any of the requested information, the expert system will provide explanations of what is required or will recommend a course of action. The human expertise that is encoded into an expert system includes the knowledge, experience, judgment, problem-solving abilities, and communication skills that have been acquired by an expert through years of training and personal experience.

Although expert systems are computer programs, there are significant differences between expert systems and conventional computer programs. The most obvious difference is that expert systems are designed to operate interactively with a user through almost all stages involved in completing a task. Typically, this includes (1) prompting the user for information such as objectives of the study, type of data required, and their values; (2) providing the user with assistance or recommendations in obtaining values or choosing a course of action; and (3) aiding in the interpretation of the results of the study, which may include a discussion of the reasoning methodology.

The second major difference between an expert system and a conventional computer program concerns the type of problem solved and the manner in which it is solved. Conventional computer programs execute a prescribed set of procedures as defined by the programmer and thus are designed for solving routine (i.e., repetitive) and exacting (i.e., mathematical calculations) tasks. For example, a numerical model, which is representative of a conventional computer program, will input quantitative data (typically numbers), manipulate these data according to a prescribed set of mathematical programming statements, and present the results in a specific format. Expert systems solve aspects of a problem that are traditionally solved by experience and judgment and thus are often more qualitative than quantitative in nature. For example, a typical expert system will interact with a user to gain information that is then used by decision-making and interpretive coding to recommend a course of action, diagnose a problem, or present explanations and justifications for the particular decision. Unlike conventional computer programs, expert systems are able to undertake this type of task because they contain an extensive amount of knowledge, as well as a decision-making and/or an interpretive ability within the code.

Information about expert systems can be obtained from a number of text books, such as Hayes-Roth et al. (1983) and Harmon and King (1985). The three main components of an expert system are (1) an inference component (the inference engine), (2) a linkage between the user and the expert system (the user-system interface), and (3) an extensive collection of knowledge (the knowledge base).

The inference engine controls the execution of all aspects of an expert system. Functions typically undertaken by an inference engine include (1) linking all of its operations through a number of modules in response to input provided by a user; (2) determining how, and in what order, the procedures are to be undertaken; (3) executing the reasoning strategy, using the rules and information stored in the knowledge base; and (4) providing the user with assistance in responding to prompts for information.

The user-system interface conveys the expertise encoded within the expert system to the user through an interactive terminal session or a dialogue format, which is analogous to a conversation between an expert and a client. This dialogue format takes the form of either a series of prompts or questions to the user for required data or a choice of options and corresponding responses from the user, or a fill-in-the-blank format (known as frames) in which the expert system requests that information be supplied or selected in a tabular format. By entering data in this manner, the user is not required to have an extensive knowledge of computer operations or computer modelling.

The knowledge base contains all the information that is used to analyze or solve a problem and consists of both factual and procedural knowledge. Factual knowledge consists of all the quantitative information for a given domain and is generally stored in data bases. Procedural knowledge is more qualitative in nature and consists of relationships among facts, concepts, and procedures used to describe a specific domain or a reasoning methodology. Procedural knowledge can be classified as either tacit or taxonomic. Tacit knowledge is based upon research and experience that has been shown to produce reasonably reliable conclusions. Taxonomic knowledge is a carefully structured representation of information and relationships. In addition to exact rules and relationships, an expert system includes heuristic knowledge, which is inexact knowledge and insight derived from years of problem-solving experience.

The knowledge required for the construction of an expert system (both factual and procedural) is placed in explicit and uniform structures that will permit the application of consistent methods of processing. This representation of knowledge, including the linkage between factual and procedural knowledge, within an expert system is essentially based on three structures: production rules, semantic nets, and frames.

Production rules make use of **IF** ... **THEN** ... inferences to form the reasoning methodology of the expert system and to represent tacit knowledge. When data accumulated for a particular problem matches the conditions stated in the **IF** part of the rule (known as the condition or premise), the statements in the **THEN** part of the rule (known as the action or consequence) are executed. For example, ***IF** aldicarb is detected in groundwater **THEN** the groundwater is contaminated.*

The semantic net is used to represent non-rule-based knowledge (i.e., taxonomic knowledge) according to an association among data, objects, events, and concepts. Data are associated by **IS A** or **IS A PART OF** links within hierarchal networks that depict the pathway through which a user can obtain and associate a series of related information. For example, from the links *aldicarb **IS A** pesticide*, and *a pesticide **IS A** hazardous chemical*, we can conclude, *aldicarb **IS A** hazardous chemical*.

Frames are used to group or categorize a collection of taxonomic knowledge that is characterized by similar attributes or related parameters and which is typically used together in a single unit. Frames provide a convenient method by which the user can enter a considerable amount of related facts, or allow the expert system to display large amounts of data conveniently and efficiently. These data could consist of facts, concepts, and/or questions. An example of information that is readily grouped within a frame is meteorological data, where daily temperature, precipitation, and such data for several meteorological stations can be accessed easily.

The reasoning strategy within an expert system, which represents its problem-solving or decision-making ability, involves both choosing and following a path of reasoning and retrieving considerable information. The reasoning strategy is constructed by combining semantic nets and frames with production rules. The most common way to form a reasoning strategy is by linking, or chaining, production rules. A forward-chaining approach links the production rules to form a predictive reasoning strategy and is used to determine a consistent and correct interpretation or to reach a conclusion from an analysis of data and/or ideas. Backward-chaining of production rules represents a diagnostic reasoning strategy and is used to determine if a specific option or interpretation is viable, based upon a series of favourable responses to a set sequence of conditions. Once a choice of a particular method of reasoning is determined by the production rules, semantic nets can quickly route the expert system through the selection of all the necessary options and data (stored as frames) required to solve the problem. Thus, the combination of production rules and semantic nets can represent links between groups of rules, nets, and frames that contain information that is focused towards a specific aspect of a problem.

The characteristics of a problem that favour a successful application of an expert system include the following:

- The knowledge domain is well defined, concise, and has distinct bounds.
- The solution requires knowledge that is not only exact and factual, but is also heuristic in nature (requiring judgment and interpretation).
- The problem is sufficiently complex that it requires specialized expertise or knowledge from several fields.
- The problem will occur often, and the frequent use of the expert system will justify its developmental cost.

- There are a sufficient number of case studies with which to verify the expert system.
- A consistent solution is required even though both quality and quantity of the input may be variable.
- An expert systems approach will clearly be beneficial to the solution of the problem (e.g., increase staff productivity).

With regard to groundwater contamination investigations, additional factors that would make this field an ideal candidate for solution by an expert systems approach include the following:

- The solutions to many groundwater problems are based on both scientific principles and regulatory constraints.
- Decisions are generally performed with sparse or incomplete data and hence are generally based on judgment (heuristic knowledge).
- Groundwater investigations often must rely upon expertise from a variety of diverse fields (e.g., geology, mathematics, biology, chemistry).
- Although many groundwater contamination problems require the same type of evaluation (e.g., is it necessary to remediate this particular site?), the type and quantity of information available upon which to base the assessment is often highly variable (e.g., available data, site characteristics, contaminants present).
- Much of the scientific research in hydrogeology has widespread applicability but is beyond the expertise of most practising hydrogeologists and engineers.

An expert systems approach can account for these aspects of a problem, thus providing hydrogeologists, engineers, and regulatory personnel with the necessary expertise to understand and effectively solve groundwater problems.

Expert systems have been in use in numerous fields, such as medicine, process control, and engineering, for over 20 years (Hayes-Roth et al. 1983, Hushon 1990a and 1990b). Their application to hydrogeological studies has occurred only during the last few years. Several expert systems have been developed for aiding in groundwater-focused problems in such areas as regulatory support, site assessment and remediation, risk assessment, groundwater contaminant modelling, and water resources. Reviews of these expert systems are provided by Rossman and Siller (1987), Hushon (1990a,b), and Crowe and McClymont (1992). EXPRES can be grouped with similar expert systems designed to aid a user in conducting simulations with groundwater contaminant models such as Expert Rokey (McClymont and Schwartz 1991a,b) and OASIS (Newell et al. 1990). This group of expert systems generally functions as an intelligent front end for complex groundwater contaminant transport models. Specifically, these models assist a novice user in preparing input data sets, executing the model, and interpreting the results of a simulation.

# The Development of the EXPRES Expert System

EXPRES (**EX**pert system for **P**esticide **R**egulatory **E**valuations and **S**imulations) is an expert system designed to provide regulatory personnel with an additional tool to aid in their assessment of the fate of pesticides in the subsurface environment. EXPRES helps sustain the quality of groundwater in agricultural areas by identifying potential groundwater contamination problems that may be associated with new pesticides submitted for registration. The objective for the expert system approach is to allow those not proficient in the use of pesticide assessment models, or in the theory of contaminant hydrogeology, to assess the fate of pesticides in the unsaturated zone with confidence and accuracy. EXPRES has been designed as a management tool to be used as an aid in making policy decisions regarding the benefits and risks associated with the use of a pesticide in different agricultural regions across Canada. EXPRES is not intended to be used in place of any portion of the current regulatory procedures (i.e., field or laboratory testing) but in conjunction with them to

- provide a quick and general assessment of the potential groundwater hazards associated with a pesticide
- identify whether further field or laboratory study is warranted
- define specific regions or sites where field testing may be required
- identify locations where post-registration monitoring may be needed

EXPRES is a knowledge-based system that couples three existing pesticide models to a text/graphical user-system interface and extensive geographical and pesticide data bases. The inclusion of three models (one screening and two mathematical models) in the expert system allows pesticide assessments to be conducted at several levels, according to the objectives of the assessment and the availability of input characterization data. EXPRES provides a range of assessments of varying complexity, including

- a review of the pesticide properties and characteristics of agricultural regions that influence the fate of pesticides in the subsurface
- a simple relative assessment (with respect to other pesticides) of the potential for a pesticide to leach to the water table
- a quantitative prediction of the concentration, distribution, and migration rates of a pesticide and its daughter products in the subsurface with respect to both time and depth
- a determination of the concentration of the pesticide at, and the time required to reach, the water table

- a detailed evaluation of the processes controlling the fate of pesticides in the unsaturated zone

EXPRES can be classified as an intelligent front-end system for groundwater contamination models. Generally, EXPRES functions by encoding the decision-making abilities of a specialist, or "expert," in the fields of contaminant hydrogeology, environmental fate of pesticides, and solute transport modelling into a computer program. The program is structured in such a way that through an interactive process between the expert system and the user, the user can be guided through the steps required to operate the three pesticide assessment models. This encoded expertise includes

- rules for selecting the most appropriate pesticide assessment model according to information supplied by the user
- the information required by the models to characterize the farm management techniques and the physical, meteorological, hydrogeological, and pedological conditions of agricultural regions across Canada
- the information required by the models to characterize the chemical properties of the pesticides being simulated
- estimation techniques for pesticide and site parameter values
- rules for ensuring the accuracy, consistency, and completeness of the input characterization data
- the computing and modelling expertise required to operate the pesticide assessment models
- assistance in the interpretation of the assessment results

One of the major factors considered in the development of EXPRES was that it should be easy to use by those not experienced in the use of numerical models that simulate the fate of pesticides in the subsurface. Several important criteria were established for the design and construction of the expert system, as follows:

- The system must be easy to use by those with minimal computer skills and little knowledge of pesticide transport in the subsurface.
- Upon introduction to the expert system, the user should be able to use the system effectively in a relatively short time.
- EXPRES must run efficiently on a DOS-based personal computer.
- Parameters required for a simulation must be readily available from data bases, or easily entered into the system by means of a dialogue format.
- The data bases should be easy to modify and update.
- Corrections and changes during data entry must be easy to make.
- Output from the models must be informative and easily understood.

## COMPUTING REQUIREMENTS FOR EXPRES

EXPRES has been designed to operate within a personal computer environment. Minimum hardware requirements include (1) an 80286-based computer, (2) an 80286 math co-processor, (3) a 20MB hard disk (with approximately 8MB of free space), (4) a monochrome monitor with a CGA graphics card, and (5) 640KB of RAM memory (with 560KB of it accessible). However, it is recommended that EXPRES be operated on a 80386- or 80486-based machine with a corresponding math co-processor to minimize the execution times with the mathematical assessment models. A VGA colour monitor and graphics card are also recommended to enhance the visual presentation of the User-System Interface, including the plots of the assessment results.

Software for EXPRES is implemented within a DOS environment. The simulation models (PRZM and LEACHM) were compiled with Microsoft® FORTRAN, while the User-System Interface and Inference Engine were developed with Microsoft® C.

## STRUCTURE OF THE EXPRES EXPERT SYSTEM

EXPRES is composed of three primary components, the Inference Engine, the User-System Interface, and the Knowledge Base, and the general architecture of EXPRES is illustrated in Figure 2.

### The Inference Engine

The main component of the EXPRES expert system is the Inference Engine (IE). It is virtually transparent to the user but acts to control the operation of EXPRES through the application of appropriate production rules. The IE is divided into seven modules (Fig. 2), each controlling specific operations within EXPRES. The Program Control Module regulates the basic computer operations, determining how, and in what order, the procedures are undertaken, and provides a link between the various components of EXPRES. The Reasoning Control Module performs the "reasoning strategy," using the rules and information stored in the data bases to provide the User-System Interface with the necessary information to guide the user through the pesticide assessment. The Data Analysis Module helps the user to interpret the simulation results. The IE allows the user to view the information contained in both the pesticide and agricultural region data bases with the Data-Base Display Module. The System Introductory Module provides access to text files that discuss (1) the basic instructions required to operate EXPRES, (2) an overview of the expert system, and (3) example files that contain a complete input data set (for all three models) and the corresponding results.

The IE also contains an Integrity Checking Module that performs consistency checks on the input data set used in the assessment, and passes any resulting error and warning messages to the User-System Interface, which in turn displays the messages to the user. The integrity checks ensure that the data set is complete, that the values assigned to the model parameters are within an acceptable range, and that they are consistent with previously entered data and with the objectives of the simulation. The integrity checking procedure is undertaken on four levels. Level 1 and 2 checks are performed as the information is being entered by the user. Level 1 (Operational) checks ensure that the operation of EXPRES is smooth and logical. For example, the integrity checks alert the user to any conflicts that occur between the options selected by the user,

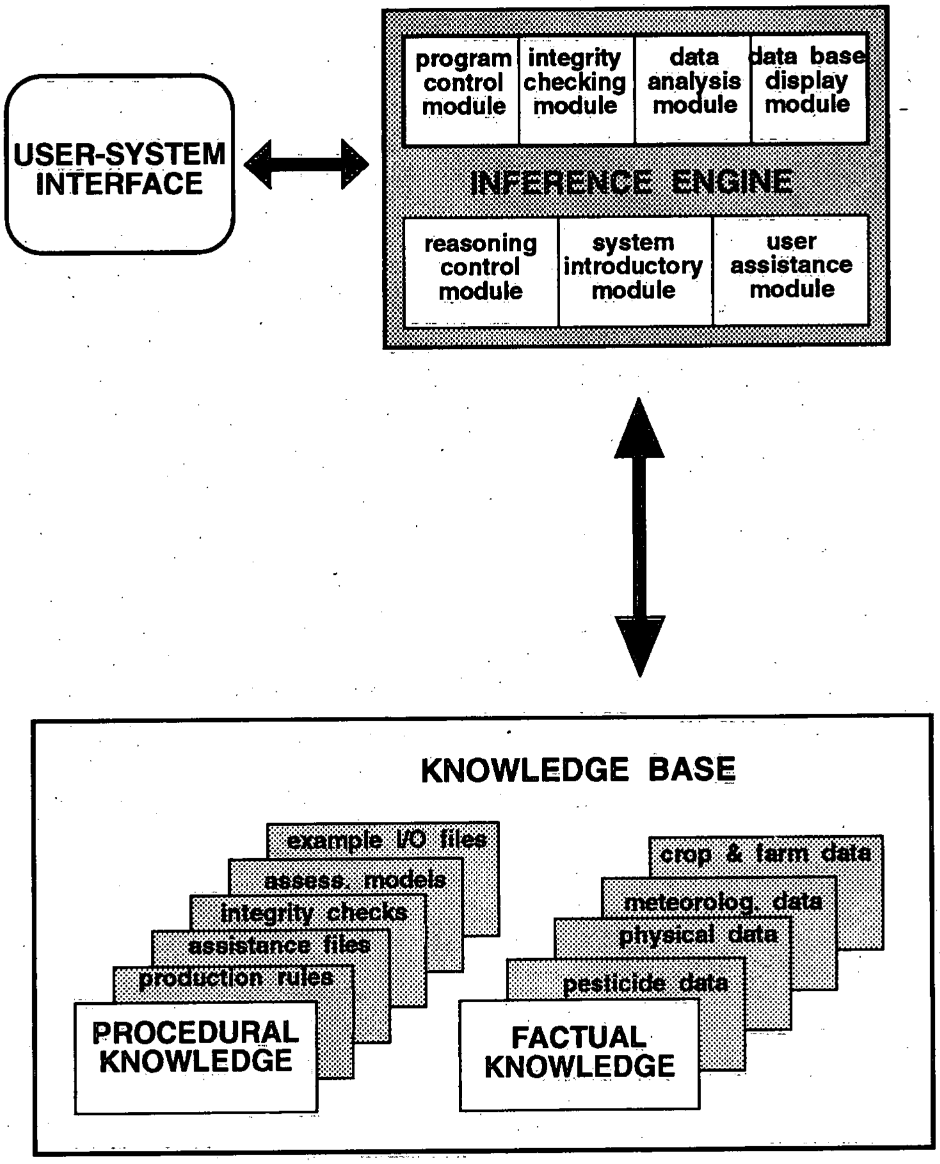



Figure 2. General architecture of the EXPRES expert system.

and will not allow the user to proceed with the assessment until the conflicts are resolved. Operational integrity checks also ensure that only the appropriate screens appear and that the user is locked out of input data fields that are not required for the selected options. Level 2 (Correct Type and Format) checks ensure that the data entered are of the correct type (e.g., alphanumeric values vs. numeric values) and that the data are entered in the correct format. Integrity checks on Level 3 and Level 4 are undertaken immediately before the execution of the assessment models. Level 3 (Appropriate Range) checks ensure that the values assigned to the model parameters are within an acceptable range (e.g., the pan evaporation coefficient should be between 0.60 and 0.80). The Level 4 (Consistency) checks are undertaken to ensure that all the input data for the assessment models are consistent with previously entered values and with the simulation objectives (e.g., the field capacity of a soil horizon may not exceed its saturated water content, the bulk density of a sandy loam soil should be between 1.25 and 1.80 g/cm$^3$). The Level 3 and Level 4 integrity checks produce warning and error messages that indicate to the user which model parameter values should be checked before the selected pesticide assessment model is executed.

The User Assistance Module (or Help facility) is designed to provide the user with assistance in responding to a prompt from EXPRES to provide values or options for the pesticide assessment models. EXPRES contains five levels of assistance (Fig. 3). Level 1 assistance provides a brief definition of the parameter or option of interest. Level 2 is a more detailed description of the parameter, including references for further information. Level 3 provides methods for estimating values for the parameter, such as empirical estimation techniques. Level 4 is a list of typical values that may be used for the model parameter, and Level 5 provides a method for allowing the user to store and recall user-supplied information for any parameter or option within EXPRES.

## The User-System Interface

The component of the expert system that is most apparent to the user is the User-System Interface (USI). The USI is the interactive program that communicates with users to guide them through the selection and entry of data required by the pesticide assessment models. The USI also displays the results of an assessment, and provides assistance in the interpretation of results obtained from the assessment models.

Generally, the USI presents information to or obtains data from a user by means of screens on the monitor. Screens allow considerable information to be entered quickly and efficiently, and require much less time and effort than to enter the same data with a series of question-and-answer prompts. Screens also allow the user to enter information in any order and to review previously entered values quickly. All screens used within EXPRES are shown in Appendix B.

It is through the USI that the Inference Engine prompts the user for the objectives of the assessment and for selection of the pesticide and agricultural region of interest. The user may then review the default data loaded by the expert system and modify any or all the data to customize the input data set to the conditions that are to be simulated. If the user has any difficulties throughout the assessment, either in understanding the information that is being requested or in determining a value for the requested model parameter, the USI provides the user with access to the Help facility.

The USI displays any warning or error messages that are produced when the integrity checks are performed on the input data set. The USI also presents the results of the simulation as either tabular or graphical output, which assists the user in visualizing trends, relationships, and/or anomalies that may exist in the predicted results.

## LEVEL 1: Definition

The Organic Carbon Partition Coefficient (Koc) is a proportionality factor that describes the partitioning of the pesticide between the amount of the pesticide that is dissolved in the soil water and the amount of the pesticide that is sorbed to the organic matter in the soil.

## LEVEL 2: Explanation

The Organic Carbon Partition Coefficient is used to determine the amount of pesticide that becomes sorbed to the soil matrix. The transport of pesticides in the unsaturated zone may be attenuated by the adsorption, and desorption, of pesticide molecules to clay particles and/or organic matter content of the soil. The concentration of a pesticide that becomes sorbed to the soil (Cs) is often assumed to be linearly related to the dissolved pesticide concentration (Cw) through a partition or distribution coefficient (Kd):

$$Cs = Kd \cdot Cw$$

It is also assumed that an instantaneous and reversible equilibrium exists between the amount of pesticide that is being adsorbed and the amount being desorbed.

For most non-ionic pesticides (without a permanent charge), the correlation between the amount of pesticide sorbed and the organic matter content of the soil is much higher than the correlation with the clay fraction of the soil. As a result, the partition coefficient is often normalized to the fractional organic carbon content of the soil (foc):

$$Kd = Koc \cdot foc$$

The adsorbed concentration of the pesticide is determined with the equation:

$$Cs = Koc \cdot foc \cdot Cw$$

*etc.*

## LEVEL 3: Estimation Formulae

Koc can be estimated by the following empirically derived equations, based on the octanol water partition coefficient (Kow), aqueous solubility (S) and molecular weight (MW):

$\log Koc = 0.72 \cdot \log Kow + 0.49$ (Schwarzenbach and Westall, 1981)
$\log Koc = -0.54 \cdot \log S + 0.44$ (Karickhoff et al., 1979)
$\log Koc = 0.0085 \cdot MW + 0.132$ (Kanazawa, 1989)

*etc.*

## LEVEL 4: Typical Values

The following table lists typical values for Koc for some common pesticides:

| Pesticide | Koc (L/kg) | Reference |
|---|---|---|
| Alachlor | 180 | 6,7 |
| Atrazine | 120 | 6,7 |
| Chlordane | 27,000 | 6,7 |
| Chlorpyrifos | 6,000 | 6,7 |
| etc. | | |

## LEVEL 5: User-Supplied

Enter any additional information you may want to record about this variable in the file "KOC.USR". Any word processor editor that can save files as ASCII text may be used. The line length should not exceed 65 characters; there is no limit to the total number of lines.

Figure 3. Representation of the five levels of assistance available for the organic carbon partition coefficient through the EXPRES Help facility.

**The Knowledge Base**

The third, and perhaps most important, component of the EXPRES expert system is the Knowledge Base. It contains two types of knowledge (see Fig. 2). The first is the quantitative data characterizing the pesticides and the agricultural regions, and is known as Factual Knowledge. The second, known as Procedural Knowledge, contains information that is more qualitative in nature, and consists of relationships among facts, concepts, and rules used to describe a specific domain or reasoning strategy. This knowledge is based on the experience, judgment, and problem-solving abilities acquired by an expert through a high level of study, training, insight, and personal experience.

*Procedural Knowledge*

Procedural Knowledge in EXPRES consists of production rules, assistance files, integrity checking information, pesticide assessment models, and example input and output files. The production rules are used to relate facts and concepts in describing a domain or reasoning strategy. As an example of a set of production rules in EXPRES, Figure 4 illustrates the rule-based reasoning strategy used to select the most appropriate pesticide model. The appropriate production rules are accessed by the Reasoning Control Module of the Inference Engine whenever a particular procedure is required to be performed. The production rules that comprise the encoded expertise include

- rules for controlling the operation of EXPRES
- rules for selecting and executing a pesticide assessment model
- rules for ensuring accuracy and consistency of user-supplied input data
- assistance in selecting appropriate values for model parameters
- guidance and assistance in interpreting the critical output from the models

Procedural Knowledge also includes assistance files, which consist of encoded explanations, definitions, examples, parameter estimation techniques, and recommended values that are accessed by the user through the User-System Interface through the Help facility. This knowledge is used to clarify the meaning of the information being requested by the expert system and provide the user with recommended values and/or heuristic or derived estimation techniques for the modelling parameters that are required for a simulation (see Fig. 3).

The integrity checking information consists of the data and relationships used by the Inference Engine to ensure that an input data set is accurate and consistent. Specifically, this information includes (1) rules for checking the operational flow of the expert system, (2) rules for checking the type and format of entered data, (3) an appropriate range of values for model parameters, and (4) rules for checking the consistency among model parameter values.

```
rules
       set MODEL = PRZM

1 a    if (COMPUTER = 80286) then
           set CUTOFF_DAYS = 150
1 b    elseif (COMPUTER = 80386 or COMPUTER = 80486) then
           set CUTOFF_DAYS = 600
       endif

2 a    if (SIMULATION_LENGTH <= CUTOFF_DAYS) then
           set MODEL = LEACHM
2 b    elseif (SIMULATION_LENGTH > CUTOFF_DAYS) then

3 a        if (DAUGHTER_PRODUCTS = YES  and
              QUICK_RESULTS = NO ) then
               set MODEL = LEACHM
3 b        elseif (DAUGHTER_PRODUCTS = YES and
              QUICK_RESULTS = YES ) then
               write "Simulation of daughter products takes > 1 hour.
                      Do you require: (A) results quickly or
                                      (B) daughter products? "
4a             if (ANSWER = A) then
                   set MODEL = PRZM
4b             elseif (ANSWER = B) then
                   set MODEL = LEACHM
               endif
           endif

5 a        if (PERFORM_UNCERTAINTY_ANALYSES = YES  and
              QUICK_RESULTS = NO) then
               set MODEL = LEACHM
5 b        elseif (PERFORM_UNCERTAINTY_ANALYSES = YES  and
              QUICK_RESULTS = YES) then
               write "Uncertainty analyses should be done with detailed
                      model to be informative, but this will take > 1 hour.
                      Do you still require results quickly: YES or NO? "
6 a            if (ANSWER = YES) then
               set MODEL = PRZM
6 b            elseif (ANSWER = NO) then
                   set MODEL = LEACHM
               endif
           endif
       endif
```

Figure 4. Production rules invoked in selecting the most appropriate pesticide assessment model.

*Factual Knowledge*

The Factual Knowledge stored in the EXPRES data base is composed of detailed quantitative information that describes the chemical properties of pesticides and the physical, pedological, meteorological, hydrogeological and agricultural characteristics of agricultural regions across Canada. This information can be viewed by the user and incorporated into the input data sets that are required by the pesticide models to test the environmental effects of applying pesticides in different agricultural regions across Canada. These two groups of data are discussed in detail below.

Pesticide Data

The pesticide data base in EXPRES currently contains information for approximately 175 pesticides that are or were in use in Canada. The data base is expandable in that both additional pesticide information can be added as it becomes available and new pesticides can be incorporated into the data base. The pesticides included in the data base are listed in Appendix A. Table 1 summarizes the types of information contained in this data base. This information is divided into two groups.

Table 1. Information Included in the Pesticide Data Base

General information

- pesticide name (active ingredient)
- synonym (trade names)
- pesticide chemical family
- type of pesticide
- Chemical Abstracts Service registration number
- mode of application
- references for data

Chemical parameters

- molecular weight (g/mole)
- specific gravity (dimensionless)
- aqueous solubility (mg/L)
- vapour pressure (mPa)
- vapour density (mg/L)
- octanol-water partition coefficient (dimensionless)
- organic carbon partition coefficient (L/kg)
- Henry's Law constant (dimensionless)
- half-life of the pesticide in soil (days)

The first group of pesticide information identifies and classifies the pesticide. For example, information for the pesticide diazanon includes its CAS registration number, 333-41-5; its family, organophosphate; the type of pesticide, insecticide; and its synonyms, Basudin, Knox-Out, Diazol, and Spectracide. The pesticide name is often referred to as the active ingredient, and the synonyms include the trade names of the pesticide (names under which the pesticide is sold). Because a pesticide listed as a trade name will often contain two or more active ingredients, synonyms in the data base also identify which active ingredients are incorporated into the pesticide. For example, the pesticide Primextra is a mixture of the active ingredients atrazine and metolachlor.

The second group consists of values describing the chemical and biological properties of the pesticide. The values for the chemical properties of the pesticides were obtained from several sources, and both the reference from which the values were obtained and the temperature at which a parameter was measured are displayed. In addition, suggested values are provided for the properties of most pesticides. The data in the pesticide data base were obtained from 17 compilations of pesticide data and are reported as presented in these references (without corrections). The source compilations are Khan (1980), Laskowski et al. (1982), Verschueren (1983), Carsel et al. (1984), Jury et al. (1984, 1987), Rao et al. (1985), Sax and Lewis (1987), Suntio et al. (1988), Worthing and Walker (1987), Gustafson (1989), the Merck Index (1989), U.S. EPA (1989), Taylor and Spencer (1990), Howard et al. (1991), Worthing and Hance (1991), and Wauchope et al. (1992). The data in each compilation were derived from a number of sources, and the value for a particular pesticide property was often listed in more than one reference. In some instances, the values reported in different compilations were obtained from the same source. All repeated values have been included in the pesticide data base to indicate that several experts in the field agree on a value reported for a particular parameter. The values contained in the pesticide data base are listed in Crowe and Mutch (1991b).

Even though these pesticides have been assembled from 17 source compilations, many of the parameter values are missing. In some instances, the values contained in the data base show considerable variability among values assigned to a single parameter, which unfortunately is typical of values reported in the literature. For example, (1) of the nine values reported for the solubility of lindane, seven are different, with the values ranging from 0.0 to $7.5 \times 10^{+2}$ mg/L; (2) five of the seven values reported for the vapour pressure of dieldrin are different, and values range from $2.4 \times 10^{-2}$ to $4.0 \times 10^{+5}$ mPa; and (3) the three log Koc values reported for dicamba are -0.40, 0.34, and 2.71 L/kg. The variability that is evident in the reported values may be due to (1) improvements in analytical instrumentation over time, (2) different analytical methods used in obtaining these values, (3) measurements conducted at various temperatures (e.g., solubility values for atrazine were reported at five different temperatures, and several values do not have a reference temperature reported), (4) typographical errors, (5) clerical errors made by the authors of the 17 compilations in copying these values from the original reference source, (6) incorrect unit conversions in converting values from one unit of measurement in the original source to a different unit of measurement in the compilation lists (e.g., from mm Hg to mPa, or from atm to Pa), or (7) incorrect conversions in the magnitude of a unit (e.g., using $10^{-3}$ rather than $10^{+3}$ to convert from Pa to mPa). The latter three are the most probable causes for the variability extremes in the reported data, especially for those values that differ by a few orders of magnitude.

## Agricultural Region Data

EXPRES also contains a data base that comprises detailed information that describes the physical, pedological, meteorological, hydrogeological, and agricultural setting of different agricultural regions across Canada. Currently, descriptions of 22 agricultural regions are available in the EXPRES data base (Table 2 and Fig. 5).

Table 2. Agricultural Regions Included in the EXPRES Data Base (numbers refer to location of the agricultural regions in Fig. 5)

| | |
|---|---|
| 1. | A raspberry field in the lower Fraser River valley, B.C. |
| 2. | An apple orchard in the Okanagan Valley, B.C. |
| 3. | A barley field in the Peace River District of Alberta |
| 4. | A barley field in central Alberta |
| 5. | Rangeland in southwestern Alberta |
| 6. | A sugar beet field in southern Alberta |
| 7. | A barley field in central Saskatchewan |
| 8. | A wheat field in southern Saskatchewan |
| 9. | A flax field in southern Manitoba |
| 10. | A sugar beet field in southern Manitoba |
| 11. | A corn field in southwestern Ontario |
| 12. | A tobacco field in southwestern Ontario |
| 13. | A grape vineyard in the Niagara region of Ontario |
| 14. | Rangeland in eastern Ontario |
| 15. | An apple orchard in southwestern Quebec |
| 16. | Rangeland in southwestern Quebec |
| 17. | A corn field in the Yamaska River valley, Quebec |
| 18. | A potato field in the Saint John River valley, N.B. |
| 19. | A forest zone in east-central New Brunswick |
| 20. | A potato field in Prince Edward Island |
| 21. | An apple orchard in the Annapolis Valley, Nova Scotia |
| 22. | A potato field on the Avalon Peninsula, Newfoundland |

These regions were selected to represent both areas of significant agricultural activity in Canada and the important crops that are grown in each of these agricultural regions. Thus, these agricultural regions represent rural areas where it would be expected that the potential for groundwater contamination by pesticides is high. The focus of this section is to describe the parameters that are required to characterize the agricultural regions, and

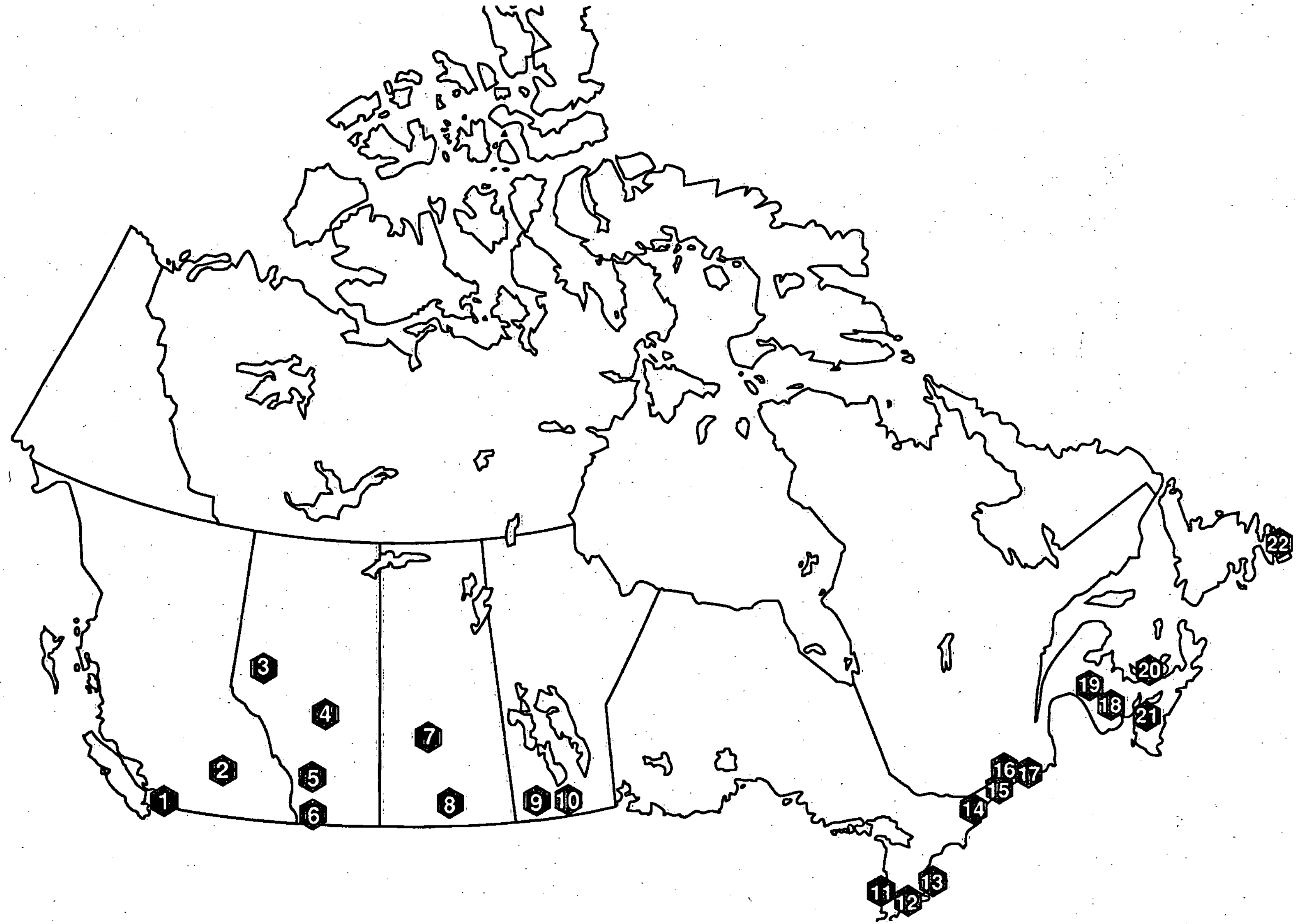



Figure 5. Location of agricultural regions included in the EXPRES data base (See Table 2 for names of these regions).

not to describe the specific conditions that are found within each of the agricultural regions included in EXPRES. A more detailed description of the agricultural regions currently available within EXPRES, as well as the values selected for the model parameters in each region, is presented in Mutch and Crowe (1991). The information stored in the agricultural data base is divided into three areas: (1) the soil profile characteristics, (2) the crops grown and farm management practices employed, and (3) the meteorological conditions of the different agricultural regions (Table 3).

The characterization of each of the typical agricultural regions (i.e., the values assigned to the soil, crop, and meteorological parameters) is hypothetical to the extent that the basic model parameters were not derived from an actual field site within the agricultural region. The model parameter values chosen to define the agricultural regions were, however, guided by experience from a variety of field studies undertaken within the particular agricultural region. The values assigned to the model parameters are representative of typical or common conditions in the agricultural region.

The general descriptions of the agricultural regions and the model parameter values selected for the regions were derived from a number of sources. In general, the physical and chemical parameters characterizing the soils in each of the agricultural regions were selected from soil survey reports that are available for most areas of the country. These reports are available through the provincial agricultural departments or through the national soils data base (CanSIS - Canadian Soil Information System).

Cropping and farm management details required by EXPRES were obtained primarily through conversations with personnel from Agriculture Canada (CDA) research stations and provincial crop extension personnel in each of the agricultural regions. Local farm managers may also be able to provide insights into the crop and farm practice patterns used in a region. Provincial agricultural publications (e.g., the AGDEX series in Alberta) are also useful in selecting parameter values.

Meteorological data were obtained from the Atmospheric Environment Services for weather stations located within each of the agricultural regions. The 22 meteorological stations currently in EXPRES are listed in Table 4. Daily precipitation, temperature, and pan evaporation values (when available) were obtained for the period January 1, 1970, to December 31, 1989, for each meteorological station. These data have been reformatted for use by EXPRES. Missing precipitation values were estimated by taking the 19-year average precipitation for that day, while missing temperature data were estimated with the average of the temperature on the previous and following days.

Those using EXPRES should be aware that it is very difficult to describe a large agricultural region, such as a wheat field in southern Saskatchewan, with one set of model parameters. An effort has been made to select values for the Knowledge Base that represent the typical conditions of each agricultural region. However, the user should be aware that conditions can vary greatly within a region, and analyses performed with EXPRES on new pesticides submitted for registration should include simulations performed over a wide range of model parameter values.

Table 3. Parameters Included in the Agricultural Region Data Base

Soil profile parameters
- soil horizon type (Surface, Root, Below root zone)
- horizon thickness (cm)
- bulk density of the soil (g/cm$^3$)
- percent organic carbon content
- percent silt content
- percent clay content
- saturated hydraulic conductivity (mm/day)
- field capacity
- wilting point
- air entry value (kPa)
- Universal Soil Loss Equation erodibility factor
- Universal Soil Loss Equation support practice factor
- Universal Soil Loss Equation length of slope factor
- depth to the water table (m)
- profile drainage conditions

Crops grown and farm management parameters
- crops grown in the agricultural zone
- crop rotation schedule
- maximum interception storage (cm)
- maximum root depth (cm)
- crop cover fraction
- pesticide uptake by the plant factor
- plant density (plants/m$^2$)
- Soil Conservation Service curve number
- Universal Soil Loss Eqn. soil cover/crop management factor
- date on which plants are planted (dd/mm/yy)
- date on which plants emerge from the soil (dd/mm/yy)
- date on which the plant roots mature (dd/mm/yy)
- date on which plants mature (dd/mm/yy)
- date on which the crop is harvested (dd/mm/yy)

Meteorological parameters
- total daily pan evaporation (cm)
- total daily precipitation (cm)
- average daily temperature (°C)
- 20-year average daily precipitation
- 20-year average daily temperature
- 20-year average daily pan evaporation
- annual summary of meteorological data
- minimum depth of evaporation (cm)
- pan evaporation coefficient
- snow melt coefficient (cm/degree day)
- erosive storm duration (h)
- irrigation applied (cm)

Table 4. Meteorological Stations Included in the EXPRES Data Base

| Name of station | Province | Latitude | Longitude |
|---|---|---|---|
| Vancouver UBC | B.C. | 49°15' | 123°15' |
| Summerland CDA | B.C. | 49°34' | 119°39' |
| Beaverlodge CDA | Alberta | 55°12' | 119°24' |
| Calgary Int'l Airport | Alberta | 51°06' | 119°24' |
| Lacombe CDA | Alberta | 52°28' | 113°45' |
| Lethbridge CDA | Alberta | 49°42' | 112°47' |
| Saskatoon SRC | Saskatchewan | 52°09' | 106°36' |
| Regina Airport | Saskatchewan | 50°26' | 104°40' |
| Glenlea - Univ. of Manitoba | Manitoba | 49°39' | 97°07' |
| Morden CDA | Manitoba | 49°11' | 98°05' |
| Delhi CDA | Ontario | 42°52' | 80°33' |
| Harrow CDA | Ontario | 42°02' | 82°54' |
| Hamilton RBG | Ontario | 43°17' | 79°53' |
| Kemptville | Ontario | 45°00' | 75°38' |
| L'Assomption CDA | Quebec | 45°59' | 73°26' |
| Ormstown | Quebec | 45°07' | 74°02' |
| St. Hyacinthe 2 | Quebec | 45°37' | 72°58' |
| Chatham Airport | New Brunswick | 47°01' | 65°27' |
| Fredericton CDA | New Brunswick | 45°55' | 66°37' |
| Charlottetown CDA | P.E.I. | 46°15' | 63°08' |
| Kentville CDA | Nova Scotia | 45°04' | 64°29' |
| St. John's West CDA | Newfoundland | 47°31' | 52°47' |

# Operation of the EXPRES Expert System

The basic operations available within EXPRES, their order of implementation, and whether the operations require prompts from the user or are handled internally by EXPRES are discussed in this chapter. The reader is referred to Appendix E for the type conventions used in this chapter and to Appendix B to view each of the screens.

## A GENERAL OVERVIEW OF THE EXPRES EXPERT SYSTEM

The overall organization and operation of EXPRES are illustrated in Figure 6 and will be discussed in general terms in this section. The general operation of EXPRES, including movement between screens, is controlled through a command line located at the top of each screen. To provide a framework in which a novice user can rapidly become familiar with the operation of EXPRES, the first input data screen (**SESSION INFORMATION**) provides the user with access to a series of introductory text files. These files provide (1) a description of the instructions required to operate EXPRES; (2) an overview of the structure, application, design criteria, pesticide models, and data bases used in EXPRES; and (3) example files that allow the user to view a complete input data set required by the three pesticide models, as well as the associated output that may be obtained with each of the models. The selection of the most appropriate pesticide model for an assessment is performed by EXPRES, based upon the objectives supplied by the user on the **ASSESSMENT OBJECTIVES** screen. Three options are available: the user may (1) select the **Data Display** option, (2) perform a **Screening Assessment**, or (3) perform a **Simulation** with one of the mathematical models.

The **Data Display** option allows the user to view the information stored in the EXPRES data bases quickly. The first data base, **Pesticide Data**, currently contains the physical and chemical properties of approximately 175 pesticides. The second data base, **Agricultural Region Data**, currently contains soil, crop, and meteorological characteristics for 22 agricultural regions across Canada. The **Data Display** option may be useful in estimating values for model parameters or in comparing and contrasting different pesticides and/or agricultural regions.

The **Screening Assessment** option provides the user with a relative ranking (with respect to other pesticides stored in the pesticide data base) of the potential for a pesticide to leach to the water table, using the LP/LI model. The LP/LI model does not simulate the processes involved in controlling the fate of a pesticide in the subsurface. If this option is selected, the user must enter four chemical properties of the pesticide of interest. EXPRES will then retrieve similar properties for the other pesticides stored in its data base and will provide a relative assessment by comparing the results of the test pesticide to the results for the other pesticides stored in the data base. Currently, there are 128 reference pesticides available for use with the LP/LI model. A list of the pesticides is given in Appendix A.

Selection of the **Simulation** option enables EXPRES to simulate the transport and transformation of a pesticide within the unsaturated zone with either the PRZM or LEACHM models. The user is required to enter further information to enable EXPRES to select the most appropriate simulation model. EXPRES guides the user through the required branches of the **Simulation** option and allows the user to enter or modify the input data required by the selected model. The user may choose to load default data for both the pesticide (**Existing Pesticides**) and **Agricultural Region** of interest from the data contained in the EXPRES data bases.

After these choices have been made, default values for the model parameters are loaded into the appropriate screens in the **Pesticide, Soil, Crop,** and **Meteorological** branches. The user may then review these data and change any or all the data to more site-specific values, if this information is available. Because the specifics of a pesticide application may vary significantly according to the crop, location, and timing of the application, default information for the pesticide application information cannot be supplied from the data base. Therefore, values required for the **Pesticide Application Parameters** branch must be supplied by the user (as indicated in Fig. 6).

The user must also enter the type of output that is desired for the simulation. If an uncertainty analysis is required, the user must select the parameter of interest and specify a modification value for the parameter. The user can execute the selected model from any screen within the **Simulation** option, once the entry of data is complete. Before executing the selected model, EXPRES subjects the input data set to a series of integrity checks and alerts the user to any errors or warnings that may have been detected. The user may ignore the warning messages generated but must resolve any conflicts that result in error messages before EXPRES will execute the model.

After the execution of the model is complete, the Data Analysis portion of EXPRES is invoked. Within Data Analysis, EXPRES assembles the results produced by the models and presents them to the user in a manner that can be easily understood and interpreted. There are two general types of plots available with EXPRES: (1) concentration profiles, which show a snapshot of the vertical distribution of the pesticide concentration through the soil profile at specified times and (2) time series plots, which depict the value of a selected parameter at a specific depth within the soil profile as it varies over time. The **Simulation** option may be used to determine (1) the concentration of the pesticide within the soil profile; (2) the leaching rates and/or travel times required for the pesticide to reach the water table; (3) the dissolved, sorbed, and total pesticide storage in the soil profile; and (4) the water storage and flux in the soil profile.

A more detailed discussion of the basic operation of EXPRES follows.

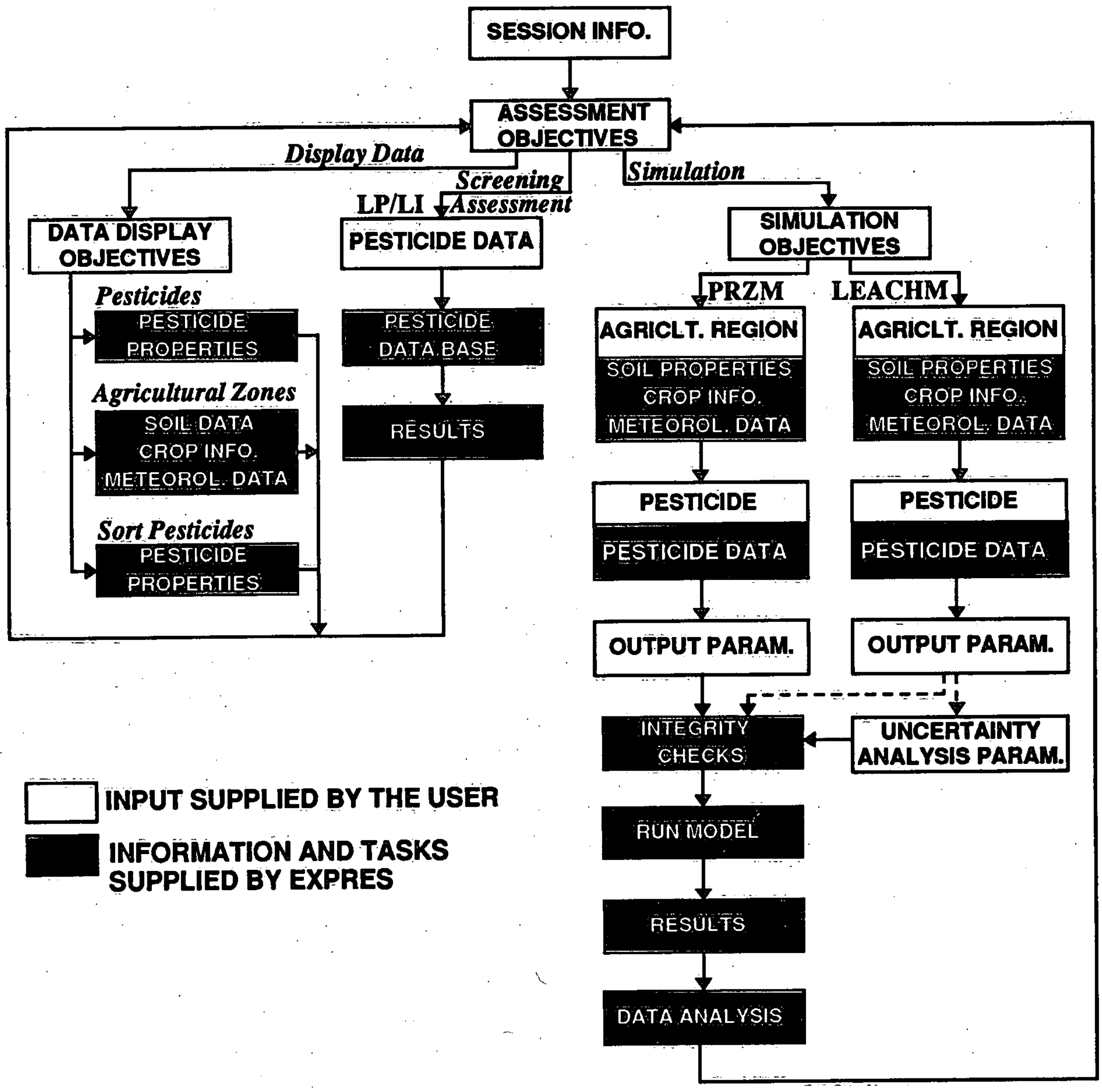



Figure 6. Structure and operation of the EXPRES expert system.

## THE EXPRES COMMAND LINE

All interactions between the user and EXPRES take place by way of the screens. A command line located at the top of each screen (see screens in Appendix B) provides the user with access to a series of commands and pull-down menus that control the operation of EXPRES. The user can gain access to the command line by using either the <Tab> and left and right arrow keys, or the function keys (e.g., *F1 = NEXT-SCRN, F2 = PREVIOUS-SCRN*). The commands are discussed below.

### The Next-Scrn (F1) and Previous-Scrn (F2) Commands

Movement between screens is handled with the *NEXT-SCRN* (*F1*) and *PREVIOUS-SCRN* (*F2*) commands.

### The Default-Data (F3) Command

The *DEFAULT-DATA* (*F3*) command provides the user with access to the default data stored in the EXPRES data base. There are five options available with this command: (1) *Return to Screen*, (2) *Highlight Changed Values*, (3) *Display Default Values*, (4) *Restore Screen to Defaults*, and (5) *Help: Default Data*.

The first option (*Return to Screen*) exits the user from the command line and returns control to the underlying input data screen.

If the user loads the default data for a particular agricultural region, modifies any of the default data, and later wishes to see which values have been modified from the original default values, the user may execute the second option, *Highlight Changed Values*. EXPRES will highlight the values on the current screen that differ from their corresponding original default values that are stored in the EXPRES data base.

If the user wishes to view the difference between the modified parameter values and the original default values, the user can view the original default values with the *Display Default Values* option. EXPRES will display the original default values for the selected agricultural region. The corresponding original values for the parameters that were changed by the user will be highlighted when the *Display Default Values* option is issued, to allow for an easy identification and comparison of the values.

If the user wishes to restore the parameters on a screen to their original default values, the fourth option (*Restore Screen to Defaults*) will replace all the model parameter values on the screen with the original default values for the selected agricultural region. In some instances, it may be necessary to restore more than one screen to the original default data to maintain consistency between associated screens. If this is the case, EXPRES will produce a warning message for the user before it restores the model parameters to their default values. If all the data associated with a screen cannot be viewed on one screen, a *MORE* message will appear on the screen, and the user may use the <PgUp> and <PgDn> keys to view the additional data.

The fifth option (*Help: Default Data*) provides on-line help that describes the function and operation of the *DEFAULT DATA* command.

**The Run (F4) Command**

The *RUN* (*F4*) command provides the user with access to the five commands associated with running a simulation model. The available options are (1) *Return to Screen*, (2) *View Error File*, (3) *Run Model*, (4) *Run Data Analysis*, and (5) *Help: Run*. Each option is discussed below.

The *Return to Screen* option exits the user from the command line and returns control to the underlying input data screen.

The second option (*View Error File*) allows the user to view the error or warning messages, produced during the integrity checks, from any location within the data entry portion of EXPRES. This option is useful if a number of error and/or warning messages are produced, and the user wishes to return to resolve these conflicts.

After all the input data are entered, the user can issue the third option (*Run Model*) to initiate the execution of the selected simulation model. The *Run Model* option can be issued from anywhere within the **Simulation** portion of EXPRES. However, before starting the execution of the selected model (either PRZM or LEACHM), EXPRES invokes a series of integrity checks (over 140 rules) to check the completeness, validity, and consistency of the data entered in the input data set. These integrity checks will ensure that the data entered are (1) of the correct type and format, (2) within an appropriate range for the model parameters, and (3) consistent with other data in the data set. EXPRES will indicate the number of warning and error messages that were generated during the integrity checks. If any error messages are produced, the user must return to the data-entry screens and resolve all the conflicts that resulted in an error message before EXPRES will execute the model. If only warning messages are produced, EXPRES presents the user with three options: (1) view the warning messages (*View Error File*), (2) return to the data-entry screens to resolve the conflicts (*Return to Screen*), or (3) ignore the warning messages and proceed directly with the execution of the model (*Ignore Warning Messages*).

The Data Analysis portion of EXPRES is accessed in two ways. After the execution of the simulation model (*Run Model*) is complete, EXPRES will automatically enter Data Analysis. Direct access is also provided to Data Analysis with the *Run Data Analysis* option. An integrity check is performed before entering Data Analysis to ensure that the available output results are consistent with the current input data set. If the input and output data sets are consistent, *Run Data Analysis* will bypass the execution of the model and enter Data Analysis. If the input data set is not consistent with the output results, EXPRES will warn the user and will allow the user to load the original input data set that was used to create the output results (*Load Original Data*) or to enter Data Analysis (*Continue*) even though the current input and output data sets do not correspond. If the *Load Original Data* option is selected, the current input data set will be overwritten by the original data set used to create the output results.

The fifth option (*Help: Run*) provides on-line help that describes the function and operation of the *RUN* command.

**The File (F5) Command**

The *FILE* (*F5*) command allows the user to save the input data file and exit from EXPRES at any time. Four options are available: (1) *Return to Screen*, (2) *Save as:* FILENAME, (3) *Exit*, and (4) *Help: Files*. Only the third option (*Exit*) is available within the Data Display and Data Analysis portions of EXPRES.

The *Return to Screen* option exits the user from the command line and returns control to the underlying input data screen.

The second option (*Save as:*FILENAME) allows the user to save the input data file at any time during the completion of the data set without exiting from EXPRES. If the user is creating a new data set, no default FILENAME will be provided, and the user must enter a FILENAME for the input data set. The FILENAME provided must be limited to a maximum of eight characters, with no DOS file extension. However, if a FILENAME currently exists for the input data set, it will appear as the default FILENAME. If the user wishes to save the input data set under a different FILENAME (preserving the old FILENAME), the user simply types the new FILENAME over the top of the default FILENAME. If the specified FILENAME already exists, EXPRES will seek confirmation from the user before the existing file is overwritten.

The user may exit EXPRES at any time during the creation of an input data set with the third option, *Exit*. A user selecting this option is provided with three additional options: (1) *Return to Screen*, (2) *Exit Without Saving*, and (3) *Exit as:*FILENAME. The *Return to Screen* option returns control to the underlying input data screen. The *Exit Without Saving* option exits the user from EXPRES without saving the input data file. Any changes that were made to the file during the session with EXPRES (or since the last saving of the file) will be lost. The *Exit as:*FILENAME option exits the user from EXPRES, saving any changes that have been made to the input data set. The process for saving a file with this option is the same as that for the *Save as:*FILENAME option, previously discussed.

The fourth option (*Help: File*) provides on-line help that describes the function and operation of the *FILE* command.

**The Notes (F6) Command**

The *NOTES* (*F6*) command allows the user to record pertinent information about the input and output data sets. This information is stored in a file that is associated with the input data set and will be accessible through the *NOTES (F6)* command whenever the user loads the input data set into EXPRES. In this file, users may wish to record, for future reference, the objective of the simulation, the type of pesticide being evaluated, any special conditions that are being simulated, and any other pertinent information about the simulation or the results produced. The users can then refer to the *NOTES* command to refresh their memory on the specifics of a given simulation, should they return to the data set at some time in the future. The *NOTES* (*F6*) command allows users to access their own editor or word processor. Thus, users have access to all the features they are normally accustomed to with their own editor or word processor. To invoke their own word processor, the users must modify their AUTOEXEC.BAT file to include an additional environment variable. An example of the statement that must be added is shown below.

*SET XEDIT=C:\WP51\WP*

In this example, the environment variable would invoke WordPerfect®. The statement must include the path to the directory in which the word processor is located (i.e., C:\WP51\), as well as the command that is used to invoke the word processor (i.e., WP).

There are three options available with the *NOTES* command: (1) *Return to Screen*, (2) *Edit File*, and (3) *Help: Notes*.

The *Return to Screen* option exits the user from the command line and returns control to the underlying input data screen.

The *Edit File* option will invoke the user's own word processor and will load the "Notes" file that is linked to the current input data set. The user may record or review pertinent information about the particular session or data set in the associated file.

The *Help: Notes* option provides on-line help that describes the function and operation of the *NOTES* command.

**The Help (F7) Command**

An important feature of EXPRES is that it is designed with an on-line Help facility to aid the user in the selection and entry of data. EXPRES provides the user with three options through the *HELP* (*F7*) command: (1) a *Definition*, (2) an *Explanation*, and (3) *User Supplied* information.

The *Definition* option gives a brief definition of the parameter or option being requested by EXPRES (Fig. 7a).

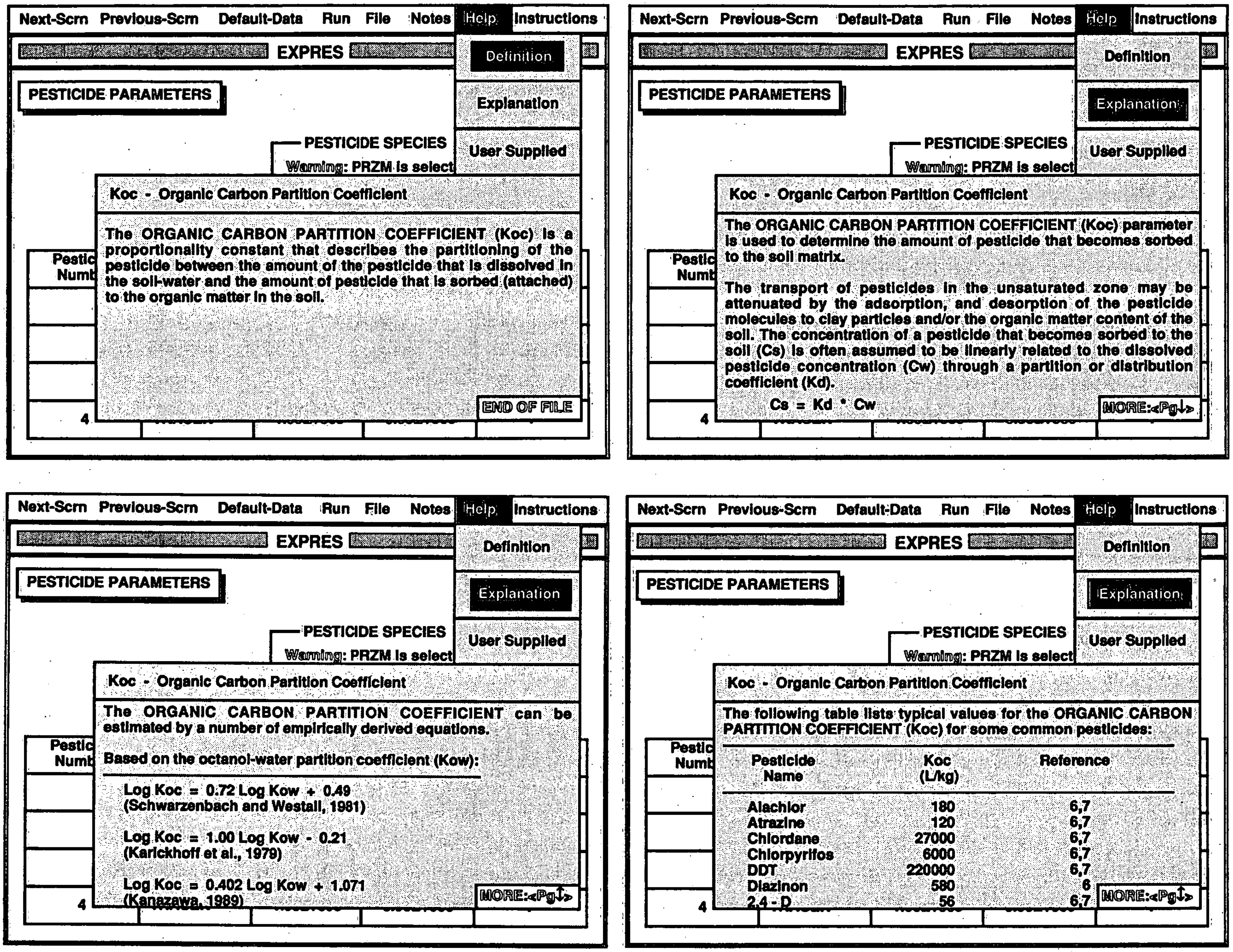



Figure 7. Example of screens showing the assistance that is available through the EXPRES Help facility: (a) a definition, (b) a more detailed explanation, (c) empirical estimation techniques, and (d) typical values.

The *Explanation* option provides additional information on the model parameter or option in question. This information discusses in more detail where or how a value may be used or obtained (Fig. 7b). Examples of empirical estimation techniques (Fig. 7c) and/or typical values (Fig. 7d) that may be used to obtain an estimate for the value of the model parameter are also given.

The *User Supplied* option provides the user of EXPRES with access to any additional information that may have been provided by previous users of EXPRES. If EXPRES users have additional information that they feel may be useful to subsequent users, they may enter this information in the *User Supplied* Help file. The *User Supplied* information cannot be added using this option; it can only be viewed. To add information, the users are given the appropriate filename (e.g., EXPRES\HELP\KOC.USR) and may simply add information to this file with any editor or word processor that can save a file in an ASCII format. The information added will then be accessible to future users of EXPRES through the *HELP* command.

### The Instructions (F8) Command

The *INSTRUCTIONS* (*F8*) command provides a brief on-line description of the all the commands discussed in this section. In addition, a conversion table is provided to allow for the conversion of data between SI and U.S. customary or imperial units. The advantage of the *INSTRUCTIONS* command is that a user can access a description of the EXPRES commands from any screen within the data entry portion of EXPRES.

### The Options (F9) Command

The *OPTIONS* (*F9*) command is specific to the Data Analysis portion of the EXPRES expert system. This command allows the user to send the output to various hardware devices (monitor, printer, or a file). It also allows the user to specify the hardware configuration for the output device (whether colour or monochrome monitor, serial or parallel printer, HPGL® or PostScript® file formats).

## A GENERAL DESCRIPTION OF THE EXPRES SCREENS

This section contains a description of each of the screens used within the EXPRES expert system. The order in which the descriptions are presented is in accordance with the order in which EXPRES presents the screens to the user as the user moves through the various branches of the expert system. EXPRES begins by presenting the user with a series of introductory screens. Based on the assessment objectives provided by the user, EXPRES will follow one of three branches of screens: (1) **Data Display**, (2) **Screening Assessment**, and (3) **Simulation.** Within each of these three branches, there are a series of sub-branches, consisting of one or more screens. The screens in each of these branches and sub-branches will be discussed in the following sections. The titles and overall order of appearance of the screens are shown in Figure 8, and a representation of each screen is presented in Appendix B.

### Introductory Screens

The four screens within this group are designed to provide the user with background information about EXPRES and to allow the user to enter information and objectives for the assessment. The four screens in this group are

| | |
|---|---|
| **TITLE** | Screen 1 |
| **DISCLAIMER** | Screen 2 |
| **SESSION INFORMATION** | Screen 3 |
| **ASSESSMENT OBJECTIVES** | Screen 4 |

EXPRES begins with a **TITLE** and a **DISCLAIMER** screen. However, the first screen on which the user is required to enter information is the **SESSION INFORMATION** screen. This screen provides the user with three types of introductory information that enable a novice user to become familiar with the basic operation and intent of EXPRES. The first option, **Instructions**, provides access to a text file that discusses the instructions used in the basic operation of EXPRES, including movement between and within screens, data entry, execution of the simulation models, and display of the output results. The second option, **Overview**, provides the user with both a short and a long overview of EXPRES. These text files discuss the purpose, operation, application, and limitations of EXPRES, as well as the application and limitations of the three pesticide assessment models in EXPRES. The third option, **Load Example File**, allows the user to view a complete data set with both the pesticide and site-specific data, as well as output from the assessment models, for a simulation of an application of the pesticide aldicarb to a potato field on Prince Edward Island. This screen also has a feature that will allow the user to change the colours of the different screen elements (**Screen Setup**). Once the user has entered the **Screen Setup** option, the desired screen element (e.g., background colour, text colour) is selected with the up and down arrow keys. The left and right arrow keys are then used to change the colour or monochrome aspects of the screen element. The colour changes that are made will be reflected in the window that appears to the left of the list of screen elements.

The user may choose to load an existing file with the **Load Existing File** option on the **SESSION INFORMATION** screen. Once this option has been selected, the user is required to enter the name of the existing input data file, which was previously created and saved with EXPRES. The data in this file are then loaded into the appropriate EXPRES screens.

There are two ways in which a user can create a new file for a screening assessment or simulation. First, the user simply continues using the *NEXT-SCRN (F1)* command. EXPRES will automatically set the numerical and alphanumerical values of the model parameters to zero and a temporary word, respectively. These values are not

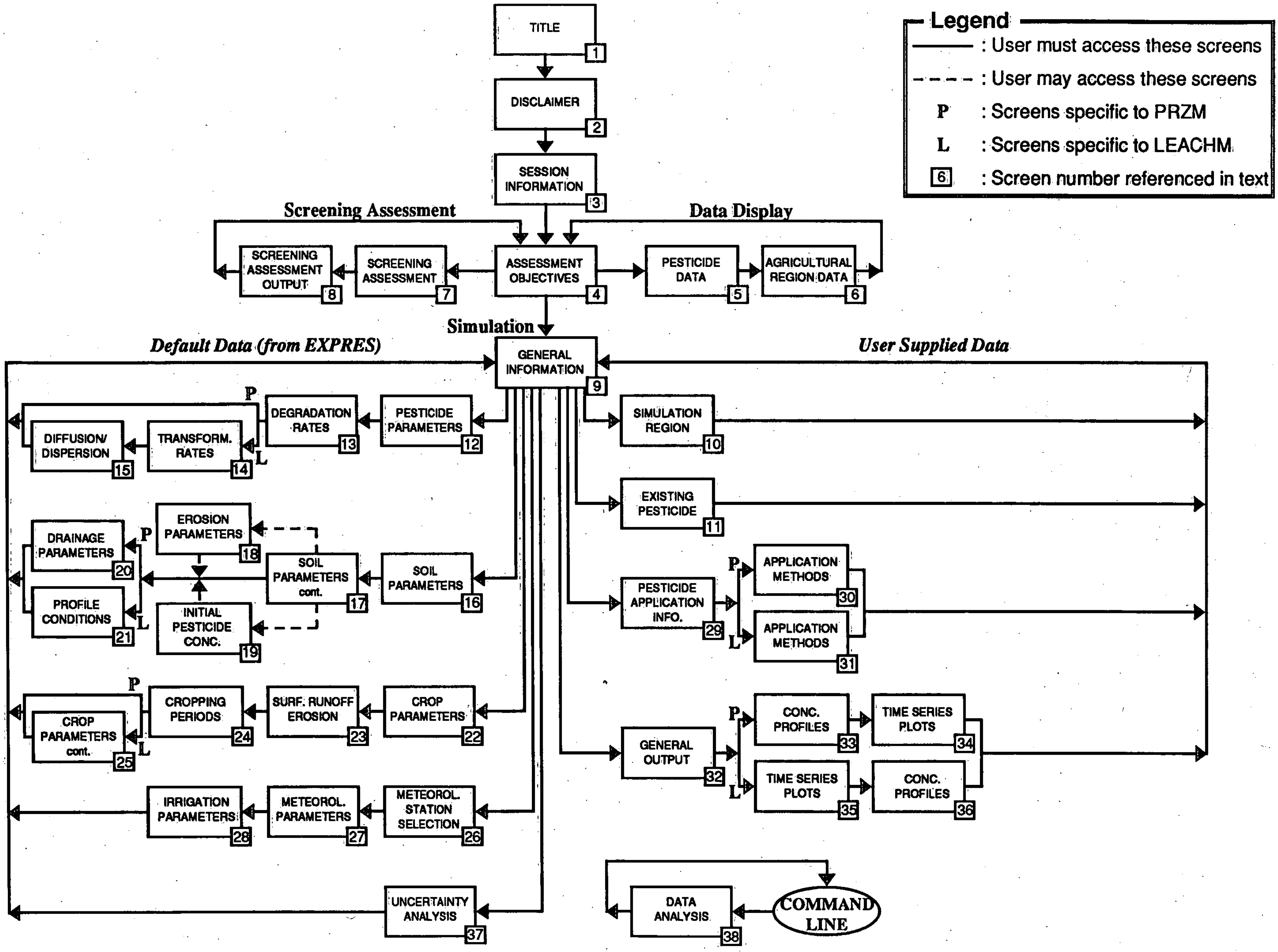



Figure 8. Flow chart showing the order of appearance of the input data screens for the EXPRES expert system.

intended to be default values for any of the model parameters. They simply indicate to the user which fields require input data and what type or format is expected for the parameter. The user is required to replace the zeros with appropriate values for each of the model parameters. The file can then be saved and named at any time using the *Save As:* option in the *FILE (F5)* command. Second, the user may load an existing file by selecting either the **Load Existing File** option or the **Load Example File** option on the **SESSION INFORMATION** screen. The values of the model parameters that have been previously created and saved will be loaded. The user must then use the *Save As:* option in the *FILE (F5)* command to rename the file before proceeding. The user can then change any of the values of the model parameters, thus creating a new input data file.

On the following screen (**ASSESSMENT OBJECTIVES** - Screen 4), EXPRES prompts the user for the objectives of the assessment, and based on these objectives, decides which is the most appropriate assessment method for the simulation. When specifying the objectives of the assessment, the user has the option of

- reviewing the data contained in the EXPRES data bases (**Data Display**)
- performing a quick and general relative assessment of the leaching potential of the pesticide, with a screening model (**Screening Assessment**)
- quantifying the migration rates and concentration distribution of a pesticide in the subsurface with the mathematical models (**Simulation**)

These are the three main options available within EXPRES. However, before proceeding with the **Simulation** option, the user is required to enter additional information about the objectives of the assessment. EXPRES requires this information to choose the most appropriate mathematical model (PRZM or LEACHM) for the intended simulation and also to determine what type of data should be requested from the user. The user must define the type of simulation that is desired by choosing between a single simulation (**Run a Scenario**) with the pesticide model or a series of simulations (**Uncertainty Analysis**), where the value of an individual model parameter is varied systematically over a plausible range to determine the response of the system to a small error in the value of the model parameter. The user must also specify whether the results are desired within an hour (**Quickly**) or can be produced over several hours (**No Preference**), and whether daughter products are to be simulated (**Simulated** or **Not Simulated**) by the pesticide model. The user also identifies the PC's processor (**80286** or **80386/80486**) and the **Approximate Simulation Length**. The **Approximate Simulation Length** need only be a rough estimate (within 20%) of the actual simulation period. Based on this information EXPRES will select the most appropriate model for the simulation. Once these options have been selected, the user can execute the *NEXT-SCRN (F1)* command to proceed to the selected option.

**Screens of the Data Display Branch**

Only two screens are contained within the **Data Display** branch:

| | |
|---|---|
| **PESTICIDE DATA** | Screen 5 |
| **AGRICULTURAL REGION DATA** | Screen 6 |

The first screen to appear in this branch of the expert system is the **PESTICIDE DATA** screen. It presents a list of the pesticides that are contained in the EXPRES data base. The user can view the chemical properties stored in the data base for a selected pesticide by using the <up> and <down> arrow keys and/or the <PgUp> and <PgDn> keys to move to the pesticide of interest and then hitting the <Enter> key. EXPRES produces a window displaying information that identifies the family and type of pesticide (e.g., organophosphate and herbicide), other trade names by which the pesticide is known, common application modes, and the Chemical Abstracts Service (CAS) registration number (Screen 5a). This screen also presents recommended values for eight commonly reported pesticide properties (molecular weight, specific gravity, $K_{oc}$, $K_{ow}$, solubility, vapour pressure, Henry's Law constant, and half-life). If more information is required, the user may invoke the **View Additional Values** option on this screen; it opens a second window (Screen 5b), where additional chemical properties are displayed for the selected pesticide. Two lines of reference information are available within the window. The first (**Temp:**) contains references for the temperature at which the values were determined (Screen 5b). The second line (**Ref:**) contains a list of the publication references from which the data were obtained (Screen 5c). The letters and numbers on these two lines correspond to the letters that follow a value in the table and to the number under the "Ref" column. The user can move along the two lines with the arrow keys. The Help facility can only be accessed after exiting from the window (by hitting any key). The Help file available for the underlying screen also contains information describing the information presented in the window.

There are two additional options listed on the **PESTICIDE DATA** screen that are available for viewing and obtaining pesticide information. These options are accessed by using the arrow keys and the <Enter> key to move to and select the required option.

The **Search For** option allows the user to search the pesticide data base in EXPRES for a particular pesticide, given a synonym, a common name for the pesticide, or its CAS registration number. Once the **Search For** option has been selected, a window will appear that displays the three search options, **Synonym**, **Name,** and **CAS Number** (Screen 5d). To initiate a search, use the <up> and <down> arrow keys and hit the <Enter> key to select the desired option. Then use the <right> arrow key to move to the box and enter the synonym, name, or CAS registration number, or their first few characters. The search is initiated by moving to the **SEARCH** button and hitting the <Enter> key. If the synonym, name, or CAS registration number is found during the search, the common name of the pesticide (Screen 5d), or all pesticides contained in that synonym (e.g., when there is more than one active ingredient) (Screen 5e) are displayed to the user. The user can exit from the window, find the pesticide of interest in the list on the **PESTICIDE DATA** screen, and view the data for that pesticide.

The **Sort By** option allows the user to sort either all the pesticides in the data base or a few selected pesticides, according to a chemical parameter. Once the **Sort By** option has been selected, a window will appear in which the user selects whether to sort **All Pesticides** in the data base or to sort only **Selected Pesticides**. If the **Selected Pesticides** option is chosen, another window will appear that enables the user to move through the list of pesticides in the data base with the <up> and <down> arrow keys and select the required pesticides by hitting the <Enter> key (Screen 5g). The chemical parameter by which the pesticides will be sorted is selected by moving to the chemical parameter of interest with the <left>, <right>, <up>, and <down> arrow keys and hitting the <Enter> key. The pesticides and corresponding values of the chemical parameter will be listed below in order (Screen 5f).

The final screen in the branch is the **AGRICULTURAL REGION DATA** screen (Screen 6). It presents the user with a list of the default agricultural regions included in the EXPRES data base. The user may quickly view the information stored in the data base for these agricultural regions by moving to the agricultural region of interest with the arrow keys and then pressing the <Enter> key. A window (Screen 6a) will appear, displaying the soil parameter data for the selected agricultural region. Two additional windows (Screens 6b and 6c) list the crop information and meteorological data for the selected agricultural region. The <PgUp> and <PgDn> keys are used to move between the three windows. Within each window, the user may move the cursor along the header of each column to obtain a full description of the abbreviations found in the column headings. A description of the information stored in the particular column appears at the bottom of the window. The Help facility for this screen can only be accessed after exiting from the window. The user can leave this branch with the *Exit* (*F5*) command.

### Screens of the Screening Assessment Branch

The screening assessment branch allows the user to conduct a relative assessment of the potential for a pesticide to leach to the water table based on four chemical properties of the pesticide. The two screens in this branch are

| | |
|---|---|
| **SCREENING ASSESSMENT** | Screen 7 |
| **SCREENING ASSESSMENT OUTPUT** | Screen 8 |

The first screen that appears (**SCREENING ASSESSMENT** - screen 7) requests information required by the LP/LI screening model to conduct an assessment. The user must first choose whether the screening assessment is to be undertaken using only **Existing Pesticides** contained in the data base or using a **New Pesticide,** not in the data base, to be ranked against existing pesticides. If a **New Pesticide** is being assessed, the user must supply its name and values of aqueous solubility, vapour pressure, half-life, and $K_{oc}$ before moving to the next screen. The results of the screening assessment are displayed on the second screen in the branch (**SCREENING ASSESSMENT OUTPUT** - Screen 8a). The user can perform either a **Leaching Potential** assessment or a **Leaching Index** assessment, and the ranking and "score" of the test pesticide are displayed in relation to the ranking and score of the other pesticides stored in the data base. The user can control which pesticides are included in the relative comparison. If the **All Pesticides** option is selected, all pesticides in the data base (to a maximum of 200) with sufficient data will be included in the comparison (Screen 8a). The user may limit the number of pesticides included in the comparison by individually choosing pesticides from a list of pesticides displayed through the **Selected Pesticides** option (Screen 8b). After the pesticides of interest are selected, the user exits the window by hitting the <Esc> key and chooses either the **Leaching Potential** or **Leaching Index**. The **Leaching Potential** assessment ranks the pesticide on its potential to leach to the water table, and in the example shown in Screen 8a, the test pesticide (TEST-PEST) ranked 125$^{th}$ when compared to all the pesticides in the data base (currently a total of 128 pesticides for the LP/LI model). An example of a Leaching Potential assessment is shown in Screen 8c, where the test pesticide (TEST-PEST) is compared to only 11 other pesticides that were chosen by the user through the **Selected Pesticides** option. The **Leaching Index** ranks the potential migration distance of the pesticide prior to its degradation. Interpretations drawn from the screening assessment model should be made with a full knowledge of the limitations inherent in the model (discussed in Chap. 3).

**Screens of the Simulation Branch**

The first screen in the **Simulation** branch is the **GENERAL INFORMATION** screen (Screen 9a), and it acts as the central pivot, or general control screen, for the remaining portion of the EXPRES expert system. The simulation **Starting** and **Ending Dates** that appear on this screen are the actual dates over which the simulation will be run. There are two versions of the **GENERAL INFORMATION** screen (Screens 9a and 9b). The only difference between the two is that one (Screen 9b) provides access to the **Uncertainty Analysis Parameter** branch, which will be discussed later in the chapter.

The screens within the **Simulation** option are divided into two categories (default data and user supplied data), as shown in Figure 8. For the screens in the default data category, the user has the option to load default data from the EXPRES data base that describe both the chemical properties of the pesticide and the physical, hydrogeological, and meteorological conditions of the agricultural region. Currently, default data are available for approximately 175 existing pesticides, and for 22 agricultural regions. If this option is selected, the default values are automatically loaded into the appropriate screens. The user may then view the default values that were loaded for the pesticide and agricultural region, and may change any or all of these values.

Default data are not supplied by EXPRES for the model parameters within the user supplied category. Because the specifics pertaining to the application of the pesticide may be varied, EXPRES does not provide the user with default data for this branch of the expert system. In addition, because no one set of output parameters will be adequate for all possible simulations, the user will also be responsible for choosing the output that is required for the simulation. Should the user have any difficulties in choosing these parameters (referred to as **User Supplied Parameters**), the Help facility in EXPRES will assist the user in selecting the appropriate model parameters. The user ***must*** proceed through all the screens requiring user supplied data and enter appropriate values for all the model parameters before a simulation can be run. It is also ***strongly*** recommended that the user review all the default data that were loaded by EXPRES before proceeding with the execution of the simulation model.

Many of the parameters required by the two mathematical models are common, and as a result, a number of the input data screens are common to the two models. Screens requesting information specific to only one of the models will appear only if that model has been selected for the given simulation. The process of determining which data and therefore which screens are required for an assessment is handled internally by EXPRES and is transparent to the user.

Both the user-supplied and default data are entered through sub-branches of screens, with each containing between one and five input data screens (Fig. 8). The description of the remaining EXPRES screens is divided according to the nine sub-branches of EXPRES (see Fig. 8). The nine sub-branches are

**Agricultural Regions**
**Existing Pesticides**
**Pesticide Parameters**
**Soil Parameters**
**Crop Parameters**
**Meteorological Parameters**
**Pesticide Application Info.**
**Output Parameters**
**Uncertainty Analysis Parameters**

*The Agricultural Regions Sub-branch*

The **Agricultural Regions** sub-branch has only one screen (**SIMULATION REGION** - Screen 10), where the user selects the **Agricultural Region** of interest (e.g., a wheat field in southern Saskatchewan) from the list of agricultural regions currently included in the EXPRES data base. The user moves the highlight bar to the desired region and hits the <**Enter**> key. EXPRES will then load the default data (soil, crop, and meteorological data) for the selected agricultural region into the appropriate screens.

*Existing Pesticides Sub-branch*

The **Existing Pesticides** sub-branch also contains only one screen (**EXISTING PESTICIDES** - Screen 11). On this screen, the user may choose to load default chemical data for a pesticide of interest from the list of pesticides. To load the default data for a pesticide, the user must move the highlight bar to the pesticide of interest and hit the <Enter> key. EXPRES will then load the default data for the pesticide into the screens within the **Pesticide Parameter** sub-branch. If simulating a new pesticide, skip this option and the pesticide parameter screens will appear as blank screens where the user must enter values for the pesticide parameters.

*The Pesticide Parameters Sub-branch*

The **Pesticide Parameters** sub-branch contains either two or four screens, depending upon which model is selected (Fig. 8). The screens are

| | |
|---|---|
| **PESTICIDE PARAMETERS** | Screen 12 |
| **DEGRADATION RATES** | Screen 13 |
| **TRANSFORMATION RATES** | Screen 14 |
| **DIFFUSION/DISPERSION** | Screen 15 |

Default values will be supplied from the EXPRES data base for all of the parameters on the screens in this sub-branch when the user selects a pesticide on the **EXISTING PESTICIDES** screen. The first two screens within this sub-branch are common to the two simulation models, but differ slightly depending on which model is selected. The **PESTICIDE PARAMETERS** screen (Screen 12) prompts the user for the number and names of the pesticides being simulated, as well as for the solubility and $K_{oc}$ values for each of the pesticides. The user must also specify whether the pesticide is a parent pesticide or a daughter product. If the PRZM model is selected, only one pesticide species can be simulated, and the user must specify the **Pesticide Number** for the pesticide of interest. However, because the LEACHM model can simulate up to four pesticide species, the user must specify the number of species to be considered in the simulation. The **DEGRADATION RATES** screen (Screen 13) allows the user to enter the **Degradation Rates** for the parent pesticide and for any daughter products (LEACHM only) that may be generated. Individual **Degradation Rates** are entered for each soil horizon, allowing the user to vary the **Degradation Rates** with depth.

If the LEACHM model is selected by EXPRES, two additional screens appear. The **TRANSFORMATION RATES** screen (Screen 14) supplies, or prompts the user to enter, **Transformation Rates** for each soil horizon. These rate constants control the rate of transformation from the parent pesticide to its subsequent daughter products. The second LEACHM-specific screen (**DIFFUSION/DISPERSION** - Screen 15) requires parameter values that describe the molecular diffusion and dispersion of the pesticide in both the water- and air-filled portions of the soil.

*The Soil Parameters Sub-branch*

When the **Agricultural Region** is selected on the **SIMULATION REGION** screen (Screen 10), default values are supplied for all the soil parameters required by the simulation models on the six screens in this branch. The six screens are

| | |
|---|---|
| **SOIL PARAMETERS** | Screen 16 |
| **SOIL PARAMETERS cont.** | Screen 17 |
| **EROSION PARAMETERS** | Screen 18 |
| **INITIAL PESTICIDE CONCENTRATIONS** | Screen 19 |
| **DRAINAGE PARAMETERS** | Screen 20 |
| **PROFILE CONDITIONS** | Screen 21 |

The **SOIL PARAMETERS** screen (Screen 16) provides the user with default data for the **Depth to Water Table**, the thickness of the soil horizons (**Horizon Thickness**), and the **Bulk Density** and **Percent Organic Carbon** content of the soil horizons. **SOIL PARAMETERS cont.** (Screen 17) supplies default values for the **Field Capacity, Wilting Point**, and the **Initial Soil-Water Content** of the soil horizons. It also characterizes the texture of each soil horizon by supplying values for the particle size distribution of the soil (i.e., **Percent Silt** and **Percent Clay**). The user may also specify if **Erosional Losses** or initial pesticide concentrations (**Pesticide Residues**) are to be simulated. The **EROSION PARAMETERS** screen (Screen 18) will only appear if the user indicates that **Erosional Losses** are important (i.e., *Y*) on the previous screen (Screen 17). The **EROSION PARAMETERS** screen will provide default values for the parameters in the Universal Soil Loss Equation (**USLEK, USLEP,** and **USLELS**). **Particle Bulk Densities** and the **Erosive Storm Duration** are also provided. If the user indicates that **Pesticide Residues** are present (i.e., *Y*) in the soil profile at the beginning of the simulation, an **INITIAL PESTICIDE CONCENTRATION** screen (Screen 19) will appear and allow the user to enter the initial pesticide concentration found within the soil profile at the beginning of the simulation. If the PRZM model is selected, the **DRAINAGE PARAMETER** screen (Screen 20) allows the user to select either a **Free Draining** (e.g., coarse soil types) or a **Restricted Draining** (e.g., tight clay type soils) simulation. If the restricted drainage option is selected, the user must supply empirical **Drainage Parameters** that slow the infiltration through the soil profile to approximate more closely the flow of water through a tight soil. (See Fig. C-2, App. C.) If the **Free Draining** option is selected the user will be locked out of the **Drainage Parameter** field on this screen. The **PROFILE CONDITIONS** screen (Screen 21) is specific to the LEACHM model. It provides values that more accurately describe the flow of water in the soil profile. The saturated hydraulic conductivity (**Ks**), air entry value (**AEV**), and an additional empirical constant (**BCAM**) are specified to approximate Richards equation for the flow of water in the unsaturated zone. The **Root Fraction** distribution within each soil horizon is also specified to simulate the transpiration of water from the soil profile.

*The Crop Parameters Sub-branch*

Default values will also be supplied for the crop parameters required by the screens in this sub-branch, when the agricultural region is selected on the **SIMULATION REGION** screen. The four screens that make up this branch are

| | |
|---|---|
| **CROP PARAMETERS** | Screen 22 |
| **SURFACE RUNOFF/EROSION** | Screen 23 |
| **CROPPING PERIODS** | Screen 24 |
| **CROP PARAMETERS cont.** | Screen 25 |

The **CROP PARAMETERS** screen (Screen 22a and 22b) presents default values for the number of crops grown in the simulated crop rotation (**Number of Different Crops**). The name of the crop (**Crop Name**), its **Maximum Interception Storage, Maximum Root Depth, Crop Cover Fraction**, and a **Pesticide Uptake Factor** are supplied for a typical crop rotation in each agricultural region. The PRZM model also requires the **Maximum Dry Foliage** weight (Screen 22a), while the LEACHM model requires the **Plant Density** (Screen 22b). The **SURFACE RUNOFF/EROSION** screen (Screen 23) requires parameter values for the Soil Conservation Service curve number method (**CN**) and for the cover management factor (**USLEC**) of the Universal Soil Loss Equation. These parameters are used in the prediction of surface runoff and erosion. The user can also indicate the initial condition of the field at the start of the simulation (**Init. Condition)** and the condition of the field after the harvest of each of the crops in the simulated crop rotation (**Cond. After Harvest**). The three options for the condition of the field after harvest are (1) fallow (**F**), (2) residue (**R**), and (3) cropping (**C**). The **CROPPING PERIODS** screen (Screen 24) specifies the cropping dates for each of the crops in the planting rotation for the duration of the simulation. The **Crop Year** (yy) is entered separately, and dates for the planting, emergence, maturity, and harvesting of each of the crops must be supplied in the format (ddmm), where the day (dd) and month (mm) are entered as two-digit numbers (e.g., July 3 is entered as 0307). The final screen in this branch, **CROP PARAMETERS cont.** (Screen 25), is specific to the LEACHM model and will only appear if LEACHM has been selected. It defines in more detail the transpiration processes of the plant in the soil profile. The user can choose a static representation (**Constant Root Length**) or a simulated growth of the plant root system (**Growing**). Parameter values must be given for the total **Root Length**, the **Minimum** and **Maximum Root Water Potentials** (all of which determine when water uptake will occur), and a **Root Flow Resistance Factor** that accounts for an increased resistance to the flow of water in the root system. Also specified is a **Maximum Actual Transpiration** enhancement factor that will increase the amount of transpiration if the amount of actual evaporation falls below the amount of potential evaporation.

*The Meteorological Parameters Sub-branch*

The **Meteorological Parameters** sub-branch contains three screens that are common to the two models:

| | |
|---|---|
| **METEOROLOGICAL STATIONS** | Screen 26 |
| **METEOROLOGICAL PARAMETERS** | Screen 27 |
| **IRRIGATION PARAMETERS** | Screen 28 |

The **METEOROLOGICAL STATIONS** screen (Screen 26) allows the user to select the **Meteorological Station** (meteorological data file) that will be used in the simulation. If an agricultural region is selected from the **AGRICULTURAL REGION** screen, the corresponding **Meteorological Station** will automatically be selected. The **Meteorological Station** that is selected will be identified by having a diamond placed in the box to the left of the list of stations on the **METEOROLOGICAL STATIONS** screen. If desired the user can change the **Meteorological Station** by moving the position of the diamond with the up and down arrow keys. The **Meteorological Station** is chosen by moving the cursor to the desired station, and hitting the <Enter> key. The meteorological data file associated with the station name contains the daily precipitation, temperature, and pan evaporation values (when available) that are used by the two models in the simulation. The **METEOROLOGICAL PARAMETERS** screen (Screen 27) allows the user to specify a value for the **Minimum Depth of Evaporation** and to enter a **Pan Evaporation Coefficient** and **Snowmelt Coefficient** for the simulation. The user is also given the option of using either the file containing the actual daily meteorological values or a data file containing 20-year mean (precipitation) and median (pan evaporation and temperature) data for the selected meteorological station. The **IRRIGATION PARAMETERS** screen (Screen 28) defines the **Number of Irrigation Applications** and the **Total Amount of Water Applied** by irrigation that occur over the growing season for each of the crops in the cropping rotation.

*The Pesticide Application Parameters Sub-branch*

The **Pesticide Application Parameters** sub-branch contains three screens that accept information that must be provided by the user:

| | |
|---|---|
| **PEST. APPLICATION INFO.** | Screen 29 |
| **APPLICATION METHODS** (PRZM) | Screen 30 |
| **APPLICATION METHODS** (LEACHM) | Screen 31 |

The **PEST. APPLICATION INFO.** screen (Screen 29) is common to both models. It requests data on the timing (dates), amount, and depth of incorporation of each of the pesticide applications that are to be simulated. Two versions of this screen are available and differ slightly depending upon whether PRZM (Screen 29a) or LEACHM (Screen 29b) has been selected. If the PRZM model has been selected by EXPRES, the

PRZM **APPLICATION METHODS** screen (Screen 30) appears, and the user is asked to supply information on the pesticide application method (Foliar or Soil Application). The user must supply the **Pesticide Decay Rate on Foliage**, as well as two empirical constants if a **Foliar Application** is being simulated. The user is allowed access to the **Foliar Application** portion of the screen only if one of the **Foliar Applications** (**Linear** or **Exponential**) is selected. If the LEACHM model is selected, the user must choose between a **Soil** application and a linear **Foliar** application on the LEACHM **APPLICATION METHODS** screen (Screen 31). At present, the LEACHM model has a simplified Foliar Application routine that accounts for a small amount of permanent interception of the pesticide by the plant canopy. The user is responsible for entering a **Washoff Factor** that represents the fraction of the pesticide that is washed off the plant canopy and hence reaches the soil surface.

*The Output Parameters Sub-branch*

EXPRES provides three general types of output for the LEACHM and PRZM models: (1) answers to commonly asked questions, (2) concentration profiles, and (3) time series plots. The **Output Parameters** sub-branch contains five screens that allow the user to specify the type, frequency, and level of detail that is required for the output files generated by the pesticide assessment models. These screens are

| | |
|---|---|
| **GENERAL OUTPUT** | Screen 32 |
| **CONCENTRATION PROFILES** (PRZM) | Screen 33 |
| **TIME SERIES PLOTS** (PRZM) | Screen 34 |
| **TIME SERIES PLOTS** (LEACHM) | Screen 35 |
| **CONCENTRATION PROFILES** (LEACHM) | Screen 36 |

The **GENERAL OUTPUT** screen (Screen 32) allows the user to generate answers to basic questions that are commonly asked during a pesticide assessment. The first question that will be answered by EXPRES is, "At what time does the concentration of the pesticide first reach or exceed the specified dissolved concentration at the specified depth?" The user may select up to four depths of interest (the water table depth and/or three depths specified by the user) and up to five pesticide concentrations of interest (1$^{st}$ non-zero, maximum, and/or three specified by the user). If the user wishes to specify depths or concentrations of interest, a *Y* must be entered in front of the appropriate **Other** parameter. This will provide the user with access to the appropriate columns on the right-hand side of the question where either the specified depths or concentrations can be entered. Answers will be provided in the Data Analysis portion of EXPRES for each combination of depth and concentration specified by the user, for each pesticide that is being simulated.

The second question that will be answered is, "What is the maximum depth of leaching of the pesticide at the following dissolved concentrations at the specified time?" The user may select up to five dissolved pesticide concentrations (1$^{st}$ non-zero, maximum, and/or three specified by the user) and up to three specific time periods of interest.

Answers will be provided in the Data Analysis portion of EXPRES for each combination of time and concentration specified by the user, for each pesticide that is being simulated. Again the user must enter a *Y* for the **Other** or **Time** parameters before access is provided to the **Conc.** and **Time (mmyy)** columns to the right of the question.

Three types of profile summary files are available with the PRZM model (Screen 33): (1) the hydrological characteristics of the site (e.g., infiltration into a soil compartment, water content), (2) the pesticide conditions (amount of pesticide applied, leaching rates, etc.), and (3) the pesticide concentrations in the soil profile (concentrations of pesticide in soil compartments). The user has the choice in generating these files. If a *Y* (Yes) is entered in the **Generate Files** column, the file will be included in the output results produced by the PRZM model. The user may also select the frequency for which this summary information will be reported, by entering either a *D* (Daily), *M* (Monthly), or *Y* (Yearly) in the **Output Time Step** column. The **Compartment Print Frequency** column allows the user to select the column frequency with which the results will be reported (e.g., if a *5* is entered, results will be reported for every fifth compartment in the soil profile). These output summary files are discussed in more detail in a later section of this chapter.

The second type of output data available with the PRZM model are time series plots. The user has the option of selecting a maximum of seven time series plots (from a total of 29 different time series plots) for any one simulation. The **TIME SERIES PLOT** screen (Screen 34) displays the time series plots that have been selected. To add to or modify any of these selections, the user must move to the appropriate location within the **Plot Type** column and hit the <Enter> key. This will bring up a window (Screen 34a) that displays the different groups of time series plotting parameters that are available. The user then moves to the group of interest and hits the <Enter> key, which produces a second window (Screen 34b), on which the user can select the desired individual time series plotting parameter. After the time series parameter is selected, the user is returned to the **TIME SERIES PLOTS** screen, and the selected plotting parameter is automatically entered in the appropriate location. The **Cum** column allows the user to have the results reported as either actual daily values (*N*), or as cumulative totals from the beginning of the simulation (*Y*). The **Observation Depth** refers to the depth within the soil profile at which the time series plots should be reported (e.g., report the water content in the soil compartment at a depth of 1 m). However, some of the time series plotting parameters do not require an **Observation Depth**, and in such cases, a *None* will automatically appear in the **Observation Depth** column.

Concentration profiles and time series plots are also available with the LEACHM model. The **TIME SERIES PLOTS** screen (Screen 35) allows the user to specify the conditions for the time series plots generated by LEACHM. The **Variables of Interest** option allows the user to choose which time series files are to be generated, while the **Print Frequency** option controls how often the results are sent to the output files. The three observation depths at which the variables will be reported may be specified with the

**Observation Depths for the Time Series File** option. The **Units** option controls whether the total pesticide content will be reported as µg/kg or $mg/m^2$.

Similar to the PRZM model, the LEACHM **CONCENTRATION PROFILES** screen (Screen 36) allows the user to select the frequency of reporting with respect to both time (**Print Options** - either **Constant Interval/Print** or **Print on Specific Days**) and depth (**Compartment Print Frequency**). The user may also choose to generate a report on the plant growth simulation (**Print Plant/Root Table**).

*The Uncertainty Analysis Parameters Sub-branch*

The **Uncertainty Analysis Parameters** sub-branch will only appear on the **GENERAL INFORMATION** screen (Screen 9b) if the **Uncertainty Analysis** option is selected on the **ASSESSMENT OBJECTIVES** screen (Screen 4). The **UNCERTAINTY ANALYSIS** screen (Screen 37) allows the user to select the model parameter for the **Uncertainty Analysis** from a list of approximately 30 model parameters. It also allows the user to enter the modification value (**n**) desired for the uncertainty analysis. It provides the user with a suggested range for the modification factor (**n**) for the uncertainty analysis and will automatically adjust the value of the model parameter once the modification factor (**n**) is specified and the LEACHM model is executed. Only one simulation is performed at a time because of the potential time and memory requirements associated with an execution of the LEACHM model.

The user is strongly advised to view all screens in each branch of the expert system before the start of a simulation. The model parameter values should be reviewed to ensure that values are appropriate for the conditions that are being simulated.

**Data Analysis**

All output from the three pesticide assessment models is provided in the form of ASCII text files. EXPRES accesses some of these files after the simulation is complete and allows the user to view a portion of this data in either a graphical or a text format. EXPRES displays the results of the simulation through the **DATA ANALYSIS** screen (Screens 38a and 38b). The first of the two methods by which the user can gain access to this screen is to execute a run with one of the models. After the simulation is complete, EXPRES will automatically place the user in the **DATA ANALYSIS** screen. The second method of gaining access to the **DATA ANALYSIS** screen is through the *RUN* (F4) command. The user can gain direct access to the **DATA ANALYSIS** screen (bypassing the execution of the model) by issuing the *Run Data Analysis* sub-command. Before the user enters Data Analysis, EXPRES will ensure that the input data set corresponds to the output results available in Data Analysis. If the input and output data sets are not consistent, EXPRES will warn the user and allow them either to load the original input data set that was used to generate the output results (*Load Original Data*) or to enter Data Analysis (*Continue*) even though the current input and output data set do not correspond. If the *Load Original Data* option is selected, the contents of the current input data set will be overwritten. The user has control over which output or plotting files are generated (see **Output Parameter** sub-branch - Screens 32 to 36), and only the plots associated with the generated files will be available within Data Analysis.

The **DATA ANALYSIS** screen (Screen 38a and b) is divided into four sections (**General Output**, **Concentration Profiles**, **Time Series Plots**, and **Plot Title**). Answers to the questions posed on the **GENERAL OUTPUT** screen (Screen 32) are accessed by moving to the **General Output** parameter on Screen 38a (or 38b) and hitting the <Enter> key. A window will appear with a series of answers (Screen 38c) to the two questions posed on the **GENERAL OUTPUT** screen. The <PgUp> and <PgDn> keys provide movement within the window. Answers are provided in the following generic formats, where ?.?? are values determined by EXPRES:

ANSWER TO QUESTION 1

At a depth of ?.?? metres, PESTICIDE NAME first reaches a dissolved concentration of

| | | | |
|---|---|---|---|
| First non-zero | (?.??E+??? mg/L) | on | Day ??? |
| Maximum | (?.??E+??? mg/L) | on | Day ??? |
| Specified Concen. #1 | (actual #1) | on | Day ??? |
| Specified Concen. #2 | (actual #2) | on | Day ??? |
| Specified Concen. #3 | (actual #3) | on | Day ??? |

ANSWER TO QUESTION 2

In MONTH/YEAR, the maximum depth of leaching for PESTICIDE NAME at a dissolved concentration of

| | | | |
|---|---|---|---|
| First non-zero | (?.??E+??? mg/L) | is | ?.?? metres. |
| Maximum | (?.??E+??? mg/L) | is | ?.?? metres. |
| Specified Concen. #1 | (actual #1) | is | ?.?? metres. |
| Specified Concen. #2 | (actual #2) | is | ?.?? metres. |
| Specified Concen. #3 | (actual #3) | is | ?.?? metres. |

If the answer to Question 1 is "Day 0," this indicates that the pesticide did not reach the specified depth at the specified dissolved concentration during the simulation period. The concentrations reported for the two questions may not exactly match the concentrations specified by the user in the question. For example, in the first question, the user may wish to know when the dissolved pesticide concentration reaches or exceeds 1.0 mg/L at a depth of 1.0 m. The concentration at a depth of 1.0 m may be 0.88 mg/L on Day 90, while on Day 91 it may jump to a concentration of 1.21 mg/L. In this case, the pesticide would first reach or exceed the specified concentration of 1.0 mg/L at a depth of 1.0 m on Day 91, and the answer would appear as follows:

At a depth of 1.0 metre, PESTICIDE first reaches or exceeds a dissolved concentration of: 1.00E+000 mg/L (actual 1.21E+000) on Day 91.

Similarly, for Question 2, if the reported depth is "0.0 metres," this indicates that the pesticide does not exceed the specified concentration at any point within the soil profile on the specified date. The reported concentration may not exactly match the specified concentration in Question 2 either. The user may wish to know the maximum depth of leaching for a pesticide at a dissolved concentration of 1.0 mg/L at a specified time. The concentration of the dissolved pesticide may be 1.21 mg/L at a depth of 4.2 m, while the concentration in the next compartment (i.e., a depth of 4.3 m) is 0.88 mg/L. In this case the maximum depth of leaching of the pesticide at a dissolved concentration of 1.0 mg/L will be reported as 4.3 m. The answer will be given as

In MAY/78, the maximum depth of leaching for PESTICIDE at a dissolved concentration of: 1.00E+000 mg/L (specified 8.80E-001) is 4.3 metres.

The two types of plots that are available through the **DATA ANALYSIS** screen (Screen 38a and b) are **Concentration Profiles** and **Time Series Plots**. To select a plot, the user simply positions the highlight bar over the type of plot desired and hits the <Enter> key. A series of windows will appear, allowing the user to define further the type of plot that is desired. If `More` appears in the lower right-hand corner of a window (Screen 38d), it indicates that there are additional parameters that must be specified on subsequent windows before a plot can be produced. The additional windows are accessed by moving the cursor to the `More` position and hitting the <Enter> key (Screen 38e). If `Plot` appears in the window (Screen 38f), this indicates that this is the final window and that once the parameters have been selected on this window, EXPRES is ready to produce a plot of the output results. To produce a plot, move the cursor to the `Plot` position and hit the <Enter> key. If the plot is displayed on the monitor, simply hit the <Enter> key when you are finished viewing the plot to return to the **DATA ANALYSIS** screen. The number of windows that appear and the type of parameters that are specified before producing a plot vary with the model selected and the type of plot desired. The user may also enter a title (maximum of 50 characters) for the plot in the **Plot Title** section of the screen. The user should be aware that EXPRES limits the number of individual plot lines that can be displayed on any one plot to a maximum of five lines per graph. Only the plots for the current model will be available within Data Analysis. If the user wishes to view the results from the other model, they must return to **ASSESSMENT OBJECTIVES** screen (Screen 4), and change the selection of the model.

In addition to plotting the results on the monitor, the user may send the results to another plotting device. The choice of a plotting device is made by the user through the *OPTIONS* (*F9*) command. The options available to the user are to send the output to (1) a *Monitor*, (2) a *HP LaserJet Printer*, (3) a *HP 7475A Plotter*, (4) a *PostScript* laser printer, (5) an *IBM ProPrinter* (dot matrix), or (6) a *File*. A second window is accessible from the *OPTIONS* window that allows the user to *Configure* the system for the hardware that is in use. The user may select a colour or a monochrome monitor, a serial or parallel connection for the printer or plotter, and an HPGL® or Encapsulated PostScript® (EPS) format for the plot to a file.

The format and type of output data available with the PRZM and LEACHM models differ slightly; however, plots of the pesticide **Concentration Profiles** and various **Time Series Plots** are available with both models. Tables 5 and 6 provide a list of the plots that are available with the PRZM and LEACHM models. Figures 9 and 10 are examples of typical **Concentration Profiles** and **Time Series Plots** produced by EXPRES.

There are 29 time series plotting parameters available with the PRZM model as indicated in Table 5. A maximum of seven of these plotting parameters may be specified during any one simulation.

**Numerical Output Data Files**

All output files generated by EXPRES are in the form of ASCII text files. In most cases, the information in these files is organized in tables that are easily read and interpreted. The files may be viewed or printed with any word processor or ASCII text editor or printed with the DOS <Print> command. A list of the files generated by EXPRES is given in Table 7, and a brief description of each of the output files follows. In the following description of the output files available with EXPRES, the root portion of the filename (e.g., FILENAME.) represents the name assigned to the input data set used in the simulation. For example, if the user assigns the name NS-TEST1 to the input data set, the output files would appear as NS-TEST1.ECP, NS-TEST1.HYD, etc., in a subdirectory of the same name. If the user initiates EXPRES from the directory C:\EXPRES, and creates the input data file NS-TEST1, both the input data file and the associated output files will be sent to the directory C:\EXPRES\NS-TEST1\.

FILENAME.ECP (PRZM) and FILENAME.ECL (LEACHM) are files that contain an echo of the input data read by the pesticide models. The files are available should the user wish to check whether the input data were read correctly by the two simulation models.

FILENAME.PID (PRZM) and FILENAME.LID (LEACHM) are files that store the original input data set that was used to create the current output data files for the two simulation models. Whenever the simulation models are executed and output data files are created, the input data file that was used in the simulation is copied to either the FILENAME.PID or the FILENAME.LID file. These files are used in the integrity check that is performed when the user attempts to enter Data Analysis through the RUN (F4) - Run Data Analysis command. EXPRES compares the current input data set to either FILENAME.PID or FILENAME.LID, and if they are not identical, it warns the user that the results available in Data Analysis may not correspond to the current input data set.

Table 5. List of Plots Available with the PRZM Model from within EXPRES

| **Pesticide Concentration Profiles (PRZM)** |
|---|
| • Total pesticide concentration in the soil profile (sum of dissolved and adsorbed concentrations - mg/kg) |
| • Dissolved pesticide concentration in the soil profile (mg/L) |
| • Adsorbed pesticide concentrations in the soil profile (concentration of pesticide that is attached to the soil particles - mg/kg) |
| **Time Series Plots (PRZM)** |
| Water Storage |
| • Amount of precipitation intercepted by the plant canopy before reaching the soil surface (cm) |
| • Amount of water stored in a soil compartment (reported as depth of water in cm) |
| • Depth of snow accumulated on soil surface (cm) |
| • Water content of a soil compartment (reported as a volume fraction, e.g., cm3/cm3) |
| Water Flux |
| • Amount of precipitation (cm/day) |
| • Amount of precipitation falling as snow (cm/day) |
| • Amount of precipitation reaching soil surface (i.e., precipitation minus canopy interception) (cm/day) |
| • Amount of water infiltrating into a soil compartment |
| • Amount of water lost from the soil surface by surface runoff (reported as depth of water, cm/day) |
| • Amount of water lost from the plant canopy by evaporation (reported as depth of water, cm/day) |
| • Amount of water lost from a soil compartment by evapotranspiration (reported as depth of water, cm/day) |
| • Amount of water lost from entire soil profile by evapotranspiration (reported as depth of water, cm/day) |
| Pesticide Storage/Concentration |
| • Mass of pesticide stored on the plant canopy (g/cm$^2$) |
| • Total mass of pesticide (both dissolved and adsorbed) stored in a soil compartment (g/cm$^2$) |
| • Mass of dissolved pesticide stored in a soil compartment (g/cm$^2$) |
| • Dissolved pesticide concentration in a soil compartment (mg/L) |
| Pesticide Flux (compartmental) |
| • Net mass of pesticide leaving a soil compartment due to diffusion/dispersion (g/cm$^2$/day) |
| • Mass of pesticide leaving a soil compartment due only to the bulk flow of water (g/cm$^2$/day) |
| • Mass of pesticide lost from the soil compartment due to degradation of the pesticide (g/cm$^2$/day) |
| • Mass of pesticide lost from the soil compartment due to pesticide uptake by the plant (g/cm$^2$/day) |
| • Net mass of pesticide moving past the bottom of the root zone (g/cm$^2$/day) |
| Pesticide Flux (total profile) |
| • Total mass of pesticide applied to the system via both foliar and soil applications (g/cm$^2$/day) |
| • Mass of pesticide lost from the plant canopy via degradation of the pesticide (g/cm$^2$/day) |
| • Mass of pesticide washed off the plant canopy onto the soil surface (g/cm$^2$/day) |
| • Total mass of pesticide lost from the entire soil profile via degradation of the pesticide (g/cm$^2$/day) |
| • Total mass of pesticide lost from the entire soil profile via pesticide uptake by the plant (g/cm$^2$/day) |
| • Mass of pesticide lost from the soil profile via surface runoff (g/cm$^2$/day) |
| • Mass of pesticide lost from the soil profile via soil erosion (g/cm$^2$/day) |
| Sediment Flux |
| • Mass of soil lost from the soil surface via soil erosion (t/day) |

If the user chooses to replace the current input data set with the original data set that was used to create the output data, either the FILENAME.PID or the FILENAME.LID files are copied into the current input data set.

Table 6. List of Plots Available with the LEACHM Model from within EXPRES

**Pesticide Concentration Profiles (LEACHM)**

- Total pesticide concentration in the soil profile (sum of dissolved, adsorbed and vapour concentrations - $mg/m^2$ or µg/kg)
- Dissolved pesticide concentration in the soil profile (mg/L)
- Vapour phase pesticide concentration within the soil profile (µg/L)

**Time Series Plots (LEACHM)**

- Total pesticide content in a soil compartment (sum of the dissolved, adsorbed and vapour phase concentrations - $mg/m^2$ or µg/kg)
- Total pesticide flux past a specified soil compartment ($mg/m^2$)
- Precipitation (mm)
- Evaporation (mm)
- Transpiration (mm)
- Water flux past a specified soil compartment (mm)
- Cumulative water flux past a specified soil compartment (mm)
- Water content in a specified soil compartment (mm)

Table 7. Output Files Created by EXPRES

| PRZM OUTPUT FILES | LEACHM OUTPUT FILES | LP/LI OUTPUT FILES | OTHER OUTPUT FILES |
|---|---|---|---|
| FILENAME.ECP | FILENAME.ECL | FILENAME.LP | FILENAME.ERR |
| FILENAME.PID | FILENAME.LID | FILENAME.LI | FILENAME.NTS |
| FILENAME.HYD | FILENAME.OUT | | PLOT.EPS |
| FILENAME.PES | FILENAME.PCN | | PLOT.HPG |
| FILENAME.CNC | FILENAME.PFX | | FILENAME.GEN |
| FILENAME.TSP | FILENAME.WFX | | |
| | FILENAME.RET | | |
| | FILENAME.PLT | | |

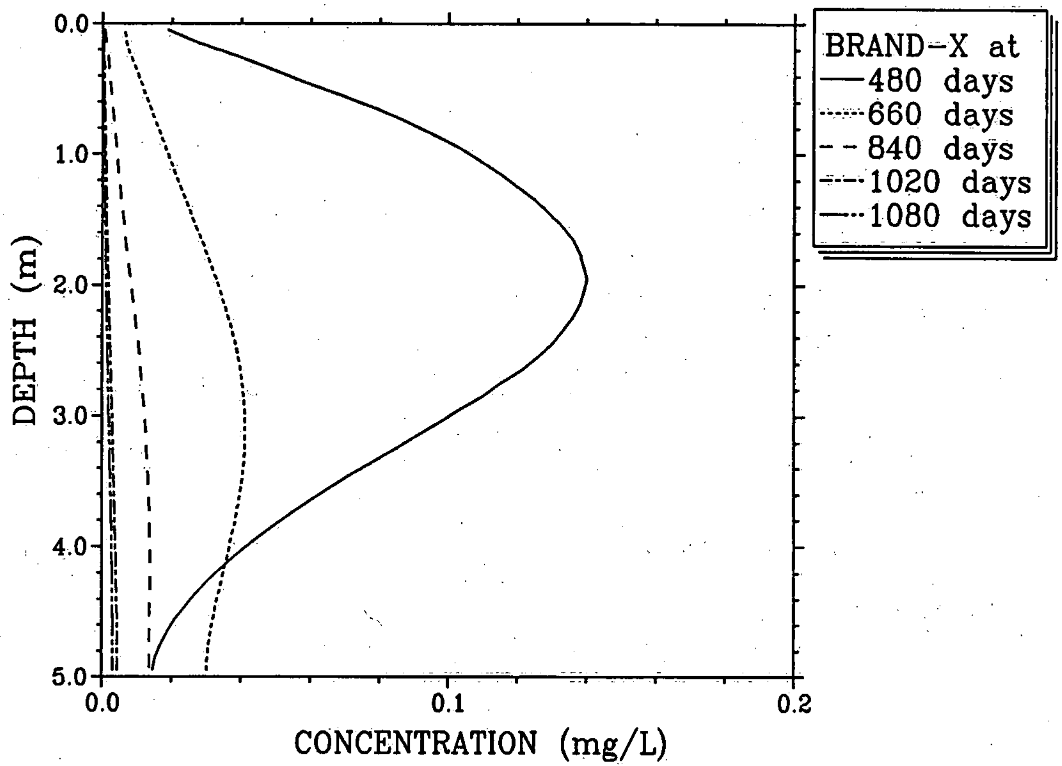



Figure 9. Typical concentration profile available through the EXPRES expert system.

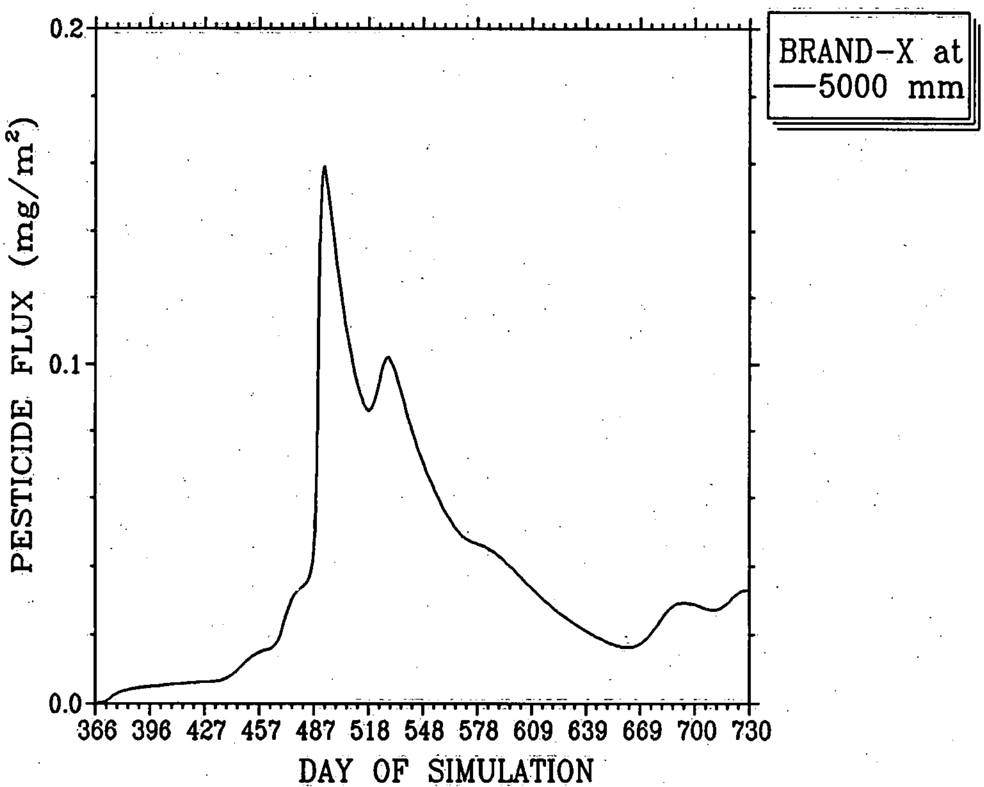



Figure 10. Typical time series plot available through the EXPRES expert system.

**FILENAME.HYD** (PRZM) contains a hydrological output summary for the PRZM simulations. The information contained in this file includes precipitation, evaporation, snowfall, runoff, and infiltration summaries, as well as current and previous water contents, leaching inputs and outputs, and transpirational losses from the various soil compartments. The file also contains profile summaries for eroded sediment, evapotranspiration, and recharge below the root zone. The information listed in this file is not accessed through the Data Analysis but can be viewed with a ASCII text editor.

The **FILENAME.PES** (PRZM) file provides the user with a pesticide output summary. The file summarizes the amount of the pesticide applied to the soil and plant canopy, pesticide leaching inputs and outputs, and plant uptake from each of the soil compartments; the profile totals for the amount of pesticide involved in plant uptake, decay, erosion, runoff, and leaching below the root zone; and pesticide mass balance totals. It indicates the current and previous pesticide storage on, and the amount of pesticide decay and washoff from, the plant canopy. The information listed in this file is not accessed through the Data Analysis, but can be viewed with an ASCII text editor.

The **FILENAME.CNC** (PRZM) file contains the predicted values of the total adsorbed and dissolved pesticide concentrations in the soil profile. The data in this file are accessed to generate the pesticide concentration plots for the PRZM model that are available in the Data Analysis portion of the expert system.

The **FILENAME.TSP** (PRZM) file contains the predicted values that produce the time series plots for the PRZM model within the Data Analysis portion of EXPRES. The time series plotting parameters (a maximum of seven) that will be included in this file are specified by the user in the **Output Parameter** branch of EXPRES.

The **FILENAME.OUT** (LEACHM) file contains a summary of the predicted retentivity and conductivity data used by LEACHM to characterize water movement in the soil. Profile totals are given for the initial and current storages and the additions of both water and pesticide. Losses of both pesticide and water through drainage, evaporation, volatilization, transformation, degradation, plant uptake, and runoff and erosion are also reported. Values for the water content, potential, and flux within the soil compartments are reported. The file also contains the information for the total dissolved and vapour phase concentration plots of the pesticide in the soil profile that are available in the Data Analysis portion of EXPRES. Mass balance checks are also provided.

The **FILENAME.PCN** (LEACHM) file contains the predicted values required to produce the time series plots of the pesticide concentrations within the soil profile that are available in the Data Analysis portion of EXPRES.

The **FILENAME.PFX** (LEACHM) file contains the predicted values required to produce the available time series plots of the pesticide flux in the soil profile.

The **FILENAME.WFX** (LEACHM) file contains the output data required to produce the time series plots of the water flux within the soil profile that are available in the Data Analysis portion of EXPRES.

The **FILENAME.RET** (LEACHM) file contains predicted values used to produce the time series plots of rainfall, evaporation, and transpiration that are available in the Data Analysis portion of EXPRES.

The **FILENAME.PLT** (LEACHM) file contains a summary of the plant growth, transpiration, and uptake of pesticide by the plant simulated by EXPRES. Currently this information is not accessed by the Data Analysis portion of EXPRES.

The **FILENAME.LP** and **FILENAME.LI** (LP/LI) files contain the relative ranking and scores calculated by the LP/LI screening model for the test pesticide, as well as for all the other pesticides in the EXPRES data base that are used for comparison purposes. The **FILENAME.LP** file can provide a relative assessment of the potential for the test pesticide to leach to the water table. To obtain the assessment, the user should compare the ranking and score assigned to the test pesticide to those listed for other pesticides in the data base. The user is given the option to select which pesticides are to be included in the comparison by selecting from a list of pesticides in the EXPRES data base. The **FILENAME.LI** file is similar to the **FILENAME.LP** file. However, in the **FILENAME.LI** file, the pesticides are ranked according to the potential migration distance that they may travel before degrading in the subsurface environment. These files are created (and may be viewed) through the **SCREENING ASSESSMENT OUTPUT** screen.

The **FILENAME.ERR** file contains a list of all the error and warning messages produced by the integrity checks performed on the input data set for the selected simulation model (PRZM or LEACHM). It is created when the user initiates an execution of the model with the ***RUN*** command.

The **FILENAME.NTS** file contains the notes entered by the user during a session through the *NOTES* (*F6*) facility. EXPRES can be set up to invoke the user's own DOS-based word processor. Therefore, the format of this file will depend on how the user's word processor saves its files (it may not be an ASCII file).

The **PLOT.EPS** and **PLOT.HPG** files are the default filenames for the plotting files that can be produced by the Data Analysis portion of the expert system. If the user chooses to send the output of a plot to a **File** and specifies a **PostScript** file, the resulting plot will be sent to the file PLOT.EPS (EPS for Encapsulated PostScript). If the user chooses an HPGL® format for the output plotting file, the plot will be sent to the file PLOT.HPG. The user is given the option to specify an eight-character root FILENAME for the plotting file. However, the extensions for the FILENAME are predetermined (e.g., FILENAME.EPS for a PostScript® file, or FILENAME.HPG for an HPGL® file).

The FILENAME.GEN file contains answers to the two questions posed on the **GENERAL OUTPUT** screen. The answers will indicate to the user when the concentration of the pesticide will first reach or exceed a specified concentration, at a specified depth. Additional answers may specify the maximum depth of leaching of the pesticide at a specified concentration at a specified time.

# Evaluation and Applications of EXPRES

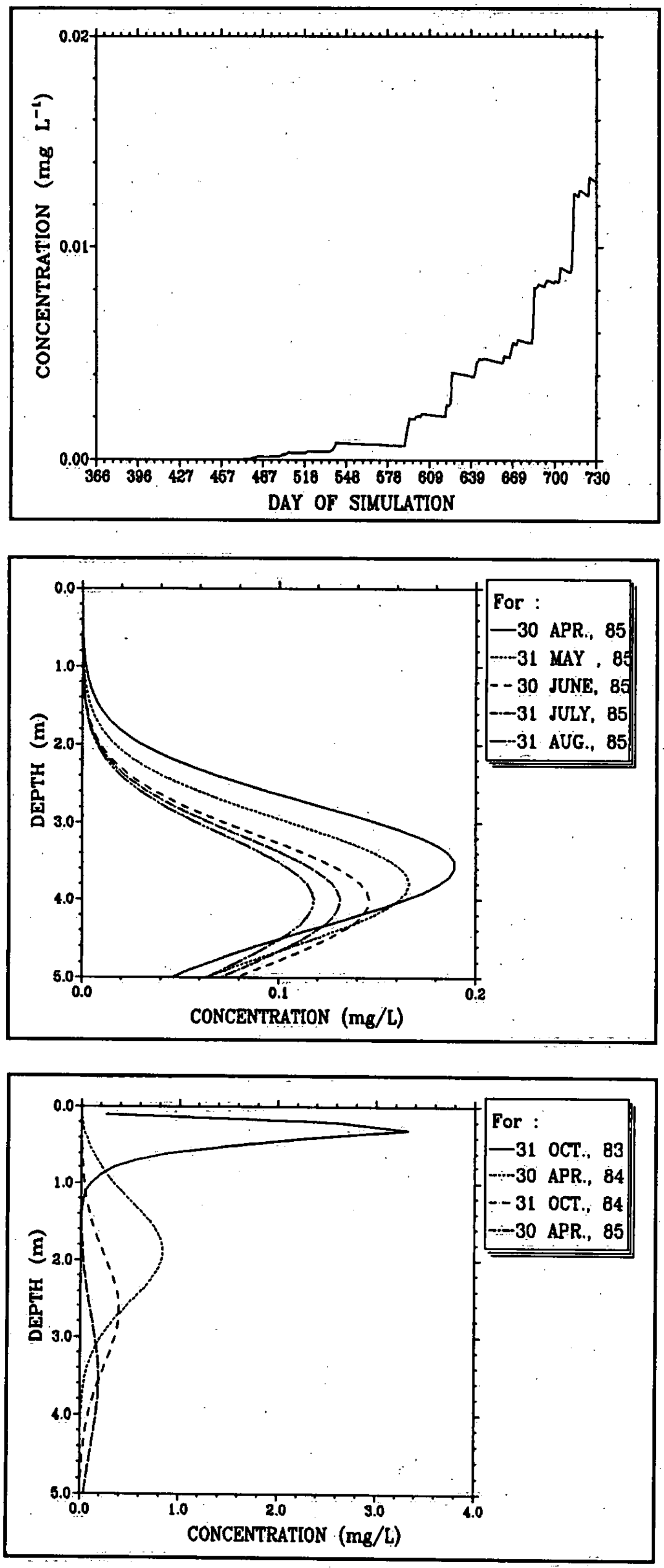
## EVALUATION OF EXPRES

For the expert system to be of value, non-experts must be able to undertake a pesticide assessment as accurately and as quickly as an expert. An evaluation of the capability of EXPRES to achieve these requirements was conducted by comparing the results of an assessment obtained by persons with little expertise in pesticide contamination and groundwater modelling but with the aid of EXPRES to results of the same assessment obtained by an expert (i.e., without the aid of EXPRES). The evaluation of EXPRES was undertaken by ten novice users whose experience and education ranged from only a couple of basic groundwater courses (no courses relating to groundwater modelling, pesticides, or organic chemistry) and no practical experience in this area to several pertinent university courses and several years of related experience.

The evaluation exercise consisted of four case studies that are typical of a pesticide assessment. The first case required an assessment with the screening model where the test subjects were asked to identify which of the pesticides in a given list had the potential to leach to the water table in the region of interest. The three remaining cases required assessments with the simulation models. All test subjects were given the same pesticide scenario to assess. However, the amount of information provided ranged from having all the data required to enter into EXPRES to having the user estimate values for many of the pesticide and site parameters using additional information that was provided (Table 8). The test subjects were asked to answer the following questions:

- Does the pesticide leach to the water table, and if so, how long does it take the dissolved pesticide to reach the water table?
- If the pesticide leaches to the water table, what is its maximum concentration at the water table, and when does it occur?
- How far does the centre of mass of the dissolved pesticide travel downward through the soil profile in 0.5, 1, and 2 years?

The subjects were given three hours to complete their assessments, following a 30-minute presentation on the operation of EXPRES. The results obtained by the experts are shown in Figure 11. Figure 11a indicates that the pesticide is first observed at the water table (5 m) on approximately Day 460. The peak pesticide concentration reaching the water table is approximately 0.08 mg/L, and occurs on June 30, 1985 (Fig. 11b). Figure 11c shows the depth to the centre of mass of the pesticide.




(a) the time of the first occurrence (≈ day 460) of the pesticide at the water table (5 m)

(b) the maximum concentration of the pesticide at the water table (≈ 0.08 mg/L on June 30, 1985)

(c) the distribution of the pesticide in the soil profile, 0.5, 1.0, 1.5, and 2.0 years after the pesticide application date

Figure 11. Results obtained by an expert in the assessment conducted for the evaluation of EXPRES.

Table 8. Data Sets Used to Evaluate the EXPRES Expert System

| | Given | User's Tasks |
|---|---|---|
| Case 1 | • some pesticide data | · estimate additional pesticide data<br>· select assessment objectives & type of output<br>· conduct relative assessments of the pesticides |
| Case 2 | • all pesticide data<br>• agricultural region of interest | · enter pesticide data<br>· select assessment objectives & type of output<br>· select agricultural zone |
| Case 3 | • some pesticide data<br>• agricultural region of interest | · estimate additional pesticide data<br>· select assessment objectives & type of output<br>· select agricultural zone |
| Case 4 | • some pesticide data<br>• agricultural region of interest<br>• new soil profile data | · estimate additional pesticide data<br>· select assessment objectives & type of output<br>· select agricultural zone<br>· estimate/modify some agr. region data |

In the first case, the missing values of the organic carbon partition coefficient ($K_{oc}$), vapour pressure, and aqueous solubility of the pesticides were correctly estimated by the users through the on-line Help facility from the additional data provided (e.g., $K_{oc}$ estimated from a value for $K_{ow}$) or obtained from the **Data Display** option. Although there were slight differences in the estimated values between the expert and the novice users, and therefore slightly different LP/LI scores, the relative ranking of the pesticides and the identification of the potential leachers were correctly determined by the users.

In Case 2, the test subjects were required to select the correct assessment options and agricultural region, and to enter the given pesticide data and simulation dates into EXPRES. The users were also required to select the type of output that would provide them with the necessary information to answer the assessment questions. The users successfully completed these tasks and obtained the same answers as the expert within the allotted three hours.

For Case 3, the novice users were given the agricultural region of interest, some of the required pesticide data, and a few additional pesticide properties. The users were able to select the correct model, enter the appropriate "given data," and estimate additional pesticide parameters required by the model, using the on-line help facility. The test subject obtained essentially the same solution as the expert within three hours.

The final case assessed the users' ability to estimate characteristics of the site with the assistance of EXPRES. Most of the required pesticide data, as well as a few additional pesticide properties, were provided. Although the users were required to undertake the assessment in the same agricultural region as above, they were provided with a different soil profile. Thus, the users had to obtain, estimate, and/or change the values of the pertinent soil parameters in the agricultural region to agree with information provided in a soils report. Within the three hours allotted for this test, the subjects successfully obtained and entered the correct values for the pesticide parameters and most of the data corresponding to the new soil profile. The test subjects were able to get the correct type of output but not the correct results. However, the users indicated that with more time and familiarity with the system they could have obtained the correct results.

These tests demonstrated that an expert systems approach can be used successfully in assessing the potential for groundwater contamination by pesticides as follows:

- All users were able to choose the correct pesticide assessment model to attain the objectives of their evaluation.
- The on-line Help facility of EXPRES enabled all users to obtain estimates for the values of the missing pesticide and soil parameters.
- The users were able to successfully compose an input data set for, and obtain meaningful results from, a complex mathematical simulation model.
- All of these tasks were undertaken by users (including ones with minimal experience or education related to the contamination of groundwater by pesticides) within three hours of being introduced to the system (without EXPRES, the selection of PRZM or LEACHM, collection of data, compilation of an input data set, successful execution of the model, and interpretation of results may take several weeks).
- All users indicated that EXPRES was a valuable educational tool.

Regulatory personnel who are required to assess the potential for a pesticide to contaminate groundwater typically do not have the data, modelling experience, estimation techniques, or the time required to conduct an assessment with mathematical models. EXPRES provides a method for transferring much of the expertise required for an assessment from a complex science to a practical tool, allowing even a novice user to conduct an assessment with these pesticide models within a reasonable period of time.

## APPLICATIONS OF EXPRES

EXPRES was developed to provide a tool through which non-specialists could obtain the necessary expertise (e.g., data, modelling experience, integrity checking, interpretation) required to undertake a modelling assessment of the potential for pesticides to contaminate groundwater. The actual occurrence and extent of contamination by pesticides are localized from site to site because of the variation in the characteristics of the soil profiles, meteorological conditions, amount of pesticide used, and application procedures. Because the number of sites that can be assessed through field programs or modelling studies is limited by practical considerations, a regionalized approach to assess the potential for a pesticide to contaminate groundwater has been adopted. Currently, a data base containing descriptions of 22 agricultural regions across Canada has been created for these regional assessments. The examples presented in this section are intended to illustrate how EXPRES may be used to answer typical questions that may be asked during a regulatory assessment of a new pesticide, which in the following scenarios is called Brand-X. Specifically, the assessment scenarios described here are designed to address the following questions:

- Does the pesticide Brand-X have a high or low potential to leach to the water table compared to pesticides that are, or have been, used in the region?
- What are the leaching rates to, and the peak concentration of Brand-X at, the water table in a given region?
- Will the leaching rate and concentration profile of Brand-X vary from region to region?
- What are the principal factors/processes affecting the leaching rate and distribution of Brand-X within the subsurface?

### Scenario #1: Relative Assessment of Leaching Potential

The objectives of Scenario #1 are to provide a general assessment of the potential risks that Brand-X will present to the groundwater environment and to undertake this assessment quickly. A screening assessment can fulfill both of these requirements because (1) the input data set required for the screening model consists of only four chemical properties of the pesticide, and therefore, the input data can be composed very quickly, and (2) it produces a relative assessment (with respect to other pesticides applied in the region) of the potential for the pesticide of interest to leach to the water table. Pesticides currently being used, or which have previously been used, in the region have been categorized as either "leachers" (atrazine, dinoseb, dicamba, picloram) or "non-leachers" (toxaphene, pronamide, endrin, chlordane), depending upon whether they are known to cause groundwater contamination (i.e., quantities of the pesticide have been detected in groundwater samples obtained from local domestic wells).

To meet the objectives of Scenario #1, the user would select the **Screening Assess.** option on the **ASSESSMENT OBJECTIVES** screen. EXPRES would then select the LP/LI model and request that the user enter the aqueous solubility, vapour pressure, organic carbon partition coefficient, and half-life of the pesticide in soil (i.e., 15.0 mg/L, 0.0085 mPa, 25 L/kg, and 125 days, respectively, for Brand-X) for the pesticide of interest. EXPRES would then execute the LP/LI model to obtain the Leaching Potential and Leaching Index scores, as well as the ranking of the test pesticide.

The results of the LP/LI assessment indicate that Brand-X has a high potential to leach to the water table relative to the other eight pesticides. The results of the screening assessment are shown in Figure 12. Brand-X has the second highest LP and third highest LI score of the pesticides in the EXPRES data base. Because the LP and LI scores for Brand-X rank it among the pesticides that are known to have leached to the water table, there is a high probability that if Brand-X is applied in the field, it will cause groundwater

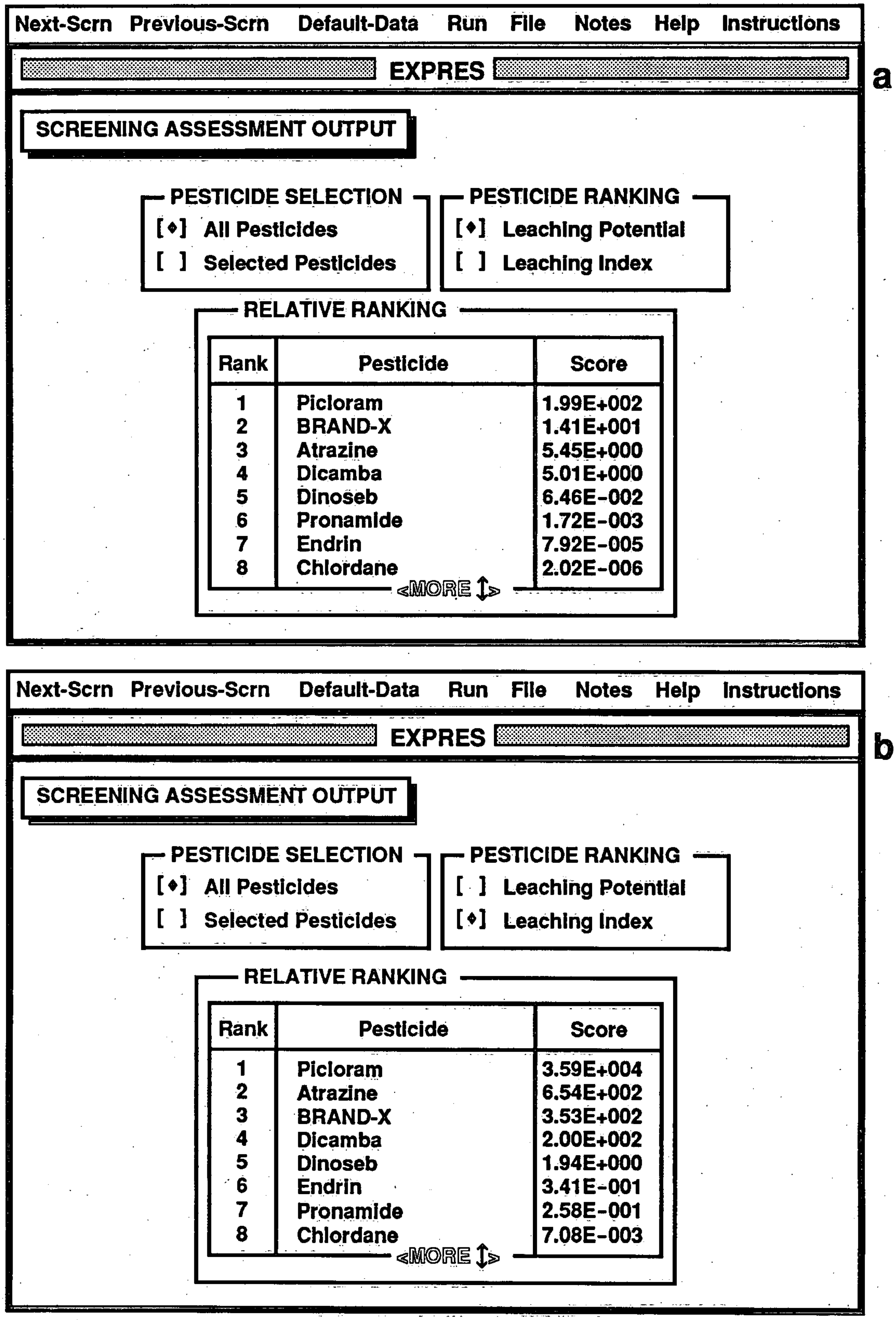



Figure 12. Ranking of the pesticide Brand-X as determined by the LP/LI screening model: (a) LP ranking and score, (b) LI ranking and score.

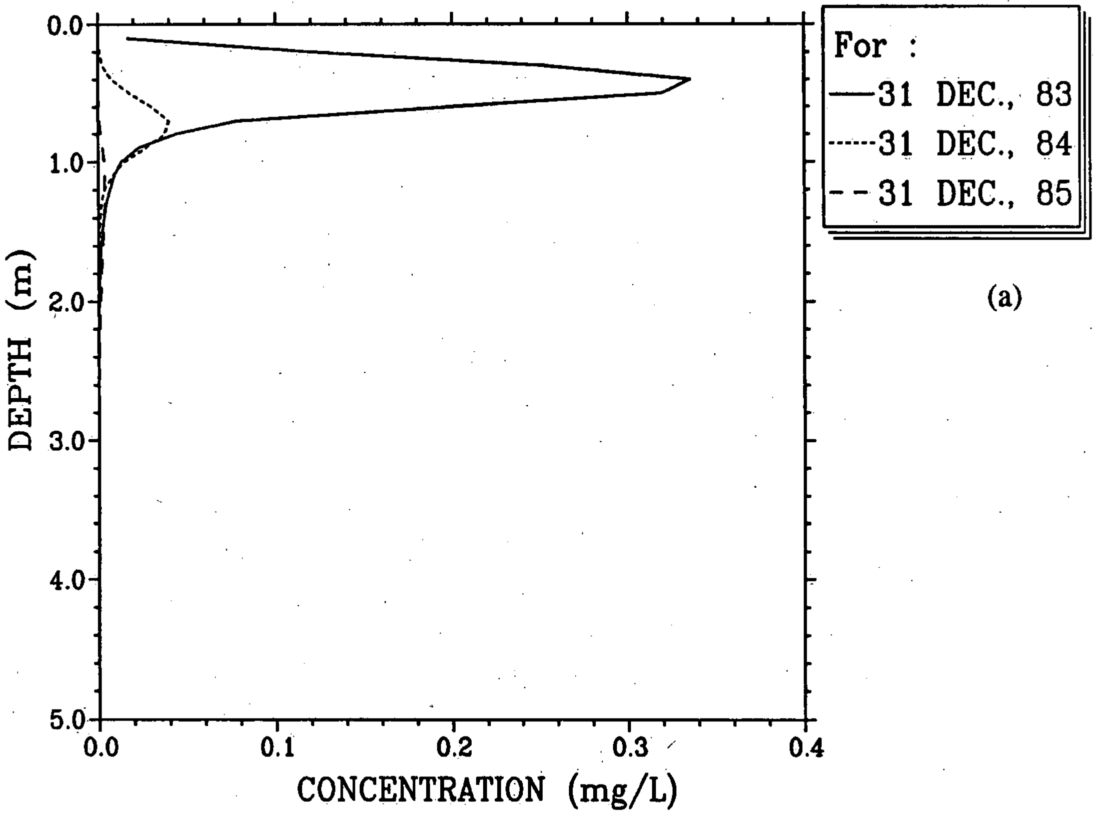
contamination. Thus, based on this quick and simple analysis, additional and more detailed studies should be undertaken on Brand-X to confirm these results.

### Scenario #2: Leaching Rate and Peak Concentration at the Water Table

In the previous scenario, the pesticide of interest, Brand-X, was determined to be a potential "leacher" and therefore to have a high potential of causing groundwater contamination. Before undertaking costly field or laboratory studies to gain further insight into the fate of Brand-X in the soil profile of several regions, a more economical method may be to conduct tests with models that simulate the migration of the pesticide in the subsurface. Simulations should never replace field and laboratory studies, in terms of obtaining direct evidence of the potential for the pesticide to contaminate (or not contaminate) the groundwater. However, simulations can be very useful for quickly narrowing the scope of the field investigations that are necessary. Screening assessments do not simulate the migration and fate of the pesticide in the subsurface, nor do they consider any of the characteristics of the site that influence pesticide mobility and persistence. Therefore, the application of a simulation model is required to determine, first, whether the use of this pesticide will have the potential to result in groundwater contamination within a selected agricultural region when the physical and chemical characteristics of the region are considered, and second, how long the pesticide will potentially take to migrate to, and what its peak concentration will be at, the water table. Because of the objectives of the simulation, the PRZM model was selected by EXPRES.

The agricultural region selected for study (i.e., the area and crop to which Brand-X will be applied) is a sugar beet field in southern Alberta. This region and data are described in Mutch and Crowe (1991). Once this region is selected on the **SIMULATION REGION** screen by the user, all the site-characterizing information, including the pedological, hydrogeological, physical, meteorological, and crop information, is loaded into the appropriate screens from the EXPRES data base. EXPRES also requires the user to enter the actual dates for the simulation (between Jan. 1, 1970, and Dec. 31, 1989). In this and the following two scenarios the three-year simulation period was chosen arbitrarily to run from Jan. 1, 1983, to Dec. 31, 1985. To complete the input data set, the user enters the chemical properties of Brand-X, the pesticide application information, and the type of output required, obtaining assistance, if required, through the ***HELP (F7)*** command.

The results of the analysis show that Brand-X fails to reach the water table to any significant degree during the three-year simulation undertaken. The concentration profile (Fig. 13a) indicates that the centre of mass of the pesticide has reached a depth of only 1.2 m by the end of the third year. The time series plot (Fig. 13b), showing the pesticide advective flux, indicates that only a very small amount of the pesticide moves past the water table during the third year of the simulation. Thus, although the screen model assessment indicated that the pesticide had a high potential to leach to the water table, when the characteristics of the site (a sugar beet field in Alberta) are considered, the




(a)

BRAND-X

(b)

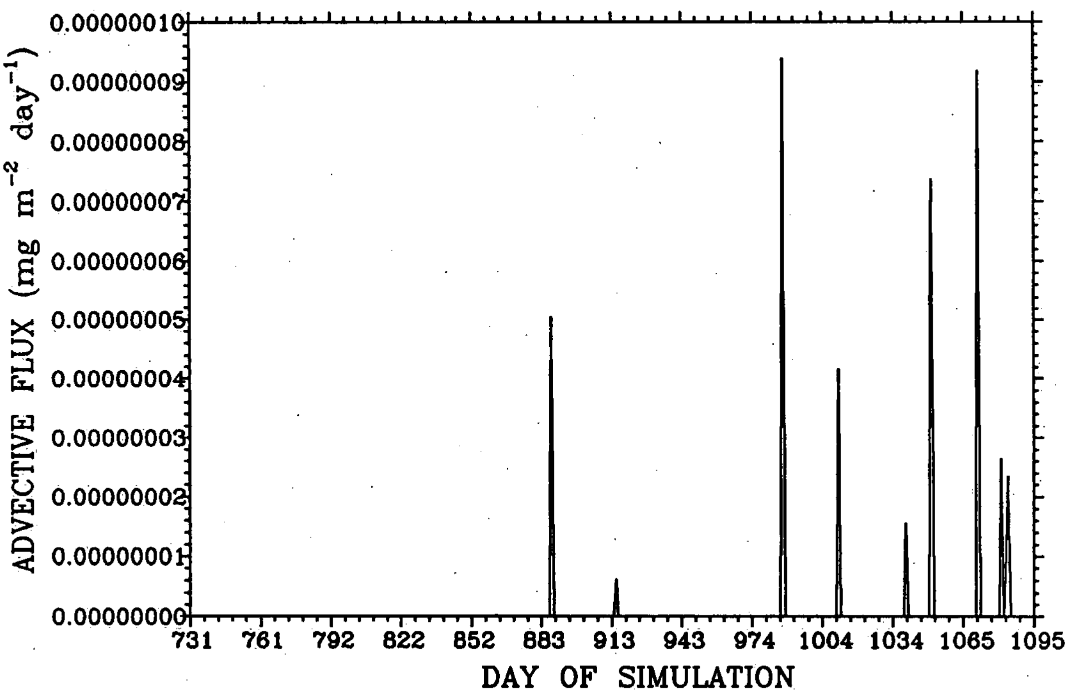



Figure 13. Plot of (a) concentration profiles and (b) pesticide advective flux at the water table for the pesticide Brand-X applied to a sugar beet field in southern Alberta.

simulation assessment with the PRZM model indicates that Brand-X will not be a significant problem under the conditions represented by this agricultural region.

### Scenario #3: Regional Comparison of Leaching Rates and Concentrations

The third scenario is designed to assess whether Brand-X will behave differently when applied in agricultural regions other than a sugar beet field in southern Alberta. The specific focus of this example is to determine whether the leaching rates and concentration profiles of the pesticide of interest will vary between various agricultural regions. The additional agricultural regions chosen for this analysis are a potato field in Prince Edward Island and a corn field in southwestern Ontario. These regions and site-characterizing data are described in Mutch and Crowe (1991).

All data comprising the input data set for the sugar beet field had been compiled and saved (Scenario #2). The information required by the input data sets for the simulations to assess the fate of Brand-X within the two other agricultural regions can be undertaken quickly. By recalling the previous data set (Scenario #2), the values corresponding to the chemical properties of Brand-X will be loaded into the appropriate screens. Then, by selecting the new agricultural region, the default data characterizing the newly selected agricultural region will overwrite the site-characterizing data of the previous agricultural region. The only change that the user is required to make to these input data is to change the application dates of the pesticide to match the planting dates and emergence dates, etc., for the crop being simulated in the new agricultural region.

The results of these analyses demonstrate that Brand-X is a potential "leacher" when applied to a potato field in Prince Edward Island and might be one when applied to a corn field in southwestern Ontario. The concentration profiles in Figure 14a reveal that the maximum concentration of the pesticide reaching the water table in Prince Edward Island is approximately 0.0022 mg/L. This occurs approximately two years (June 30, 1985) after the application of the pesticide (May 1, 1983). The concentration profiles in Figure 14b indicate that the pesticide has not yet reached the water table to any significant degree by the end of the three-year simulation under the corn field in southwestern Ontario. However, the centre of mass of the pesticide remains above the water table (at approximately the 2.0 m depth on December 31, 1985). Concentrations at the water table would continue to rise if the simulation were to continue beyond December 31, 1985. The time series plots of the pesticide advective flux (Fig. 15a and b) reveal that a greater amount of the applied pesticide is reaching the water table in the Ontario and Prince Edward Island scenarios than did in the Alberta scenario (Fig. 13b). Figure 15b indicates that the pesticide is just starting to reach the water table under the corn field in Ontario at the end of the three-year simulation. Therefore, the results of this analysis indicated that Brand-X has the potential to contaminate groundwater in the agricultural regions representing a potato field in PEI and a corn field in southwestern Ontario.

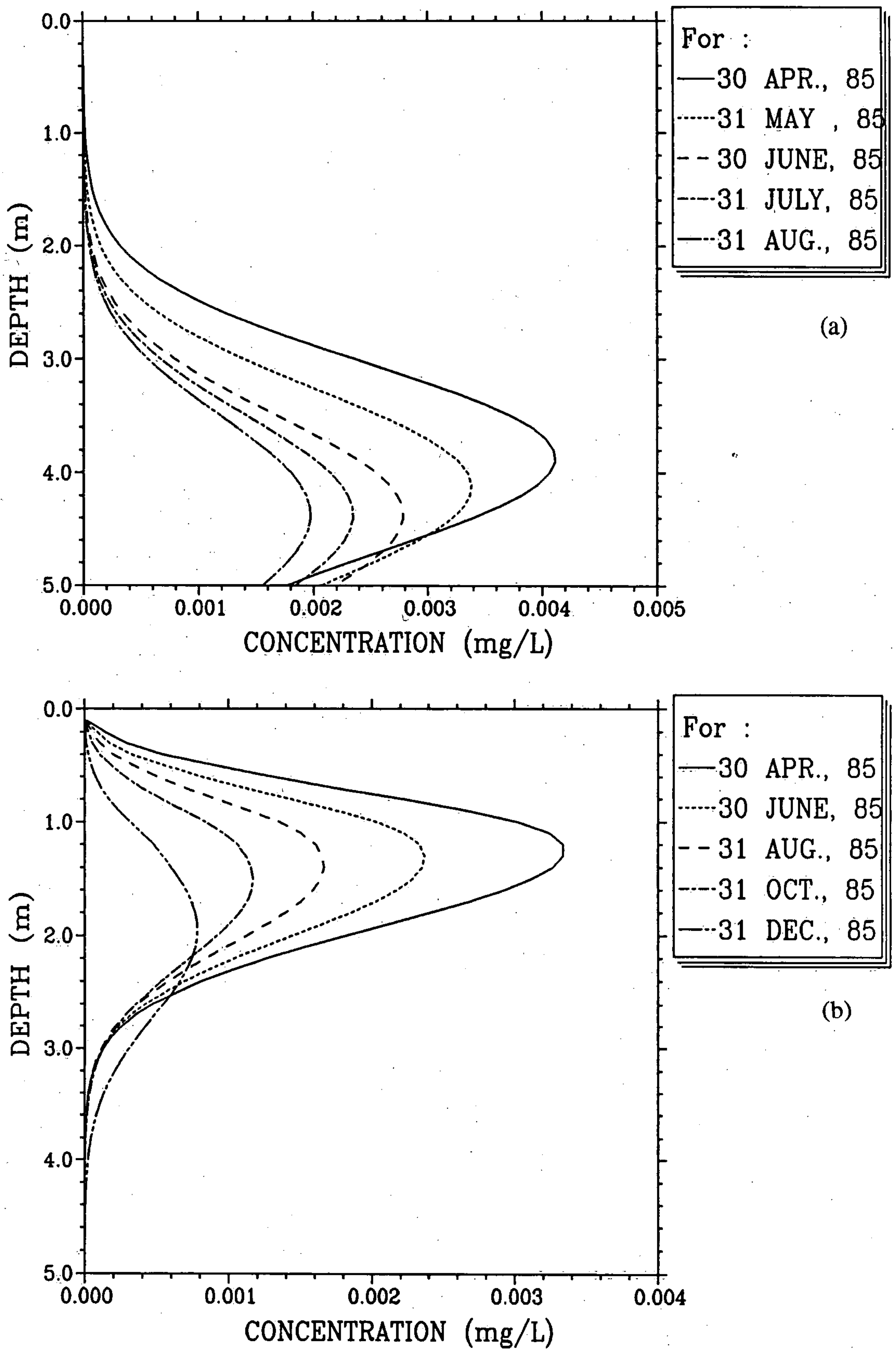
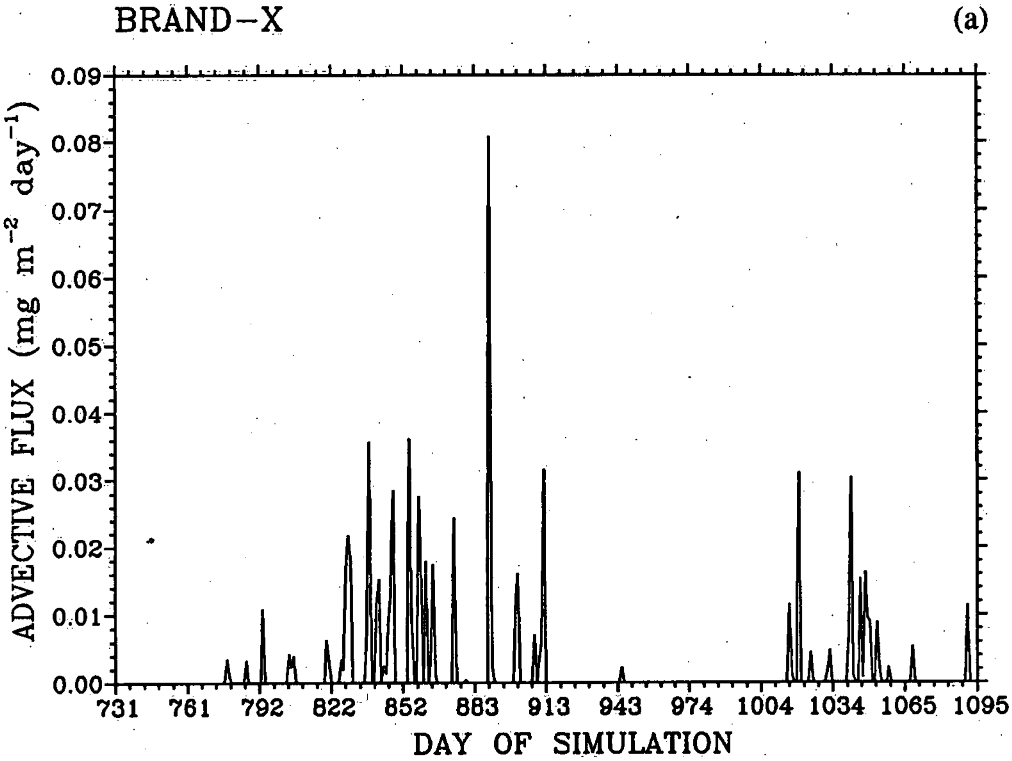



Figure 14. Concentration profiles for an application of pesticide Brand-X to (a) a potato field in Prince Edward Island and (b) a corn field in southwestern Ontario.



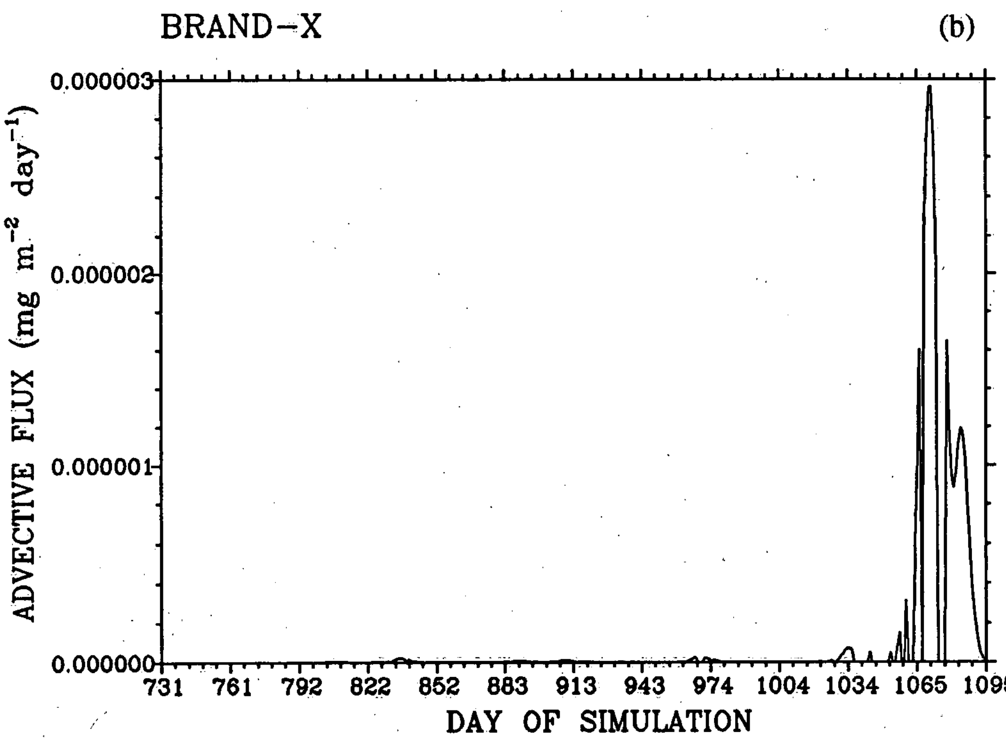




Figure 15. Time series plots of the pesticide advective flux at the water table (5 m) for the pesticide Brand-X applied to (a) a potato field in Prince Edward Island and (b) a corn field in southwestern Ontario.

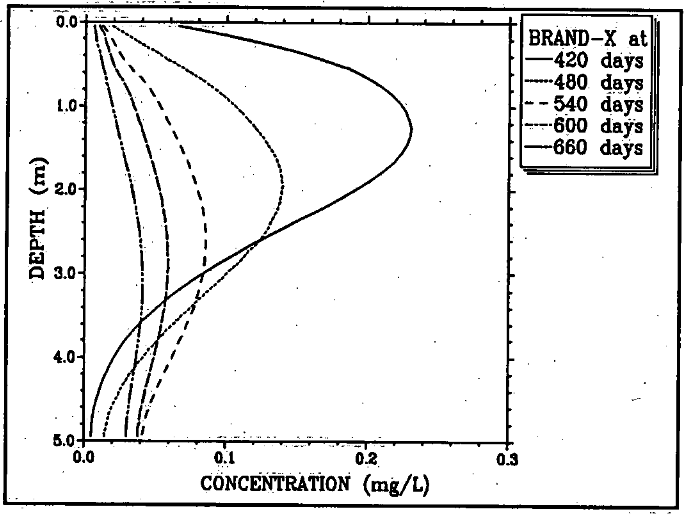
**Scenario #4: Controls on Pesticide Leaching Rates and Concentrations**

The analyses undertaken in Scenario #3 indicated that Brand-X has a high potential to cause groundwater contamination in the PEI agricultural region and possibly in the Ontario region but not in the Alberta region. To understand the reasons for this, the analyses undertaken as part of Scenario #4 involve conducting detailed studies into the nature of the problem by undertaking uncertainty analyses on some of the primary factors that influence the mobility, persistence, and retention of Brand-X in the unsaturated zone. An uncertainty analysis is used here within a context of assessing how the system would respond to variations in a parameter that are typical of the range that would be expected within natural conditions for the parameter. For example, we will consider a worst-case/best-case scenario by varying the hydraulic conductivity by two orders of magnitude, the precipitation by ± 20%, and the organic matter content by an absolute change of ± 2.0%. The specific method for undertaking an uncertainty analysis on a given parameter is to select the **Uncertainty Analysis** option on the **GENERAL INFORMATION** and **ASSESSMENT OBJECTIVES** screens. The second step is to enter the modification factor for the parameter on which the uncertainty analysis will be conducted on the **UNCERTAINTY ANALYSIS** screens.

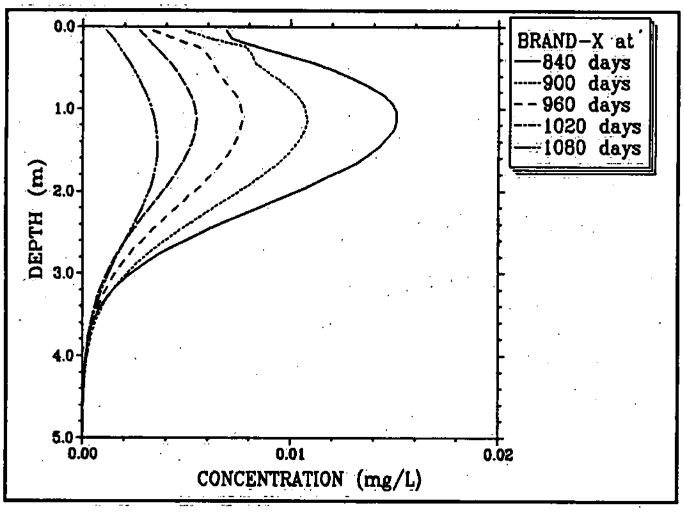
Uncertainty analyses should be undertaken with a simulation model that best simulates the actual physical, chemical, and biological processes that occur in a soil profile. PRZM treats the movement of water in the soil profile with a lumped parameter approach, whereas LEACHM simulates the flow of water much more realistically with Richards equation and attempts to simulate the processes that are occurring in the soil. Therefore, EXPRES will select the LEACHM model for this task. EXPRES allows the user to choose among 30 parameters that influence the fate of a pesticide in the subsurface and recommends a range of typical values over which the parameter of interest should be varied for use in the uncertainty analyses.

The primary difference between the Ontario and Prince Edward Island (PEI) regions and the Alberta agricultural region is (1) the amount of precipitation (considerably less in Alberta), (2) the percent organic carbon content of the soil profile (lower in Alberta), and (3) the saturated hydraulic conductivity of the soil profile (high in Alberta). Uncertainty analyses undertaken for this scenario are designed to determine which is the controlling parameter (e.g., whether precipitation is more important than hydraulic conductivity in influencing the extent and rate of pesticide leaching).

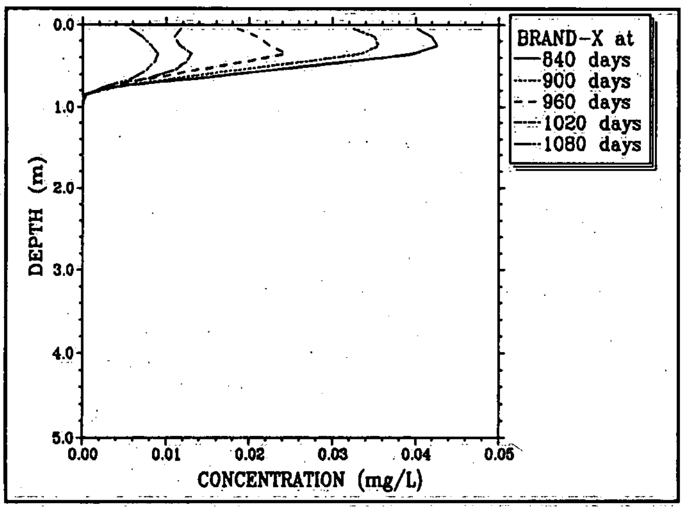
In the following LEACHM simulations for an application of the pesticide Brand-X to the three agricultural regions (PEI, Ontario, and Alberta), identical chemical properties were used in all simulations. The individual default values for the three agricultural regions (stored in the EXPRES data base) were used to describe the soil profile and agricultural practices in each of the agricultural regions. Uncertainty analyses were conducted by changing the selected parameter by the modification factor as indicated. All other parameters in the simulations remained unchanged. The results shown in Figure 16 represent the pesticide concentration profiles predicted by the LEACHM model for the initial default conditions (i.e., no model parameters were modified) for each of the




(a) a potato field in Prince Edward Island




(b) a corn field in southwestern Ontario




(c) a sugar beet field in southern Alberta

Figure 16. Pesticide concentration profiles predicted by the LEACHM model for an application of the pesticide Brand-X.

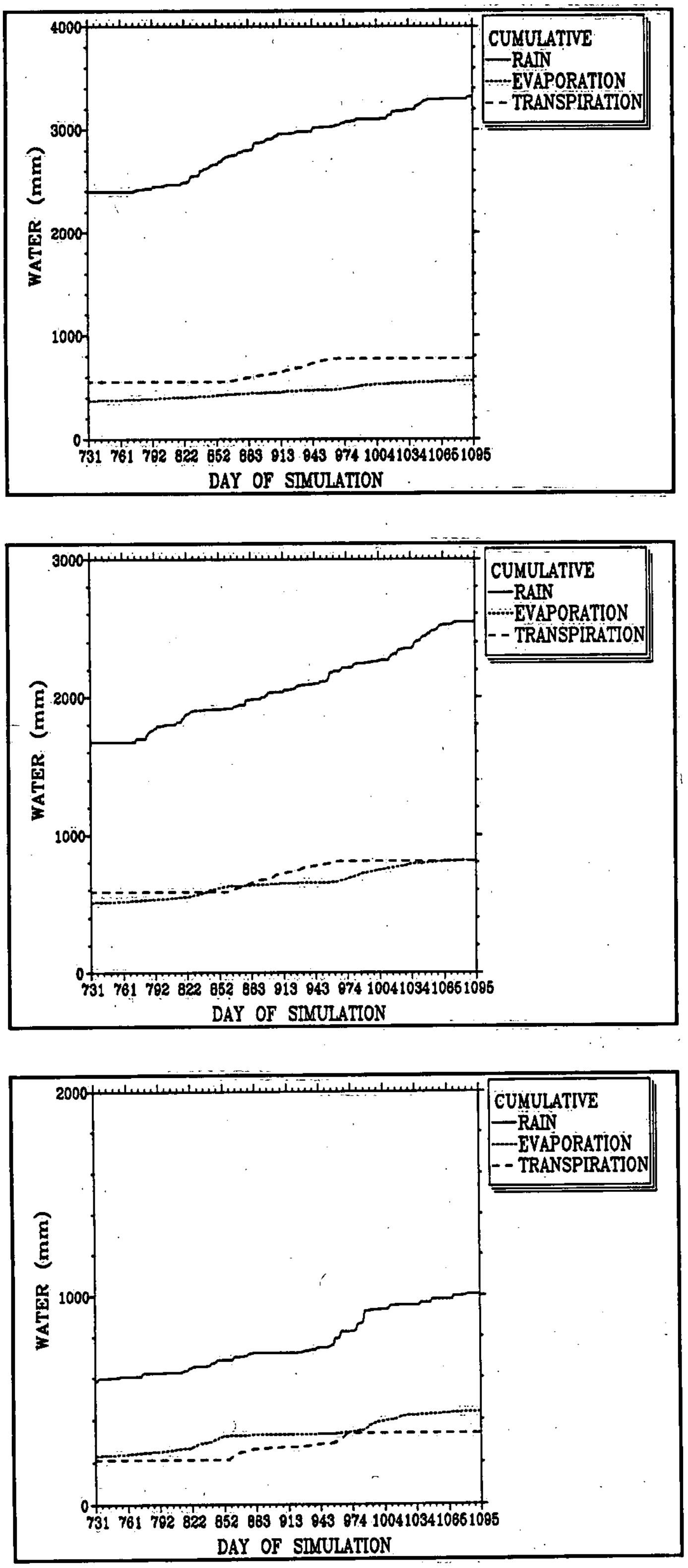
three agricultural regions. The time periods displayed in the concentration profiles (in both Fig. 16 and those that follow) represent the times at which the pesticide concentrations just above the water table (i.e., at 5.0 m) were at a maximum. In the cases in which the pesticide did not leach to the water table, the time periods selected for display in the concentration profiles are representative of the pesticide distribution in the profile during the final year of the simulation (i.e., at two-month intervals running from Day 840 to Day 1080). The precipitation, evaporation, and transpiration amounts simulated in each of the three agricultural regions (under the initial default conditions) are presented in Figure 17 and are based on recorded meteorological data taken from a climatic station within each agricultural region (1983-1985). Figure 17 illustrates that precipitation amounts were much higher in PEI and Ontario than in Alberta. However, leaching of the pesticide Brand-X to the water table was predicted in only the PEI soil (Fig. 16) for the initial default conditions stored in the EXPRES data base.

*Precipitation*

The simulations that were conducted in Scenarios 2 and 3 served to highlight the importance of climatic variability on the leaching rates and leaching depths of the pesticide Brand-X. To investigate the influence of the amount of precipitation on the model predictions, simulations were conducted where the precipitation values were multiplied by factors of 0.8 and 1.2 for each of the three agricultural regions. Table 9 gives an indication of the amount of, and variation in, the precipitation and evaporation that is typical in each of the agricultural regions. Values for the simulation period (1983-1985) used in the uncertainty analyses are also shown. The evaporation values are actual amounts predicted by PRZM, based on daily precipitation, temperature, and pan evaporation values, and are less than the potential evaporation expected in each of the agricultural regions. The predicted concentration profiles for the factors 0.8 and 1.2 are shown in Figure 18, while those for a factor of 1.0 are presented in Figure 16.

Table 9. Average Annual Precipitation (mm) and Evaporation (mm) in the Three Agricultural Regions in PEI, Ontario, and Alberta (1970-1989)

| | PEI | | ONTARIO | | ALBERTA | |
|---|---|---|---|---|---|---|
| | Precip. | Evap. | Precip. | Evap. | Precip. | Evap. |
| Mean (1970-1989) | 1153.8 | 396.2 | 908.9 | 387.6 | 375.4 | 213.4 |
| Std. deviation | 141.8 | 47.3 | 114.3 | 49.2 | 102.8 | 31.9 |
| Maximum | 1484.9 | 475.0 | 1178.8 | 481.1 | 714.1 | 277.4 |
| Minimum | 947.2 | 295.3 | 712.8 | 306.7 | 237.0 | 165.0 |
| VALUES FOR THE SIMULATION PERIOD (1983-1985) (mm) | | | | | | |
| 1983 | 1158.6 | 211.8 | 997.0 | 398.7 | 272.1 | 206.9 |
| 1984 | 1249.8 | 315.2 | 831.0 | 404.5 | 326.9 | 197.0 |
| 1985 | 947.2 | 251.4 | 995.9 | 386.1 | 406.1 | 221.5 |
| Mean (1983-1985) | 1118.5 | 259.5 | 941.3 | 396.4 | 335.0 | 208.5 |

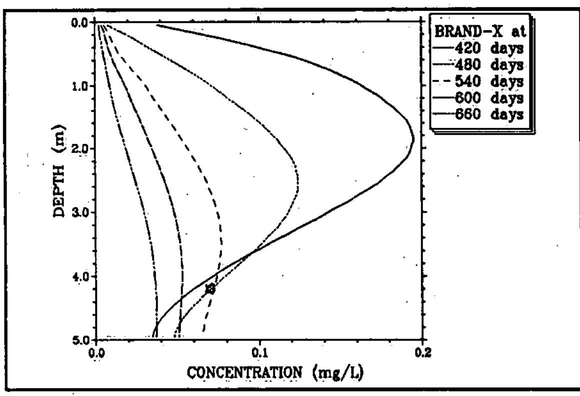



(a) a potato field in Prince Edward Island

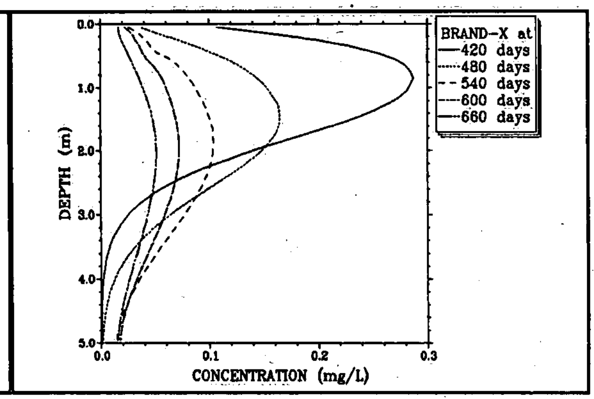
(b) a corn field in southwestern Ontario

(c) a sugar beet field in southern Alberta

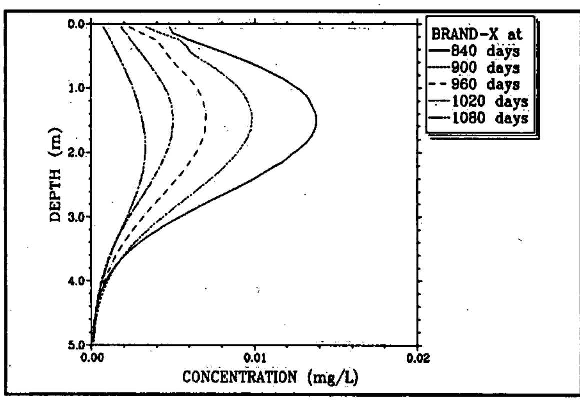
Figure 17. Cumulative rain, evaporation, and transpiration calculated by the LEACHM model for the third year of a three-year simulation.



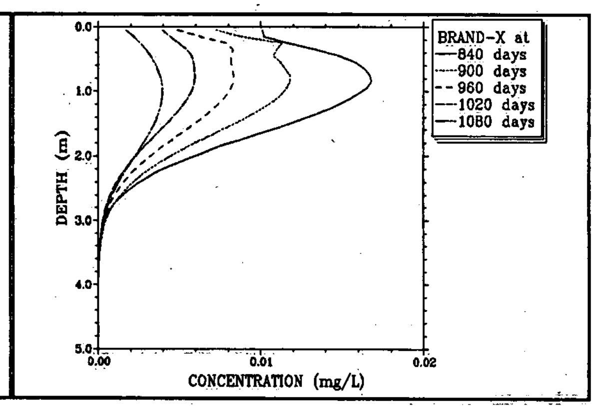

(a) n = 1.2



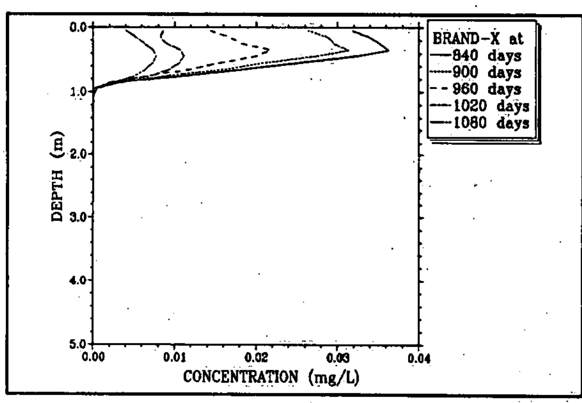

(b) n = 0.8



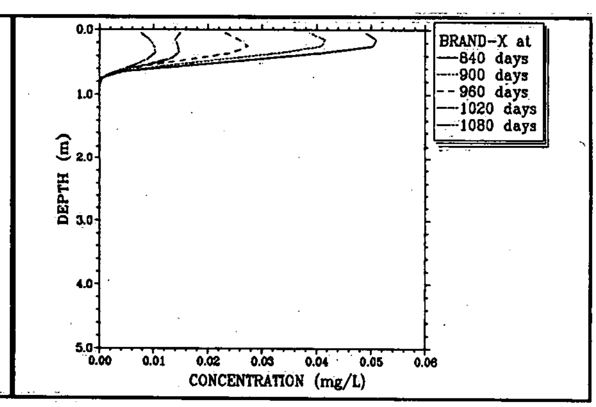

(c) n = 1.2




(d) n = 0.8




(e) n = 1.2




(f) n = 0.8

Figure 18. Dissolved pesticide concentration profiles for an application of Brand-X to (a) and (b) a potato field in Prince Edward Island, (c) and (d) a corn field in southwestern Ontario, and (e) and (f) a sugar beet field in southern Alberta, where the actual amount of precipitation (P) simulated is multiplied by a modification factor (n =), indicated below each plot (i.e., P = P * n).

Because of the large amount of precipitation that occurs in PEI (Fig. 17a), the pesticide Brand-X leaches to the water table even when the amount of precipitation is reduced to 80% of the recorded values (Fig. 18b). It is difficult to see the influence of the change in precipitation on the leaching depth in PEI because the pesticide leaches to the water table in both cases (whether increasing or decreasing the precipitation by 20%). However, a measure of the variation in the predicted results can be obtained by comparing the peak pesticide concentrations just above the water table. Concentrations just above the water table are approximately half the normal values with a 20% reduction in precipitation (Figs. 16a and 18b), while concentrations increase by approximately 50% with a 20% increase in precipitation (Figs. 16a and 18a).

Precipitation values are slightly less in Ontario than in PEI and under normal conditions (Fig. 16b) the pesticide does not leach to the water table by the end of the three-year simulation. However the maximum leaching depth (defined arbitrarily as the depth where the concentration rises above 0.0001 mg/L) is approximately 4.2 m. An increase of 20% in the amount of precipitation applied to the Ontario scenario will cause the leading edge of the pesticide concentration profile to reach the water table (maximum leaching depth increases from 4.2 m to 5.0 m) at the end of the three-year simulation (Fig. 18c). A decrease of 20% will cause the leaching depth to decrease by approximately 0.8 m (from 4.2 m to 3.4 m) (Fig. 18d).

Because of the relatively small amount of precipitation in Alberta, increasing or decreasing the amount of precipitation by 20% had a relatively minor impact on the depth of leaching of the pesticide. Increasing or decreasing the amount of precipitation by 20% will result in a change in the leaching depth of only approximately 0.2 m. The maximum leaching depth for the pesticide is approximately 1 m at the end of the three-year simulation (Fig. 18e).

The results indicate that, between regions, the depth of leaching of the pesticide depends on the total amount of precipitation a region receives rather than on the relative variation in the amount of precipitation. For example, a 20% change in precipitation for a region that receives 1000 mm of precipitation a year will be more significant in that region than a change of 20% in a region that receives only 400 mm of precipitation a year. However, the variations in the results within a given region to a change in the precipitation are applicable only on a region-by-region basis. They serve only to highlight what may happen in a year where conditions are wetter or drier than average within each of the three regions.

The previous simulations show the influence that a change in the amount of precipitation has on the leaching patterns within a region. However, they do not indicate whether the amount of precipitation is more or less important than the soil characteristics in determining the leaching rates and depths of a pesticide. To test the importance of the amount of precipitation on the leaching rates and depths of the pesticide Brand-X, simulations were conducted in which the meteorological data for a region were replaced with the meteorological record from another region (i.e., what the concentrations and leaching depths would be in Alberta if it received as much precipitation as PEI). Two simulations were conducted for each agricultural region, using the meteorological data from one of the other two agricultural regions in each simulation. The results indicated that the pesticide Brand-X would leach to the water table in Alberta if either the PEI or Ontario meteorological conditions existed in Alberta (Fig. 19e and f). Figure 19, b and d, also suggests that the pesticide Brand-X would not leach to the water table in either the PEI or Ontario soils if they were subjected to the meteorological conditions found in southern Alberta. The pesticide leached to the water table in all three agricultural regions (see Figs. 19, c and e, and 16a) when subjected to the PEI meteorological conditions (mean annual precipitation for the simulation period = 1119 mm). However, it did not leach to the water table in any of the three agricultural regions (Figs. 19, b and d, and 16c) when subjected to the Alberta meteorological conditions (mean annual precipitation for the simulation period = 335 mm). This suggests that a significant amount of precipitation is required to leach the pesticide Brand-X to the water table, regardless of the soil, crop, and farming conditions found within an agricultural region.

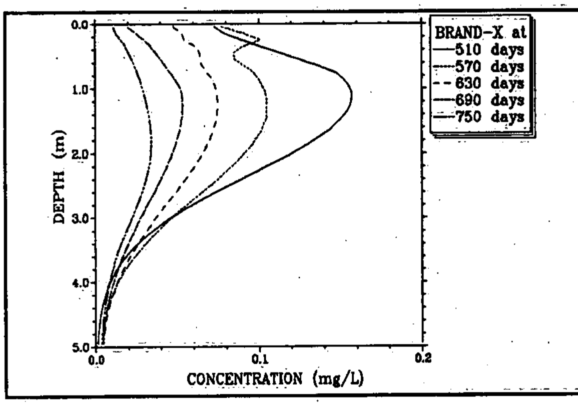
*Hydraulic Conductivity*

Natural soil profiles are highly heterogeneous and often exhibit a wide spatial variability in many of the properties used to define the physical and chemical characteristics of the soil profile. The hydraulic conductivity of a soil profile is one such property. It is often difficult to obtain values of hydraulic conductivity that are representative of the various depths within a single soil profile, let alone obtain field-averaged values that are representative of some larger area. The uncertainty that may exist in the hydraulic conductivity of a soil profile was investigated by both increasing and decreasing the value of the hydraulic conductivity by a maximum of two orders of magnitude (x $10^2$ and x $10^{-2}$). The initial values for the hydraulic conductivities of the soil horizons in the three agricultural regions are listed in Table 10, and the results of the simulations are presented in Figure 20.

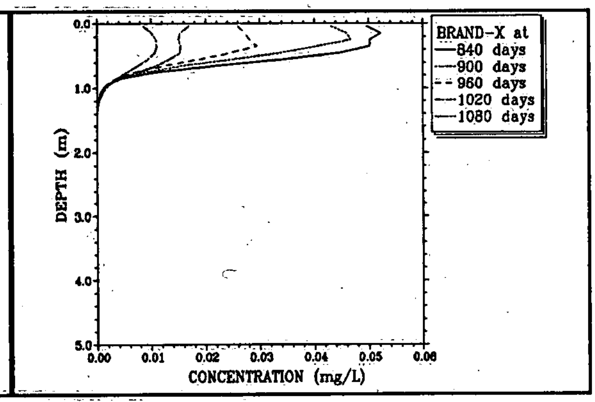
Table 10. Hydraulic Conductivities and Organic Carbon Content Values of the Three Agricultural Regions in PEI, Ontario, and Alberta

| PRINCE EDWARD ISLAND | | | ONTARIO | | | ALBERTA | | |
|---|---|---|---|---|---|---|---|---|
| Depth (cm) | K (mm/day) | OC (%) | Depth (cm) | K (mm/day) | OC (%) | Depth (cm) | K (mm/day) | OC (%) |
| 0-10 | 779 | 0.40 | 0-20 | 24 | 2.50 | 0-20 | 1530 | 1.00 |
| 10-20 | 2780 | 2.55 | 20-50 | 12 | 1.00 | 20-60 | 915 | 0.50 |
| 20-40 | 300 | 0.70 | 50-100 | 12 | 0.60 | 60-100 | 1530 | 0.30 |
| 40-60 | 50 | 0.10 | 100-120 | 12 | 0.40 | 100-500 | 1830 | 0.10 |
| 60-90 | 200 | 0.01 | 120-500 | 18 | 0.10 | | | |
| 90-500 | 200 | 0.01 | | | | | | |

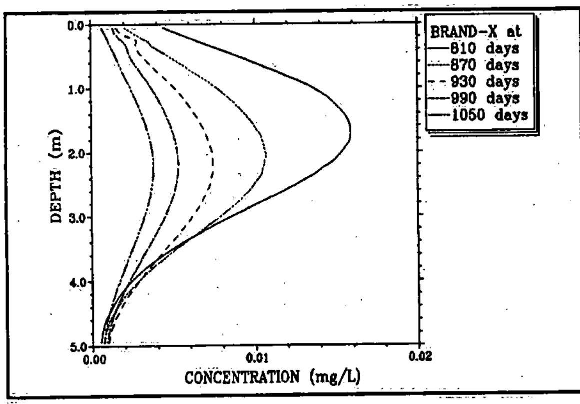
Depth = depth of soil horizon, K = hydraulic conductivity, OC = organic carbon



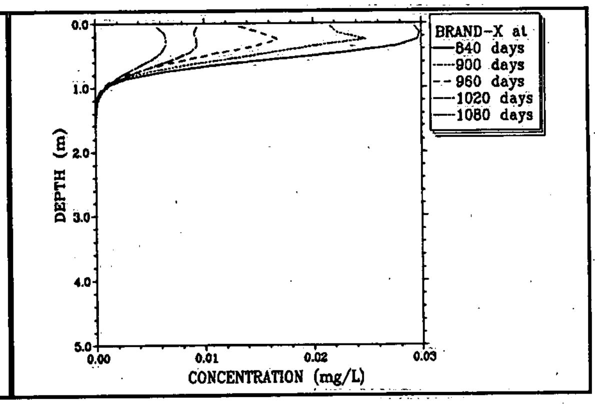

(a) PEI Soil with Ontario Precipitation



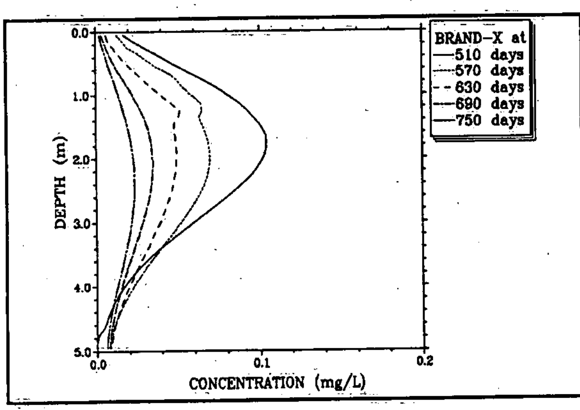

(b) PEI Soil with Alberta Precipitation



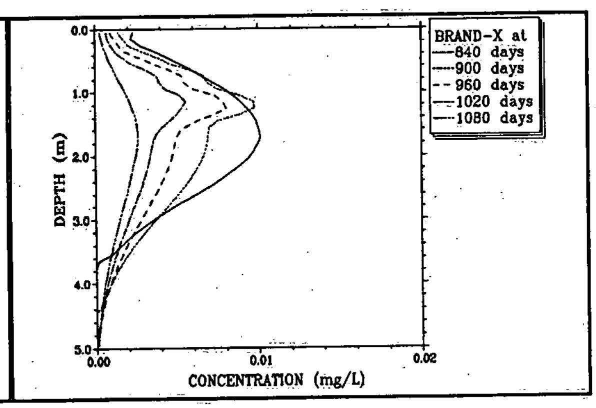

(c) Ontario Soil with PEI Precipitation




(d) Ontario Soil with Alberta Precipitation

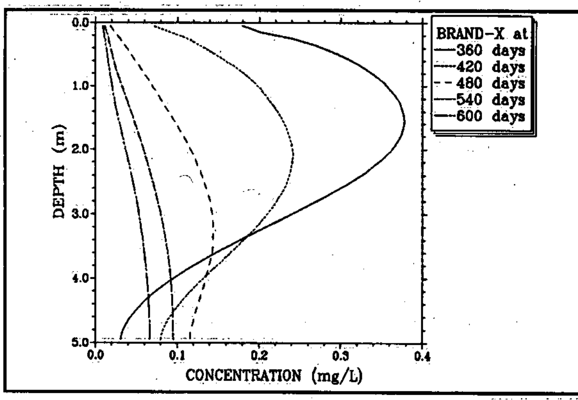



(e) Alberta Soil with PEI Precipitation

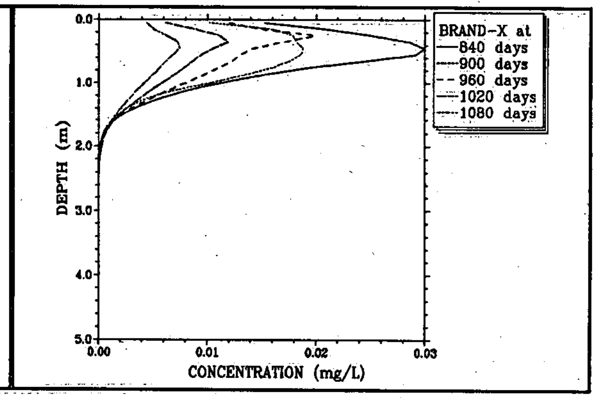



(f) Alberta Soil with Ontario Precipitation

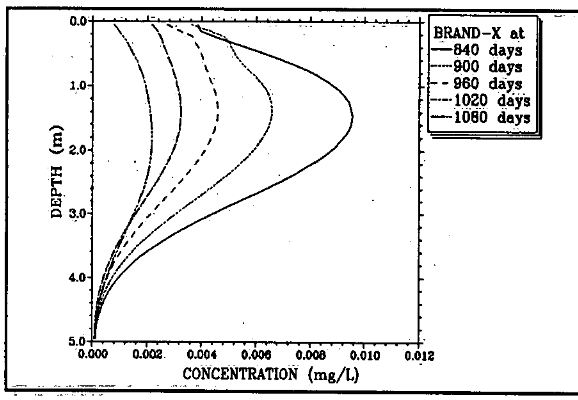
Figure 19. Dissolved pesticide concentration profiles for an application of Brand-X to (a) and (b) a potato field in Prince Edward Island, (c) and (d) a corn field in southwestern Ontario, and (e) and (f) a sugar beet field in southern Alberta, where the local meteorological conditions were replaced by the meteorological conditions found in other regions (as indicated below each plot).




(a) n = 2




(b) n = -2

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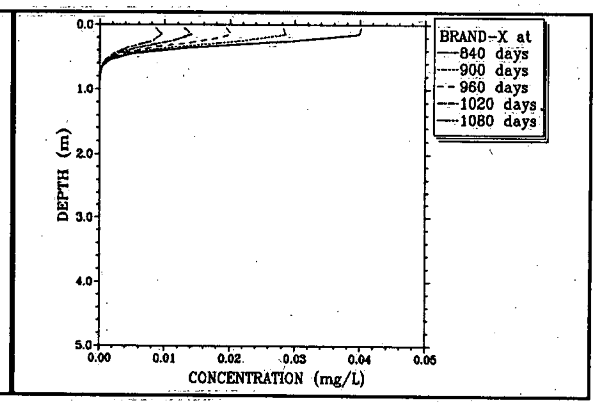
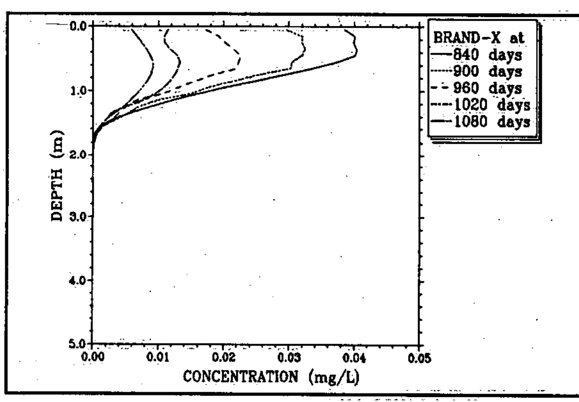
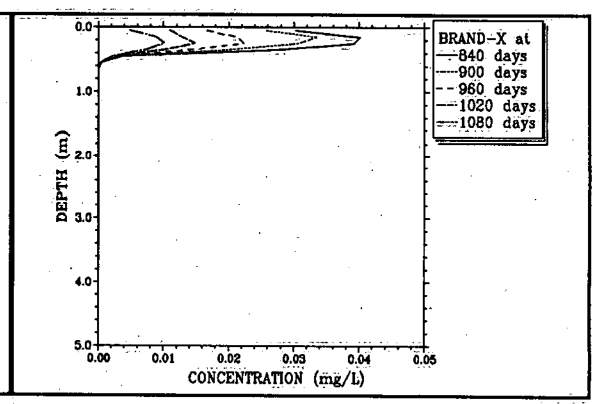



(d) n = -2




(e) n = 2




(f) n = -2

Figure 20. Dissolved pesticide concentration profiles for an application of Brand-X to (a) and (b) a potato field in Prince Edward Island, (c) and (d) a corn field in southwestern Ontario, and (e) and (f) a sugar beet field in southern Alberta, where the value of the hydraulic conductivity (K) of the soil horizons was changed by a factor equal to the modification factor (n =), as indicated below each plot (i.e., $K = K * 10^n$).

In all cases where the hydraulic conductivity was decreased by two orders of magnitude, the pesticide did not leach to the water table (Fig. 20b, d, and f). In the case of the PEI and Ontario soils (Fig. 20b and d), there was a significant reduction in the leaching depth of the pesticide when compared to the normal conditions shown in Figure 16, a and b. The leaching depth varied less in the Alberta scenario, showing approximately a 10% change in the leaching depth for a two order-of-magnitude decrease in the hydraulic conductivity (Figs. 16c and 20f). These results are primarily due to the amount of water actually infiltrating into the soil profile, which is a function of the amount of precipitation and the hydraulic conductivities in the surface horizons. The LEACHM model assumes that if the precipitation that is applied on a given day does not infiltrate by the end of that day, the water that has not yet infiltrated will be lost as additional runoff. Because of the large amount of precipitation and the low hydraulic conductivities of the surface horizons in PEI and in Ontario, a larger amount of the precipitation was being lost as additional runoff (approximately 75% in Ontario, and 50% in PEI) and was not infiltrating past the surface horizon. The amount of precipitation lost as additional runoff in Alberta was much less (approximately 15%) due to the higher hydraulic conductivity in the surface horizon and the smaller amount of precipitation. With the decrease in the hydraulic conductivity, the amount of precipitation actually infiltrating in the Ontario soil (≈ 650 mm) is less than the infiltration in Alberta (≈ 860 mm). The amount of infiltration in PEI (≈ 1600 mm) is still approximately twice as high as in Alberta but is substantially less than the amount received with the original hydraulic conductivity value (≈ 3300 mm).

The concentration of the pesticide reaching the water table in all three regions increased in response to a two order-of-magnitude increase in the hydraulic conductivity. The peak concentrations reaching the water table in the PEI soil were approximately three times larger than under the normal conditions (Figs. 20a and 16a). When the hydraulic conductivity in the Alberta soil was increased, the leaching depth of the pesticide more than doubled, increasing from approximately 0.9 m under normal conditions to approximately 1.9 m (Figs. 20e and 16c). Because of the low initial hydraulic conductivities in the Ontario scenario (Table 10), it was expected that this soil would be more sensitive to the increase than the other two soils. However, the increase in the concentration at the water table due to an increase in the hydraulic conductivity in the Ontario soil was dampened by an increase in the amount of evaporation that occurred (an extra 200 mm over the three-year simulation) due to the greater mobility of the water and pesticide in the soil profile. The pesticide reached the water table at approximately Day 840 (Fig. 20c), as opposed to just reaching the water table on Day 1080 under normal conditions (Fig. 16b). However, the increased hydraulic conductivity also allowed more water to be drawn to the soil surface, where it was lost to the atmosphere in meeting the evaporative demand. Although there was an increase in the cumulative water flux to the water table (from approximately 665 to 750 mm), there was a decrease in the cumulative amount of water flux past the 1-m depth in the soil (from 595 to 425 mm). The sensitivity of the model to the hydraulic conductivity was reduced in the soil layers influenced by the evaporative loss. As a result, the change in the concentration due to an increase in the hydraulic conductivity was less than might be expected in this agricultural region.

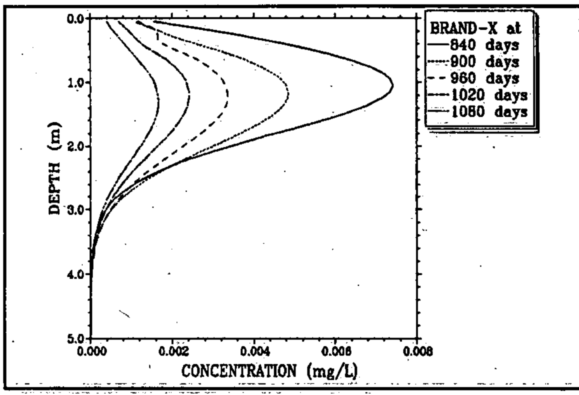
*Organic Carbon Content*

The attenuation of a pesticide in a soil profile is primarily related to the organic carbon content of the soil profile. However, the amount of organic carbon in a soil profile is also highly variable (see Table 10), and therefore uncertainty is created when field-averaged values are used to describe the areal distribution of the organic carbon content in a field situation. For this reason, the influence of the organic carbon content of the soil horizons on the potential for the pesticide to leach was investigated in the three agricultural regions. The initial organic carbon contents of the soil horizons in the three agricultural regions are shown in Table 10, and the results are presented in Figure 21.

When the organic carbon contents of the soil horizons were increased by 2%, the pesticide Brand-X did not leach to the water table in the three agricultural regions (Fig. 21a, c, and e). The leaching depths of the pesticide were affected more in the PEI (>5.0 m to 3.5 m) and Ontario (4.2 m to 2.3 m) soils than in the Alberta soil (0.9 m to 0.7 m). Increasing the organic carbon content of the soil horizons will affect the leaching of the pesticide in the PEI and Ontario soils to a greater extent than in the Alberta soil, because under normal conditions there is sufficient precipitation to drive the pesticide into the lower soil horizons in these two regions. The pesticide in both the PEI and Ontario soils will, therefore, interact with a larger amount of the additional organic carbon in the soil horizon. The organic carbon that was added to the lower horizons in the Alberta soil will have no effect on the leaching of the pesticide because there is not sufficient precipitation in the Alberta scenario to drive the pesticide into these lower soil horizons. The same reasoning can be applied to the situation in which organic carbon content is reduced by 2% (set to zero if the original value was less than 2%). Because the pesticide will encounter more of the soil horizons in the PEI and Ontario soils than in the Alberta soil, the overall reduction in the organic carbon content in each of the soil horizons will have a greater affect on the leaching patterns in the PEI and Ontario soils. The pesticide concentration at the water table in the PEI soil increased by approximately 50%, while the maximum leaching depth in the Ontario soil moved from approximately 4.2 m to 5.0 m (Fig. 21b and d). The change in the leaching depth in the Alberta was less noticeable than in the other two agricultural regions because the initial organic carbon contents of the soil horizons were lower and therefore less affected by a decrease in the amount of organic carbon. The change in the leaching depth was approximately 0.2 m (Figs. 21f and 16c) in Alberta. In all three agricultural regions, the concentration profiles varied more due to an increase in the organic carbon content of the soil horizons than to a decrease. This result is observed because many of the soil horizons had initial organic carbon contents that were less than 2%. Therefore, the actual reduction that occurred in the organic carbon content was less than 2% in many of the soil horizons.

*Discussion of Analyses*

In the preceding discussions, comparisons were made between agricultural regions as to which regions were more or less affected by variations in the parameter being investigated. In the following discussions, a comparison will be made within each region as to which parameter (precipitation, hydraulic conductivity, or organic carbon) has the

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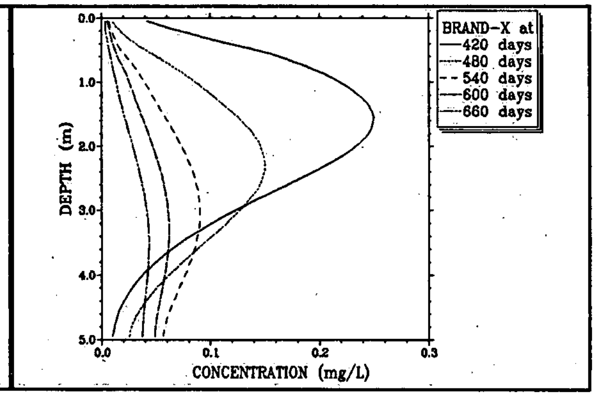
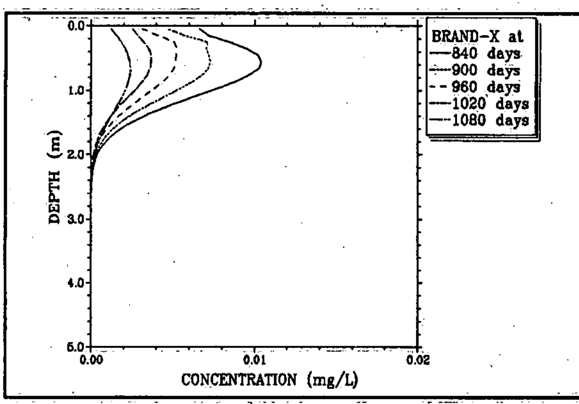
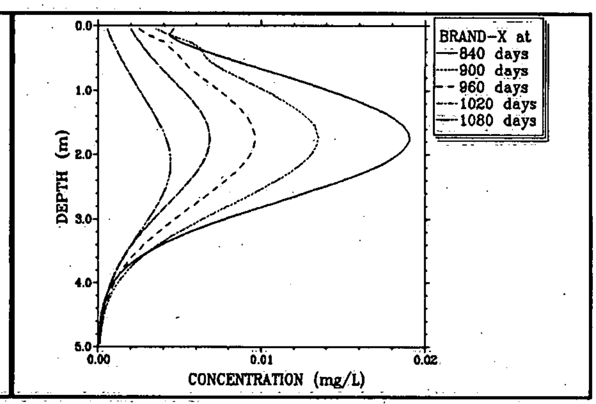


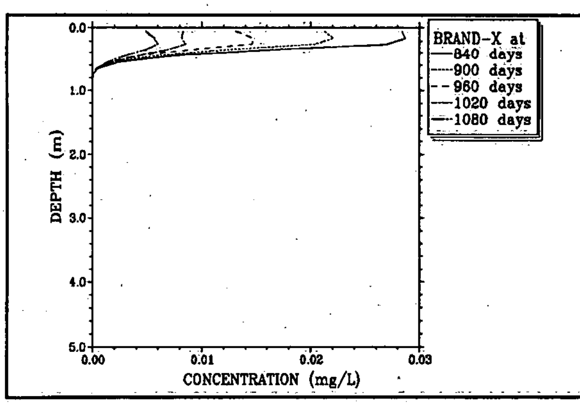

(b) n = -2




(c) n = 2




(d) n = -2

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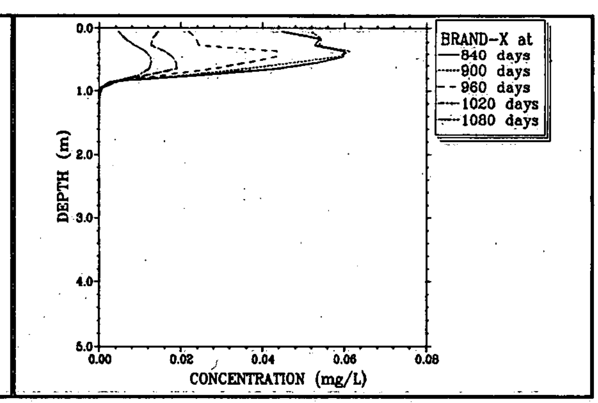


(f) n = -2

Figure 21. Dissolved pesticide concentration profiles for an application of the pesticide Brand-X to (a) and (b) a potato field in Prince Edward Island, (c) and (d) a corn field in southwestern Ontario, and (e) and (f) a sugar beet field in southern Alberta, where the value of the organic carbon (OC) content in the soil profile was changed by the modification factor (n =), as indicated below each plot (i.e., OC = OC + n).

greatest influence on the leaching of the pesticide. Because of the natural variability in the soil parameters and uncertainties in their measurement, these analyses can be used to indicate which parameter measurements require special attention. Table 11 has been compiled as a summary of the studies in each region. This table lists the maximum leaching depth of the pesticide, and if the pesticide leached past the water table, it also records the maximum pesticide concentration that was observed at the water table.

The analyses indicate that within the PEI agricultural region, the leaching of the pesticide Brand-X is affected most by the value of the hydraulic conductivity (Fig. 20a and b), followed by the organic carbon content (Fig. 21a and b), and then by a change in the amount of precipitation (Fig. 18a and b) for the range of values that were investigated. Although the maximum concentration observed at the water table was slightly higher for an increase of 20% in the precipitation (0.063 mg/L) (see Table 11) than for a reduction of 2% in the organic carbon content (0.055 mg/L), the concentration was much lower when the organic carbon content was increased by 2% (the pesticide did not reach the water table) than when the precipitation was decreased by 20% (0.018 mg/L). In turn, the leaching of the pesticide is affected more by the hydraulic conductivity than by the organic carbon content. The pesticide concentration was higher at the water table when the hydraulic conductivity was increased (0.118 mg/L) than when the organic carbon was decreased by 2% (0.055 mg/L). The leaching depth was also less when the hydraulic conductivity was decreased (2.2 m) than when organic carbon was increased (3.5 m).

The situation in Ontario is essentially the same as in PEI. The leaching of the pesticide Brand-X was affected most by changes in the value of the hydraulic conductivity and least by changes in the value for organic carbon content and precipitation. Referring to Table 11, the maximum leaching depth for all three parameters in Ontario was close to 5.0 m. However, the minimum leaching depth for the hydraulic conductivity in Ontario was 0.70 m, while the minimum leaching depths for organic carbon and precipitation were 2.3 and 3.4 m, respectively. Although the leaching depth was most sensitive to the hydraulic conductivity, all three parameters investigated (precipitation, hydraulic conductivity, and organic carbon content) can influence whether the pesticide Brand-X will leach to the water table when varied over the range of values investigated in these studies. Figures 18c, 20c, and 21d all suggest that the pesticide will leach to the water table when more favourable conditions are specified for the leaching of the pesticide in the Ontario soil. Figures 18d, 20d, and 21c, however, suggest that under the less favourable circumstances, the pesticide will not leach to the water table during the three-year simulation. Thus, changing the precipitation, organic carbon content, and hydraulic conductivity values can have a significant result on the leaching depth of the pesticide under conditions simulated for the Ontario agricultural region.

Leaching of the pesticide in the Alberta soil was also affected most by the value of the hydraulic conductivity and to a lesser degree by changes in the organic carbon content and precipitation. The difference between the maximum leaching depth due to changes in the hydraulic conductivity was 1.3 m (Table 11), while differences for precipitation and organic carbon were 0.2 and 0.4 m, respectively. Although the leaching

Table 11. Summary of the Leaching Depths and Maximum Pesticide Concentrations at the Water Table Predicted by the LEACHM Model for the Uncertainty Analyses Conducted in the PEI, Ontario, and Alberta Agricultural Regions

PRINCE EDWARD ISLAND

| | Precipitation | | | Hydraulic Conductivity | | | Organic Carbon | | |
|---|---|---|---|---|---|---|---|---|---|
| | n = 1.2 | n = 1.0 | n = 0.8 | n = 2 | n = 0 | n = -2 | n = 2 | n = 0 | n = -2 |
| Max. leaching depth (m) | > 5 | > 5 | > 5 | > 5 | > 5 | 2.2 | 3.5 | > 5 | > 5 |
| Max. concentration at water table (mg/L) | 0.063 | 0.040 | 0.018 | 0.118 | 0.040 | - | - | 0.040 | 0.055 |

ONTARIO

| | Precipitation | | | Hydraulic Conductivity | | | Organic Carbon | | |
|---|---|---|---|---|---|---|---|---|---|
| | n = 1.2 | n = 1.0 | n = 0.8 | n = 2 | n = 0 | n = -2 | n = 2 | n = 0 | n = -2 |
| Max. leaching depth (m) | 5.0 | 4.2 | 3.4 | 4.9 | 4.2 | 0.70 | 2.3 | 4.2 | 5.0 |
| Max. concentration at water table (mg/L) | - | - | - | - | - | - | - | - | - |

ALBERTA

| | Precipitation | | | Hydraulic Conductivity | | | Organic Carbon | | |
|---|---|---|---|---|---|---|---|---|---|
| | n = 1.2 | n = 1.0 | n = 0.8 | n = 2 | n = 0 | n = -2 | n = 2 | n = 0 | n = -2 |
| Max. leaching depth (m) | 1.0 | 0.9 | 0.8 | 1.9 | 0.9 | 0.6 | 0.7 | 0.9 | 1.1 |
| Max. concentration at water table (mg/L) | - | - | - | - | - | - | - | - | - |

n = modification factor ($K = K * 10^n$, $P = P * n$, $OC = OC + n$)

of the pesticide is affected least by a change in the amount of precipitation, it can also be concluded from these analyses that the amount of precipitation received in Alberta is the limiting factor in determining the leaching depth of the pesticide Brand-X. Even when the hydraulic conductivity and organic carbon content values were set to values representative of more favourable conditions for leaching, the pesticide leached to the water table only when the precipitation was dramatically increased by substituting either the PEI or Ontario meteorological conditions for the Alberta data. The amount of precipitation that this region receives appears to be the primary factor in determining whether Brand-X will leach to the water table. In support of this conclusion, it was observed that when the Alberta meteorological data were substituted in either PEI or Ontario scenarios, the pesticide did not leach to the water table (Fig. 19b and d).

The amount of precipitation received will also govern the change of the leaching depth of the pesticide to changes in the hydraulic conductivity and organic carbon content values. Because the amount of precipitation is limiting in Alberta, the leaching depth was affected less by large changes in the hydraulic conductivity or organic carbon content values (Figs. 20e and f and 21e and f) when compared to similar changes made in either the PEI or Ontario scenarios (Figs. 20a–d and 21a–d). Because the amount of precipitation is high in PEI, the pesticide leaches to the water table even when the amount of precipitation is reduced by 20% (Fig. 18b). Therefore, in this situation, the major concern would be how fast it leaches and what the maximum concentration at the water table is. Ontario also has an ample amount of precipitation to leach the pesticide Brand-X to the water table in sandy soils (see Fig. 19, a and f). However, the soil characterized in the Ontario agricultural region is much tighter than in either the PEI or Alberta situations, restricting the percolation of water through the soil profile. As a result, the influence of the amount of precipitation on the leaching of the pesticide may not be so pronounced as in more permeable soils.

In general, the leaching depth of the pesticide Brand-X within a region was affected most by changes in the values for the hydraulic conductivity and least by changes in the amount of precipitation that occurs within the region. However, when comparing differences between regions, the amount of infiltration (the amount of precipitation minus the amount of evaporation) is found to be the main controlling factor in the leaching depth of the pesticide Brand-X. Regardless of the differences in the soil profile characteristics between the three regions (e.g., different hydraulic conductivities and organic carbon contents), the pesticide leached to the water table when the regions were subjected to the meteorological conditions found in PEI (specifically, the large amount of precipitation). In the same respect, the pesticide will not leach to the water table in any of the regions when the meteorological data from Alberta is applied (specifically, low levels of precipitation, high evaporation). However, ample precipitation is not solely sufficient in determining whether the pesticide Brand-X will leach to the water table. In PEI, which has ample precipitation to leach the pesticide to the water table under normal conditions (Fig. 16a), the pesticide did not leach to the water table (Figs. 20b and 21a) when the hydraulic conductivity and organic carbon were set to unfavourable values (i.e., hydraulic conductivity reduced by two orders of magnitude and organic carbon contents increased by 2%). There must be an adequate balance between the amount of infiltration occurring and the degree to which the soil profile properties are conducive to leaching, to result in the leaching of the pesticide to the water table.

These analyses may be used to alert pesticide regulatory personnel to the key factors that may be important in determining the leaching potential of a pesticide seeking registration both within a region and between different regions. If regulatory personnel are given results from a field test with the pesticide in Alberta, they may want to scrutinize closely the amount of precipitation or irrigation water that was applied to determine how closely the values approximate the maximum rainfall and irrigation that might be expected for the conditions under which the new pesticide is used. Similarly, if the field test results were from PEI or Ontario, regulatory personnel should perhaps be more concerned with how well the hydraulic conductivity and organic carbon contents of the field test compare with the worst-case scenario that might reasonably be expected for the conditions under which the pesticide will be applied. With these analyses, it is possible to identify the parameters that require special attention in obtaining accurate measurements from the field. It is also possible to take conditions present during the field test and subject them to the meteorological conditions from another region to get an indication on how the leaching patterns may change in another agricultural region.

The results of these analyses for the pesticide Brand-X within a region, in general, can be applied to other pesticides that may be seeking registration in the same region. However, because the chemical properties of the pesticide influence the results produced by the model, these chemical properties will influence the way in which a pesticide reacts with a soil profile. For example, the leaching of a pesticide with a high organic pesticide partition coefficient will be affected more by changes in the value of the organic carbon content of the soil than a pesticide with a lower organic carbon partition coefficient. However, the relative leaching depths may remain the same. Therefore, the results obtained for a pesticide within a region cannot be applied to all pesticides being used within that region. Individual uncertainty analyses must be conducted for each new pesticide because each has different chemical properties that influence its transport and fate in the unsaturated zone.

# Summary and Recommendations

## SUMMARY

Within a regulatory framework, the widespread use of existing pesticide models for assessing the fate of pesticides in the subsurface may be limited because (1) the application of these models requires a high level of expertise in numerical modelling and in the theory of pesticide transport, (2) considerable pesticide and site-characterizing data are typically required to undertake a simulation but are often not available, and (3) there are no means of ensuring that the input data and the results calculated by the models are accurate and meaningful. The EXPRES expert system was developed to enable regulatory personnel to gain the knowledge and experience necessary to assess confidently and accurately the potential for pesticides to contaminate groundwater. EXPRES couples three pesticide assessment models with extensive data bases on the chemical properties of pesticides and site characteristics of agricultural regions across Canada (physical, pedological, hydrogeological, meteorological data, crops grown, and agricultural practices) within an expert system framework. This approach enables EXPRES to guide the user through the selection of the information required to choose the most appropriate pesticide assessment model, compose the input data set, execute the model, and interpret the results.

The use of the EXPRES expert system by regulatory personnel for assessing the potential for groundwater contamination will improve the efficiency and productivity of the organization. The advantages of using EXPRES include

(1) complex modelling codes that can be used by those not familiar with this technology
(2) reduced costs and time associated with not having to contact an outside consultant
(3) a test of the integrity of user-supplied data and suggestions for missing or inconsistent data
(4) an evaluation and interpretation of critical output from the simulation models
(5) data bases containing knowledge, facts, and information that can be stored for future reference
(6) assurance that all evaluations are undertaken on a consistent basis both from pesticide to pesticide by a single user, or among several users
(7) rapid and easy distribution of this aspect of the pesticide assessment process throughout the organization
(8) its possible use as an educational tool for teaching basic concepts about the fate and transport of pesticides in the subsurface

EXPRES has a data base that contains information that characterizes 22 typical agricultural regions across Canada. The information stored in this data base is used as default data for these agricultural regions. However, those using EXPRES should be aware that it is very difficult to describe a large agricultural region, such as a wheat field in southern Saskatchewan, with one set of model parameters. An effort has been made to select values that are representative of the typical conditions that may exist within an agricultural region. However, the user should be aware that conditions can vary greatly within an agricultural region and that analyses performed with EXPRES on new pesticides seeking registration should include simulations performed over a wide range of model parameter values.

## RECOMMENDATIONS

All the initial objectives of the project were met during the two years it took to develop the EXPRES expert system. During this time, EXPRES grew considerably from what was originally envisioned, in terms of both its form (e.g., design and operation of the screens, menus) and its content (e.g., additional assessment models, data bases, integrity checks). The nature of the development of EXPRES is typical of an expert system. Although EXPRES is currently a complete and operational expert system, there are additional modifications, improvements, and additions that could be undertaken to enhance its usefulness and applicability. Therefore, it is recommended that the following tasks be considered to enhance the EXPRES expert system.

(1) Although the information stored in the EXPRES data bases is extensive, the coupling of EXPRES to a geographical information system (GIS) represents a very attractive method for expanding the amount of data that could be accessed by the user. It would also allow for a geographical display of the results (i.e., maps). Coupling EXPRES to a GIS system could provide the user with a much larger data base for model parameters, such as those representing the soil profile. For example, the user might be able to access a GIS data base containing data on all the soil series in a particular province and select from the individual soil series the soil that best represents the site where the pesticide is to be applied. The GIS would also simplify the selection of these data for the user.

(2) Adding more agricultural regions to the data base of EXPRES would allow regulatory personnel to conduct assessments in additional agricultural regions across the country.

(3) Loading EXPRES on to a work station environment may also be beneficial. The increased speed of the work station would allow the user to take full advantage of the capabilities of EXPRES. The research model, LEACHM, incorporated into EXPRES is most effectively employed when used to conduct uncertainty analyses to determine which model parameters and processes are most influential in controlling the fate of pesticides in the subsurface. However, a large number of simulations are required for these uncertainty analyses, and the execution times

with the LEACHM model are lengthy. The decreased execution times on a work station may be conducive to performing more uncertainty analyses with EXPRES. EXPRES was originally designed to operate on an 80286-based PC. However, computing technology has developed rapidly during the past two years, and the cost of a work station is becoming affordable.

(4) The decrease in execution time on a work station would also open up the possibility of conducting stochastic simulations with EXPRES. The stochastic simulations would allow the user to more accurately define the uncertainty associated with predictions made with the EXPRES simulations. Stochastic modelling requires a large number of simulations to be conducted so that statistical probabilities can be attached to the predicted results.

(5) The possibility of incorporating a more detailed surface runoff model in the EXPRES expert system could also be investigated. A more detailed surface runoff model could provide the necessary link required to couple EXPRES to existing surface water quality models, thereby enhancing the overall evaluation of the fate of pesticides in the aquatic environment.

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# References


Aller, L., T. Bennet, J. Lehr, and R. Petty. 1985. DRASTIC: A standardized system for evaluating groundwater pollution potential using hydrogeologic settings. U.S. EPA 600/2-85/018, Ada, Okla. 384 pp.

Bohn, H.L., B.L. McNeal, and G.A. O'Connor. 1979. Soil chemistry. New York: John Wiley and Sons. 329 pp.

Bonazountas, M., and J.M. Wagner. 1984. "SESOIL" - A seasonal soil compartment model. Cambridge, Mass.: Arthur D. Little Consultants.

Carsel, R.F., C.N. Smith, L.A. Mulkey, J.D. Dean, and P. Jowise. 1984. User's manual for the pesticide root zone model (PRZM), Release 1. U.S. EPA 600/3-84/109, Athens, Ga. 216 pp.

Carsel, R.F., L.A. Mulkey, M.N. Lorber, and L.B. Baskin. 1985. The pesticide root zone model (PRZM): a procedure for evaluating pesticide leaching threats to groundwater. Ecol. Modell. 30:49-69.

Carsel, R.F., R.L. Jones, J.L. Hansen, R.L. Lamb, and M.P. Anderson. 1988. A simulation procedure for groundwater quality assessments of pesticides. J. Contam. Hydrol. 2:125-138.

Cohen, S.Z., S.M. Creeger, R.F. Carsel, and C.G. Enfield. 1984. Potential for pesticide contamination of groundwater resulting from agricultural uses. *In* Treatment and Disposal of Pesticide Wastes, ed. R.F. Kruger and J.N. Seiber. Am. Chem. Soc. Symp. Ser. No. 259:297-325.

Crowe, A.S., and G.L. McClymont. 1992. The application of expert systems to solving groundwater problems. *In* Proc. 1992 Can. Hydrol. Symp., Hydrology: Its Contribution to Sustainable Development, pp. 213-231, June 15-17, 1992, Winnipeg, Man.

Crowe, A.S., and J.P. Mutch. 1990. Assessing the migration and transformation of pesticides in the subsurface: the role of expert systems. Can. Water Pollut. Res. J. 25(3):293-323.

Crowe, A.S., and J.P. Mutch. 1991a. EXPRES: An expert system for assessing the fate of pesticides in the subsurface; Progress Report: Incorporation of the LP/LI screening model into EXPRES. National Water Research Institute Contrib. #91-68, Burlington, Ont. 30 pp.

Crowe, A.S., and J.P. Mutch. 1991b. EXPRES: An expert system for assessing the fate of pesticides in the subsurface; Progress Report: Incorporation of the data base display module into EXPRES. National Water Research Institute Contrib. #91-84, Burlington, Ont. 68 pp.

Donigian, A.S., and P.S.C. Rao. 1986. Overview of terrestrial processes and modeling. *In* Vadose zone modeling of organic pollutants, ed. S.C. Hern and S.M. Melancon, 1-35. Chelsea, Mich.: Lewis Publishers.

Enfield, C.G., R.F. Carsel, S.Z. Choen, T. Phan, and D.M. Walters. 1982. Method for approximating pollutant transport to ground water. Ground Water 20:711-722.

Gustafson, D.I. 1989. Groundwater ubiquity score: a simple method for assessing pesticide leachability. Environ. Toxicol. Chem. 8:339-357.

Haith, D.A., and R.C. Loehr, eds. 1979. Effectiveness of soil and water conservation practices for pollution control. U.S. EPA 600/3-79/106, Athens, Ga.

Harkin, J.M., F.A. Jones, R.N. Fathulla, E.K. Dzantor, and D.G. Kroll. 1986. Fate of aldicarb in Wisconsin groundwater. *In* Evaluation of Pesticides in Ground Water, ed. W.Y. Garner, R.C. Honeycutt, and H.N. Nigg. Am. Chem. Soc. Symp. Ser. 315(12):219-255.

Harmon, P., and D. King. 1985. Expert systems. New York: John Wiley and Sons. 283 pp.

Hayes-Roth, F., D.A. Waterman, and D.B. Lenat, eds. 1983. An overview of expert systems. *In* Building Expert Systems, 3-29. Reading, Mass.: Addison-Wesley Publishers.

Hess, P.J. 1986. Groundwater use in Canada, 1981. NHRI Pap. No. 26, IWD Tech. Bull. No. 140, National Hydrology Research Institute, Inland Waters Directorate, Environment Canada, Ottawa. 43 pp.

Hillel, D. 1980a. Applications of soil physics. San Diego, Calif.: Academic Press. 385 pp.

Hillel, D. 1980b. Fundamentals of soil physics. San Diego, Calif.: Academic Press. 413 pp.

Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko. 1991. Handbook of environmental degradation rates. Chelsea, Mich.: Lewis Publishers. 725 pp.

Hushon, J.M. 1990a. The defence priority model for Department of Defence remedial site ranking. *In* Expert Systems for Environmental Applications, ed. J.M. Hushon. Am. Chem. Soc. Symp. Ser. 431:206-216.

Hushon, J.M. 1990b. Expert systems for environmental problems. Environ. Sci. Technol. 21:838-841.

Hutson, J.L., and A. Cass. 1987. A retentivity function for use in soil-water simulation models. J. Soil Sci. 38:105-113.

Jones, R.L. 1985. Effect of application methods on movement and degradation of aldicarb in Maine potato fields. Environ. Toxicol. Chem. 5:167-173.

Jones, R.L., and T.E. Marquardt. 1987. Monitoring of aldicarb residues in Long Island, New York, potable wells. Arch. Environ. Contam. Toxicol. 16:643-647.

Jones, R.L., G.W. Black, and T.L. Estes. 1986. Comparison of computer model predictions with unsaturated zone field data for aldicarb and aldoxycarb. Environ. Toxicol. Chem. 5:1027-1037.

Jones, R.L., A.G. Hornsby, P.S.C. Rao, and M.P. Anderson. 1987. Movement and degradation of aldicarb residues in the saturated zone under citrus groves on the Florida ridge. J. Contam. Hydrol. 1:265-285.

Jury, W.A. 1986. Adsorption of organic chemicals onto soil. *In* Vadose Zone Modeling of Organic Pollutants, ed. S.C. Hern and S.M. Melancon, 177-189. Chelsea, Mich.: Lewis Publishers.

Jury, W.A., and R.L. Valentine. 1986. Transport mechanisms and loss pathways for chemicals in soil. *In* Vadose Zone Modeling of Organic Pollutants, ed. S.C. Hern and S.M. Melancon, 37-60. Chelsea, Mich.: Lewis Publishers.

Jury, W.A., W.F. Spencer, and W.J. Farmer. 1984. Behavior assessment model for trace organics in soil: III. Application of screening model. J. Environ. Qual. 13(4):573-579.

Jury, W.A., D.D. Focht, and W.J. Farmer. 1987. Evaluation of pesticide groundwater pollution potential from standard indices of soil-chemical adsorption and biodegradation. J. Environ. Qual. 16:422-428.

Kanazawa, J. 1989. Relationship between the soil sorption constants for pesticides and their physiochemical properties. Environ. Toxicol. Chem. 8:477-484.

Karickhoff, S.W., D.S. Brown, and T.A. Scott. 1979. Sorption of hydrophobic pollutants on natural sediments. Water Res. 13:241-248.

Khan, S.U. 1980. Pesticides in the soil environment. New York: Elsevier Scientific Publishing Co. 240 pp.

Laskowski, D.A., C.A.I. Goring, P.J. McCall, and R.L. Swan. 1982. Terrestrial environment. *In* Environmental Risk Analysis for Chemicals, ed. R.A. Conway, 198-240. New York: Van Nostrand Reinhold Co.

Leonard, R.A., W.G. Knisel, and D.A. Still. 1987. GLEAMS: Groundwater loading effects on agricultural management systems. Trans. ASAE 30:1403-1418.

McClymont, G.L., and F.W. Schwartz. 1991a. Embedded knowledge in software: 1. Description of a system for contaminant transport modelling. Ground Water 29:648-654.

McClymont, G.L., and F.W. Schwartz. 1991b. Embedded knowledge in software: 2. Demonstration and preliminary evaluation. Ground Water 29:878-884.

Merck Index. 1989. 11th ed. Merck and Company, Inc.: Rahway, N.J. 2319 pp.

Mutch, J.P., and A.S. Crowe. 1989. An expert system for assessing the migration and transformation of pesticides in the subsurface; Phase 1 Report: A review and analysis of existing pesticide transport and transformation models. NWRI Contrib. #89-172, National Water Research Institute, Burlington, Ont. 36 pp.

Mutch, J.P., and A.S. Crowe. 1990a. An expert system for assessing the migration and transformation of pesticides in the subsurface; Phase 2 Report: Development of the basic expert system. NWRI Contrib. #90-82, National Water Research Institute, Burlington, Ont. 48 pp.

Mutch, J.P., and A.S. Crowe. 1990b. An expert system for assessing the migration and transformation of pesticides in the subsurface; Phase 4 Report: Verification of the pesticide models incorporated into EXPRES. NWRI Contrib. #90-98, National Water Research Institute, Burlington, Ont. 23 pp.

Mutch, J.P., and A.S. Crowe. 1991. An expert system for assessing the fate of pesticides in the subsurface; Phase 5 Report: Description of the agricultural zones included in EXPRES. NWRI Contrib. #92-112, National Water Research Institute, Burlington, Ont. 96 pp.

Newell, C.J., J.F. Haasbeek, and P.B. Bedient. 1990. OASIS: A graphical decision support system for ground-water contamination modeling. Ground Water 28:224-234.

Nofziger, D.L., and A.G. Hornsby. 1986. A microcomputer-based management tool for chemical movement in soil. Applied Agric. Res. 1:50-56.

Padilla, F., P. Lafrance, C. Robert, and J.-P. Villeneuve. 1988. Modeling the transport and the fate of pesticides in the unsaturated zone considering temperature effects. Ecol. Modell. 44:73-88.

Priddle, M.W., R.E. Jackson, K.S. Novakowski, S. Denhoed, B.W. Graham, R.J. Patterson, D. Chaput, and D.E. Jardine. 1987. Migration and fate of aldicarb in the sandstone aquifer of Prince Edward Island. Water Pollut. Res. J. Can. 22:173-185.

Priddle, M.W., R.E. Jackson, A.S. Crowe, and J.P. Mutch. 1988. Aldicarb and nitrogen residues in a sandstone aquifer. *In* Proc. Agricultural Impacts on Ground Water, 191-210. NWWA Conference, March 21-23, 1988, Des Moines, Iowa.

Rao, P.S.C., A.G. Hornsby, and R.E. Jessup. 1985. Indices for ranking the potential for pesticide contamination of groundwater. *In* Proc. Soil Crop Sci. Soc. Florida 44:1 8.

Rawls, W.J., and D.L. Brakensiek. 1983. A procedure to predict Green and Ampt infiltration parameters. *In* Advances in Infiltration. ASAE Publ. No. 11-83, Am. Soc. Agr. Engineers, St. Joseph, Mich.

Rossman, L.A., and T.S. Siller. 1987. Expert systems in environmental engineering. *In* Expert Systems for Civil Engineers: Technology and Applications, ed. M.L. Maher, 113-128. New York: American Society of Civil Engineers.

Sax, N.I., and J.R. Lewis. 1987. Hazardous chemicals desk reference. New York, N.Y.: Van Nostrand Reinhold Co. 1084 pp.

Steenhuis, T.S., S. Pacenka, and K.S. Porter. 1987. MOUSE: A management model for evaluating groundwater contamination from diffuse surface sources aided by computer graphics. Applied Agric. Res. 2:277-289.

Suntio, R.L., W.Y. Shiu, D. MacKay, J.N. Seiber, and D. Glotfelty. 1988. Critical review of Henry's Law constants for pesticides. Rev. Environ. Contam. Toxicol. 103:1-59.

Taylor, A.W., and W.F. Spencer. 1990. Volatilization and vapour transport processes. *In* Pesticides in the Soil Environment: Processes, Impacts, and Modeling, ed. H.H. Cheng. Soil Sci. Soc. Am. Book Ser. #2:213-269.

Tennessee Valley Authority. 1985. A review of field-scale physical solute transport in saturated and unsaturate porous media. Electrical Power Res. Inst. Project 2485-5, EPRI EA-4190:3.28-3.33.

U.S. EPA (Environmental Protection Agency). 1989. Drinking water health advisory: pesticides. Chelsea, Mich.: Lewis Publishers. 819 pp.

Valentine, R.L. 1986. Nonbiological transformation. *In* Vadose Zone Modeling of Organic Pollutants, ed. S.C. Hern and S.M. Melancon, 223-243. Chelsea, Mich.: Lewis Publishers.

Valentine, R.L., and J.L. Schnoor. 1986. Biotransformation. *In* Vadose Zone Modeling of Organic Pollutants, ed. S.C. Hern and S.M. Melancon, 191-222. Chelsea, Mich.: Lewis Publishers.

Verschueren, K. 1983. Handbook of environmental data on organic chemicals, 2nd ed. New York: Van Nostrand Reinhold Company. 1310 pp.

Villeneuve, J.-P., O. Banton, P. Lafrance, C. Blanchette, and S. Deschenes. 1987. VULPEST - Un outil pour l'évaluation de la vulnerabilité des eaux souterraines à la contamination par les pesticides - manuel d'utilisation. Rapport Scientifique INRS-Eau n°234, Sainte-Foy, Que. 88 pp.

Voss, C.I. 1984. SUTRA Saturated-Unsaturated TRAnsport. U.S. Geol. Surv. Water Resour. Investigation Rep. 84-4369, Denver, Colo. 409 pp.

Wagenet, R.J. 1986. Principles of modeling pesticide movement in the unsaturated zone. *In* Evaluation of Pesticides in Ground Water, ed. W.Y. Garner, R.C. Honeycutt, and H.N. Nigg. ACS (Am. Chem. Soc.) Symp. Ser. 315:330-341.

Wagenet, R.J., and J.L. Hutson. 1987. LEACHM: Leaching Estimation And CHemistry Model, vol. 2. Water Resources Institute Continuum, Center for Environmental Research, Cornell University, Ithaca, N.Y. 80 pp.

Walker, A. 1974. A simulation model for prediction of herbicide persistence. J. Environ. Qual. 3(4):396-401.

Wauchope, R.D., T.M. Buttler, A.G. Hornsby, P.W.M. Augustijn-Beckers, and J.P. Burt. 1992. The SCS/ARS/CES pesticide properties database for environmental decision-making. Rev. Environ. Contam. Toxicol. 123:1-155.

Wilkerson, M.R., and K.D. Kim. 1986. The Pesticide Contamination Prevention Act: setting specific numerical values. California Department of Food and Agriculture, Environmental Monitoring and Pest Management, Sacramento, Calif.

Williams, J.R., and H.D. Berndt. 1977. Sediment yield prediction based on watershed hydrology. Trans. ASAE 20:1100-1104.

Worthing, C.R., and R.J. Hance, eds. 1991. The pesticide manual: a world compendium, 9th ed. Farnham, Surrey, U.K.: British Crop Protection Council. 1141 pp.

Worthing, C.R., and S.B. Walker, eds. 1987. The pesticide manual: a world compendium. 8th ed. Farnham, Surrey, U.K.: British Crop Protection Council. 1081 pp.

Zaki, M.H., D. Moran, and D. Harris. 1982. Pesticides in groundwater: the aldicarb story in Suffolk County, N.Y. Am. J. Public Health 72:1391-1395.

# Appendix A

# Pesticides Included in the EXPRES Data Base

## Pesticides Included in the EXPRES Data Base

* Acephate
Acifluorfen
* Alachlor
* Aldicarb
Aldrin
* Ametryn
* Amitrole
* Anilazine
* Atrazine
* Azinphos-methyl
Barban
* Benomyl
* Bensulide
* Bentazon
* Bifenox
* Bromacil
Bromoxynil
* Butylate
* Captan
* Carbaryl
* Carbathiin
Carbendazim
* Carbofuran
* Chloramben
* Chlordane
Chlorfenvinphos
* Chloroneb
* Chloropicrin
* Chlorothalonil
* Chloroxuron
* Chlorpropham
* Chlorpyrifos
* Chlorsulfuron
* Chlorthal
* Clopyralid
* Cyanazine
* Cypermethrin
* 1,2-D
* 1,3-D
* 2,4-D
2,4-DB
Dalapon
Dazomet
* DBCP
* DDT
Deltamethrin
Demetron
Dialifor
* Diazinon
* Dicamba
* Dichlobenil
Dichloran
* Dichlorprop
* Diclofop-methyl
* Dicofol
* Dieldrin
* Difenzoquat-methylsulfate
* Dimethoate
* Dinoseb
* Diphenamid
Diquat
* Disulfoton
* Diuron
DNOC
* EDB
* Endosulfan
Endothall
* Endrin
* EPTC
* Ethalfluralin
* Ethion
* Ethofumesate
* Ethoprop
Ethylene-thiourea
* Fenamiphos
Fenitrothion
Fenoprop
* Fenoxaprop-ethyl
Fensulfothion
* Fenthion
* Fenvalerate
* Ferbam
Flamprop-methyl
* Fluazifop-butyl
* Fluometuron
* Fonofos
* Fosamine-ammonium
Glyphosate
* Heptachlor
* Hexazinone
* Imazamethabenz-methyl
* Iprodione
* Lindane
* Linuron
* Malathion
Maleic hydrazide
Mancozeb
Maneb
* MCPA
MCPB
* Mecoprop
* Metalaxyl
* Metam
* Methamidophos
* Methidathion
* Methomyl
Methoprene
Methoxychlor
Methyl bromide
* Methyl-isothiocyanate
* Methyl parathion
* Metiram
Metobromuron
* Metolachlor
* Metribuzin
* Metsulfuron-methyl
* Mevinphos
Monolinuron
* Monuron
* Naled
* Napropamide
Naptalam
Nitrapyrin
Nitrofen
* Oxamyl
* Oxydemeton-methyl
* Oxyfluorfen
Paraquat
* Parathion

* Pebulate
* Pendimethalin
* Permethrin
* Phorate
  Phosalone
* Phosmet
* Picloram
  Pirimicarb
  Profluralin
* Prometone
* Prometryn
* Pronamide
* Propachlor
* Propanil
* Propazine
  Propham
  Propiconazole
* Propoxur
* Pyrazon
  Quintozene
  Ronnel
* Sethoxydim
* Siduron
* Simazine
* 2,4,5-T
  TCA
* Tebuthiuron
* Terbacil
* Terbufos
* Terbutryn
* Thiabendazole
* Thiophanate-methyl
* Thiram
* Toxaphene
* Triadimefon
* Triallate
* Trichlorfon
* Triclopyr
* Trifluralin
* Vernolate
  Zineb
  Ziram

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* Pesticides accessible by the LP/LI screening model.

# Appendix B

# EXPRES Screens

Table B-1. List of Screen Titles for the EXPRES Expert System

| Screen Number | Used by LP/LI, PRZM, LEACHM, ALL | Screen Title |
|---|---|---|
| 1 | - | TITLE |
| 2 | - | DISCLAIMER |
| 3 | ALL | SESSION INFORMATION |
| 4 | ALL | ASSESSMENT OBJECTIVES |
| 5 | - | PESTICIDE DATA |
| 6 | - | AGRICULTURAL REGION DATA |
| 7 | LP/LI | SCREENING ASSESSMENT |
| 8 | LP/LI | SCREENING ASSESSMENT OUTPUT |
| 9 | PRZM, LEACHM | GENERAL INFORMATION |
| 10 | PRZM, LEACHM | SIMULATION REGION |
| 11 | PRZM, LEACHM | EXISTING PESTICIDES |
| 12 | PRZM, LEACHM | PESTICIDE PARAMETERS |
| 13 | PRZM, LEACHM | DEGRADATION RATES |
| 14 | LEACHM | TRANSFORMATION RATES |
| 15 | LEACHM | DIFFUSION/DISPERSION |
| 16 | PRZM, LEACHM | SOIL PARAMETERS |
| 17 | PRZM, LEACHM | SOIL PARAMETERS cont. |
| 18 | PRZM, LEACHM | EROSION PARAMETERS |
| 19 | PRZM, LEACHM | INITIAL PESTICIDE CONC. |
| 20 | PRZM | DRAINAGE PARAMETERS |
| 21 | LEACHM | PROFILE CONDITIONS |
| 22 | PRZM, LEACHM | CROP PARAMETERS |
| 23 | PRZM, LEACHM | SURFACE RUNOFF/EROSION |
| 24 | PRZM, LEACHM | CROPPING PERIODS |
| 25 | LEACHM | CROP PARAMETERS cont. |
| 26 | PRZM, LEACHM | METEOROLOGICAL STATION SELECTION |
| 27 | PRZM, LEACHM | METEOROLOGICAL PARAMETERS |
| 28 | PRZM, LEACHM | IRRIGATION PARAMETERS |
| 29 | PRZM, LEACHM | PESTICIDE APPLICATION INFO. |
| 30 | PRZM | APPLICATION METHODS |
| 31 | LEACHM | APPLICATION METHODS |
| 32 | PRZM, LEACHM | GENERAL OUTPUT |
| 33 | PRZM | CONCENTRATION PROFILES |
| 34 | PRZM | TIME SERIES PLOTS |
| 35 | LEACHM | TIME SERIES PLOTS |
| 36 | LEACHM | CONCENTRATION PROFILES |
| 37 | LEACHM | UNCERTAINTY ANALYSIS |
| 38 | PRZM, LEACHM | DATA ANALYSIS |

Screen: 1

EXPRES

EXPERT SYSTEM FOR PESTICIDE REGULATORY EVALUATIONS AND SIMULATIONS

Version 2.1

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NEXT

Screen: 2

DISCLAIMER

This computer system (computer program and related files) was developed to aid in pesticide regulatory decisions, and is intended only for use by the authors and the employees of the Commercial Chemicals Branch of Environment Canada, and by those individuals authorized by the developers. Anyone else using this expert system does so at their own risks, in reliance solely upon his or her inspection of the contents of the system and without reliance upon any representation concerning the contents of the system or its application. The authors make no expressed or implied warranty of any kind with regard to the contents of the system or its ability to operate on any (or all) computers. Furthermore, the authors shall not be held liable for incidental or consequential damages in connection with, or arising from, the furnishing, use, misuse, or performance of the contents of this expert system.

NEXT

Screen: 3

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

SESSION INFORMATION

INTRODUCTION
[•] Instructions
[ ] Overview of EXPRES
[ ] Screen Setup

FILES
[ ] Load Example File
[ ] Load Existing File

Screen: 4

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

ASSESSMENT OBJECTIVES

[•] Data Display
[ ] Screening Assess.
[ ] Simulation

Specific Objectives
[ ] Run a Scenario
[ ] Uncertainty Analysis

Need Results
[ ] Quickly
[ ] No Preference

Daughter Products
[ ] Simulated
[ ] Not Simulated

Computer
[ ] 80286
[ ] 80386/80486

Approximate Simulation Length (days):

Screen: 5

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

**PESTICIDE DATA**

PESTICIDE

- Acephate
- Acifluoren
- Alachlor
- Aldicarb
- Aldrin
- Ametryn
- Amitrole
- Anilazine
- Atrazine
- Azinphos-methyl
- Barban
- Benomyl
- Bensulide
- Bentazon
- Bifenox
- Bromacil

<MORE ↓>

Search For . . .

Sort By . . .

Screen: 5a

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

Pesticide : Alachlor
CAS num.: 15972-60-8
Family : Amide
Type : Herbicide
Application Mode: Soil spray, soil granular application, soil incorporated

Synonym(s)

Lasso

Recommended Values

| | |
|---|---|
| Molecular Weight (g): | 270 |
| logKoc (L/kg): | 2.23 |
| logH: | -5.89 |
| logKow: | 2.78 |
| Solubility (mg/L): | 2.4E+02 |
| Vapour Pressure (mPa): | 2.9E+00 |
| Specific Gravity: | 1.133 |
| Half-life (days): | 15 |

Return to Screen

View Additional Values

Screen: 5b

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

**PESTICIDE DATA**

Pesticide: Alachlor

Temp: * a b c d e f g h i j k m n o p q r s t u v
v w x y z A B C D E F G H I J K L M N O P Q R

Calculated at 25°C

Ref: 1 2 3 4 5 6 7 8 9 10 11 12
13 14 15 16 17 18 19 20 21 22 23 24

| m.w. g/mol | logKoc L/kg | logH | logKow | S mg/L | Vp mPa | Vd mg/L | s.g. | $t_{1/2}$ days | Ref |
|---|---|---|---|---|---|---|---|---|---|
| | | -5.89 | | 2.4E+02g | 2.9E+00g | 3.2E-04g | | | 1 |
| 2.70 | 2.28 | | 2.92 | 2.4E+02 | 2.9E+00 | | | 7 | 2 |
| | | | | 1.5E+02g | 2.7E+03u | | | | 4 |
| | | | 2.78 | 2.2E+02C | | | | 18 | 5 |
| | 2.21 | | | 2.0E+02 | | | | 14 | 6 |
| | | | | 2.4E+02g | 2.9E+00g | | 1.133g | | 7 |
| | 2.08 | | | | | | | 18 | 9 |
| | 2.28 | -5.89 | | 2.4E+02 | 2.9E+00 | | | 7 | 10 |
| | 2.23 | | | 2.4E+02 | 1.9E+00 | | | 15 | 11 |

<MORE ↓>

Screen: 5c

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

**PESTICIDE DATA**

Pesticide: Alachlor

Temp: * a b c d e f g h i j k m n o p q r s t u v
v w x y z A B C D E F G H I J K L M N O P Q R

Ref: 1 2 3 4 5 6 7 8 9 10 11 12
13 14 15 16 17 18 19 20 21 22 23 24

Verschueren (1983)

| m.w. g/mol | logKoc L/kg | logH | logKow | S mg/L | Vp mPa | Vd mg/L | s.g. | $t_{1/2}$ days | Ref |
|---|---|---|---|---|---|---|---|---|---|
| | | -5.89 | | 2.4E+02g | 2.9E+00g | 3.2E-04g | | | 1 |
| 2.70 | 2.28 | | 2.92 | 2.4E+02 | 2.9E+00 | | | 7 | 2 |
| | | | | 1.5E+02g | 2.7E+03u | | | | 4 |
| | | | 2.78 | 2.2E+02C | | | | 18 | 5 |
| | 2.21 | | | 2.0E+02 | | | | 14 | 6 |
| | | | | 2.4E+02g | 2.9E+00g | | 1.133g | | 7 |
| | 2.08 | | | | | | | 18 | 9 |
| | 2.28 | -5.89 | | 2.4E+02 | 2.9E+00 | | | 7 | 10 |
| | 2.23 | | | 2.4E+02 | 1.9E+00 | | | 15 | 11 |

<MORE ↓>

Screen: 5d

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

PESTICIDE DATA

[•] Synonym
[ ] Name
[ ] CAS Number

KNOX-OUT

SEARCH
CANCEL

Search For . . .
Sort By . . .

Diazinon

Screen: 5e

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

PESTICIDE DATA

[•] Synonym
[ ] Name
[ ] CAS Number

WEEDAR

SEARCH
CANCEL

Search For . . .
Sort By . . .

2,4-D
MCPA
2,4,5-T

Screen: 5f

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

PESTICIDE DATA

SORT:
[ ] All Pesticides
[•] Selected Pesticides

BY:
[ ] logKoc
[ ] logH
[ ] logKow
[•] Solubility
[ ] Vapour Pressure
[ ] Specific Gravity
[ ] Half-Life

| Rank | Pesticides | Solubility (mg/L) |
|---|---|---|
| 1 | Dimethoate | 2.50E+004 |
| 2 | Dicamba | 4.50E+003 |
| 3 | 1,2-D | 2.70E+003 |
| 4 | 2,4-D | 8.90E+003 |
| 5 | Alachor | 2.40E+002 |
| 6 | Malathion | 1.50E+002 |
| 7 | Carbaryl | 1.20E+002 |
| 8 | Atrazine | 3.30E+001 |

h For . . .
y . . .

Screen: 5g

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

PESTICIDE DATA

SORT:
[ ] All Pestic
[•] Selected

[•] 1,2-D
[ ] 1,3-D
[ ] 2,4,5-T
[•] 2,4-D
[ ] Acephate
[•] Alachlor
[ ] Aldicarb
[ ] Ametryn
[ ] Amitrole
[ ] Anilazine
[•] Atrazine
[•] Azinphos-methyl
[ ] Benomyl
[ ] Bensulide
[ ] Bentazon

<MORE ↓>

essure
ravity

n For . . .
y . . .

| Rank | | lubility mg/L) |
|---|---|---|
| 1 | Dim | E+004 |
| 2 | Dica | E+003 |
| 3 | 1,2- | E+003 |
| 4 | 2,4- | E+003 |
| 5 | Alac | E+002 |
| 6 | Mal | E+002 |
| 7 | Car | E+002 |
| 8 | Atra | E+001 |

Screen: 6

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

**AGRICULTURAL REGION DATA**

**AGRICULTURAL REGION**

- Apple orchard in the Okanagan Valley of central B.C.
- Raspberry field in the lower Fraser River Valley, B.C.
- Barley field in the Peace River District of Alberta
- Barley field in central Alberta (i.e. Edmonton)
- Rangeland in southwestern Alberta (i.e. Calgary)
- Sugar beet field in southern Alberta (i.e. Lethbridge)
- Wheat field in southern Saskatchewan (i.e. Regina)
- Barley Field in central Saskatchewan (i.e. Saskatoon)
- Sugar beet field in southern Manitoba (i.e. Winnipeg)
- Flax field in southern Manitoba (i.e. Morden)
- Corn field in southwestern Ontario (i.e. Harrow)

<MORE ↓>

Screen: 6a

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

**AGRICULTURAL REGION DATA**

**AGRICULTURAL REGION**

rd in the Okanagan Valley of B.C.

**SOIL PARAMETERS**

Barley field in the Peace River District of Alberta

5.0 : Depth to the water table (m)

| Horz | Thk | B.D. | %OC | %Si | %Cl | Ks | F.C. | W.P. | AEV |
|---|---|---|---|---|---|---|---|---|---|
| 1 S | 10 | 1.20 | 1.50 | 67 | 15 | 7.00E+02 | .320 | .140 | -3.94E+00 |
| 2 R | 10 | 1.30 | 1.00 | 66 | 17 | 5.00E+02 | .300 | .140 | -3.97E+00 |
| 3 R | 40 | 1.45 | 0.50 | 59 | 34 | 7.00E+01 | .370 | .210 | -4.89E+00 |
| 4 R | 30 | 1.45 | 0.30 | 60 | 32 | 5.00E+01 | .360 | .200 | -4.89E+00 |
| 5 B | 410 | 1.50 | 0.10 | 58 | 37 | 5.00E+01 | .370 | .220 | -4.89E+00 |

| K | P | LS |
|---|---|---|
| 0.42 | 0.75 | 1.30 |

Field Capacity

More <Pg↓>

Screen: 6b

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

**AGRICULTURAL REGION DATA**

**CROP PARAMETERS**

Barley field in the Peace River District of Alberta

| Crop | I.C. | R.D. | C.C.F. | P.U. | P.D. | Curve No. | USLEC |
|---|---|---|---|---|---|---|---|
| 1 canola | 0.15 | 100 | 95.0 | 0.00 | 150 | 86 / 73 / 80 | 1.0 / 0.3 / 0.7 |
| 2 barley | 0.10 | 100 | 90.0 | 0.00 | 150 | 86 / 73 / 80 | 1.0 / 0.3 / 0.7 |
| 3 wheat | 0.10 | 100 | 90.0 | 0.00 | 180 | 86 / 73 / 80 | 1.0 / 0.3 / 0.7 |

| Crop Sequence | Planting | Emergence | Root-mat. | Plant-mat. | Harvest |
|---|---|---|---|---|---|
| 1 canola | 10/05/YR1 | 15/05/YR1 | 03/08/YR1 | 13/08/YR1 | 14/08/YR1 |
| 2 barley | 15/05/YR2 | 22/05/YR2 | 10/07/YR2 | 25/08/YR2 | 26/08/YR2 |
| 3 wheat | 07/05/YR3 | 15/05/YR3 | 15/07/YR3 | 25/08/YR3 | 26/08/YR3 |
| 4 fallow | 10/05/YR4 | 10/05/YR4 | 10/05/YR4 | 10/05/YR4 | 10/05/YR4 |

Maximum Interception Storage (cm)

More <Pg↕>

Screen: 6c

F1:Next-Scrn F2:Previous-Scrn F5:Exit F6:Notes F7:Help F8:Instructions

EXPRES

**METEOROLOGICAL PARAMETERS**

Barley field in the Peace River District of Alberta

**Beaverlodge-CDA (Meteorological Station)**

- 10.0 : Minimum depth of evaporation (cm)
- 0.70 : Pan evaporation coefficient
- 0.34 : Snowmelt coefficient (cm/°C-day)
- 0.20 : Erosive storm duration (hrs)
- N : Irrigation applied

**Annual Summary (1970 - 1989)**

| | Evap.* (mm) | Precip. (mm) | Temp. (°C) |
|---|---|---|---|
| Mean | 277.0 | 453.8 | 2.2 |
| Std. Dev. | 42.7 | 85.5 | 1.2 |
| Max. (Year) | 373.3 ('89) | 587.4 ('82) | 24.3 # |
| Min. (Year) | 196.4 ('70) | 300.2 ('70) | -37.5 # |

**Mean Monthly Values**

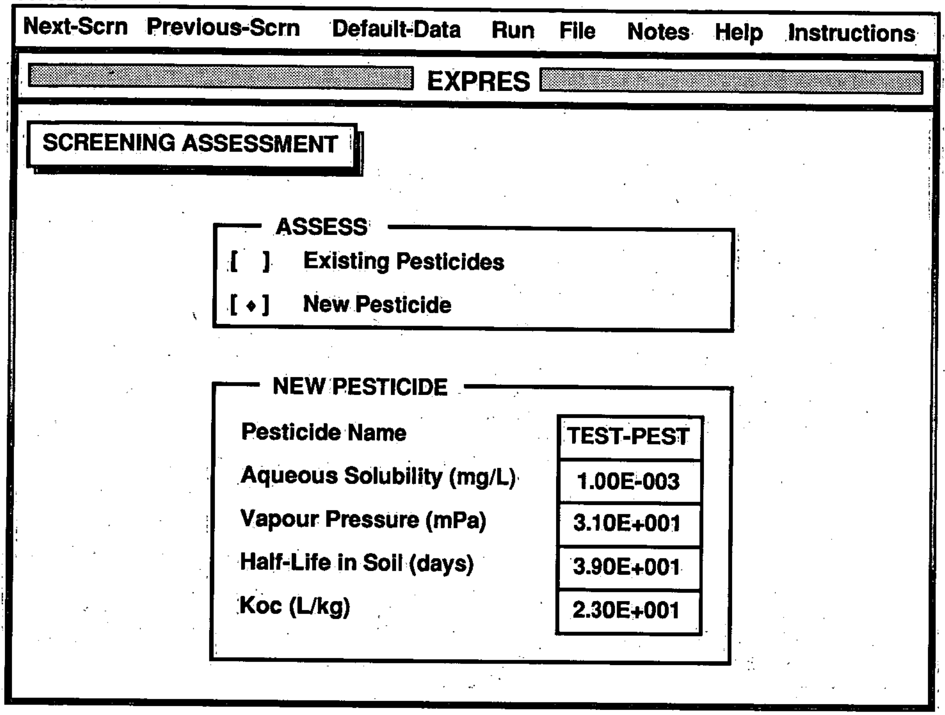
| | Evap.* (mm) | Prec. (mm) | Temp. (°C) |
|---|---|---|---|
| Jan | 5.4 | 31.0 | -12.5 |
| Feb | 8.8 | 21.4 | -10.0 |
| Mar | 12.8 | 21.8 | -4.5 |
| Apr | 22.4 | 16.4 | 3.6 |
| May | 32.4 | 37.4 | 9.7 |
| Jun | 45.9 | 66.8 | 13.4 |
| Jul | 51.8 | 69.6 | 15.3 |
| Aug | 39.8 | 64.0 | 14.3 |
| Sep | 32.9 | 50.2 | 9.5 |
| Oct | 13.6 | 24.0 | 4.5 |
| Nov | 6.2 | 21.3 | -5.8 |
| Dec | 5.0 | 29.9 | -11.3 |

* - Predicted by PRZM from Class A Pan Data # - Extreme Daily Values

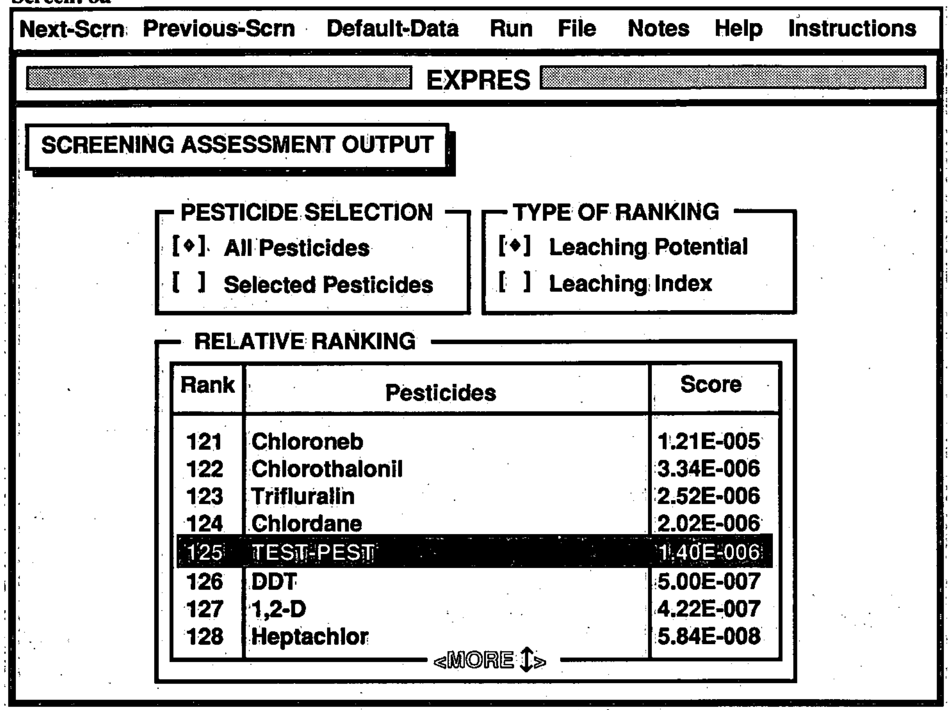
Avg. Total Monthly Precipitation (mm)

More <Pg↕>

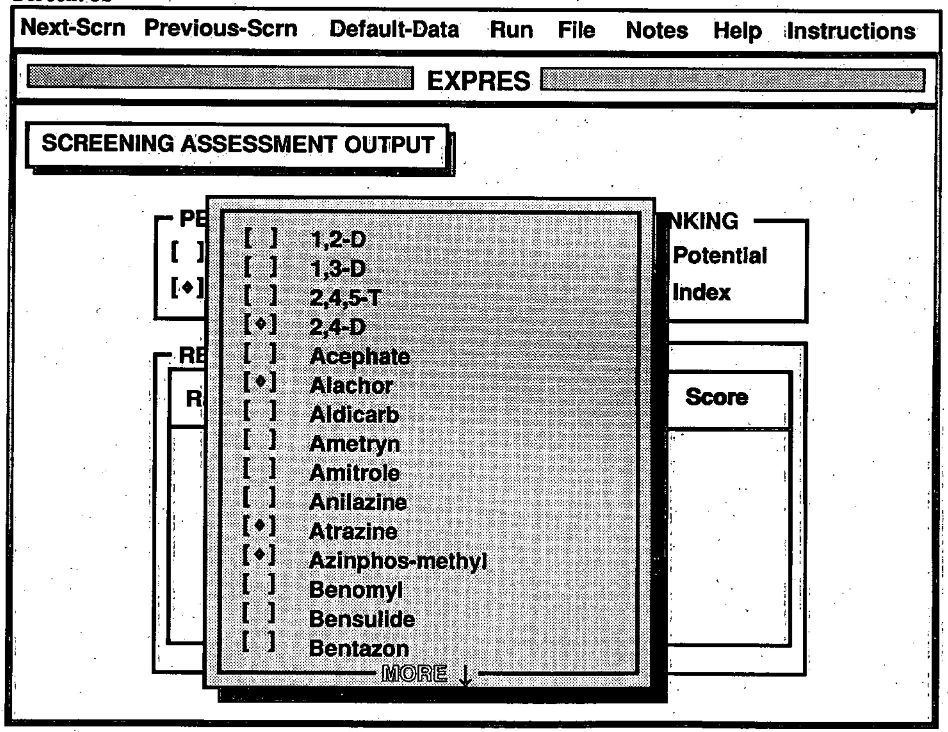
Screen: 7



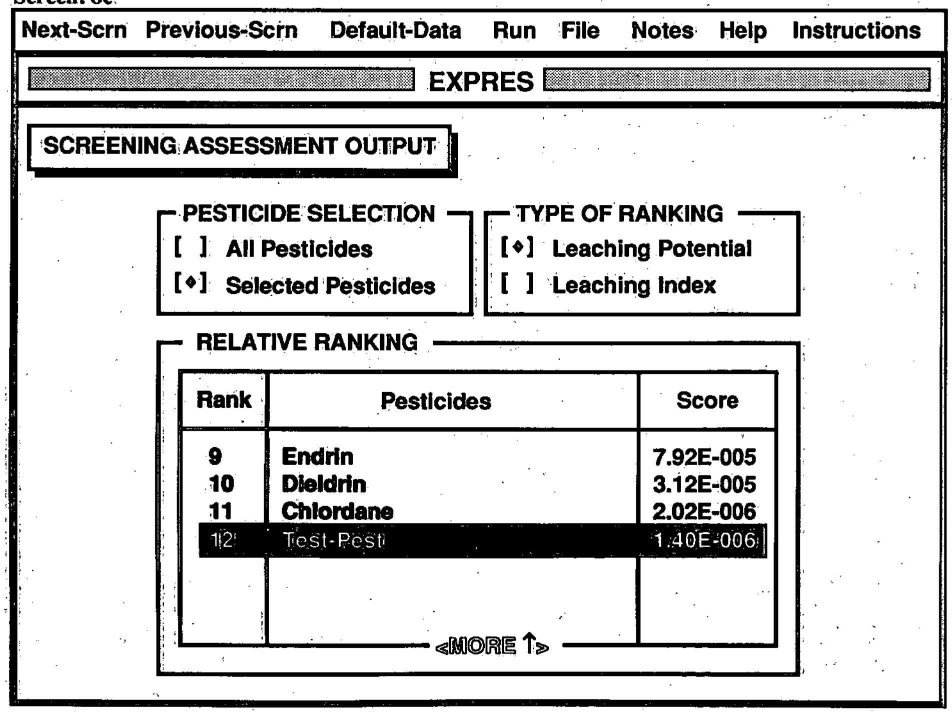

Screen: 8a




Screen: 8b




Screen: 8c



Screen: 9a

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

GENERAL INFORMATION

SIMULATION DATES (ddmmyy)

Starting 010183

Ending 311284

PARAMETER BRANCHES

Load Default Parameters

[ ] Agricultural Regions
[•] Existing Pesticides

View/Modify Default Parameters

[ ] Pesticide Parameters
[ ] Soil Parameters
[ ] Crop Parameters
[ ] Meteorological Parameters

User Supplied Parameters

[ ] Pesticide Application Parameters
[ ] Output Parameters

Screen: 9b

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

GENERAL INFORMATION

SIMULATION DATES (ddmmyy)

Starting 010183

Ending 311284

PARAMETER BRANCHES

Load Default Parameters

[ ] Agricultural Regions
[•] Existing Pesticides

View/Modify Default Parameters

[ ] Pesticide Parameters
[ ] Soil Parameters
[ ] Crop Parameters
[ ] Meteorological Parameters

User Supplied Parameters

[ ] Pesticide Application Parameters
[ ] Output Parameters
[ ] Uncertainty Analysis Parameters

Screen: 10

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

SIMULATION REGION

AGRICULTURAL REGIONS

[ ] Apple orchard in the Okanagan Valley of central B.C.
[ ] Raspberry field in the lower Fraser River Valley, B.C.
[ ] Barley field in the Peace River District of Alberta
[ ] Barley field in central Alberta (i.e. Edmonton)
[ ] Rangeland in southwestern Alberta (i.e. Calgary)
[ ] Sugar beet field in southern Alberta (i.e. Lethbridge)
[•] Wheat field in southern Saskatchewan (i.e. Regina)
[ ] Barley field in central Saskatchewan (i.e. Saskatoon)
[ ] Sugar beet field in southern Manitoba (i.e. Winnipeg)
[ ] Flax field in southern Manitoba (i.e. Morden)
[ ] Corn field in southwestern Ontario (i.e. Harrow)

MORE ↓

Screen: 11

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

EXISTING PESTICIDES

PESTICIDES

[ ] 1,2-D
[ ] 1,3-D
[ ] 2,4,5-T
[ ] 2,4-D
[ ] Acephate
[ ] Alachlor
[ ] Aldicarb
[ ] Ametryn
[ ] Amitrole
[ ] Anilazine
[•] Atrazine
[ ] Azinphos-methyl
[ ] Benomyl
[ ] Bensulide
[ ] Bentazon

MORE ↓

Screen: 12

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

PESTICIDE PARAMETERS

PESTICIDE SPECIES

Number of Pesticides and Transformation Products to Simulate (Maximum of 4): 4

| Pesticide Number | Pesticide Name | Solubility (mg/L) | Koc (L/kg) | Parent / Daughter |
|---|---|---|---|---|
| 1 | ALDICARB | 6.00E+003 | 5.00E+000 | P |
| 2 | SULFOXIDE | 2.80E+004 | 1.00E+000 | D |
| 3 | SULFONE | 7.80E+003 | 2.00E+000 | D |
| 4 | TRACER | 1.00E+003 | 0.00E+000 | P |

Screen: 13

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

DEGRADATION RATES

| Horizon Number | Degradation Rates (1/day) for: | | | |
|---|---|---|---|---|
| | ALDICARB | SULFOXIDE | SULFONE | TRACER |
| 1 | 4.81E-002 | 3.74E-003 | 9.62E-003 | 0.00E+000 |
| 2 | 4.81E-002 | 3.74E-003 | 9.62E-003 | 0.00E+000 |
| 3 | 4.81E-002 | 3.74E-003 | 9.62E-003 | 0.00E+000 |
| 4 | 9.62E-003 | 7.50E-004 | 1.92E-003 | 0.00E+000 |
| 5 | 9.62E-003 | 7.50E-004 | 1.92E-003 | 0.00E+000 |

<MORE ↓>

Screen: 14

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

TRANSFORMATION RATES

| Horizon Number | Transformation Rates (1/day) for: | | | |
|---|---|---|---|---|
| | ALDICARB | SULFOXIDE | SULFONE | TRACER |
| 1 | 9.08E-002 | 1.13E-002 | 0.00E+000 | 0.00E+000 |
| 2 | 9.08E-002 | 1.13E-002 | 0.00E+000 | 0.00E+000 |
| 3 | 9.08E-002 | 1.13E-002 | 0.00E+000 | 0.00E+000 |
| 4 | 1.82E-002 | 2.25E-003 | 0.00E+000 | 0.00E+000 |
| 5 | 1.82E-002 | 2.25E-003 | 0.00E+000 | 0.00E+000 |

<MORE ↓>

Screen: 15

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

DIFFUSION/DISPERSION

Molecular Diffusion Coefficient (Aqueous Solution) ($mm^2$/day): 1.20E+002

DIFA: 1.00E-003 DIFB: 1.00E+001

Dispersivity (mm): 1.00E+002

Diffusion Coefficient in Air ($mm^2$/day): 4.30E+005

Barometric Enhancement ($mm^2$/day): 0.00E+000

| Pesticide Name | Vapour Density (mg/L) |
|---|---|
| ALDICARB | 3.60E-005 |
| SULFOXIDE | 3.60E-005 |
| SULFONE | 3.60E-005 |
| TRACER | 0.00E+000 |

Screen: 16

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

SOIL PARAMETERS

Number of Soil Horizons: 6 Depth to Water Table (m): 4.50E+000

| Horizon Number | Horizon Thickness (cm) | Surface / Root / Below Root | Bulk Density ($g/cm^3$) | Percent Organic Carbon |
|---|---|---|---|---|
| 1 | 10.0 | S | 1.32 | 0.70 |
| 2 | 20.0 | R | 1.23 | 1.40 |
| 3 | 40.0 | R | 1.62 | 0.50 |
| 4 | 60.0 | B | 1.67 | 0.10 |
| 5 | 120.0 | B | 1.83 | 0.01 |

<MORE ↓>

Screen: 17

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

SOIL PARAMETERS cont.

( Y ) Erosional Losses ( Y ) Pesticide Residues

| Horizon Number | Field Capacity | Wilting Point | Percent Silt | Percent Clay | Initial Soil-Water Content |
|---|---|---|---|---|---|
| 1 | 0.340 | 0.030 | 37.000 | 5.000 | 0.300 |
| 2 | 0.390 | 0.140 | 38.000 | 9.000 | 0.260 |
| 3 | 0.360 | 0.120 | 37.000 | 9.000 | 0.260 |
| 4 | 0.360 | 0.120 | 37.000 | 11.000 | 0.240 |
| 5 | 0.280 | 0.190 | 34.000 | 13.000 | 0.230 |

<MORE ↓>

Screen: 18

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

EROSION PARAMETERS

SOIL LOSS EQN.

| | |
|---|---|
| USLEK | 0.25 |
| USLEP | 0.50 |
| USLELS | 1.20 |

PARTICLE BULK DENSITY

| | |
|---|---|
| Organic ($g/cm^3$) | 1.10 |
| Clay ($g/cm^3$) | 2.65 |
| Sand ($g/cm^3$) | 2.65 |

Erosive Storm Duration (hrs): 2.30

Area of the Field (ha): 20.00

Screen: 19

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

INITIAL PESTICIDE CONCENTRATIONS

| Soil Depth (cm) | Pesticide Concentrations (mg/kg) | | | |
|---|---|---|---|---|
| | ALDICARB | SULFOXIDE | SULFONE | TRACER |
| 0 - 10 | 0.00E+000 | 0.00E+000 | 0.00E+000 | 0.00E+000 |
| 10 - 20 | 0.00E+000 | 0.00E+000 | 0.00E+000 | 0.00E+000 |
| 20 - 30 | 0.00E+000 | 0.00E+000 | 0.00E+000 | 0.00E+000 |
| 30 - 40 | 0.00E+000 | 0.00E+000 | 0.00E+000 | 0.00E+000 |
| 40 - 50 | 0.00E+000 | 0.00E+000 | 0.00E+000 | 0.00E+000 |

<MORE ↓>

Screen: 20

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

DRAINAGE PARAMETERS

SOIL HYDRAULICS
[◆] Free Draining
[ ] Restricted Draining

DRAINAGE PARAMETERS

| Horizon Number | Drainage Parameter |
|---|---|
| 1 | 0.00 |
| 2 | 0.00 |
| 3 | 0.00 |
| 4 | 0.00 |
| 5 | 0.00 |

<MORE ↓>

Screen: 21

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

PROFILE CONDITIONS

TOTAL PROFILE DEPTH
If Different From Depth to Water Table Entered Earlier (m): 5.00E+000

BOTTOM BOUNDARY CONDITIONS
[ ] Constant Potential
[◆] Free Draining
[ ] Zero Flux
[ ] Lysimeter Tank

| Horizon Number | AEV (kPa) | BCAM | Ks (mm/day) | Root Fraction |
|---|---|---|---|---|
| 1 | -5.92E-001 | 3.87E+000 | 7.79E+002 | 0.250 |
| 2 | -1.03E+000 | 4.56E+000 | 2.78E+003 | 0.300 |
| 3 | -6.46E-001 | 4.51E+000 | 1.70E+002 | 0.300 |
| 4 | -5.16E-001 | 5.42E+000 | 9.70E+001 | 0.150 |

<MORE ↓>

Screen: 22a

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

CROP PARAMETERS

Number of Different Crops: 3

| Crop Number | Crop Name | Maximum Intercept. Storage (cm) | Maximum Root Depth (cm) | Crop Cover Fraction | Pesticide Uptake Factor | Maximum Dry Foliage ($kg/m^2$) |
|---|---|---|---|---|---|---|
| 1 | HAY | 0.10 | 30.00 | 0.60 | 0.00 | 0.78 |
| 2 | POTATO | 0.10 | 45.00 | 0.80 | 0.00 | 0.90 |
| 3 | BARLEY | 0.10 | 30.00 | 0.60 | 0.00 | 0.56 |
| | | | | | | |
| | | | | | | |

Screen: 22b

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

CROP PARAMETERS

Number of Different Crops: 3

| Crop Number | Crop Name | Maximum Intercept. Storage (cm) | Maximum Root Depth (cm) | Crop Cover Fraction | Pesticide Uptake Factor | Plant Density (plants per $m^2$) |
|---|---|---|---|---|---|---|
| 1 | HAY | 0.10 | 30.00 | 0.60 | 0.00 | 10.00 |
| 2 | POTATO | 0.10 | 45.00 | 0.80 | 0.00 | 2.00 |
| 3 | BARLEY | 0.10 | 30.00 | 0.60 | 0.00 | 10.00 |
| | | | | | | |
| | | | | | | |

Screen: 23

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

SURFACE RUNOFF/EROSION

Initial Crop Number: 1

INIT. CONDITION
[•] Fallow
[ ] Cropping
[ ] Residue

| Crop Name | Curve No. (CN) Cover Management Factor (USLEC) | | | | | | Cond. After Harvest (F/C/R) |
|---|---|---|---|---|---|---|---|
| | Fallow | | Cropping | | Residue | | |
| | CN | USLEC | CN | USLEC | CN | USLEC | |
| HAY | 86 | 0.45 | 69 | 0.45 | 77 | 0.45 | R |
| POTATO | 86 | 0.50 | 75 | 0.50 | 80 | 0.50 | R |
| BARLEY | 86 | 0.45 | 73 | 0.45 | 79 | 0.45 | R |

Screen: 24

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

CROPPING PERIODS

Number of Cropping Periods: 5

| Crop Period | Crop Number | Crop Year (yy) | Planting Date (ddmm) | Emergence Date (ddmm) | Maturity Date (ddmm) | | Harvest Date (ddmm) |
|---|---|---|---|---|---|---|---|
| | | | | | Roots | Plants | |
| 1 | 1 | 83 | 0105 | 1006 | 0109 | 2509 | 1010 |
| 2 | 2 | 84 | 2005 | 1506 | 1508 | 1009 | 3009 |
| 3 | 3 | 85 | 1005 | 3005 | 2009 | 3009 | 0710 |
| 4 | 1 | 86 | 0105 | 1006 | 0109 | 2509 | 1010 |
| 5 | 2 | 87 | 2005 | 3005 | 1508 | 1009 | 3009 |

Screen: 25

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

CROP PARAMETERS cont.

PLANT ROOTS
[ ] Growing
[•] Constant
Root Length (m): 5.00E+002

PLANT TRANSPIRATION

| | |
|---|---|
| Min. Root Water Potential (kPa) | -3.00E+003 |
| Max Root Water Potential (kPa) | 0.00E+000 |
| Root Flow Resistance Factor | 1.05E+000 |
| Max. Actual Transpiration | 1.10E+000 |

Screen: 26

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

METEOROLOGICAL STATIONS

STATIONS

| | Name | Prov. | Lat. | Long. | Available Data (ddmmyy) |
|---|---|---|---|---|---|
| [ ] | Vancouver UBC | BC | 49° 15' | 123° 15' | 010179 - 311289 |
| [•] | Summerland CDA | BC | 49° 34' | 119° 39' | 010179 - 311289 |
| [ ] | Beaverlodge CDA | ALTA | 55° 12' | 119° 24' | 010179 - 311289 |
| [ ] | Calgary Int'l Airport | ALTA | 51° 06' | 119° 24' | 010179 - 311289 |
| [ ] | Lacombe CDA | ALTA | 52° 28' | 113° 45' | 010179 - 311289 |
| [ ] | Lethbridge CDA | ALTA | 49° 42' | 112° 47' | 010179 - 311289 |
| [ ] | Saskatoon SRC | SASK | 52° 09' | 106° 36' | 010179 - 311289 |
| [ ] | Regina Airport | SASK | 50° 26' | 104° 40' | 010179 - 311289 |
| [ ] | Glenlea - Univ. of Manitoba | MAN | 49° 39' | 97° 07' | 010179 - 311289 |
| [ ] | Morden CDA | MAN | 49° 11' | 98° 05' | 010179 - 311289 |
| [ ] | Delhi CDA | ONT | 42° 52' | 80° 33' | 010179 - 311289 |

MORE ↓

Screen: 27

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

METEOROLOGICAL PARAMETERS

METEOROLOGICAL RECORD
[◆] Actual Daily Values
[ ] Mean and Median Values

Min. Depth of Evap. (cm) 10.00

Pan Evap. Coefficient 0.700

Snowmelt Coefficient (cm/°C-day) 0.300

Screen: 28

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

IRRIGATION PARAMETERS

| Crop Name | Number of Irrigation Applications | Total Amount of Water Applied (cm) |
|---|---|---|
| HAY | 0 | 0.00E+000 |
| POTATO | 0 | 0.00E+000 |
| BARLEY | 0 | 0.00E+000 |
| | | |
| | | |

Screen: 29a

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

PEST. APPLICATION INFO.

Number of Pesticide Applications: 4

Only applications for pesticide # 4 (TRACER) will occur.
Only one application per day is allowed.

| Application Number | Pesticide Number | Application Date (ddmmyy) | Application Rate (kg a.i./ha) | Depth of Incorp. (cm) |
|---|---|---|---|---|
| 1 | 1 | 010583 | 2.00 | 10.00 |
| 2 | 4 | 010583 | 10.00 | 10.00 |
| 3 | 4 | 010584 | 10.00 | 10.00 |
| 4 | 4 | 010585 | 10.00 | 10.00 |
| | | | | |

Screen: 29b

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

PEST. APPLICATION INFO.

Number of Pesticide Applications: 4

| Application Number | Pesticide Number | Application Date (ddmmyy) | Application Rate (kg a.i./ha) | Depth of Incorp. (cm) |
|---|---|---|---|---|
| 1 | 1 | 010583 | 2.00 | 10.00 |
| 2 | 4 | 010583 | 10.00 | 10.00 |
| 3 | 4 | 010584 | 10.00 | 10.00 |
| 4 | 4 | 010585 | 10.00 | 10.00 |
| | | | | |

Screen: 30

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

APPLICATION METHODS

PESTICIDE APPLICATION METHOD

[♦] Application to Soil Only
[ ] Foliar Application (Linear)
[ ] Foliar Application (Exponential)

FOLIAR APPLICATION

Pest. Decay Rate on Foliage (1/day) [ ]

Foliar Extraction Coeff. (1/day) [ ]

Filtration Parameter [ ]

Screen: 31

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

APPLICATION METHODS

| Application Number | Pesticide Name | Application Method (Soil/Foliar) | Washoff Factor |
|---|---|---|---|
| 1 | ALDICARB | S | 1.00 |
| 2 | TRACER | F | 0.95 |
| 3 | TRACER | F | 0.95 |
| 4 | TRACER | F | 0.95 |
| | | | |

Screen: 32

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

GENERAL OUTPUT

Q1 - At what time does the concentration of the pesticide first reach or exceed the specified dissolved concentration at the specified depth?

Specified depths:
(Y) include water table
(Y) other depths (cm)

Specified concentration:
(Y) 1st non-zero
(N) maximum
(Y) other (mg/L)

| Depth | Conc. |
|---|---|
| 50 | 5.00E-03 |
| 100 | 1.00E-02 |
| 200 | 1.00E-01 |

Q2 - What is the maximum depth of leaching of the pesticide at the following dissolved concentration at the specified time?

Specified concentration:
(N) 1st non-zero
(Y) maximum
(Y) other (mg/L)

Specified time:
(Y) time (mmyy)

| Conc. | Time |
|---|---|
| 1.00E-01 | 0587 |
| 5.00E-01 | 1187 |
| | 0588 |

Screen: 33

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

CONCENTRATION PROFILES

| Summary Files | Generate Files (Yes/No) | Output Time Step (Day/Month/Year) | Compartment Print Frequency |
|---|---|---|---|
| Hydrological | Y | M | 5 |
| Pesticide | Y | M | 1 |
| Conc. Profile | Y | M | 1 |

Screen: 34

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

TIME SERIES PLOTS

| Plot Type | Cum Y/N | Observation Depth (cm) |
|---|---|---|
| [•] Amount of total precipitation. | N | None |
| [•] Amount of water stored in a soil compartment. | N | 50 |
| [•] Amount of water infiltrating into a soil compartment. | Y | 50 |
| [•] Mass of dissolved pesticide stored in a soil compartment. | N | 20 |
| [•] Mass of pesticide movement due to the bulk flow of water. | N | 100 |
| [•] Mass of pesticide movement due to the bulk flow of water. | N | 200 |
| [ ] | | |

Screen: 34a

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

TIME SERIES PLOTS

| Plot Type | Cum Y/N | Observation Depth (cm) |
|---|---|---|
| [•] Amount of tota | N | None |
| [•] Amount of wat | N | 50 |
| [•] Amount of wat | Y | 50 |
| [•] Mass of dissol ... ent. | N | 20 |
| [•] Mass of pesticide movement due to the bulk flow of water. | N | 100 |
| [•] Mass of pesticide movement due to the bulk flow of water. | N | 200 |
| [ ] | | |

Return to Screen
Delete Plot Type
Water Storage
Water Flux
Pesticide Storage/Concentration
Pesticide Flux (Compartmental)
Pesticide Flux (Total Profile)
Sediment Flux

Screen: 34b

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

TIME SERIES PLOTS

| Plot Type | Cum Y/N | Observation Depth (cm) |
|---|---|---|
| [• | | e |
| [• | | 0 |
| [• | | 0 |
| [• | | 0 |
| [•] | N | 100 |
| [•] Mass of pesticide movement due to the bulk flow of water. | N | 200 |
| [ ] | | |

Interception - Amount of precipitation intercepted by the plant canopy before reaching the soil surface (cm).
Water Storage - Amount of water stored in a soil compartment (reported as depth of water in cm).
Snowpack - Depth of snow accumulated on the soil surface (cm).
Water Content - Water content of a soil compartment (reported as a volume fraction, i.e. cm3/cm3).

Screen: 35

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

TIME SERIES PLOTS

UNITS
[•] μg/kg
[ ] mg/m²

Print Frequency (days): 5

Observation Depths for Time Series File (cm)

| Depth 1 | Depth 2 | Depth 3 |
|---|---|---|
| 100 | 150 | 200 |

VARIABLES OF INTEREST (choose any or all)
(Y) Pesticide Contents
(Y) Pesticide Flux Past a Specific Depth
(Y) Water Flux / Cumulative Water Flux / Water Content
(Y) Cumulative Rain / Transpiration / Evaporation

Screen: 36

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

**CONCENTRATION PROFILES**

PRINT PLANT/ROOT TABLE

(N) Include Plant Growth and Uptake Data

PRINT OPTIONS

[♦] Constant Interval/Print

Print Interval (days): 30.00

[ ] Print on Specific Days

Total No. of Prints:

Compartment Print Frequency: 5

IF PRINT ON SPECIFIC DAYS

| Print Number | Specific Dates (ddmmyy) |
|---|---|
| | |
| | |
| | |
| | |
| | |

Screen: 37

Next-Scrn Previous-Scrn Default-Data Run File Notes Help Instructions

EXPRES

**UNCERTAINTY ANALYSIS**

[♦] SOLUBILITY
[ ] Koc
[ ] APPLICATION RATE
[ ] APPLICATION DEPTH
[ ] DEPTH OF INCORPORATION
[ ] DEGRADATION RATES
[ ] TRANSFORMATION RATES
[ ] MOLECULAR DIFFUSION
[ ] VAPOUR DENSITY
[ ] DIFFUSION COEFFICIENT IN AIR
[ ] DISPERSIVITY
[ ] CN - CURVE NUMBER
[ ] AEV - AIR ENTRY VALUE
[ ] BCAM - CAMPBELL'S B VALUE
[ ] Ks - SAT. HYDRAULIC CONDUCT.
[ ] STARTING THETA
[ ] FIELD CAPACITY
[ ] WILTING POINT

<MORE ↓>

Modify SOLUBILITY:
SOLUBILITY = SOLUBILITY * n
(i.e. n = 0.1, 0.2, 1.0, 5.0, 10.0)

where n = 1.0

NOTE: - The value will be modified upon the running of the model.
- EXPRES will only run one (1) simulation at a time.

Screen: 38a

File Name: EXAMPLE F5:EXIT F6:NOTES F7:HELP F9:OPTIONS

EXPRES

**DATA ANALYSIS**

CONTAMINATION INFORMATION

GENERAL OUTPUT →

CONCENTRATION PROFILES

TOTAL →
ADSORBED →
DISSOLVED →

TIME SERIES PLOTS

SOIL WATER CONTENT @ 10 cm →
RUNOFF →
DISSOLVED PESTICIDE STORAGE @ 500 cm →
DISSOLVED PESTICIDE STORAGE @ 100 cm →
PESTICIDE RUNOFF FLUX →
DISSOLVED PESTICIDE CONCENTRATION @ 100 cm →
DISSOLVED PESTICIDE CONCENTRATION @ 500 cm →

PLOT TITLE

Screen: 38b

File Name: EXAMPLE F5:EXIT F6:NOTES F7:HELP F9:OPTIONS

EXPRES

**DATA ANALYSIS**

CONTAMINATION INFORMATION

GENERAL OUTPUT →

CONCENTRATION PROFILES

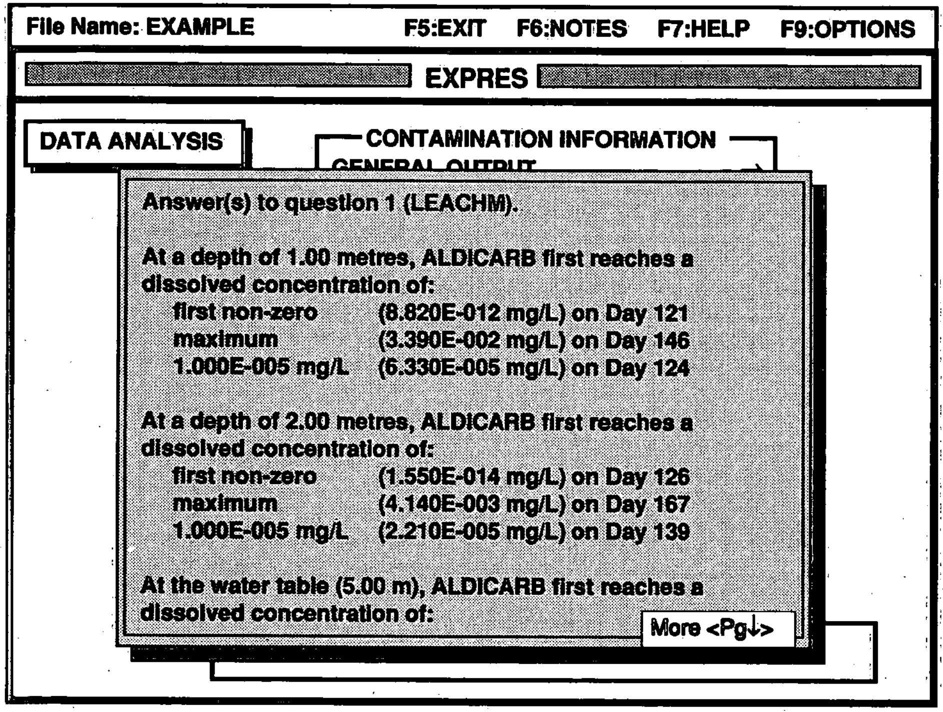
TOTAL →
DISSOLVED →
VAPOUR →

TIME SERIES PLOTS

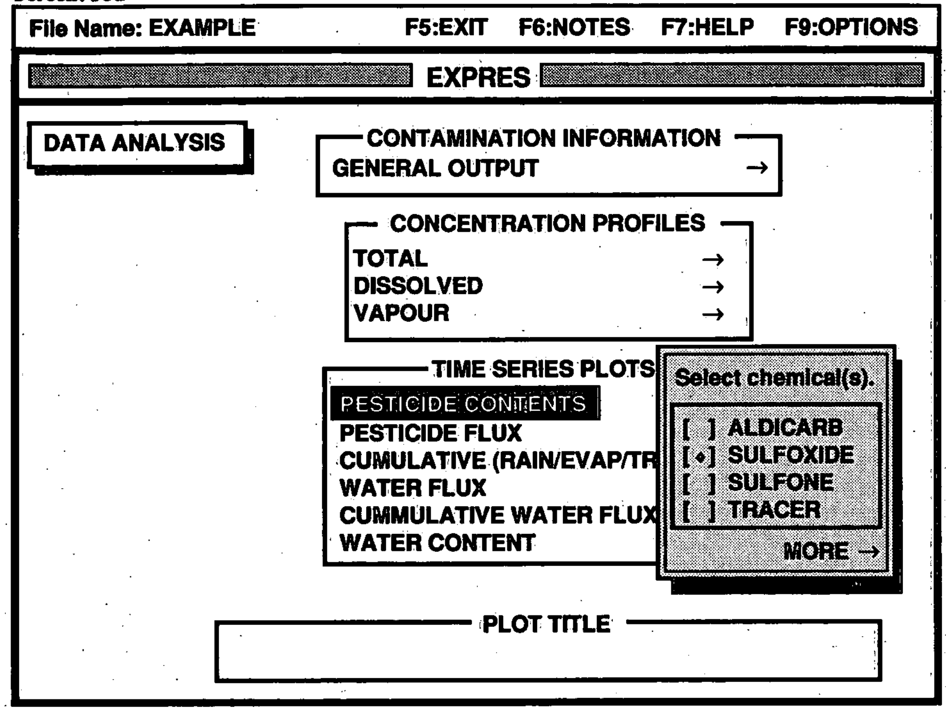
PESTICIDE CONTENTS →
PESTICIDE FLUX →
CUMULATIVE (RAIN/EVAP/TRANS) →
WATER FLUX →
CUMMULATIVE WATER FLUX →
WATER CONTENT →

PLOT TITLE

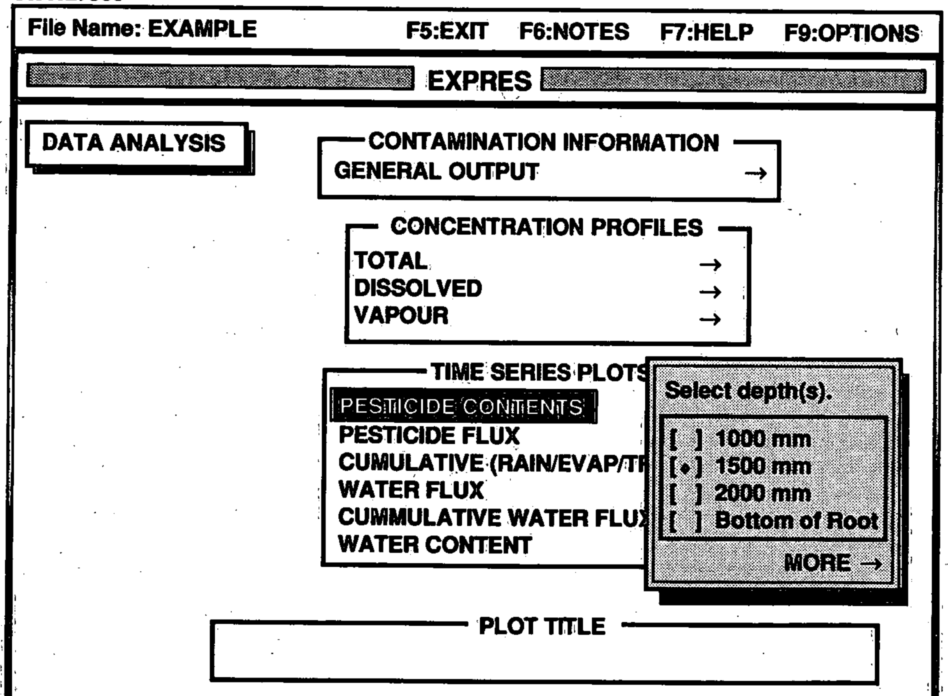
Screen: 38c



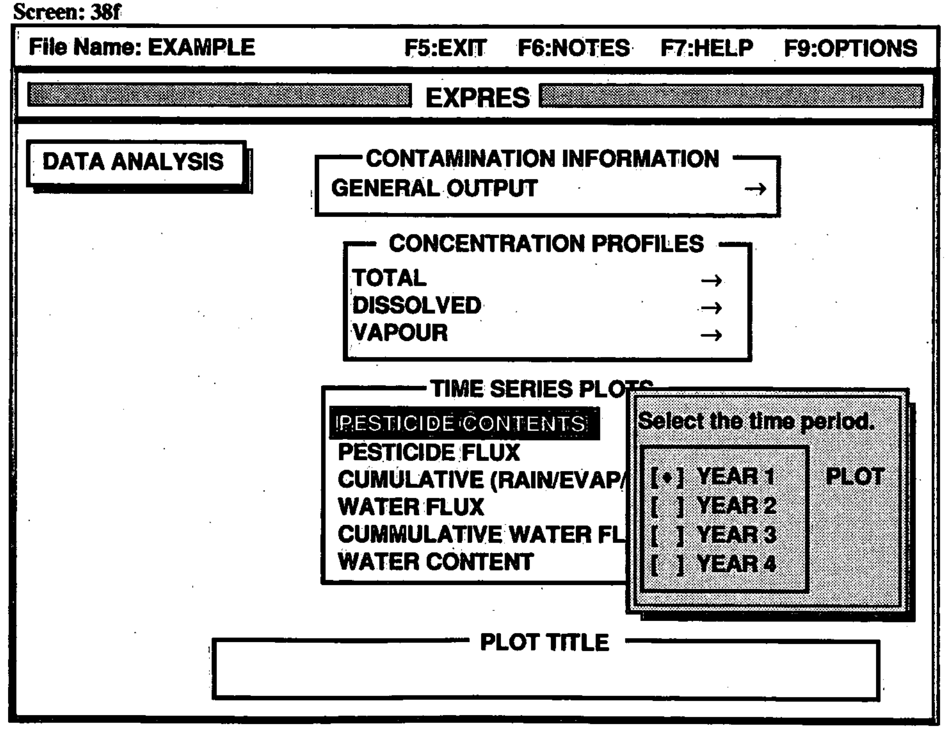

Screen: 38d




Screen: 38e




Screen: 38f



# Appendix C

## Figures Referred to in the EXPRES Help Facility

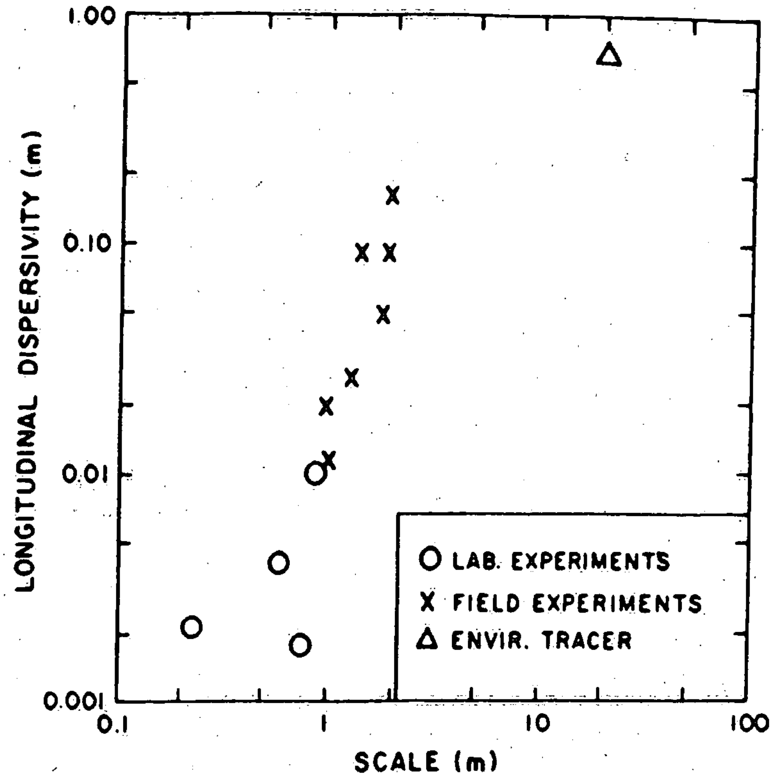



Figure C-1. Longitudinal dispersivity versus scale of observation for the unsaturated zone. (After Tennessee Valley Authority 1985)

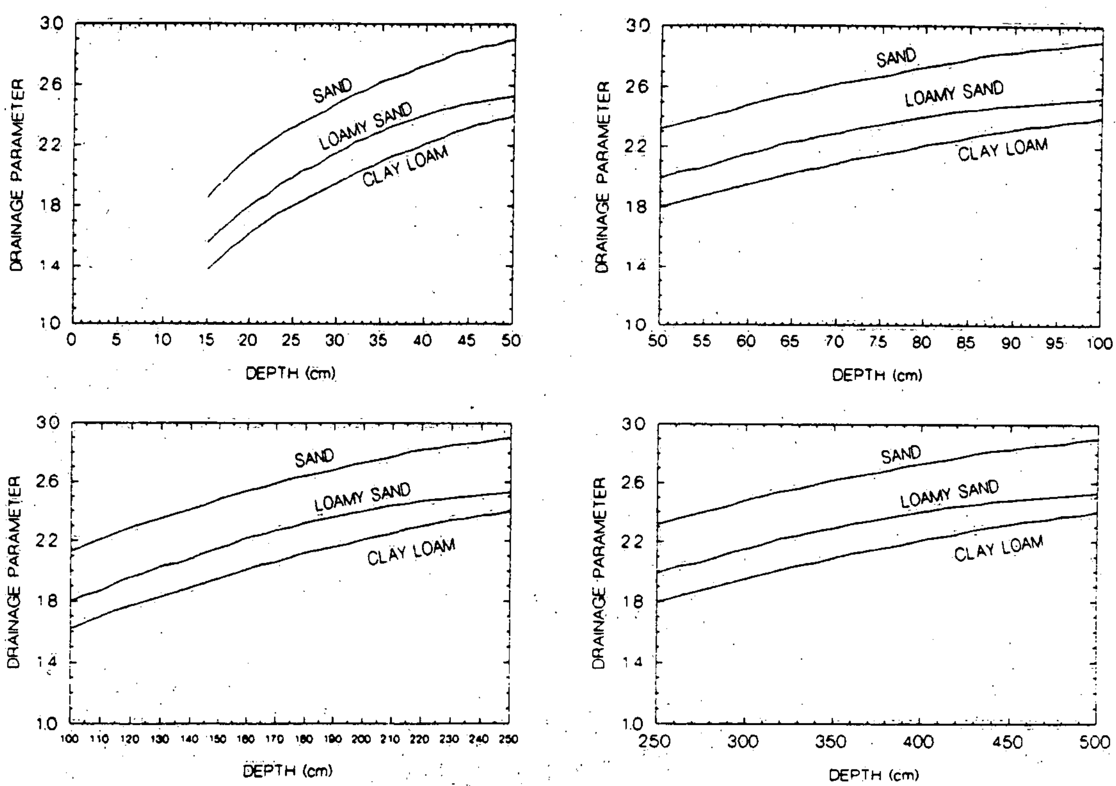



Figure C-2. Estimation of the restricted drainage parameter versus the depth of the soil profile.

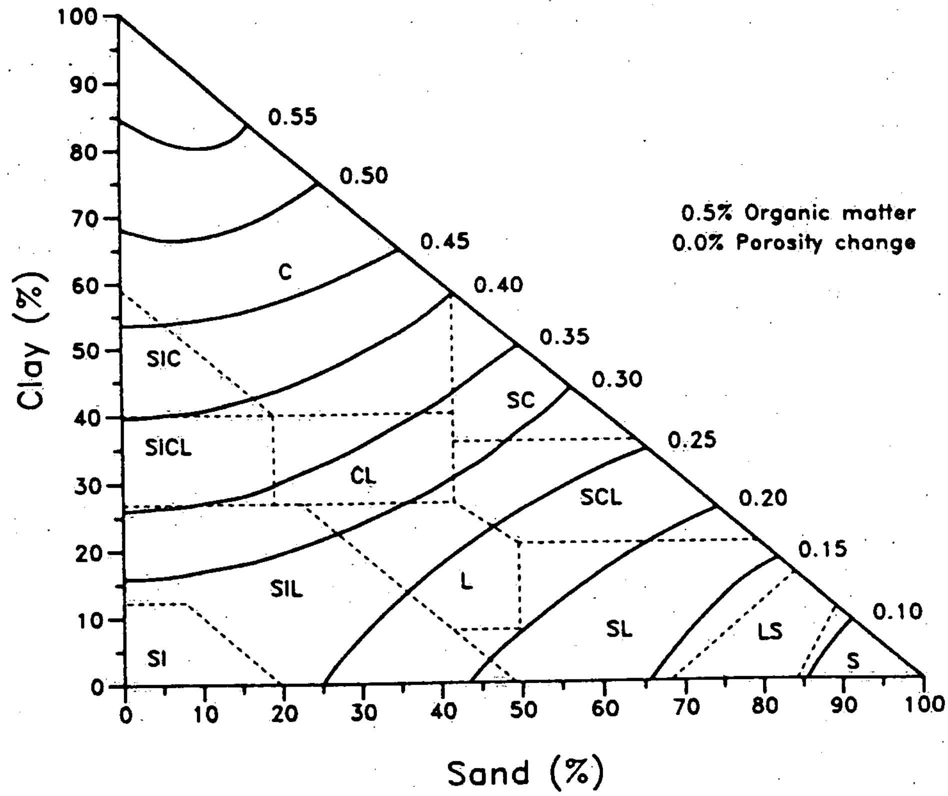



Figure C-3. 1/3-bar (i.e., field capacity) soil moisture by volume. (After Carsel et al. 1984)

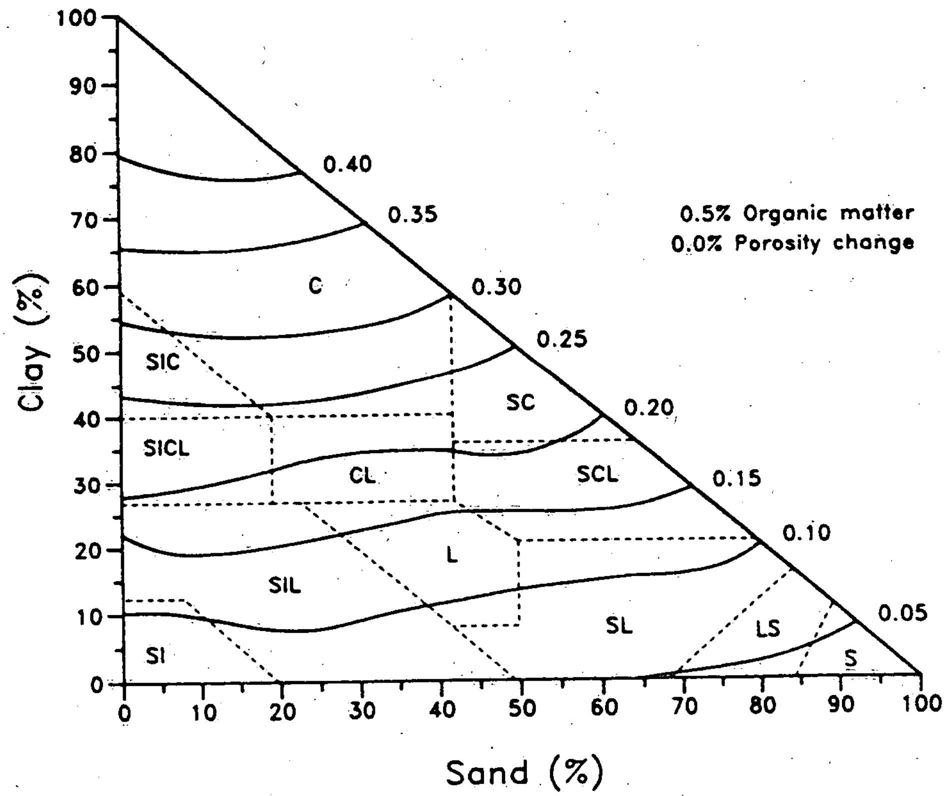



Figure C-4. 15-bar soil moisture (i.e., wilting point) by volume. (After Carsel et al. 1984)

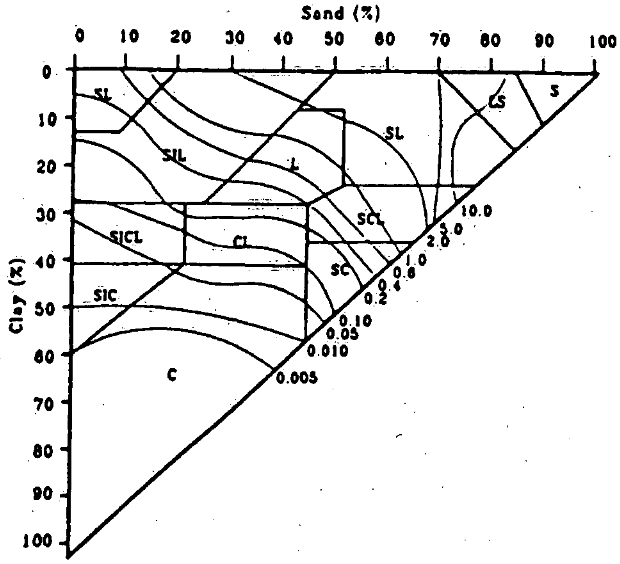



Figure C-5. Nomograph for the saturated hydraulic conductivity (cm/h). (After Rawls and Brakensiek 1983)

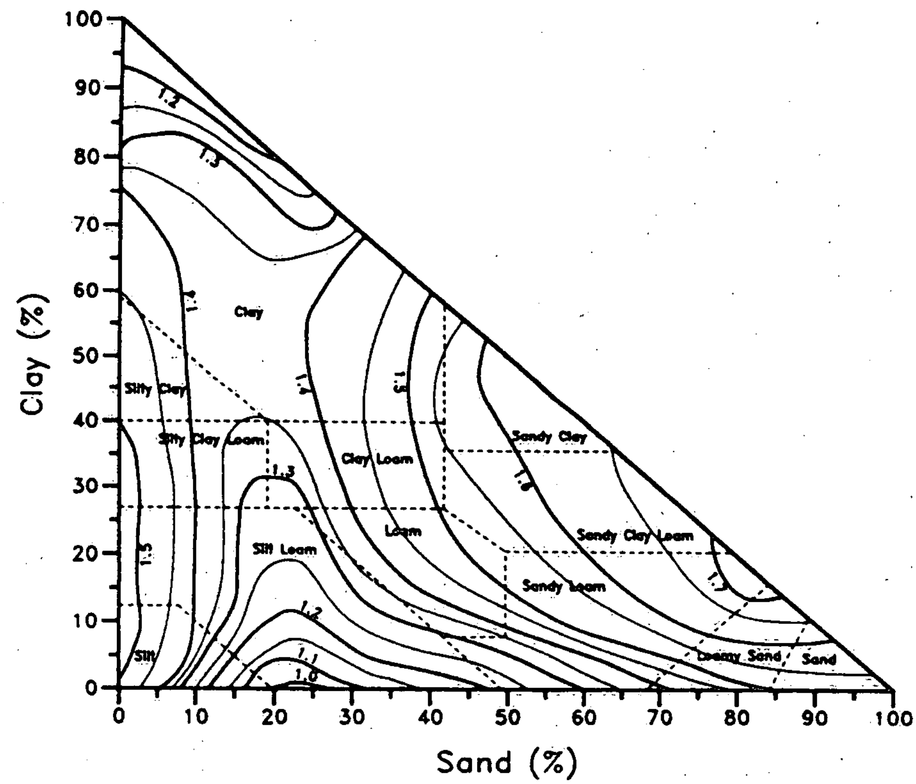



Figure C-6. Mineral bulk density (g/cm³). (After Carsel et al. 1984)

# Appendix D

# List of Files in the EXPRES Expert System

## PATH TO C:\EXPRES\

| | | | | |
|---|---|---|---|---|
| ANALYSIS.EXE | DATADISP.EXE | DB-REGNS.EXE | ERRORS.EXE | EXPRES.EXE |
| FILTER.EXE | LEACHP.EXE | NOTES.EXE | PRZM.EXE | USI.EXE |

## PATH TO C:\EXPRES\INI\

| | | | |
|---|---|---|---|
| EXPRES.DAT | EXPRES.INI | EX-DAT.OLD | OUTPUT.OPT |

## PATH TO C:\EXPRES\DATABASE\

| | | | | | |
|---|---|---|---|---|---|
| BERRY-BC.INF | BERRY-BC.DAT | VANC-UBC.EXE | APPLE-BC.INF | APPLE-BC.DAT | SUMM-CDA.EXE |
| BARLY-AL.INF | BARLY-AL.DAT | BEAV-CDA.EXE | B-EDM-AL.INF | B-EDM-AL.DAT | LAC-CDA.EXE |
| RANGE-AL.INF | RANGE-AL.DAT | CALG-IA.EXE | SUGRB-AL.INF | SUGRB-AL.DAT | LETHBRDG.EXE |
| BARLY-SK.INF | BARLY-SK.DAT | SASK-SRC.EXE | WHEAT-SK.INF | WHEAT-SK.DAT | REGINA-A.EXE |
| FLAX-MAN.INF | FLAX-MAN.DAT | MORD-CDA.EXE | SUGRB-MN.INF | SUGRB-MN.DAT | GLEN-UOM.EXE |
| CORN-ONT.INF | CORN-ONT.DAT | HARR-CDA.EXE | TOBAC-ON.INF | TOBAC-ON.DAT | DELHICDA.EXE |
| GRAPE-ON.INF | GRAPE-ON.DAT | HAMILTON.EXE | DAIRY-ON.INF | DAIRY-ON.DAT | KEMPTV.EXE |
| ORCH-QUE.INF | ORCH-QUE.DAT | ORMSTOWN.EXE | DAIRY-QU.INF | DAIRY-QU.DAT | LASS-CDA.EXE |
| CORN-QUE.INF | CORN-QUE.DAT | ST-HY2.EXE | POTAT-NB.INF | POTAT-NB.DAT | FRED-CDA.EXE |
| FORST-NB.INF | FORST-NB.DAT | CHATHA-A.EXE | POTAT.PE.INF | POTAT-PE.DAT | CHARLOTT.EXE |
| APPLE-NS.INF | APPLE-NS.DAT | KENT-CDA.EXE | POTAT.NF.INF | POTAT-NF.DAT | STJW-CDA.EXE |
| PEST.TXT | PEST.SEL | PEST.SRT | PEST.ASS | MET-STAT.TXT | AG-REGNS.TXT |

## PATH TO C:\EXPRES\EXAMPLE\

| | | | | | |
|---|---|---|---|---|---|
| EXAMPLE.CNC | EXAMPLE.DAT | EXAMPLE.ECL | EXAMPLE.ECP | EXAMPLE.GEN | EXAMPLE.HYD |
| EXAMPLE.HYD | EXAMPLE.LID | EXAMPLE.LI | EXAMPLE.LP | EXAMPLE.NTS | EXAMPLE.OUT |
| EXAMPLE.PCN | EXAMPLE.PES | EXAMPLE.PLT | EXAMPLE.RET | EXAMPLE.TSP | EXAMPLE.WFX |

## PATH TO C:\EXPRES\HELP\

| | | | | | |
|---|---|---|---|---|---|
| AEV.DEF | AEV.EXP | AEV.USR | AG-ZONE1.DEF | AG-ZONE1.EXP | AG-ZONE1.USR |
| AG-ZONE2.DEF | AG-ZONE2.EXP | AG-ZONE2.USR | AGZN-DAT.DEF | AGZN-DAT.EXP | AGZN-DAT.USR |
| AIR-DIFF.DEF | AIR-DIFF.EXP | AIR-DIFF.USR | APP-DATE.DEF | APP-DATE.EXP | APP-DATE.USR |
| APP-METH.DEF | APP-METH.EXP | APP-METH.USR | APP-RATE.DEF | APP-RATE.EXP | APP-RATE.USR |
| APPLE-BC.DEF | APPLE-BC.EXP | APPLE-BC.USR | APPLE-NS.DEF | APPLE-NS.EXP | APPLE-NS.USR |
| APPRXSIM.DEF | APPRXSIM.EXP | APPRXSIM.USR | AREA.DEF | AREA.EXP | AREA.USR |
| B-EDM-AL.DEF | B-EDM-AL.EXP | B-EDM-AL.USR | BAR-EN.DEF | BAR-EN.EXP | BAR-EN.USR |
| BARLY-AL.DEF | BARLY-AL.EXP | BARLY-AL.USR | BARLY-SK.DEF | BARLY-SK.EXP | BARLY-SK.USR |
| BBC.DEF | BBC.EXP | BBC.USR | BCAM.DEF | BCAM.EXP | BCAM.USR |
| BD-CLAY.DEF | BD-CLAY.EXP | BD-CLAY.USR | BD-OM.DEF | BD-OM.EXP | BD-OM.USR |
| BD-SAND.DEF | BD-SAND.EXP | BD-SAND.USR | BERRY-BC.DEF | BERRY-BC.EXP | BERRY-BC.USR |
| BULK-D.DEF | BULK-D.EXP | BULK-D.USR | CHIP-286.DEF | CHIP-286.EXP | CHIP-286.USR |
| CHIP-386.DEF | CHIP-386.EXP | CHIP-386.USR | CLIMATE.DEF | CLIMATE.EXP | CLIMATE.USR |
| COMP-FRQ.DEF | COMP-FRQ.EXP | COMP-FRQ.USR | COND-HAR.DEF | COND-HAR.EXP | COND-HAR.USR |
| CORN-ONT.DEF | CORN-ONT.EXP | CORN-ONT.USR | CORN-QUE.DEF | CORN-QUE.EXP | CORN-QUE.USR |
| CROP-NUM.DEF | CROP-NUM.EXP | CROP-NUM.USR | CROP-PAR.DEF | CROP-PAR.EXP | CROP-PAR.USR |
| CROP-PER.DEF | CROP-PER.EXP | CROP-PER.USR | CROP-YR.DEF | CROP-YR.EXP | CROP-YR.USR |
| CROPDATE.DEF | CROPDATE.EXP | CROPDATE.USR | CRP-FRAC.DEF | CRP-FRAC.EXP | CRP-FRAC.USR |
| CRP-NAME.DEF | CRP-NAME.EXP | CRP-NAME.USR | CURV-NUM.DEF | CURV-NUM.EXP | CURV-NUM.USR |
| DAIRYONT.DEF | DAIRYONT.EXP | DAIRYONT.USR | DAIRYQUE.DEF | DAIRYQUE.EXP | DAIRYQUE.USR |
| DATA-DIS.DEF | DATA-DIS.EXP | DATA-DIS.USR | DATES.DEF | DATES.EXP | DATES.USR |
| DEG-RATE.DEF | DEG-RATE.EXP | DEG-RATE.USR | DEPTH-IN.DEF | DEPTH-IN.EXP | DEPTH-IN.USR |
| DIFAB.DEF | DIFAB.EXP | DIFAB.USR | DISPER.DEF | DISPER.EXP | DISPER.USR |
| DRAIN-P.DEF | DRAIN-P.EXP | DRAIN-P.USR | DRY-FOL.DEF | DRY-FOL.EXP | DRY-FOL.USR |
| EMERGE.DEF | EMERGE.EXP | EMERGE.USR | ERO-LOSS.DEF | ERO-LOSS.EXP | ERO-LOSS.USR |
| EX-SESSN.DEF | EX-SESSN.EXP | EX-SESSN.USR | EXIST-P.DEF | EXIST-P.EXP | EXIST-P.USR |
| EXP-APP.DEF | EXP-APP.EXP | EXP-APP.USR | FIELD-C.DEF | FIELD-C.EXP | FIELD-C.USR |
| FIL-PARM.DEF | FIL-PARM.EXP | FIL-PARM.USR | FLAX-MAN.DEF | FLAX-MAN.EXP | FLAX-MAN.USR |
| FOL-DK.DEF | FOL-DK.EXP | FOL-DK.USR | FOL-EXTR.DEF | FOL-EXTR.EXP | FOL-EXTR.USR |
| FORST-NB.DEF | FORST-NB.EXP | FORST-NB.USR | GEN-FILE.DEF | GEN-FILE.EXP | GEN-FILE.USR |
| GEN-OUT1.DEF | GEN-OUT1.EXP | GEN-OUT1.USR | GEN-OUT2.DEF | GEN-OUT2.EXP | GEN-OUT2.USR |
| GRAPE-ON.DEF | GRAPE-ON.EXP | GRAPE-ON.USR | H-THICK.DEF | H-THICK.EXP | H-THICK.USR |
| HAF-LIFE.DEF | HAF-LIFE.EXP | HAF-LIFE.USR | HARVEST.DEF | HARVEST.EXP | HARVEST.USR |
| INSTR.DEF | INSTR.EXP | INSTR.USR | INT-CONC.DEF | INT-CONC.EXP | INT-CONC.USR |
| INT-COND.DEF | INT-COND.EXP | INT-COND.USR | INT-CROP.DEF | INT-CROP.EXP | INT-CROP.USR |

| | | | | | |
|---|---|---|---|---|---|
| INT-PRNT.DEF | INT-PRNT.EXP | INT-PRNT.USR | K-SAT.DEF | K-SAT.EXP | K-SAT.USR |
| KOC.DEF | KOC.EXP | KOC.USR | LIN-APP.DEF | LIN-APP.EXP | LIN-APP.USR |
| MAX-INT.DEF | MAX-INT.EXP | MAX-INT.USR | MAX-RDEP.DEF | MAX-RDEP.EXP | MAX-RDEP.USR |
| MAX-RWP.DEF | MAX-RWP.EXP | MAX-RWP.USR | MAX-TRAN.DEF | MAX-TRAN.EXP | MAX-TRAN.USR |
| MET-PAR.DEF | MET-PAR.EXP | MET-PAR.USR | MET-STA.DEF | MET-STA.EXP | MET-STA.USR |
| MIN-EVAP.DEF | MIN-EVAP.EXP | MIN-EVAP.USR | MIN-RWP.DEF | MIN-RWP.EXP | MIN-RWP.USR |
| MOLE-DIF.DEF | MOLE-DIF.EXP | MOLE-DIF.USR | NO-PREF.DEF | NO-PREF.EXP | NO-PREF.USR |
| NOT-SIMU.DEF | NOT-SIMU.EXP | NOT-SIMU.USR | NUM-CROP.DEF | NUM-CROP.EXP | NUM-CROP.USR |
| NUM-IRIG.DEF | NUM-IRIG.EXP | NUM-IRIG.USR | O-CARBON.DEF | O-CARBON.EXP | O-CARBON.USR |
| OB-DEPTH.DEF | OB-DEPTH.EXP | OB-DEPTH.USR | ORCH-QUE.DEF | ORCH-QUE.EXP | ORCH-QUE.USR |
| OUT-PAR.DEF | OUT-PAR.EXP | OUT-PAR.USR | OUT-STEP.DEF | OUT-STEP.EXP | OUT-STEP.USR |
| OUT-UNIT.DEF | OUT-UNIT.EXP | OUT-UNIT.USR | OVERVIEW.DEF | OVERVIEW.EXP | OVERVIEW.USR |
| P-DENSE.DEF | P-DENSE.EXP | P-DENSE.USR | P-SELECT.DEF | P-SELECT.EXP | P-SELECT.USR |
| PAN-COEF.DEF | PAN-COEF.EXP | PAN-COEF.USR | PAR-NAME.DEF | PAR-NAME.EXP | PAR-NAME.USR |
| PER-CLAY.DEF | PER-CLAY.EXP | PER-CLAY.USR | PER-SILT.DEF | PER-SILT.EXP | PER-SILT.USR |
| PEST-APP.DEF | PEST-APP.EXP | PEST-APP.USR | PEST-DAT.DEF | PEST-DAT.EXP | PEST-DAT.USR |
| PEST-INF.DEF | PEST-INF.EXP | PEST-INF.USR | PEST-NUM.DEF | PEST-NUM.EXP | PEST-NUM.USR |
| PEST-PAR.DEF | PEST-PAR.EXP | PEST-PAR.USR | PEST-RES.DEF | PEST-RES.EXP | PEST-RES.USR |
| PEST-RNK.DEF | PEST-RNK.EXP | PEST-RNK.USR | PEST-SEL.DEF | PEST-SEL.EXP | PEST-SEL.USR |
| PEST-SRT.DEF | PEST-SRT.EXP | PEST-SRT.USR | PEST-SYN.DEF | PEST-SYN.EXP | PEST-SYN.USR |
| PLANTING.DEF | PLANTING.EXP | PLANTING.USR | PLNT-MAT.DEF | PLNT-MAT.EXP | PLNT-MAT.USR |
| POTAT-NB.DEF | POTAT-NB.EXP | POTAT-NB.USR | POTAT-NF.DEF | POTAT-NF.EXP | POTAT-NF.USR |
| POTAT-PE.DEF | POTAT-PE.EXP | POTAT-PE.USR | PRECIP.DEF | PRECIP.EXP | PRECIP.USR |
| PREV-SES.DEF | PREV-SES.EXP | PREV-SES.USR | PRO-DPTH.DEF | PRO-DPTH.EXP | PRO-DPTH.USR |
| PRT-DATR.DEF | PRT-DATR.EXP | PRT-DATR.USR | PRT-FREQ.DEF | PRT-FREQ.EXP | PRT-FREQ.USR |
| PST-NAME.DEF | PST-NAME.EXP | PST-NAME.USR | PST-SPCS.DEF | PST-SPCS.EXP | PST-SPCS.USR |
| QUICKLY.DEF | QUICKLY.EXP | QUICKLY.USR | RANGE-AL.DEF | RANGE-AL.EXP | RANGE-AL.USR |
| REP-DEP.DEF | REP-DEP.EXP | REP-DEP.USR | ROOT-FRC.DEF | ROOT-FRC.EXP | ROOT-FRC.USR |
| ROOT-MAT.DEF | ROOT-MAT.EXP | ROOT-MAT.USR | ROOT-OPT.DEF | ROOT-OPT.EXP | ROOT-OPT.USR |
| ROOT-RES.DEF | ROOT-RES.EXP | ROOT-RES.USR | ROOT-TAB.DEF | ROOT-TAB.EXP | ROOT-TAB.USR |
| S-SWITCH.DEF | S-SWITCH.EXP | S-SWITCH.USR | S-THETA.DEF | S-THETA.EXP | S-THETA.USR |
| SCENARIO.DEF | SCENARIO.EXP | SCENARIO.USR | SCREEN.DEF | SCREEN.EXP | SCREEN.USR |
| SCRN-PST.DEF | SCRN-PST.EXP | SCRN-PST.USR | SEN-STUD.DEF | SEN-STUD.EXP | SEN-STUD.USR |
| SENS-PAR.DEF | SENS-PAR.EXP | SENS-PAR.USR | SENSANAL.DEF | SENSANAL.EXP | SENSANAL.USR |
| SETUP.DEF | SETUP.EXP | SETUP.USR | SIMULATE.DEF | SIMULATE.EXP | SIMULATE.USR |
| SIMULATN.DEF | SIMULATN.EXP | SIMULATN.USR | SNOW-COE.DEF | SNOW-COE.EXP | SNOW-COE.USR |
| SOIL-APP.DEF | SOIL-APP.EXP | SOIL-APP.USR | SOIL-DK.DEF | SOIL-DK.EXP | SOIL-DK.USR |
| SOIL-HOR.DEF | SOIL-HOR.EXP | SOIL-HOR.USR | SOIL-PAR.DEF | SOIL-PAR.EXP | SOIL-PAR.USR |
| SOLUBIL.DEF | SOLUBIL.EXP | SOLUBIL.USR | SPEC-DAY.DEF | SPEC-DAY.EXP | SPEC-DAY.USR |
| SPEC-PRT.DEF | SPEC-PRT.EXP | SPEC-PRT.USR | SRB.DEF | SRB.EXP | SRB.USR |
| STRM-DUR.DEF | STRM-DUR.EXP | STRM-DUR.USR | SUGRB-AL.DEF | SUGRB-AL.EXP | SUGRB-AL.USR |
| SUGRBMAN.DEF | SUGRBMAN.EXP | SUGRBMAN.USR | TEMPER.DEF | TEMPER.EXP | TEMPER.USR |
| TOBACONT.DEF | TOBACONT.EXP | TOBACONT.USR | TOT-IRIG.DEF | TOT-IRIG.EXP | TOT-IRIG.USR |
| TRF-RATE.DEF | TRF-RATE.EXP | TRF-RATE.USR | TS-CUM.DEF | TS-CUM.EXP | TS-CUM.USR |
| UPTAKE.DEF | UPTAKE.EXP | UPTAKE.USR | USLEC.DEF | USLEC.EXP | USLEC.USR |
| USLEK.DEF | USLEK.EXP | USLEK.USR | USLELS.DEF | USLELS.EXP | USLELS.USR |
| USLEP.DEF | USLEP.EXP | USLEP.USR | VAP-DEN.DEF | VAP-DEN.EXP | VAP-DEN.USR |
| VAP-PRES.DEF | VAP-PRES.EXP | VAP-PRES.USR | VAR-INT.DEF | VAR-INT.EXP | VAR-INT.USR |
| WASHOFF.DEF | WASHOFF.EXP | WASHOFF.USR | WATR-TBL.DEF | WATR-TBL.EXP | WATR-TBL.USR |
| WHEAT-SK.DEF | WHEAT-SK.EXP | WHEAT-SK.USR | WILT-PNT.DEF | WILT-PNT.EXP | WILT-PNT.USR |

# Appendix E

# Type Conventions Used in the Description of EXPRES

| Type Conventions | | |
|---|---|---|
| screen title | · bold Helvetica<br>· all letters capitalized | e.g. **SESSION OBJECTIVES** |
| screen parameter | · bold Helvetica<br>· 1st letters capitalized | e.g. **Bulk Density** |
| command line | · italics Helvetica<br>· all letters capitalized | e.g. *DEFAULT-DATA* |
| command line options | · italics Helvetica<br>· 1st letters capitalized | e.g. *Run Model* |
| DOS filename | · normal Helvetica<br>· all letters capitalized | e.g. EXAMPLE.DAT |
| key strokes | · normal Helvetica<br>· 1st letters capitalized | e.g. <PgDn> |
| user entries | · italics Times<br>· 1st letters capitalized | e.g. *Pesticide 4* |
| EXPRES response | · italics Courier<br>· 1st letters capitalized | e.g. *Warning, command is...* |

**EXPRES: An Expert System for Assessing the Fate of Pesticides in the Subsurface**    **Mutch, Crowe and Resler**